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# Supporting information for:

16OSTM10: A new open-shell transition metal conformational energies database to challenge contemporary semiempirical and force field methods

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### Tables forming the basis of Figures 2-8 in the main text

Table S1. Table forming the basis of Figure 2.

Method	PBE	PBE0	M06	ωB97X-V
min	0.42	0.68	0.65	0.36
average	0.91	0.94	0.92	0.87
max	0.99	1.00	0.99	0.99
Worst compound	LUFCIZ	LUFCIZ	LUFCIZ	LUFCIZ
Best compound	ONEHAS	ONEHAS	FUHWAG	ONEHAS

#### Pearson correlation coefficients for conformational energies

	PBE	PBE0	M06	ωB97X-V
ADULES	0.95	0.93	0.90	0.92
AJOMIX	0.81	0.89	0.81	0.71
AQINUK	0.99	0.99	0.98	0.99
AVIXIO	0.99	0.99	0.98	0.99
FIYMEI	0.83	0.83	0.74	0.54
FUDNIB	0.84	0.88	0.89	0.65
FUHWAG	0.99	0.99	0.99	0.99
LIBLEN	0.98	0.97	0.94	0.97
LUFCIZ	0.42	0.68	0.65	0.36
ONEHAS	0.99	1.00	0.98	0.99
OQOQOB	0.98	0.99	0.98	0.98
QUHVAS	0.97	0.98	0.96	0.96
ROBHUN	0.99	0.99	0.99	0.99
UZEYAA	0.93	0.96	0.91	0.93
WUDYOL	0.99	0.99	0.98	0.97
YIKLUC	0.98	0.99	0.99	0.99

Table S2. Table forming the basis of Figure 3.

Mean correlation coefficients for PBEh-3c.

	average	min	max
ADULES	0.86	0.80	0.90
AJOMIX	0.35	0.06	0.55
AQINUK	0.99	0.98	0.99
AVIXIO	0.99	0.98	0.99
FIYMEI	0.85	0.69	0.95
FUDNIB	0.92	0.78	0.98
FUHWAG	0.99	0.98	0.99
LIBLEN	0.93	0.84	0.97
LUFCIZ	0.72	0.38	0.96
ONEHAS	0.99	0.98	1.00
OQOQOB	0.91	0.87	0.95
QUHVAS	0.96	0.94	0.98
ROBHUN	0.98	0.97	0.99
UZEYAA	0.93	0.89	0.95

WUDYOL	0.98	0.96	0.99
YIKLUC	0.98	0.97	0.99

#### Mean correlation coefficients for B97-3c.

	average	min	max
ADULES	0.96	0.94	1.00
AJOMIX	0.88	0.68	0.98
AQINUK	0.99	0.98	1.00
AVIXIO	0.99	0.98	1.00
FIYMEI	0.88	0.61	0.99
FUDNIB	0.90	0.64	0.99
FUHWAG	0.99	0.99	1.00
LIBLEN	0.95	0.89	0.98
LUFCIZ	0.72	0.28	0.95
ONEHAS	1.00	0.99	1.00
OQOQOB	0.99	0.99	1.00
QUHVAS	0.98	0.97	1.00
ROBHUN	0.99	0.98	1.00
UZEYAA	0.95	0.90	1.00
WUDYOL	0.99	0.98	1.00
YIKLUC	0.99	0.98	1.00

#### Correlation coefficients for PBEh-3c.

	PBE	PBE0	M06	ωB97X-V
ADULES	0.85	0.80	0.87	0.90
AJOMIX	0.06	0.35	0.55	0.46
AQINUK	0.99	0.99	0.98	0.99
AVIXIO	0.99	0.99	0.99	0.98
FIYMEI	0.92	0.95	0.85	0.69
FUDNIB	0.95	0.98	0.98	0.78
FUHWAG	0.99	0.99	0.98	0.98
LIBLEN	0.94	0.97	0.84	0.97
LUFCIZ	0.38	0.96	0.68	0.86
ONEHAS	1.00	1.00	0.98	1.00
OQOQOB	0.87	0.92	0.91	0.95
QUHVAS	0.94	0.95	0.95	0.98
ROBHUN	0.97	0.98	0.97	0.99
UZEYAA	0.92	0.94	0.89	0.95
WUDYOL	0.98	0.99	0.99	0.96
YIKLUC	0.97	0.98	0.99	0.98

#### Correlation coefficients for B97-3c.

	PBE	PBE0	M06	ωB97X-V
ADULES	1.00	0.94	0.94	0.96
AJOMIX	0.97	0.98	0.90	0.68
AQINUK	1.00	1.00	0.98	0.99
AVIXIO	1.00	0.99	0.98	0.99
FIYMEI	0.99	0.99	0.93	0.61

FUDNIB	0.99	0.99	0.98	0.64
FUHWAG	0.99	1.00	0.99	1.00
LIBLEN	0.98	0.97	0.89	0.97
LUFCIZ	0.94	0.71	0.95	0.28
ONEHAS	1.00	1.00	0.99	1.00
OQOQOB	0.99	1.00	0.99	0.99
QUHVAS	1.00	1.00	0.97	0.97
ROBHUN	1.00	0.99	0.98	0.98
UZEYAA	1.00	0.99	0.90	0.93
WUDYOL	0.99	1.00	0.99	0.98
YIKLUC	1.00	1.00	0.98	0.98

Table S3. Table forming the basis of Figure 4.

#### Mean correlation coefficients for PM6.

	average	min	max
ADULES	0.94	0.89	0.98
AJOMIX	0.24	0.00	0.47
AQINUK	-0.14	-0.19	-0.12
OIXIVA	0.61	0.56	0.65
FIYMEI	-0.42	-0.65	-0.05
FUDNIB	0.46	0.38	0.54
FUHWAG	0.60	0.53	0.65
LIBLEN	0.63	0.58	0.68
LUFCIZ	0.16	-0.59	0.79
ONEHAS	0.69	0.67	0.75
OQOQOB	0.02	-0.02	0.07
QUHVAS	0.93	0.91	0.97
ROBHUN	0.82	0.78	0.85
UZEYAA	0.84	0.78	0.90
WUDYOL	0.94	0.92	0.96
YIKLUC	0.72	0.65	0.78

#### Mean correlation coefficients for PM7.

	average	min	max
ADULES	0.94	0.89	0.97
AJOMIX	0.51	0.28	0.73
AQINUK	-0.11	-0.17	-0.08
AVIXIO	0.95	0.94	0.95
FIYMEI	-0.03	-0.26	0.16
FUDNIB	0.34	-0.07	0.57
FUHWAG	0.97	0.96	0.97
LIBLEN	0.09	0.05	0.20
LUFCIZ	0.33	-0.36	0.86
ONEHAS	0.95	0.93	0.97
OQOQOB	0.83	0.81	0.84
QUHVAS	0.81	0.75	0.85
ROBHUN	0.64	0.61	0.65

UZEYAA	0.71	0.69	0.75
WUDYOL	0.05	0.03	0.10
YIKLUC	0.82	0.79	0.87

#### Correlation coefficients for PM6.

	PBE	PBE0	M06	ωB97X-V
ADULES	0.98	0.92	0.89	0.97
AJOMIX	0.47	0.24	0.00	0.25
AQINUK	-0.12	-0.12	-0.12	-0.19
AVIXIO	0.63	0.61	0.65	0.56
FIYMEI	-0.60	-0.65	-0.38	-0.05
FUDNIB	0.38	0.50	0.54	0.43
FUHWAG	0.65	0.65	0.53	0.57
LIBLEN	0.68	0.64	0.58	0.63
LUFCIZ	0.79	-0.09	0.52	-0.59
ONEHAS	0.68	0.69	0.75	0.67
OQOQOB	-0.02	0.00	0.07	0.05
QUHVAS	0.93	0.92	0.91	0.97
ROBHUN	0.83	0.85	0.78	0.84
UZEYAA	0.84	0.85	0.78	0.90
WUDYOL	0.96	0.94	0.95	0.92
YIKLUC	0.65	0.72	0.74	0.78

#### Correlation coefficients for PM7.

	PBE	PBE0	M06	ωB97X-V
ADULES	0.93	0.97	0.89	0.96
AJOMIX	0.73	0.60	0.43	0.28
AQINUK	-0.11	-0.10	-0.08	-0.17
AVIXIO	0.95	0.95	0.94	0.94
FIYMEI	0.05	-0.06	0.16	-0.26
FUDNIB	0.57	0.46	0.39	-0.07
FUHWAG	0.97	0.97	0.96	0.97
LIBLEN	0.07	0.06	0.20	0.05
LUFCIZ	0.86	0.12	0.68	-0.36
ONEHAS	0.93	0.94	0.97	0.94
OQOQOB	0.84	0.83	0.81	0.83
QUHVAS	0.81	0.85	0.82	0.75
ROBHUN	0.65	0.63	0.61	0.65
UZEYAA	0.69	0.70	0.75	0.69
WUDYOL	0.10	0.05	0.04	0.03
YIKLUC	0.79	0.83	0.81	0.87

Table S4. Table forming the basis of Figure 5.

#### Mean correlation coefficients for GFN1-xTB.

	average	min	max	
ADULES	0.95	0.93	0.97	

AJOMIX	0.57	0.20	0.82
AQINUK	0.25	0.24	0.26
AVIXIO	0.97	0.95	0.98
FIYMEI	0.35	-0.05	0.55
FUDNIB	0.78	0.40	0.92
FUHWAG	0.96	0.95	0.98
LIBLEN	-0.01	-0.06	0.05
LUFCIZ	0.62	0.19	0.88
ONEHAS	0.98	0.98	0.99
OQOQOB	0.91	0.90	0.92
QUHVAS	0.95	0.94	0.96
ROBHUN	0.78	0.73	0.82
UZEYAA	0.76	0.66	0.80
WUDYOL	0.93	0.90	0.95
YIKLUC	_	_	-

#### Mean correlation coefficients for GFN2-xTB.

	average	min	max
ADULES	0.97	0.93	0.98
AJOMIX	0.77	0.42	0.91
AQINUK	0.31	0.27	0.33
AVIXIO	0.92	0.89	0.93
FIYMEI	0.81	0.46	0.93
FUDNIB	0.76	0.45	0.89
FUHWAG	0.97	0.95	0.98
LIBLEN	0.62	0.56	0.66
LUFCIZ	0.25	-0.40	0.72
ONEHAS	0.97	0.96	0.97
OQOQOB	0.76	0.74	0.79
QUHVAS	0.96	0.95	0.97
ROBHUN	0.77	0.73	0.80
UZEYAA	0.87	0.82	0.91
WUDYOL	0.97	0.95	0.99
YIKLUC	0.95	0.94	0.95

#### Mean correlation coefficients for GFN-FF.

	average	min	max
ADULES	0.93	0.90	0.97
AJOMIX	-0.10	-0.35	0.11
AQINUK	0.49	0.48	0.50
AVIXIO	0.90	0.88	0.91
FIYMEI	0.40	0.02	0.58
FUDNIB	0.13	0.04	0.24
FUHWAG	0.98	0.98	0.98
LIBLEN	0.30	0.15	0.36
LUFCIZ	0.06	-0.60	0.75
ONEHAS	0.98	0.97	0.99
OQOQOB	0.96	0.94	0.98
OUHVAS	0.82	0.78	0.84

ROBHUN	0.58	0.55	0.61
UZEYAA	0.83	0.78	0.86
WUDYOL	0.93	0.90	0.95
YIKLUC	0.76	0.69	0.81

#### Correlation coefficients for GFN1-xTB.

	PBE	PBE0	M06	ωB97X-V
ADULES	0.97	0.96	0.93	0.96
AJOMIX	0.82	0.69	0.56	0.20
AQINUK	0.26	0.26	0.25	0.24
AVIXIO	0.98	0.98	0.95	0.97
FIYMEI	0.52	0.55	0.38	-0.05
FUDNIB	0.92	0.91	0.88	0.40
FUHWAG	0.95	0.96	0.97	0.98
LIBLEN	0.05	-0.06	0.03	-0.06
LUFCIZ	0.19	0.88	0.60	0.80
ONEHAS	0.98	0.99	0.98	0.99
OQOQOB	0.92	0.92	0.90	0.91
QUHVAS	0.95	0.94	0.95	0.96
ROBHUN	0.73	0.79	0.77	0.82
UZEYAA	0.80	0.80	0.66	0.78
WUDYOL	0.95	0.94	0.94	0.90
YIKLUC	-	-	_	-

#### Correlation coefficients for GFN2-xTB.

				- 0=
	PBE	PBE0	M06	ωB97X-V
ADULES	0.98	0.97	0.93	0.97
AJOMIX	0.91	0.89	0.84	0.42
AQINUK	0.33	0.33	0.32	0.27
AVIXIO	0.92	0.93	0.89	0.92
FIYMEI	0.93	0.93	0.91	0.46
FUDNIB	0.89	0.89	0.84	0.45
FUHWAG	0.95	0.95	0.98	0.98
LIBLEN	0.66	0.63	0.56	0.61
LUFCIZ	-0.40	0.58	0.10	0.72
ONEHAS	0.97	0.97	0.96	0.97
OQOQOB	0.79	0.75	0.75	0.74
QUHVAS	0.96	0.95	0.95	0.97
ROBHUN	0.73	0.76	0.78	0.80
UZEYAA	0.87	0.91	0.82	0.90
WUDYOL	0.99	0.98	0.98	0.95
YIKLUC	0.94	0.95	0.95	0.95

#### Correlation coefficients for GFN-FF.

	PBE	PBE0	M06	ωB97X-V
ADULES	0.97	0.90	0.91	0.96
AJOMIX	-0.35	-0.12	0.11	-0.06
AQINUK	0.50	0.49	0.48	0.50

AVIXIO	0.91	0.90	0.88	0.91
FIYMEI	0.52	0.58	0.47	0.02
FUDNIB	0.04	0.14	0.10	0.24
FUHWAG	0.98	0.98	0.98	0.98
LIBLEN	0.36	0.36	0.15	0.33
LUFCIZ	0.75	-0.25	0.34	-0.60
ONEHAS	0.98	0.98	0.97	0.99
OQOQOB	0.98	0.97	0.96	0.94
QUHVAS	0.82	0.78	0.84	0.83
ROBHUN	0.55	0.57	0.59	0.61
UZEYAA	0.86	0.85	0.78	0.83
WUDYOL	0.95	0.93	0.94	0.90
YIKLUC	0.69	0.75	0.78	0.81

Table S5. Table forming the basis of Figure 6.

	Q3	Q1	max	min	median
PBE-D3(BJ)	0.99	0.91	0.99	0.42	0.98
PBE0-D3(BJ)	0.99	0.92	1.00	0.68	0.98
M06	0.98	0.90	0.99	0.65	0.97
ωB97X-V	0.99	0.87	0.99	0.36	0.97
PBEh-3c	0.98	0.90	0.99	0.35	0.94
B97-3c	0.99	0.94	1.00	0.72	0.99
PM6	0.83	0.22	0.94	-0.42	0.62
PM7	0.86	0.27	0.97	-0.11	0.67
GFN1-xTB	0.95	0.59	0.98	-0.01	0.78
GFN2-xTB	0.96	0.76	0.97	0.25	0.84
GFN-FF	0.93	0.37	0.98	-0.10	0.79

Table S6. Table forming the basis of Figure 7.

	0
	T,S
PBE-D3(BJ)	191.554
PBE0-D3(BJ)	2833.729
M06	2985.011
ωB97X-V	5083.924
B97-3c	89.404
PBEh-3c	732.035
GFN1	0.102
GFN2	0.045
GFN-FF	0.002
PM6	0.06
PM7	0.06

Computer architecture: Intel(R) Core(TM) i5-10600K CPU @ 4.10GHz, 12 Gb RAM. Single core was utilized.

Table S7. Table forming the basis of Figure 8.

# Pearson correlation coefficients for the compounds of 16OSTM10 database.

$\rho$ (PBE/ $\lambda$ 2, PBE-D3/ $\lambda$ 2)
0.98
0.83
0.97
-0.03
0.43
0.57
0.82
0.96
0.90
0.99
0.36
0.97
0.97
0.96
0.98
1.00

#### Absolute energies of the conformations.

	$E(PBE/\lambda 2)$ , Hartree	$E(PBE-D3/\lambda 2)$ , Hartree
AQINUK_13	-14773.18958987	-14773.39572320
AQINUK_15	-14773.18909685	-14773.39552260
AQINUK_17	-14773.19006450	-14773.39754890
AQINUK_20	-14773.18209972	-14773.39202320
AQINUK_22	-14773.18803601	-14773.39488890
AQINUK_29	-14773.18532039	-14773.39373860
AQINUK_32	-14773.19374792	-14773.39866630
AQINUK_6	-14773.19137329	-14773.39682680
AQINUK_7	-14773.18870787	-14773.39502500
AQINUK_9	-14773.19005499	-14773.39643980
AVIXIO_10	-9169.07080765	-9169.39987730
AVIXIO_13	-9169.06718954	-9169.41365544
AVIXIO_14	-9169.05921435	-9169.39063622
AVIXIO_18	-9169.06941891	-9169.38825686
AVIXIO_1	-9169.06659658	-9169.40484071
AVIXIO_20	-9169.07301828	-9169.39140229
AVIXIO_21	-9169.05871940	-9169.39329549
AVIXIO_29	-9169.06583520	-9169.40183112
AVIXIO_6	-9169.06861715	-9169.37467736
AVIXIO_7	-9169.06432069	-9169.39715459
FUHWAG_14	-5610.75066424	-5611.06911273
FUHWAG_15	-5610.76285951	-5611.08308297
FUHWAG_27	-5610.76084649	-5611.08836039
FUHWAG_31	-5610.75217648	-5611.05050731

	1	1
FUHWAG_32	-5610.72998715	-5611.05610486
FUHWAG_33	-5610.75733521	-5611.07626111
FUHWAG_34	-5610.72692895	-5611.03402162
FUHWAG_3	-5610.75776431	-5611.07501040
FUHWAG_6	-5610.75241487	-5611.05682053
FUHWAG_8	-5610.76168456	-5611.07307748
OQOQOB_10	-6284.93613798	-6285.28693455
OQOQOB_13	-6284.93992218	-6285.30791036
OQOQOB_17	-6284.93206104	-6285.26427936
OQOQOB_1	-6284.93906166	-6285.28292884
OQOQOB_22	-6284.92968058	-6285.27806728
OQOQOB_26	-6284.93884803	-6285.26721225
OQOQOB_30	-6284.93421247	-6285.28266902
OQOQOB_3	-6284.93443704	-6285.28502328
OQOQOB_6	-6284.95258933	-6285.27274288
OQOQOB_8	-6284.95766487	-6285.30261991
WUDYOL_0	-3365.92567093	-3366.04385828
WUDYOL_16	-3365.92633909	-3366.04424275
WUDYOL_19	-3365.92465111	-3366.04352511
WUDYOL_20	-3365.92458616	-3366.04153828
WUDYOL_21	-3365.92417380	-3366.04217666
WUDYOL_32	-3365.91831691	-3366.03715427
WUDYOL_34	-3365.91526920	-3366.03412316
WUDYOL_3	-3365.92274571	-3366.03971021
WUDYOL_7	-3365.91766403	-3366.03718520
WUDYOL_8	-3365.91824895	-3366.03746748
YIKLUC_15	-2947.60179050	-2947.76280711
YIKLUC_18	-2947.60146966	-2947.76289800
YIKLUC_19	-2947.60191833	-2947.76320955
YIKLUC_27	-2947.60490643	-2947.76733277
YIKLUC_29	-2947.59464934	-2947.75565699
YIKLUC_30	-2947.60490877	-2947.76644897
YIKLUC_32	-2947.59925495	-2947.75987496
YIKLUC_33	-2947.60087199	-2947.76217573
YIKLUC_34	-2947.59694240	-2947.75763625
YIKLUC_9	-2947.60617699	-2947.76834241
LIBLEN_16	-2728.89037254	-2729.03958725
LIBLEN_18	-2728.89052564	-2729.03964391
LIBLEN_1	-2728.89612672	-2729.04336249
LIBLEN_23	-2728.89052627	-2729.04016380
LIBLEN_24	-2728.88899990	-2729.03526877
LIBLEN_25	-2728.88368277	-2729.03230438
LIBLEN_26	-2728.89053615	-2729.03910705
LIBLEN_31	-2728.88409753	-2729.03322960
LIBLEN_33	-2728.89502980	-2729.04172213
LIBLEN_3	-2728.89564956	-2729.04289863
ONEHAS_12	-3244.41006970	-3244.63082024
ONEHAS_14	-3244.41199479	-3244.63092203
ONEHAS_17	-3244.40329840	-3244.62429939
ONEHAS_22	-3244.40357900	-3244.62417748

ONEHAS_23	-3244.39875918	-3244.61790303
ONEHAS_27	-3244.38353377	-3244.60588665
ONEHAS_30	-3244.38208145	-3244.60409414
ONEHAS_31	-3244.38635711	-3244.61205569
ONEHAS_33	-3244.40131212	-3244.62495600
ONEHAS_34	-3244.38245547	-3244.60442146
UZEYAA_14	-3891.83024091	-3892.07160777
UZEYAA_19	-3891.83008407	-3892.07012319
UZEYAA_20	-3891.84112263	-3892.07972428
UZEYAA_22	-3891.83113304	-3892.07100437
UZEYAA_23	-3891.84015508	-3892.07572665
UZEYAA_30	-3891.83533515	-3892.07400234
UZEYAA_31	-3891.83922215	-3892.07743790
UZEYAA_33	-3891.83133269	-3892.07168807
UZEYAA_3	-3891.83425407	-3892.07288898
uzeyaa_7	-3891.84129394	-3892.07888925
ADULES_14	-3092.51201732	-3092.69304940
ADULES_16	-3092.52774329	-3092.70314664
ADULES_20	-3092.52530924	-3092.70151279
ADULES_23	-3092.51665397	-3092.69640612
ADULES_25	-3092.51669377	-3092.69508230
ADULES_28	-3092.50555616	-3092.68821415
ADULES_2	-3092.52173770	-3092.69886801
ADULES_31	-3092.51448295	-3092.69242929
ADULES_6	-3092.51951173	-3092.69592108
ADULES_9	-3092.51132739	-3092.69093187
AJOMIX_11	-4476.60604917	-4476.81202450
AJOMIX_14	-4476.60348911	-4476.81010973
AJOMIX_17	-4476.60267220	-4476.81039517
AJOMIX_18	-4476.60739914	-4476.81403947
AJOMIX_19	-4476.60713589	-4476.81409206
AJOMIX_26	-4476.60701163	-4476.81387462
AJOMIX_31	-4476.60462004	-4476.81035596
AJOMIX_4	-4476.60592395	-4476.80938065
AJOMIX_7	-4476.60351552	-4476.80952930
_AJOMIX_9	-4476.60756533	-4476.81400623
FIYMEI_10	-6434.49058795	-6434.80956262
FIYMEI_12	-6434.48044361	-6434.79860198
FIYMEI_17	-6434.48150501	-6434.79525908
FIYMEI_18	-6434.47772465	-6434.79617935
FIYMEI_21	-6434.47954657	-6434.81717111
FIYMEI_28	-6434.47881272	-6434.80670693
FIYMEI_31	-6434.48669340	-6434.80573867
FIYMEI_32	-6434.47364428	-6434.79594755
FIYMEI_5	-6434.47955659	-6434.80067479
FIYMEI_6	-6434.48020046	-6434.79970603
QUHVAS_16	-3411.99095636	-3412.18980991
QUHVAS_20	-3411.98806832	-3412.18811247
QUHVAS_21	-3411.98453617	-3412.18689936
QUHVAS_24	-3411.97124149	-3412.17404124

QUHVAS_25	-3411.98184796	-3412.18497682
QUHVAS_26	-3411.97995692	-3412.17903192
QUHVAS_27	-3411.97377877	-3412.17897882
QUHVAS_28	-3411.99235346	-3412.19024210
QUHVAS_29	-3411.96954857	-3412.17393631
QUHVAS_6	-3411.98243012	-3412.18372402
FUDNIB_18	-4541.58506057	-4541.80985694
FUDNIB_21	-4541.58556205	-4541.80770346
FUDNIB_23	-4541.58607438	-4541.80607285
FUDNIB_24	-4541.58461327	-4541.80242194
FUDNIB_26	-4541.58238413	-4541.80499325
FUDNIB_27	-4541.58650860	-4541.81286286
FUDNIB_2	-4541.58745213	-4541.80775509
FUDNIB_32	-4541.58676239	-4541.81300568
FUDNIB_3	-4541.58645492	-4541.81243594
FUDNIB_5	-4541.58549864	-4541.80523584
LUFCIZ_25	-3592.17307904	-3592.42059437
LUFCIZ_27	-3592.16736935	-3592.41030929
LUFCIZ_28	-3592.16649064	-3592.41602369
LUFCIZ_29	-3592.16753941	-3592.41892177
LUFCIZ_2	-3592.18077240	-3592.43006424
LUFCIZ_30	-3592.16113583	-3592.41396696
LUFCIZ_32	-3592.16062592	-3592.41046575
LUFCIZ_6	-3592.17104859	-3592.42273467
LUFCIZ_9	-3592.17379822	-3592.42547364
ROBHUN_10	-5594.49325700	-5594.70774467
ROBHUN_12	-5594.49457945	-5594.70950435
ROBHUN_13	-5594.48992405	-5594.70308577
ROBHUN_14	-5594.49696543	-5594.71206300
ROBHUN_29	-5594.49617789	-5594.71073301
ROBHUN_2	-5594.49655413	-5594.71025193
ROBHUN_34	-5594.48978930	-5594.70282712
ROBHUN_3	-5594.49595350	-5594.70885132
ROBHUN_4	-5594.50058495	-5594.71432033
ROBHUN_8	-5594.49378397	-5594.70896207

Table S8. T1/T2 diagnostic values for 10 compounds of 16OSTM10 database

	Т1	Т2
LUFCIZ	0.011	0.063
ONEHAS	0.012	0.047
ROBHUN	0.012	0.058
ADULES	0.012	0.080
AQINUK	0.012	0.078
AVIXIO	0.013	0.071
FUHWAG	0.013	0.072
OQOQOB	0.013	0.073
QUHVAS	0.013	0.094
WUDYOL	0.017	0.093

# **FOD** plots

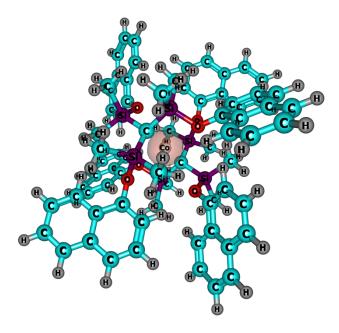


Figure S1. Qualitative FOD diagnostics for FIYMEI. The isosurface value is  $\sigma = 0.005$  e/Bohr<sup>3</sup>.

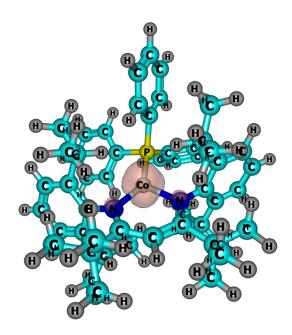


Figure S2. Qualitative FOD diagnostics for UZEYAA. The isosurface value is  $\sigma$  = 0.005 e/Bohr³.

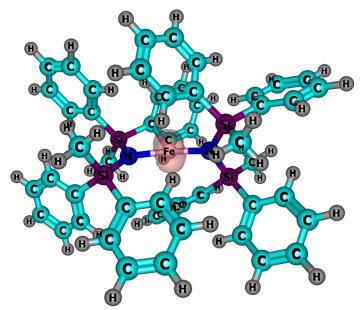


Figure S3. Qualitative FOD diagnostics for FUDNIB. The isosurface value is  $\sigma = 0.005$  e/Bohr³.

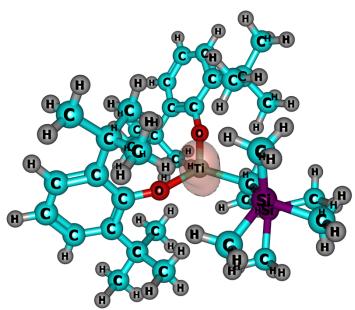


Figure S4. Qualitative FOD diagnostics for YIKLUC. The isosurface value is  $\sigma = 0.005$  e/Bohr<sup>3</sup>.

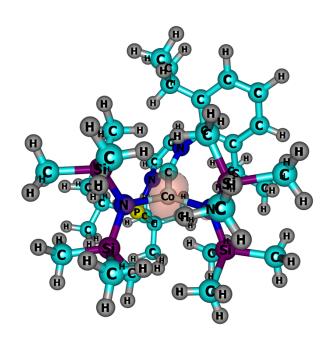


Figure S5. Qualitative FOD diagnostics for AJOMIX. The isosurface value is  $\sigma = 0.005$  e/Bohr<sup>3</sup>.

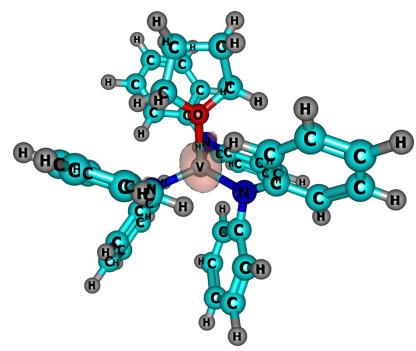


Figure S6. Qualitative FOD diagnostics for LIBLEN. The isosurface value is  $\sigma = 0.005$  e/Bohr³.

## Composition of the $\lambda 1$ and $\lambda 2$ basis sets used in the Priroda calculations

Elements	Primitive and contracted functions
λ1	
Н	$(6s2p) \rightarrow [2s1p]$
B, C, N, O, F	(10s7p3d) → [3s2p1d]
Al, Si, P, S, Cl	(14s11p3d) → [4s3p1d]
Ti, V, Cr, Fe, Co, Cu	(19s15p11d5f) → [6s5p3d1f]
Br	(19s15p11d) → [5s4p2d]
λ2	
Н	(8s4p2d) → [3s2p1d]
B, C, N, O, F	$(12s8p4d2f) \rightarrow [4s3p2d1f]$
Al, Si, P, S, Cl	(18s13p5d2f) → [5s4p2d1f]
Ti, V, Cr, Fe, Co, Cu	(23s18p13d8f4g) → [8s7p5d3f1g]
Br	(23s18p13d2f) → [6s5p3d1f]
λ1 (relativistic)	
Н	$(6s2p) \rightarrow [2s1p]$
B, C, N, O, F	(10s7p3d) → [3s2p1d]
Al, Si, P, S, Cl	(15s11p3d) → [4s3p1d]
Ti, V, Cr, Fe, Co, Cu	(21s16p11d5f) → [6s5p3d1f]
Br	(21s17p11d) → [5s4p2d]
λ2 (relativistic)	
Н	(8s4p2d) → [3s2p1d]
B, C, N, O, F	$(12s8p4d2f) \rightarrow [4s3p2d1f]$
Al, Si, P, S, Cl	$(19s13p5d2f) \rightarrow [5s4p2d1f]$
Ti, V, Cr, Fe, Co, Cu	$(25s20p14d8f4g) \rightarrow [8s7p5d3f1g]$
Br	(25s21p14d2f) → [6s5p3d1f]

# Tabulated absolute conformational energies and optimized Cartesian coordinates for the compounds of 16OSTM10 database.

				С	-0.250105	0.535799	-4.074476
				H	-0.763873	1.247450	-4.756630
ADU]	LES.			С	0.792684	-0.201098	-4.931942
HDU				H	0.316835	-0.807591	-5.728421
~ .				H	1.416539	-0.872134	-4.310604
	nation 14. .icity: 4			H C	1.474901 0.450869	0.527122 1.396366	-5.417566 -3.012058
Charge:				Н	-0.276842	1.891299	-2.339416
	sc) = -3093.966599	795127 Hartree		H	1.037861	2.198291	-3.506303
	lef2-TZVP) = -3093		tree	Н	1.159806	0.809979	-2.395038
	· D3(BJ)/def2-TZVE			C	-2.488712	-2.708615	-0.679725
	- D3(BJ)/def2-TZV			H	-1.467590	-2.636781	-0.249650
E (PBEh-	-3c) = -3089.87101	.5364763 Hartree		C	-2.807603	-4.199331	-0.885013
	= 12.97362  Kcal/m			H	-2.117054	-4.674421	-1.609518
	= 12.80835  Kcal/m			H	-3.840494	-4.344316	-1.263772
	I-V/def2-TZVP) = -		Hartree	H	-2.727442	-4.750555	0.074456
	xTB) = -132.17764			C	-3.465796	-2.079235	0.329026
	$^{\circ}$ XTB) = -130.92520 $^{\circ}$ F) = -18.18289164			H H	-3.227010 -3.429388	-1.013610 -2.611091	0.509993 1.302246
E (GEN-E	r) = -10.10209109	10000 Hartree		H	-4.509958	-2.126696	-0.043150
Coordin	ates:			C	1.210134	1.359027	1.580302
Со	-0.524023	0.313364	-0.282308	C	0.843076	0.867344	2.870175
С	-2.133803	1.496291	-0.467672	C	0.721206	1.779623	3.929786
H	-1.885718	2.421581	-1.037301	H	0.447976	1.414599	4.930645
H	-2.737215	0.868477	-1.165412	C	0.938092	3.152000	3.732622
C	-2.960112	1.852405	0.768044	H	0.834320	3.852825	4.574451
H	-3.914745	2.347536	0.460819	С	1.272801	3.625259	2.458670
H	-3.283656	0.922686	1.283221	H	1.432264	4.704286	2.307020
C	-2.241343	2.774228	1.759163	C	1.414087	2.751100	1.365505
H H	-1.892325 -1.312586	3.668343 2.279700	1.197422 2.111553	C H	0.530905 1.177417	-0.612974 -1.170619	3.044842 2.335994
С	-3.047517	3.251715	2.977195	C C	-0.926774	-0.888373	2.636852
Н	-2.527274	4.140281	3.395558	Н	-1.135867	-1.973474	2.550979
Н	-4.046778	3.618969	2.646296	Н	-1.174833	-0.412112	1.656423
С	-3.230838	2.248123	4.129660	H	-1.634891	-0.446111	3.366475
H	-3.564957	2.813945	5.026994	С	0.815389	-1.155293	4.449636
H	-2.233387	1.832789	4.398267	H	0.665530	-2.253540	4.476553
C	-4.221634	1.104073	3.893184	H	0.135835	-0.717177	5.209427
H	-5.209805	1.490946	3.566660	H	1.857514	-0.943205	4.763664
H	-4.383751	0.516331	4.820223	C	1.794549	3.293760	-0.006493
H	-3.877448	0.396101	3.113341	H	1.864000	2.421809	-0.687888
N N	-0.193693 1.261664	-1.125092 0.452191	-1.564675 0.491321	C H	0.711082 -0.274651	4.234078 3.732425	-0.559190 -0.586230
C	1.172595	-3.136628	-2.400775	H	0.962707	4.561167	-1.588980
C	0.966794	-1.789674	-1.625786	Н	0.609586	5.143800	0.068567
Ċ	2.081135	-1.382393	-0.846847	C	3.166170	3.990625	0.005303
H	2.970236	-1.992633	-1.008613	H	3.967192	3.321125	0.376908
C	2.257583	-0.379150	0.141297	H	3.158239	4.892654	0.652057
C	3.714114	-0.322241	0.722379	H	3.444819	4.318072	-1.017528
C	0.118053	-3.461210	-3.476531				
H	0.385397	-4.430334	-3.945119		rmation 16.		
H H	0.077745 -0.899252	-2.701035 -3.561911	-4.276030 -3.064004	Charge	plicity: 4		
С	2.554657	-3.189671	-3.095874		-3c) = -3093.978690	751810 Hartree	
Н	2.632155	-4.125965	-3.684598		def2-TZVP) = -3093		rtree
Н	3.402319	-3.187106	-2.384218		- D3(BJ)/def2-TZVP		
H	2.694836	-2.339826	-3.792481	E (PBE)	) - D3(BJ)/def2-TZV	P) = -3092.84138	6704271 Hartree
C	1.117613	-4.256407	-1.329418		n-3c) = -3089.87640		
H	1.255726	-5.248237	-1.808515		= 2.70757  Kcal/mo		
H	0.139735	-4.264463	-0.809129		= 7.79350  Kcal/mo		
H	1.906917	-4.126367	-0.563122 -0.424048		7X-V/def2-TZVP) = -		6 Hartree
C H	4.635564 5.686728	0.161935 0.218005	-0.424048		1-xTB) = $-132.188632-xTB$ ) = $-130.93852$		
H	4.336170	1.172173	-0.769264		-FF) = $-18.19561164$		
Н	4.598871	-0.515881	-1.298575	D (0111	11, 10.13301101	OJIZ HATCICC	
C	4.153855	-1.733521	1.185755	Coord	inates:		
H	3.460877	-2.130136	1.955512	Co	-0.083465	0.571433	-0.016518
H	5.165451	-1.677084	1.637105	C	-1.800136	1.560192	0.155315
H	4.201937	-2.470665	0.362276	H	-1.565215	2.246802	1.006881
С	3.942461	0.607754	1.929271	H	-1.900516	2.206356	-0.746340
H	3.358359	0.301635	2.816456	C	-3.073567	0.772835	0.436997
H	3.701488	1.663132	1.720189	H	-3.318847	0.122016	-0.432285 1.284263
H	5.016559	0.557527	2.201671	H	-2.901365	0.075823	
C C	-1.329529 -1.378847	-1.191209 -0.376396	-2.407251 -3.579841	C H	-4.300600 -4.471405	1.647972 2.341815	0.749746 -0.102629
C	-2.558004	-0.399984	-4.348459	п Н	-4.066228	2.298523	1.623695
Н	-2.601337	0.218870	-5.259371	C	-5.585162	0.857775	1.033978
C	-3.673491	-1.160411	-3.977066	Н	-6.446753	1.560979	1.083726
H	-4.582161	-1.152192	-4.597417	H	-5.798140	0.184001	0.172055
С	-3.631248	-1.903568	-2.791816	С	-5.548256	0.026184	2.321303
H	-4.517519	-2.477101	-2.478042	H	-5.325270	0.700382	3.179163
С	-2.479099	-1.926152	-1.988248	H	-4.699695	-0.689393	2.280543

С	-6.843769	-0.740114	2.588916	H	-1.362398	-1.294019	-1.222027
H	-7.712748	-0.054270	2.678191	H	-2.809163	-2.348889	-1.187060
Н	-6.787415	-1.331118	3.526013	H	-1.445828	-2.732425	-2.297303
H	-7.069823	-1.447493	1.763092				
N	1.357685	0.848207	-1.248164	Confo	rmation 2.		
N	0.575051	-1.022831	0.839738		olicity: 4		
C	3.610446	0.257804	-2.346332	Charge			
C	2.453494	0.076663	-1.310169		-3c) = -3093.97373	8702698 Hartree	
Č	2.614237	-1.024329	-0.430809		/def2-TZVP) = -3093		rt.ree
Н	3.555048	-1.564362	-0.563563		- D3(BJ)/def2-TZV		
С	1.771055	-1.572780	0.568709		0 - D3(BJ)/def2-TZ		
C	2.383034	-2.806448	1.318911		h-3c) = -3089.8725		
C	3.613275	-0.985225	-3.269076		= 6.30908  Kcal/m		
Н	4.432803	-0.904604	-4.013155		) = 12.43891 Kcal/r		
Н	2.656427	-1.067194	-3.823012		7X-V/def2-TZVP) = -		8 Hartree
H	3.755649	-1.925975	-2.703200		1-xTB) = $-132.1809$		
С	3.519960	1.503005	-3.248019		2-xTB) = -130.9308		
Н	4.383408	1.487715	-3.943989		-FF) = -18.1910797		
H	3.570489	2.446513	-2.675606	•	•		
H	2.600690	1.532924	-3.858428	Coord	inates:		
С	4.960290	0.353733	-1.594062	Co	0.452602	0.297322	0.045668
Н	5.782290	0.515453	-2.321194	С	0.782289	2.247110	-0.224105
H	5.200268	-0.560524	-1.018598	Н	0.724814	2.728845	0.777499
H	4.958957	1.208070	-0.887031	H	1.863152	2.279272	-0.510358
С	1.523232	-3.403488	2.449873	С	-0.082912	2.963848	-1.250804
Н	2.118385	-4.188463	2.959526	Н	-0.042824	2.431923	-2.226364
H	0.595477	-3.875897	2.082546	H	-1.145058	2.909470	-0.942683
Н	1.236939	-2.655591	3.210739	С	0.309133	4.433009	-1.501086
С	3.721361	-2.358298	1.961873	H	1.387384	4.451346	-1.774358
Н	4.456497	-2.008253	1.212712	H	0.237601	5.007606	-0.549015
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				H	1.836643	1.500194	-3.264264
Conform	mation 20.			H	2.152073	3.206820	-3.711235
Multip	licity: 4			H	0.580319	2.461567	-4.109509
Charge:				C	0.167960	4.356838	-2.114941
_	3c) = -3093.97659	2267044 H		Н	-0.333777	4.671370	-1.179395
	,	3.641615779439 Ha		H	-0.586319	4.382435	-2.928271
E(PBE -	- D3(BJ)/def2-TZV	P) = -3092.615921	271834 Hartree	H	0.945381	5.114203	-2.348366
E(PBE0	- D3(BJ)/def2-TZ	VP) = -3092.83926	3194862 Hartree	C	-1.490589	-1.897959	-0.434465
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	= 4.82982 Kcal/m			С	-0.724310	-4.202473	-0.585229
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		-3095.70120859139	b Hartree	С	-1.277764	-4.313580	-1.866573
	-xTB) = $-132.1868$			H	-1.189035	-5.255621	-2.428228
E (GFN2-	-xTB) = -130.9354	27281578 Hartree		C	-1.938076	-3.214027	-2.433637
E (GFN-I	FF) = -18.1954902	42084 Hartree		H	-2.366477	-3.304111	-3.443151
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Coordin	nates:				-2.058022		-1./41992
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	0.240518	0.095806	-0.354780	H	-0.186205 -0.277289	-2.921266 -1.866259	1.538113 1.869272
C	0.240518 1.647642	-0.838363	-1.396767	H C	-0.186205 -0.277289 1.310594	-2.921266 -1.866259 -3.270084	1.538113 1.869272 1.513815
	0.240518			H	-0.186205 -0.277289	-2.921266 -1.866259	1.538113 1.869272
C	0.240518 1.647642	-0.838363	-1.396767	H C	-0.186205 -0.277289 1.310594	-2.921266 -1.866259 -3.270084	1.538113 1.869272 1.513815
C H H	0.240518 1.647642 1.316596 1.443900	-0.838363 -1.898850 -0.496887	-1.396767 -1.344256 -2.442000	H C H H	-0.186205 -0.277289 1.310594 1.758104 1.861174	-2.921266 -1.866259 -3.270084 -3.147069 -2.615170	1.538113 1.869272 1.513815 2.520997 0.812650
C H H C	0.240518 1.647642 1.316596 1.443900 3.124062	-0.838363 -1.898850 -0.496887 -0.686425	-1.396767 -1.344256 -2.442000 -1.058468	H C H H	-0.186205 -0.277289 1.310594 1.758104 1.861174 1.479222	-2.921266 -1.866259 -3.270084 -3.147069 -2.615170 -4.320880	1.538113 1.869272 1.513815 2.520997 0.812650 1.199732
C H H C H	0.240518 1.647642 1.316596 1.443900 3.124062 3.410733	-0.838363 -1.898850 -0.496887 -0.686425 0.388065	-1.396767 -1.344256 -2.442000 -1.058468 -1.079016	H C H H C	-0.186205 -0.277289 1.310594 1.758104 1.861174 1.479222 -0.933312	-2.921266 -1.866259 -3.270084 -3.147069 -2.615170 -4.320880 -3.805916	1.538113 1.869272 1.513815 2.520997 0.812650 1.199732 2.552076
C H H C H H	0.240518 1.647642 1.316596 1.443900 3.124062 3.410733 3.300141	-0.838363 -1.898850 -0.496887 -0.686425 0.388065 -1.013919	-1.396767 -1.344256 -2.442000 -1.058468 -1.079016 -0.009458	H C H H C	-0.186205 -0.277289 1.310594 1.758104 1.861174 1.479222 -0.933312 -0.500992	-2.921266 -1.866259 -3.270084 -3.147069 -2.615170 -4.320880 -3.805916 -3.689460	1.538113 1.869272 1.513815 2.520997 0.812650 1.199732 2.552076 3.567299
С Н С Н С	0.240518 1.647642 1.316596 1.443900 3.124062 3.410733 3.300141 4.095247	-0.838363 -1.898850 -0.496887 -0.686425 0.388065 -1.013919 -1.476103	-1.396767 -1.344256 -2.442000 -1.058468 -1.079016 -0.009458 -1.963819	H C H H C H	-0.186205 -0.277289 1.310594 1.758104 1.861174 1.479222 -0.933312 -0.500992 -0.860219	-2.921266 -1.866259 -3.270084 -3.147069 -2.615170 -4.320880 -3.805916 -3.689460 -4.878770	1.538113 1.869272 1.513815 2.520997 0.812650 1.199732 2.552076 3.567299 2.277208
С Н С Н С Н	0.240518 1.647642 1.316596 1.443900 3.124062 3.410733 3.300141 4.095247 5.131309	-0.838363 -1.898850 -0.496887 -0.686425 0.388065 -1.013919	-1.396767 -1.344256 -2.442000 -1.058468 -1.079016 -0.009458	H C H H C	-0.186205 -0.277289 1.310594 1.758104 1.861174 1.479222 -0.933312 -0.500992	-2.921266 -1.866259 -3.270084 -3.147069 -2.615170 -4.320880 -3.805916 -3.689460	1.538113 1.869272 1.513815 2.520997 0.812650 1.199732 2.552076 3.567299
С Н С Н С	0.240518 1.647642 1.316596 1.443900 3.124062 3.410733 3.300141 4.095247	-0.838363 -1.898850 -0.496887 -0.686425 0.388065 -1.013919 -1.476103	-1.396767 -1.344256 -2.442000 -1.058468 -1.079016 -0.009458 -1.963819	H C H H C H	-0.186205 -0.277289 1.310594 1.758104 1.861174 1.479222 -0.933312 -0.500992 -0.860219	-2.921266 -1.866259 -3.270084 -3.147069 -2.615170 -4.320880 -3.805916 -3.689460 -4.878770	1.538113 1.869272 1.513815 2.520997 0.812650 1.199732 2.552076 3.567299 2.277208
С Н С Н С Н Н	0.240518 1.647642 1.316596 1.443900 3.124062 3.410733 3.300141 4.095247 5.131309 4.019930	-0.838363 -1.898850 -0.496887 -0.686425 0.388065 -1.013919 -1.476103 -1.242336 -1.098734	-1.396767 -1.344256 -2.442000 -1.058468 -1.079016 -0.009458 -1.963819 -1.634972 -3.009165	H C H H C H H	-0.186205 -0.277289 1.310594 1.758104 1.861174 1.479222 -0.933312 -0.500992 -0.860219 -2.010152 -2.720154	-2.921266 -1.866259 -3.270084 -3.147069 -2.615170 -4.320880 -3.805916 -3.689460 -4.878770 -3.551636	1.538113 1.869272 1.513815 2.520997 0.812650 1.199732 2.552076 3.567299 2.277208 2.610330 -2.394847
С Н Н С Н С Н С С	0.240518 1.647642 1.316596 1.443900 3.124062 3.410733 3.300141 4.095247 5.131309 4.019930 3.891193	-0.838363 -1.898850 -0.496887 -0.686425 0.388065 -1.013919 -1.476103 -1.242336 -1.098734 -3.004023	-1.396767 -1.344256 -2.442000 -1.058468 -1.079016 -0.009458 -1.963819 -1.634972 -3.009165 -1.954568	H C H H C H H C H	-0.186205 -0.277289 1.310594 1.758104 1.861174 1.479222 -0.933312 -0.500992 -0.860219 -2.010152 -2.720154 -3.025323	-2.921266 -1.866259 -3.270084 -3.147069 -2.615170 -4.320880 -3.805916 -3.689460 -4.878770 -3.551636 -0.789089 -0.099764	1.538113 1.869272 1.513815 2.520997 0.812650 1.199732 2.552076 3.567299 2.277208 2.610330 -2.394847 -1.580717
С Н С Н С Н С Н С Н	0.240518 1.647642 1.316596 1.443900 3.124062 3.410733 3.300141 4.095247 5.131309 4.019930 3.891193 4.871999	-0.838363 -1.898850 -0.496887 -0.686425 0.388065 -1.013919 -1.476103 -1.242336 -1.098734 -3.004023 -3.512957	-1.396767 -1.344256 -2.442000 -1.058468 -1.079016 -0.009458 -1.963819 -1.634972 -3.009165 -1.954568 -2.084651	Н С Н Н С Н Н С Н Н С Н С С Н С С Н С С С С С С С С С С С С С С С С С С С С	-0.186205 -0.277289 1.310594 1.758104 1.861174 1.479222 -0.933312 -0.500992 -0.860219 -2.010152 -2.720154 -3.025323 -1.701060	-2.921266 -1.866259 -3.270084 -3.147069 -2.615170 -4.320880 -3.805916 -3.689460 -4.878770 -3.551636 -0.789089 -0.099764 -0.029859	1.538113 1.869272 1.513815 2.520997 0.812650 1.199732 2.552076 3.567299 2.277208 2.610330 -2.394847 -1.580717 -3.262775
С Н С Н С Н С Н С Н	0.240518 1.647642 1.316596 1.443900 3.124062 3.410733 3.300141 4.095247 5.131309 4.019930 3.891193 4.871999 3.533003	-0.838363 -1.898850 -0.496887 -0.686425 0.388065 -1.013919 -1.476103 -1.242336 -1.098734 -3.004023 -3.512957 -3.314349	-1.396767 -1.344256 -2.442000 -1.058468 -1.079016 -0.009458 -1.963819 -1.634972 -3.009165 -1.954568 -2.084651 -0.945668	Н С Н Н С Н Н С Н Н С Н Н С Н Н С Н Н С Н Н С Н Н С С Н С Н Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н Н С Н С Н С Н С Н Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н Н С Н Н С Н Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н В Н В	-0.186205 -0.277289 1.310594 1.758104 1.861174 1.479222 -0.933312 -0.500992 -0.860219 -2.010152 -2.720154 -3.025323 -1.701060 -0.820689	-2.921266 -1.866259 -3.270084 -3.147069 -2.615170 -4.320880 -3.805916 -3.689460 -4.878770 -3.551636 -0.789089 -0.099764 -0.029859 0.269178	1.538113 1.869272 1.513815 2.520997 0.812650 1.199732 2.552076 3.567299 2.277208 2.610330 -2.394847 -1.580717 -3.262775 -2.655993
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С Н С Н С Н С Н С Н	0.240518 1.647642 1.316596 1.443900 3.124062 3.410733 3.300141 4.095247 5.131309 4.019930 3.891193 4.871999 3.533003	-0.838363 -1.898850 -0.496887 -0.686425 0.388065 -1.013919 -1.476103 -1.242336 -1.098734 -3.004023 -3.512957 -3.314349	-1.396767 -1.344256 -2.442000 -1.058468 -1.079016 -0.009458 -1.963819 -1.634972 -3.009165 -1.954568 -2.084651 -0.945668	Н С Н Н С Н Н С Н Н С Н Н С Н Н С Н Н С Н Н С Н Н С С Н С Н Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н Н С Н С Н С Н С Н Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н Н С Н Н С Н Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н В Н В	-0.186205 -0.277289 1.310594 1.758104 1.861174 1.479222 -0.933312 -0.500992 -0.860219 -2.010152 -2.720154 -3.025323 -1.701060 -0.820689	-2.921266 -1.866259 -3.270084 -3.147069 -2.615170 -4.320880 -3.805916 -3.689460 -4.878770 -3.551636 -0.789089 -0.099764 -0.029859 0.269178	1.538113 1.869272 1.513815 2.520997 0.812650 1.199732 2.552076 3.567299 2.277208 2.610330 -2.394847 -1.580717 -3.262775 -2.655993
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СННСННСННСННСННИЙСССНС	0.240518 1.647642 1.316596 1.443900 3.124062 3.410733 3.300141 4.095247 5.131309 4.019930 3.891193 4.871999 3.533003 2.929024 3.347114 1.964807 2.665621 3.606312 1.986841 2.191037 0.142877 -1.440368 -1.065339 -0.924642 -2.061791 -2.867818 -2.333654	-0.838363 -1.898850 -0.496887 -0.6866425 0.388065 -1.013919 -1.476103 -1.242336 -1.098734 -3.004023 -3.512957 -3.314349 -3.549652 -3.329238 -3.002135 -5.048939 -5.636920 -5.422741 -5.280123 1.768822 -0.634213 3.580789 2.175282 1.338879 1.777790 0.025572	-1.396767 -1.344256 -2.442000 -1.058468 -1.079016 -0.009458 -1.963819 -1.634972 -3.009165 -1.954568 -2.084651 -0.945668 -3.019399 -4.027169 -2.970571 -2.881545 -2.938667 -3.675017 -1.904393 0.573120 0.205192 1.951799 1.278199 1.418706 2.012422 0.957987	H C H H C H H C H H C H H H C H H H E (B97- E(M06/ E(B98- E(PBE0	-0.186205 -0.277289 1.310594 1.758104 1.861174 1.479222 -0.933312 -0.500992 -0.860219 -2.010152 -2.720154 -3.025323 -1.7701060 -0.820689 -2.145002 -1.333558 -3.981378 -4.709509 -3.749302 -4.481312  mation 23.  licity: 4 :: 0 :3c) = -3093.97067' def2-TZVP) = -309' - D3(BJ)/def2-TZVI) - D3(BJ)/def2-TZVI	-2.921266 -1.866259 -3.270084 -3.147069 -2.615170 -4.320880 -3.805916 -3.689460 -4.878770 -3.551636 -0.789089 -0.099764 -0.029859 0.269178 0.890477 -0.666161 -1.141345 -1.709925 -1.751134 -0.218017	1.538113 1.869272 1.513815 2.520997 0.812650 1.199732 2.552076 3.567299 2.277208 2.610330 -2.394847 -1.580717 -3.262775 -2.655993 -3.695593 -4.094138 -3.195125 -2.581601 -4.092461 -3.552135
СННСННСННСННКИМСССНСС	0.240518 1.647642 1.316596 1.443900 3.124062 3.410733 3.300141 4.095247 5.131309 4.019930 3.891193 4.871999 3.533003 2.929024 3.347114 1.964807 2.665621 3.606312 1.986841 2.191037 0.142877 -1.440368 -1.065339 -0.924642 -2.061791 -2.867818 -2.333654 -3.693498	-0.838363 -1.898850 -0.496887 -0.686425 0.388065 -1.013919 -1.476103 -1.242336 -1.098734 -3.004023 -3.512957 -3.314349 -3.549652 -3.329238 -3.002135 -5.048939 -5.636920 -5.422741 -5.280123 1.768822 -0.634213 3.580789 2.175282 1.338879 1.777790 0.025572 -0.569641	-1.396767 -1.344256 -2.442000 -1.058468 -1.079016 -0.009458 -1.963819 -1.634972 -3.009165 -1.954568 -2.084651 -0.945668 -3.019399 -4.027169 -2.970571 -2.881545 -2.938667 -3.675017 -1.904393 0.573120 0.205192 1.951799 1.278199 1.418706 2.012422 0.957987 1.444153	H C H H C H H C H H C H H H C H H H C E (B97- E(M06/ E(PBE0) E(PBE0) E(PBE0)	-0.186205 -0.277289 1.310594 1.758104 1.861174 1.479222 -0.933312 -0.500992 -0.860219 -2.010152 -2.720154 -3.025323 -1.701060 -0.820689 -2.145002 -1.333558 -3.981378 -4.709509 -3.749302 -4.481312  mation 23.  plicity: 4 10 3c) = -3093.97067 def2-TZVP) = -3093.97067 def2-TZVP) = -3093.97067	-2.921266 -1.866259 -3.270084 -3.147069 -2.615170 -4.320880 -3.805916 -3.689460 -4.878770 -3.551636 -0.789089 -0.099764 -0.029859 0.269178 0.890477 -0.666161 -1.141345 -1.709925 -1.751134 -0.218017	1.538113 1.869272 1.513815 2.520997 0.812650 1.199732 2.552076 3.567299 2.277208 2.610330 -2.394847 -1.580717 -3.262775 -2.655993 -3.695593 -4.094138 -3.195125 -2.581601 -4.092461 -3.552135
СННСННСННСННСННИЙСССНССС	0.240518 1.647642 1.316596 1.443900 3.124062 3.410733 3.300141 4.095247 5.131309 4.019930 3.891193 4.871999 3.533003 2.929024 3.347114 1.964807 2.665621 3.606312 1.986841 2.191037 0.142877 -1.440368 -1.065339 -0.924642 -2.061791 -2.867818 -2.333654 -3.693498 0.158414	-0.838363 -1.898850 -0.496887 -0.686425 0.388065 -1.013919 -1.476103 -1.242336 -1.098734 -3.004023 -3.512957 -3.314349 -3.549652 -3.329238 -3.002135 -5.048939 -5.636920 -5.422741 -5.280123 1.768822 -0.634213 3.580789 2.175282 1.338879 1.777790 0.025572 -0.569641 4.508136	-1.396767 -1.344256 -2.442000 -1.058468 -1.079016 -0.009458 -1.963819 -1.634972 -3.009165 -1.954568 -2.084651 -0.945668 -3.019399 -4.027169 -2.970571 -2.881545 -2.938667 -3.675017 -1.904393 0.573120 0.205192 1.951799 1.278199 1.418706 2.012422 0.957987 1.444153 1.831316	H C H H C H H C H H C H H C H H C E (B97- E (M06/ E (PBE E (PBE) E (PBE) E (PBE) E (PBE) E	-0.186205 -0.277289 1.310594 1.758104 1.861174 1.479222 -0.933312 -0.5500992 -0.860219 -2.010152 -2.720154 -3.025323 -1.701060 -0.820689 -2.145002 -1.333558 -3.981378 -4.709509 -3.749302 -4.481312  mation 23. plicity: 4 10 10 10 10 10 10 10 10 10 10 10 10 10	-2.921266 -1.866259 -3.270084 -3.147069 -2.615170 -4.320880 -3.805916 -3.689460 -4.878770 -3.551636 -0.789089 -0.099764 -0.029859 0.269178 0.890477 -0.666161 -1.141345 -1.709925 -1.751134 -0.218017	1.538113 1.869272 1.513815 2.520997 0.812650 1.199732 2.552076 3.567299 2.277208 2.610330 -2.394847 -1.580717 -3.262775 -2.655993 -3.695593 -4.094138 -3.195125 -2.581601 -4.092461 -3.552135
СННСННСННСННСНННИЙСССНСССН	0.240518 1.647642 1.316596 1.443900 3.124062 3.410733 3.300141 4.095247 5.131309 4.019930 3.891193 4.871999 3.533003 2.929024 3.347114 1.964807 2.665621 3.606312 1.986841 2.191037 0.142877 -1.440368 -1.065339 -0.924642 -2.061791 -2.867818 -2.333654 -3.693498 0.158414 -0.105338	-0.838363 -1.898850 -0.496887 -0.686425 0.388065 -1.013919 -1.476103 -1.242336 -1.098734 -3.004023 -3.512957 -3.314349 -3.549652 -3.329238 -3.002135 -5.048939 -5.636920 -5.422741 -5.280123 1.768822 -0.634213 3.580789 2.175282 1.338879 1.777790 0.025572 -0.569641 4.508136 5.489697	-1.396767 -1.344256 -2.442000 -1.058468 -1.079016 -0.009458 -1.963819 -1.634972 -3.009165 -1.954568 -2.084651 -0.945668 -3.019399 -4.027169 -2.970571 -2.881545 -2.938667 -3.675017 -1.904393 0.573120 0.205192 1.951799 1.278199 1.418706 2.012422 0.957987 1.444153 1.831316 2.275112	H C H H H C C H H C C H H H C C H H H C C H E (B97- E (M06- E)(PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E	-0.186205 -0.277289 1.310594 1.758104 1.861174 1.479222 -0.933312 -0.500992 -0.860219 -2.010152 -2.720154 -3.025323 -1.701060 -0.820689 -2.145002 -1.333558 -3.981378 -4.709509 -3.749302 -4.481312  mation 23. Dicity: 4 :: 0 :0 :0 = -3093.97067' def2-TZVP) = -309: - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - 3c) = -3089.87504 = 9.33738 Kcal/m = 9.33738 Kcal/m	-2.921266 -1.866259 -3.270084 -3.147069 -2.615170 -4.320880 -3.805916 -3.689460 -4.878770 -3.551636 -0.789089 -0.099764 -0.029859 0.269178 0.890477 -0.666161 -1.141345 -1.709925 -1.751134 -0.218017	1.538113 1.869272 1.513815 2.520997 0.812650 1.199732 2.552076 3.567299 2.277208 2.610330 -2.394847 -1.580717 -3.262775 -2.655993 -3.695593 -4.094138 -3.195125 -2.581601 -4.092461 -3.552135
СННСННСННСННСННИЙИСССНСССН	0.240518 1.647642 1.316596 1.443900 3.124062 3.410733 3.300141 4.095247 5.131309 4.019930 3.891193 4.871999 3.533003 2.929024 3.347114 1.964807 2.665621 3.606312 1.986841 2.191037 0.142877 -1.440368 -1.065339 -0.924642 -2.061791 -2.867818 -2.333654 -3.693498 0.158414 -0.105338 0.461873	-0.838363 -1.898850 -0.496887 -0.6866425 0.388065 -1.013919 -1.476103 -1.242336 -1.098734 -3.004023 -3.512957 -3.314349 -3.549652 -3.329238 -3.002135 -5.048939 -5.636920 -5.422741 -5.280123 1.768822 -0.634213 3.580789 2.175282 1.338879 1.777790 0.025572 -0.569641 4.508136 5.489697 4.684970	-1.396767 -1.344256 -2.442000 -1.058468 -1.079016 -0.009458 -1.963819 -1.634972 -3.009165 -1.954568 -2.084651 -0.945668 -3.019399 -4.027169 -2.970571 -2.881545 -2.938667 -3.675017 -1.904393 0.573120 0.205192 1.951799 1.278199 1.418706 2.012422 0.957987 1.444153 1.831316 2.275112 0.784271	H C H H H C H H C H H C H H C H H H C C H H H H C C H H H H C C H H H H H C C H H H H H C C H H H H H C C H H H H H C C H H H H H H C C H H H H H H C C H H H H H H C C H H H H H H C C H H H H H H C C H H H H H H H C C H H H H H H H C C H H H H H H H H C C H H H H H H H H H C C H H H H H H H H H H H C C H H H H H H H H H H H H H H H H H H H H	-0.186205 -0.277289 1.310594 1.758104 1.861174 1.479222 -0.933312 -0.500992 -0.860219 -2.010152 -2.720154 -3.025323 -1.701060 -0.820689 -2.145002 -1.333558 -3.981378 -4.709509 -3.749302 -4.481312  mation 23. elicity: 4 :: 0 -3c) = -3093.97067 def2-TZVP) = -3093 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - 9.33738 Kcal/m = 12.06737 Kcal/m X-V/def2-TZVP) = -	-2.921266 -1.866259 -3.270084 -3.147069 -2.615170 -4.320880 -3.805916 -3.689460 -4.878770 -3.551636 -0.789089 -0.099764 -0.029859 0.269178 0.890477 -0.666161 -1.141345 -1.709925 -1.751134 -0.218017	1.538113 1.869272 1.513815 2.520997 0.812650 1.199732 2.552076 3.567299 2.277208 2.610330 -2.394847 -1.580717 -3.262775 -2.655993 -3.695593 -4.094138 -3.195125 -2.581601 -4.092461 -3.552135
СННСННСННСННСННИЙОССНСССННН	0.240518 1.647642 1.316596 1.443900 3.124062 3.410733 3.300141 4.095247 5.131309 4.019930 3.891193 4.871999 3.533003 2.929024 3.347114 1.964807 2.665621 3.606312 1.986841 2.191037 0.142877 -1.440368 -1.065339 -0.924642 -2.061791 -2.867818 -2.333654 -3.693498 0.158414 -0.105338 0.461873 1.042059	-0.838363 -1.898850 -0.496887 -0.6866425 0.388065 -1.013919 -1.476103 -1.242336 -1.098734 -3.004023 -3.512957 -3.314349 -3.549652 -3.329238 -3.002135 -5.048939 -5.636920 -5.422741 -5.280123 1.768822 -0.634213 3.580789 2.175282 1.338879 1.777790 0.025572 -0.569641 4.508136 5.489697 4.684970 4.125448	-1.396767 -1.344256 -2.442000 -1.058468 -1.079016 -0.009458 -1.963819 -1.634972 -3.009165 -1.954568 -2.084651 -0.945668 -3.019399 -4.027169 -2.970571 -2.881545 -2.938667 -3.675017 -1.904393 0.573120 0.205192 1.951799 1.278199 1.418706 2.012422 0.957987 1.444153 1.831316 2.275112 0.784271 2.371277	H C H H H C H H C H H C H H C H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H H C C H H H H C C H H H H H C C H H H H H C C H H H H H C C H H H H H C C H H H H H C C H H H H H C C H H H H H H C C H H H H H H C C H H H H H H C C H H H H H H H C C H H H H H H H C C H H H H H H H C C H H H H H H H H H H C C H H H H H H H H H H H C C H H H H H H H H H H H C C H H H H H H H H H H H H H H H H H H H H	-0.186205 -0.277289 1.310594 1.758104 1.861174 1.479222 -0.933312 -0.500992 -0.860219 -2.010152 -2.720154 -3.025323 -1.701060 -0.820689 -2.145002 -1.333558 -3.981378 -4.709509 -3.749302 -4.481312  mation 23.  chicity: 4 chickly: 4	-2.921266 -1.866259 -3.270084 -3.147069 -2.615170 -4.320880 -3.805916 -3.689460 -4.878770 -3.551636 -0.789089 -0.099764 -0.029859 0.269178 0.890477 -0.666161 -1.141345 -1.709925 -1.751134 -0.218017	1.538113 1.869272 1.513815 2.520997 0.812650 1.199732 2.552076 3.567299 2.277208 2.610330 -2.394847 -1.580717 -3.262775 -2.655993 -3.695593 -4.094138 -3.195125 -2.581601 -4.092461 -3.552135
СННСННСННСННСННКИСССНСССННС	0.240518 1.647642 1.316596 1.443900 3.124062 3.410733 3.300141 4.095247 5.131309 4.019930 3.891193 4.871999 3.533003 2.929024 3.347114 1.964807 2.665621 3.606312 1.986841 2.191037 0.142877 -1.440368 -1.065339 -0.924642 -2.061791 -2.867818 -2.333654 -3.693498 0.158414 -0.105338 0.461873	-0.838363 -1.898850 -0.496887 -0.6866425 0.388065 -1.013919 -1.476103 -1.242336 -1.098734 -3.004023 -3.512957 -3.314349 -3.549652 -3.329238 -3.002135 -5.048939 -5.636920 -5.422741 -5.280123 1.768822 -0.634213 3.580789 2.175282 1.338879 1.777790 0.025572 -0.569641 4.508136 5.489697 4.684970	-1.396767 -1.344256 -2.442000 -1.058468 -1.079016 -0.009458 -1.963819 -1.634972 -3.009165 -1.954568 -2.084651 -0.945668 -3.019399 -4.027169 -2.970571 -2.881545 -2.938667 -3.675017 -1.904393 0.573120 0.205192 1.951799 1.278199 1.418706 2.012422 0.957987 1.444153 1.831316 2.275112 0.784271 2.371277 1.274201	H C H H H C H H C H H C H H C H H C H H C H H C H H C H H H C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H H H H C H H H H H H H H H H H H H H H H H H H H	-0.186205 -0.277289 1.310594 1.758104 1.861174 1.479222 -0.933312 -0.500992 -0.860219 -2.010152 -2.720154 -3.025323 -1.701060 -0.820689 -2.145002 -1.333558 -3.981378 -4.709509 -3.749302 -4.481312  mation 23. vlicity: 4 :0 3c) = -3093.97067 def2-TZVP) = -3093 -D3(BJ)/def2-TZVI -D3(BJ)/def2-TZVI -3c) = -3089.8750 = 9.33738 Kcal/mc = 12.06737 Kcal/mc = -xTB) = -132.1811	-2.921266 -1.866259 -3.270084 -3.147069 -2.615170 -4.320880 -3.805916 -3.689460 -4.878770 -3.551636 -0.789089 -0.099764 -0.029859 0.269178 0.890477 -0.666161 -1.141345 -1.709925 -1.751134 -0.218017	1.538113 1.869272 1.513815 2.520997 0.812650 1.199732 2.552076 3.567299 2.277208 2.610330 -2.394847 -1.580717 -3.262775 -2.655993 -3.695593 -4.094138 -3.195125 -2.581601 -4.092461 -3.552135
СННСННСННСННСННИЙОССНСССННН	0.240518 1.647642 1.316596 1.443900 3.124062 3.410733 3.300141 4.095247 5.131309 4.019930 3.891193 4.871999 3.533003 2.929024 3.347114 1.964807 2.665621 3.606312 1.986841 2.191037 0.142877 -1.440368 -1.065339 -0.924642 -2.061791 -2.867818 -2.333654 -3.693498 0.158414 -0.105338 0.461873 1.042059	-0.838363 -1.898850 -0.496887 -0.6866425 0.388065 -1.013919 -1.476103 -1.242336 -1.098734 -3.004023 -3.512957 -3.314349 -3.549652 -3.329238 -3.002135 -5.048939 -5.636920 -5.422741 -5.280123 1.768822 -0.634213 3.580789 2.175282 1.338879 1.777790 0.025572 -0.569641 4.508136 5.489697 4.684970 4.125448	-1.396767 -1.344256 -2.442000 -1.058468 -1.079016 -0.009458 -1.963819 -1.634972 -3.009165 -1.954568 -2.084651 -0.945668 -3.019399 -4.027169 -2.970571 -2.881545 -2.938667 -3.675017 -1.904393 0.573120 0.205192 1.951799 1.278199 1.418706 2.012422 0.957987 1.444153 1.831316 2.275112 0.784271 2.371277	H C H H H C H H C H H C H H C H H C H H C H H C H H C H H H C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H H H H C H H H H H H H H H H H H H H H H H H H H	-0.186205 -0.277289 1.310594 1.758104 1.861174 1.479222 -0.933312 -0.500992 -0.860219 -2.010152 -2.720154 -3.025323 -1.701060 -0.820689 -2.145002 -1.333558 -3.981378 -4.709509 -3.749302 -4.481312  mation 23.  chicity: 4 chickly: 4	-2.921266 -1.866259 -3.270084 -3.147069 -2.615170 -4.320880 -3.805916 -3.689460 -4.878770 -3.551636 -0.789089 -0.099764 -0.029859 0.269178 0.890477 -0.666161 -1.141345 -1.709925 -1.751134 -0.218017	1.538113 1.869272 1.513815 2.520997 0.812650 1.199732 2.552076 3.567299 2.277208 2.610330 -2.394847 -1.580717 -3.262775 -2.655993 -3.695593 -4.094138 -3.195125 -2.581601 -4.092461 -3.552135
СННСННСННСННСННКИСССНСССННС	0.240518 1.647642 1.316596 1.443900 3.124062 3.410733 3.300141 4.095247 5.131309 4.019930 3.891193 4.871999 3.533003 2.929024 3.347114 1.964807 2.665621 3.606312 1.986841 2.191037 0.142877 -1.440368 -1.065339 -0.924642 -2.061791 -2.867818 -2.333654 -3.693498 0.158414 -0.105338 0.461873 1.042059 -2.255387	-0.838363 -1.898850 -0.496887 -0.686425 0.388065 -1.013919 -1.476103 -1.242336 -1.098734 -3.004023 -3.512957 -3.314349 -3.549652 -3.329238 -3.002135 -5.048939 -5.636920 -5.422741 -5.280123 1.768822 -0.634213 3.580789 2.175282 1.338879 1.777790 0.025572 -0.569641 4.508136 5.489697 4.684970 4.125448 4.306483	-1.396767 -1.344256 -2.442000 -1.058468 -1.079016 -0.009458 -1.963819 -1.634972 -3.009165 -1.954568 -2.084651 -0.945668 -3.019399 -4.027169 -2.970571 -2.881545 -2.938667 -3.675017 -1.904393 0.573120 0.205192 1.951799 1.278199 1.418706 2.012422 0.957987 1.444153 1.831316 2.275112 0.784271 2.371277 1.274201	H C H H H C H H C H H C H H C H H C H H C H H C H H C H H H C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H H H H C C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H H H H C H H H H H H H H H H H H H H H H H H H H	-0.186205 -0.277289 1.310594 1.758104 1.861174 1.479222 -0.933312 -0.500992 -0.860219 -2.010152 -2.720154 -3.025323 -1.701060 -0.820689 -2.145002 -1.333558 -3.981378 -4.709509 -3.749302 -4.481312  mation 23. vlicity: 4 :0 3c) = -3093.97067 def2-TZVP) = -3093 -D3(BJ)/def2-TZVI -D3(BJ)/def2-TZVI -3c) = -3089.8750 = 9.33738 Kcal/mc = 12.06737 Kcal/mc = -xTB) = -132.1811	-2.921266 -1.866259 -3.270084 -3.147069 -2.615170 -4.320880 -3.805916 -3.689460 -4.878770 -3.551636 -0.789089 -0.099764 -0.029859 0.269178 0.890477 -0.666161 -1.141345 -1.709925 -1.751134 -0.218017	1.538113 1.869272 1.513815 2.520997 0.812650 1.199732 2.552076 3.567299 2.277208 2.610330 -2.394847 -1.580717 -3.262775 -2.655993 -3.695593 -4.094138 -3.195125 -2.581601 -4.092461 -3.552135

Coordi				С	0.657068	-1.268041	-2.818263
Со	0.005793	-0.482125	0.506378	H	0.092935	-0.642709	-2.091233
C	-1.132498	-2.122092	0.358039	С	-0.362655	-2.126968	-3.576716
H	-1.012718	-2.498634	-0.681105	H	-1.146473	-1.482309	-4.022682
H	-0.599881	-2.858785	1.010866	H	-0.862242	-2.854630	-2.907098
C	-2.600778	-2.014028	0.757400	H	0.106172	-2.692611	-4.408749
H	-2.687087	-1.607029	1.786544	C	1.374119	-0.307610	-3.780708
H	-3.111371	-1.261010	0.121187	H	0.636691	0.275806	-4.370053
C H	-3.398543	-3.332832	0.701978	H H	2.016672	-0.864976	-4.494171
н	-4.432429 -2.960215	-3.134405 -4.054053	1.063153 1.427138	C	2.012892 3.290319	0.413977 -1.904612	-3.238612 1.528343
С	-3.456889	-4.003914	-0.679198	Н	3.128187	-0.807713	1.551647
Н	-2.447710	-4.389606	-0.941629	C	2.357880	-2.521707	2.586419
H	-4.113529	-4.900034	-0.611394	Н	1.299850	-2.284665	2.360156
C	-3.947968	-3.105764	-1.825714	Н	2.587020	-2.130867	3.599484
Н	-3.973454	-3.708160	-2.759803	Н	2.457676	-3.626537	2.609205
Н	-3.199462	-2.306525	-2.012278	C	4.765307	-2.165733	1.867493
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H	-6.092291	-3.228742	-1.368787				
N	-0.390104	1.368448	0.858008	Confo	rmation 25.		
N	1.725770	-0.270607	-0.325131		plicity: 4		
C	0.170223	3.896082	0.783224	Charg	re: 0		
С	0.462696	2.369270	0.571684		(-3c) = -3093.968834		
С	1.746580	2.100844	0.036424		3/def2-TZVP) = $-3093$		
H	2.366304	2.991013	-0.088187		- D3(BJ)/def2-TZVE		
C	2.366733	0.905771	-0.410517		0 - D3(BJ)/def2-TZ\	,	0189364 Hartree
C	3.832508	1.096577	-0.931721		h-3c) = $-3089.87304$		
C	-1.168112	4.245105	1.462668		= 10.10311  Kcal/m		
H H	-1.206620	5.344527 3.775330	1.604324 2.456227		) = 10.92971 Kcal/n		2 Hartras
H H	-1.281229	3.775330			7X-V/def2-TZVP) = -		2 Hartree
С	-2.046568 1.288313	4.512013	0.860945 1.663898		(1-xTB) = -132.18180 (2-xTB) = -130.92999		
Н	1.067536	5.584810	1.839104		I-FF) = -18.18741510		
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Н	1.348634	4.010622	2.649101	Coord	linates:		
C	0.186609	4.594804	-0.598575	Co	0.397977	0.403911	0.146975
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H	4.347706	2.410831	0.772625	H	1.047013	-0.639740	5.084763
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C	-1.748420	1.428476	1.266293	C	2.200839	0.000395	6.812207
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C	-4.473255	1.355468	1.996086	N	-0.429092	1.235369	-1.408570
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C	-2.760124	1.631682	0.275607	C	-1.665106	-0.758158	-1.941728
C	-1.126776	0.823554	3.752444	Н	-2.421795	-1.142913	-2.629332
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H	3.842524	2.192485	-2.989191	H	3.823215	-0.789599	2.331728
H	3.543130	0.488362	-3.463974	C	3.784158	3.035185	0.605851
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Č	2.253863	-3.038034	-0.380666	Č	0.812582	-4.059597	-2.925357
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	-2.776409	-1.778503	3.401779		3.378383		
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С	-1.315204	0.201286	2.819108	H	1.442725	0.230185	-2.299231
H	-0.542217	0.615599	2.125957	С	0.331449	-3.563586	1.355093
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				Н	2.196357	-4.590451	1.938364
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Charge				C	-1.164267	-3.612816	1.713868
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		(VP) = -3092.83185	5513065 Hartree		-0.719652	2.283687	0.411044
		.24178142 Hartree		С	-1.216277	2.252976	1.751042
	= 19.93019 Kcal/			С	-2.276292	3.105746	2.099515
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Coordi				С	-0.657370	1.232658	2.737163
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H	-1.442320 -3.375433 -3.802132		-1.236112	С	-0.715153	1.673169	4.203760
H H	-1.442320 -3.375433 -3.802132 -3.379966	-1.462260 -2.373583 -1.702778	-1.236112 0.335028		-0.715153 -0.214491	1.673169 0.924285	4.203760 4.850115
H	-1.442320 -3.375433 -3.802132	-1.462260 -2.373583	-1.236112	С	-0.715153	1.673169	4.203760
H H	-1.442320 -3.375433 -3.802132 -3.379966	-1.462260 -2.373583 -1.702778	-1.236112 0.335028	C H	-0.715153 -0.214491	1.673169 0.924285	4.203760 4.850115
H H C	-1.442320 -3.375433 -3.802132 -3.379966 -4.341802	-1.462260 -2.373583 -1.702778 -0.296772	-1.236112 0.335028 -1.018256	C H H	-0.715153 -0.214491 -1.759035	1.673169 0.924285 1.767780	4.203760 4.850115 4.567334
Н Н С Н	-1.442320 -3.375433 -3.802132 -3.379966 -4.341802 -5.386417	-1.462260 -2.373583 -1.702778 -0.296772 -0.678370	-1.236112 0.335028 -1.018256 -1.024029	C H H H	-0.715153 -0.214491 -1.759035 -0.211752	1.673169 0.924285 1.767780 2.648733	4.203760 4.850115 4.567334 4.356535
Н Н С Н	-1.442320 -3.375433 -3.802132 -3.379966 -4.341802 -5.386417 -4.163685	-1.462260 -2.373583 -1.702778 -0.296772 -0.678370 0.082430	-1.236112 0.335028 -1.018256 -1.024029 -2.047657	C H H H	-0.715153 -0.214491 -1.759035 -0.211752 -0.937985	1.673169 0.924285 1.767780 2.648733 3.022015	4.203760 4.850115 4.567334 4.356535 -2.039519
H H C H H	-1.442320 -3.375433 -3.802132 -3.379966 -4.341802 -5.386417 -4.163685 -4.227313	-1.462260 -2.373583 -1.702778 -0.296772 -0.678370 0.082430 0.858890	-1.236112 0.335028 -1.018256 -1.024029 -2.047657 -0.015834	C H H H C H	-0.715153 -0.214491 -1.759035 -0.211752 -0.937985 0.062663	1.673169 0.924285 1.767780 2.648733 3.022015 2.544491	4.203760 4.850115 4.567334 4.356535 -2.039519 -2.065609
H H C H H C	-1.442320 -3.375433 -3.802132 -3.379966 -4.341802 -5.386417 -4.163685 -4.227313 -3.152556	-1.462260 -2.373583 -1.702778 -0.296772 -0.678370 0.082430 0.858890 1.088937	-1.236112 0.335028 -1.018256 -1.024029 -2.047657 -0.015834 0.133748	C H H C H C	-0.715153 -0.214491 -1.759035 -0.211752 -0.937985 0.062663 -1.899625	1.673169 0.924285 1.767780 2.648733 3.022015 2.544491 2.102180	4.203760 4.850115 4.567334 4.356535 -2.039519 -2.065609 -2.810397
H H C H H C H	-1.442320 -3.375433 -3.802132 -3.379966 -4.341802 -5.386417 -4.163685 -4.227313 -3.152556 -4.669184	-1.462260 -2.373583 -1.702778 -0.296772 -0.678370 0.082430 0.858890 1.088937 1.783334	-1.236112 0.335028 -1.018256 -1.024029 -2.047657 -0.015834 0.133748 -0.446966	C H H C H C	-0.715153 -0.214491 -1.759035 -0.211752 -0.937985 0.062663 -1.899625 -1.957970	1.673169 0.924285 1.767780 2.648733 3.022015 2.544491 2.102180 1.109100	4.203760 4.850115 4.567334 4.356535 -2.039519 -2.065609 -2.810397 -2.327533 -3.857835 -2.831807
Н Н С Н С Н С Н Н С Н	-1.442320 -3.375433 -3.802132 -3.379966 -4.341802 -5.386417 -4.163685 -4.227313 -3.152556 -4.669184 -4.883677	-1.462260 -2.373583 -1.702778 -0.296772 -0.678370 0.082430 0.858890 1.088937 1.783334 0.588248	-1.236112 0.335028 -1.018256 -1.024029 -2.047657 -0.015834 0.133748 -0.446966 1.346066	С Н Н С Н С Н	-0.715153 -0.214491 -1.759035 -0.211752 -0.937985 0.062663 -1.899625 -1.957970 -1.561198	1.673169 0.924285 1.767780 2.648733 3.022015 2.544491 2.102180 1.109100 1.962574	4.203760 4.850115 4.567334 4.356535 -2.039519 -2.065609 -2.810397 -2.327533 -3.857835
H H C H C H C H H	-1.442320 -3.375433 -3.802132 -3.379966 -4.341802 -5.386417 -4.163685 -4.227313 -3.152556 -4.669184 -4.883677 -4.541232	-1.462260 -2.373583 -1.702778 -0.296772 -0.678370 0.082430 0.858890 1.088937 1.783334 0.588248 1.363002	-1.236112 0.335028 -1.018256 -1.024029 -2.047657 -0.015834 0.133748 -0.446966 1.346066 2.064724	С Н Н С Н С Н Н	-0.715153 -0.214491 -1.759035 -0.211752 -0.937985 0.062663 -1.899625 -1.957970 -1.561198 -2.924195	1.673169 0.924285 1.767780 2.648733 3.022015 2.544491 2.102180 1.109100 1.962574 2.528599	4.203760 4.850115 4.567334 4.356535 -2.039519 -2.065609 -2.810397 -2.327533 -3.857835 -2.831807
Н Н С Н С Н С Н Н С Н	-1.442320 -3.375433 -3.802132 -3.379966 -4.341802 -5.386417 -4.163685 -4.227313 -3.152556 -4.669184 -4.883677 -4.541232 -4.512094	-1.462260 -2.373583 -1.702778 -0.296772 -0.678370 0.082430 0.858890 1.088937 1.783334 0.588248 1.363002 -0.380310	-1.236112 0.335028 -1.018256 -1.024029 -2.047657 -0.015834 0.133748 -0.446966 1.346066 2.064724 1.749998	С Н Н С Н С Н Н С	-0.715153 -0.214491 -1.759035 -0.211752 -0.937985 0.062663 -1.899625 -1.957970 -1.561198 -2.924195 -0.841903	1.673169 0.924285 1.767780 2.648733 3.022015 2.544491 2.102180 1.109100 1.962574 2.528599 4.394001	4.203760 4.850115 4.567334 4.356535 -2.039519 -2.065609 -2.810397 -2.327533 -3.857835 -2.831807 -2.722421

Н	-0.445012	4.282694	-3.752013	С	-2.393240	-4.390464	-1.184709	
Conform	ation 31.			H H	-3.380042 -2.535031	-4.162542 -5.234453	-1.635915 -0.478612	
	icity: 4			н Н	-1.721724	-4.751318	-1.990289	
Charge:				C	-0.449507	-3.499209	0.173942	
	c) = $-3093.96545$			H	-0.007063	-2.605849	0.676277	
		3.629400858030 Hai		H	0.291753	-3.879041	-0.558619	
	- ( - / /	P) = -3092.6066128 VP) = -3092.833781		H C	-0.581702 2.019513	-4.262188 0.964735	0.968840 -0.608907	
		51266124 Hartree	1409012 Hartree	C	2.949872	-0.120582	-0.672892	
	= 11.83661 Kcal/			С	4.262732	0.091331	-0.220276	
	= 14.50920 Kcal/			H	4.992592	-0.728093	-0.277413	
		-3095.693471187178 47326341 Hartree	Hartree	C H	4.658349 5.690984	1.322613 1.465656	0.319821 0.671586	
		31769479 Hartree		C	3.723187	2.357200	0.434846	
	F) = -18.1838564			H	4.026476	3.312191	0.890886	
				С	2.399476	2.206004	-0.014649	
Coordin	ates: -0.161102	-0.299109	0.415017	C H	2.500897 1.492075	-1.488636 -1.646965	-1.180569 -0.725369	
C	0.126946	-0.299109	2.369161	C	3.395361	-2.647238	-0.727217	
Н	-0.309662	0.903180	2.639664	Н	2.921002	-3.616235	-0.982620	
H	-0.533083	-0.851001	2.841143	H	3.579991	-2.632767	0.363890	
C H	1.558166 2.218256	-0.195536 0.526285	2.890589 2.356342	H C	4.379611 2.299540	-2.624522 -1.544886	-1.239663 -2.703281	
н	1.600369	0.107542	3.964374	Н	1.943944	-2.550027	-3.010430	
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H	1.995909	-1.926026	1.692476	H	1.551529	-0.807612	-3.042806	
H C	1.552215	-2.314576	3.361404	C	1.407463	3.348526	0.179747	
Н	3.634325 3.980955	-1.728553 -2.758132	3.093492 2.847632	H C	1.015455	3.088986 3.489552	-0.378543 1.661542	
Н	4.216469	-1.047255	2.432343	Н	0.598270	2.545266	2.055772	
C	3.986696	-1.431493	4.555311	H	0.254529	4.286792	1.792724	
H	3.381092	-2.090396	5.217546	H	1.896863	3.755437	2.281697	
H C	3.681686 5.473618	-0.392818 -1.612396	4.806999 4.863119	C H	1.930174 2.253928	4.691203 4.621105	-0.360153 -1.417267	
Н	5.805765	-2.651600	4.655473	H	2.795655	5.055612	0.230356	
H	5.707390	-1.392489	5.924578	H	1.140505	5.467452	-0.295744	
H	6.096754	-0.939345	4.237137					
N N	-1.973881 0.677060	-0.325158 0.731363	-0.260641 -0.998164		mation 6. licity: 4			
C	-3.726689	0.023674	-2.123729	Charge:				
C	-2.320330	0.194403	-1.447637		3c) = -3093.971023	3226195 Hartree		
C	-1.374568	0.888118	-2.244107		def2-TZVP) = -3093			
H	-1.784666	1.261664	-3.183351		- D3(BJ)/def2-TZVI			
C C	0.007659 0.636220	1.158780 1.957332	-2.083118 -3.281392		- D3(BJ)/def2-TZV -3c) = -3089.87660		3/10656 Hartree	
C	-3.558974	-1.019271	-3.255700		= 8.97611 Kcal/mo			
H	-4.521478	-1.161817	-3.789818		= 11.82756 Kcal/r			
H H	-3.249833	-2.001558	-2.846627 -3.993610		X-V/def2-TZVP) = -		9 Hartree	
С	-2.795685 -4.874961	-0.703867 -0.453040	-1.210872		-xTB) = $-132.18110-xTB$ ) = $-130.92908$			
Н	-5.803835	-0.482681	-1.816457		FF) = -18.19026849			
H	-5.051626	0.236150	-0.364696					
H C	-4.715313 -4.199228	-1.464489 1.366398	-0.799463 -2.736117	Coordin	nates: -0.408296	-0.002955	-0.174162	
Н	-5.220787	1.242023	-3.148860	Co C	-2.271400	0.723510	-0.205758	
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H	-4.238922	2.165834	-1.969183	H	-2.917590	-0.171065	-0.369674	
C H	0.312335 0.781155	1.228460 1.778123	-4.612485 -5.453970	C H	-2.766548 -2.836742	1.562341 0.939160	0.972756 1.891338	
H	-0.772162	1.167302	-4.821625	H	-1.996150	2.323043	1.211898	
H	0.716192	0.196988	-4.616988	С	-4.099797	2.321318	0.754672	
C	2.167432	2.129933	-3.250794	H	-4.136470	2.660848	-0.305674	
H H	2.521778 2.476561	2.744930 2.636603	-2.407726 -4.187708	H C	-4.072453 -5.415554	3.253720 1.604538	1.361314 1.098311	
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C	-0.009919	3.363567	-3.324215	H	-6.239545	2.324296	0.901223	
H	0.188706	3.930390	-2.394742 -3.455773	C	-5.717056 -5.289507	0.285771	0.359152	
H H	-1.107776 0.408661	3.307756 3.944986	-4.171661	H H	-6.815497	0.332351 0.188782	-0.666581 0.219177	
C	-2.774219	-1.078769	0.636160	C	-5.208890	-0.962630	1.083976	
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H C	-4.941228 -4.298154	-0.856134 -2.704229	3.272395 2.366220	H N	-5.390970 0.748911	-1.885748 -0.619021	0.495996 1.238127	
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C C	-2.721155 -3.644894	-2.505590 1.036488	0.520653 1.997301	C H	2.688214 3.738946	-0.722291 -1.022114	-0.164632 -0.179015	
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H	-1.873593 -3 177789	1.924256		H	1 372217	-2 267718	3 593611	
H C	-1.873593 -3.177789 -3.187519	3.076321 1.309066	1.448420 3.447692	H H	1.372217 2.104756	-2.267718 -0.703445	3.593611 4.033181	
C H	-3.177789 -3.187519 -3.710762	3.076321 1.309066 0.670899	1.448420 3.447692 4.185076	H C	2.104756 3.258232	-0.703445 -3.019143	4.033181 1.702133	
C H H	-3.177789 -3.187519 -3.710762 -3.379531	3.076321 1.309066 0.670899 2.367246	1.448420 3.447692 4.185076 3.718968	H C H	2.104756 3.258232 3.896275	-0.703445 -3.019143 -3.537373	4.033181 1.702133 2.447824	
C H H H	-3.177789 -3.187519 -3.710762 -3.379531 -2.101544	3.076321 1.309066 0.670899 2.367246 1.118812	1.448420 3.447692 4.185076 3.718968 3.553929	Н С Н Н	2.104756 3.258232 3.896275 3.789152	-0.703445 -3.019143 -3.537373 -3.026261	4.033181 1.702133 2.447824 0.730542	
C H H	-3.177789 -3.187519 -3.710762 -3.379531	3.076321 1.309066 0.670899 2.367246	1.448420 3.447692 4.185076 3.718968	H C H	2.104756 3.258232 3.896275	-0.703445 -3.019143 -3.537373	4.033181 1.702133 2.447824	

H	4.882318	-1.255685	3.131259	С	-0.450716	-2.101897	1.384869
H	4.048451	0.259665	2.662638	H	-1.509704	-2.388326	1.191987
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H H	3.992564 5.209958	1.885372 0.973865	-1.821525 -2.773506	H H	0.926281 0.012073	-1.724731 -1.441184	5.494327 6.981949
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H	-1.485707	-3.338737	-2.538928	Н	-0.502056	-3.334820	-4.862228
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C	0.087773	-2.462044	-4.663761	H	-1.210387	-4.731111	-3.997818
H	1.019204	-2.073175	-5.122820	С	3.397415	-1.395989	-0.332455
H	-0.717391	-2.385245	-5.423297	Н	2.946005	-0.404846	-0.548886
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Conforma	tion 0			H H	5.010272 5.412452	-1.193899 -2.274987	-1.826636 -0.458801
Multipli				Н	5.390243	-0.508849	-0.214529
Charge:				C	3.274691	-1.655427	1.180390
	e) = -3093.96385	6053141 Hartree		Н	2.215525	-1.648284	1.503005
		3.631833698390 Har	tree	Н	3.819951	-0.887831	1.766271
E(PBE -	D3(BJ)/def2-TZV	P) = -3092.6052652	98622 Hartree	H	3.692576	-2.648943	1.442610
		VP) = -3092.834249	570261 Hartree	С	-1.360572	1.610422	1.214818
		21068853 Hartree		С	-2.701852	1.261939	1.540585
	= 14.47656 Kcal/			С	-3.181598	1.634427	2.814858
	= 14.89500 Kcal/		II	H	-4.214751	1.361604	3.084566
		-3095.692909302862	nartree	С	-2.392712	2.320796	3.740264
		37986320 Hartree 70408595 Hartree		H C	-2.800941 -1.067897	2.591148 2.643269	4.725452 3.410867
	F(18) = -130.9217			Н	-0.440485	3.172349	4.142560
-,	,			C	-0.531529	2.288203	2.166542
Coordina	ates:			C	-3.720015	0.557437	0.632016
Со	0.052541	-0.541344	0.230928	Н	-4.245111	-0.146675	1.316140

C H H C H	-3.201197						
H H H C H	-3.201197	0 00000	0 501060		1 050015	F F C O F O O	0 051144
H H C H		-0.293608	-0.531869	H	1.359017	-5.569798	-2.851144
H C H	-4.038457	-0.891797	-0.946485	H	0.191083	-4.713496	-1.786074
C H	-2.418367	-0.999909	-0.199056	H	1.694041	-5.404845	-1.100432
H	-2.781758	0.311655	-1.358020	С	1.317436	-2.883796	-3.488030
Н	-4.791084	1.547869	0.129595	Н	1.834000	-1.958575	-3.808641
	-5.598776	1.005662	-0.403794	Н	0.263667	-2.630472	-3.271811
H							
	-4.358498	2.282554	-0.578776	H	1.327154	-3.587735	-4.347281
H	-5.252892	2.113821	0.966242	C	-2.732690	3.476409	0.270000
С	0.924087	2.578175	1.819432	Н	-1.630877	3.475242	0.341960
H	0.974788	2.724518	0.721403	Н	-3.129857	4.091884	1.104076
C	1.487814	3.844461	2.473854	Н	-2.999534	3.993604	-0.673920
H	0.857698	4.730617	2.256509	С	-3.961591	1.237999	2.075318
H	2.509474	4.048877	2.094578	H	-4.743898	0.451769	2.050513
Н	1.565484	3.745147	3.576084	H	-4.349919	2.087316	2.674609
С	1.799097	1.356831	2.144979	Н	-3.083121	0.801953	2.587053
H	1.343230	0.416823	1.753503	C	-5.167617	1.970265	-0.610149
H	1.895683	1.210620	3.240068	H	-5.026216	2.307995	-1.656844
H	2.814838	1.447579	1.710688	H	-5.741391	2.758962	-0.078403
				Н	-5.795741	1.056795	-0.623077
				С	-4.414872	-1.823432	-0.298907
$IOC_{I}$	MIX			Н	-3.984563	-2.115618	0.678624
				H	-4.728628	-2.745657	-0.831213
	mation 11.			H	-5.327926	-1.227194	-0.094628
Multip:	licity: 4			C	-1.746221	-1.915300	-1.906341
Charge	: 0			H	-1.164993	-1.345324	-2.659443
(B97-	3c) = -4478.40679	7519745 Hartree		H	-2.121237	-2.843097	-2.386731
		8.394981553469 Ha	x+x00	Н	-1.047557	-2.217030	-1.099269
		(P) = -4476.712739		C	-4.058704	-0.337756	-2.942279
		VP) = -4477.08689	9115723 Hartree	H	-4.935189	0.319770	-2.789732
	-3c) = -4473.0039			H	-4.413424	-1.266013	-3.438789
(PM6)	= -142.60181 Kca	1/mol		H	-3.364205	0.170815	-3.640889
	= -204.38983 Kca			C	1.620274	0.544057	3.851634
,		, -	0 1125+500	Н			
		-4480.43499537966	o marcies		1.883484	-0.445427	4.275127
	-xTB) = $-139.7716$			H	1.819286	1.312059	4.628542
GFN2	-xTB) = $-136.9608$	11665688 Hartree		H	2.297917	0.743861	2.999303
(GFN-	FF) = -18.0596002	03140 Hartree		C	-1.212803	0.631477	4.941081
				Н	-2.296215	0.760255	4.746667
'oordi	nates:			Н	-0.878763	1.477832	5.577733
		0 175076	0 017200				
C	0.943747	0.175276	-0.817298	H	-1.077927	-0.299813	5.526669
C	2.594591	1.031047	-2.166228	C	-0.463819	2.342764	2.551843
H	3.115699	1.809692	-2.728987	Н	-0.014221	2.433280	1.540561
С	2.815587	-0.311402	-2.063730	H	-0.005860	3.126514	3.190290
Н	3.592034	-0.935453	-2.511222	Н	-1.540249	2.575917	2.467337
C	1.021096	2.674169	-1.238478	C	-2.962656	-2.116782	3.539309
C	-0.021798	3.163833	-2.068209	H	-2.988035	-1.510090	4.465090
C	-0.318405	4.536233	-1.969508	H	-3.291363	-3.145820	3.796710
H	-1.121488	4.958629	-2.587063	H	-3.705120	-1.686868	2.837929
C	0.374118	5.373387	-1.086604	C	-1.334707	-3.493241	1.391832
H	0.111642	6.440470	-1.027103	H	-2.123028	-3.275594	0.646208
C	1.385670	4.857950	-0.271086	H	-1.584527	-4.464837	1.867508
Н	1.915072	5.522189	0.426967	Н	-0.376109	-3.600207	0.848374
С	1.742036	3.497296	-0.334774	С	-0.040746	-2.874219	4.066040
C	-0.803217	2.247123	-3.008328	Н	0.975285	-3.031175	3.649421
H	-1.078792	1.357157	-2.399013	H	-0.411467	-3.853192	4.435937
C	-2.113876	2.868423	-3.502773	H	0.057493	-2.203470	4.943575
H	-2.767996	3.182206	-2.667436	N	1.468016	1.310531	-1.396567
Н	-2.676303	2.127836	-4.103180	N	1.808052	-0.824228	-1.249366
	-1.934834	3.747112	-4.157147		-2.468070	0.515057	-0.424473
U				N			
	0.026982	1.788456	-4.223335	N	-0.676794	-0.607598	2.170342
C	0.334453	2.657737	-4.841954	Si	-3.508164	1.738098	0.299226
C H		1.117753	-4.864393	Si	2 174005		
C H	-0.581022	1.11/100		0 1	-3.174895	-0.813254	-1.325253
C H H			-3.940546				
C H H	0.940151	1.232879	-3.940546 0.506862	Si	-0.205973	0.634180	3.325519
H C H H C	0.940151 2.902337	1.232879 2.967650	0.506862	Si Si	-0.205973 -1.233710	0.634180 -2.174440	3.325519 2.749986
C H H H C H	0.940151 2.902337 2.775809	1.232879 2.967650 1.867486	0.506862 0.591926	Si Si P	-0.205973 -1.233710 1.636939	0.634180 -2.174440 -2.525314	3.325519 2.749986 -0.698943
C H H C H C	0.940151 2.902337 2.775809 4.254460	1.232879 2.967650 1.867486 3.243352	0.506862 0.591926 -0.181672	Si Si	-0.205973 -1.233710	0.634180 -2.174440	3.325519 2.749986
C H H H	0.940151 2.902337 2.775809	1.232879 2.967650 1.867486 3.243352 2.787290	0.506862 0.591926	Si Si P Co	-0.205973 -1.233710 1.636939 -0.745807	0.634180 -2.174440 -2.525314	3.325519 2.749986 -0.698943
C H H C H C	0.940151 2.902337 2.775809 4.254460	1.232879 2.967650 1.867486 3.243352	0.506862 0.591926 -0.181672	Si Si P Co	-0.205973 -1.233710 1.636939	0.634180 -2.174440 -2.525314	3.325519 2.749986 -0.698943
С Н Н С Н С Н Н	0.940151 2.902337 2.775809 4.254460 4.318654 5.089215	1.232879 2.967650 1.867486 3.243352 2.787290 2.839140	0.506862 0.591926 -0.181672 -1.186841 0.426842	Si Si P Co	-0.205973 -1.233710 1.636939 -0.745807	0.634180 -2.174440 -2.525314	3.325519 2.749986 -0.698943
C H H C H C H H H	0.940151 2.902337 2.775809 4.254460 4.318654 5.089215 4.414056	1.232879 2.967650 1.867486 3.243352 2.787290 2.839140 4.335456	0.506862 0.591926 -0.181672 -1.186841 0.426842 -0.295974	Si Si P Co Conform	-0.205973 -1.233710 1.636939 -0.745807 mation 14. licity: 4	0.634180 -2.174440 -2.525314	3.325519 2.749986 -0.698943
С н н С н С н н С н С	0.940151 2.902337 2.775809 4.254460 4.318654 5.089215 4.414056 2.932912	1.232879 2.967650 1.867486 3.243352 2.787290 2.839140 4.335456 3.540644	0.506862 0.591926 -0.181672 -1.186841 0.426842 -0.295974 1.932108	Si Si P Co Conform Multip Charge	-0.205973 -1.233710 1.636939 -0.745807 mation 14. licity: 4	0.634180 -2.174440 -2.525314 0.023505	3.325519 2.749986 -0.698943
C H H C H C H H C H H H	0.940151 2.902337 2.775809 4.254460 4.318654 5.089215 4.414056 2.932912 3.197074	1.232879 2.967650 1.867486 3.243352 2.787290 2.839140 4.335456 3.540644 4.618079	0.506862 0.591926 -0.181672 -1.186841 0.426842 -0.295974 1.932108 1.934126	Si P Co Conform Multip Charge E(B97-	-0.205973 -1.233710 1.636939 -0.745807 mation 14. licity: 4 : 0 3c) = -4478.40583	0.634180 -2.174440 -2.525314 0.023505	3.325519 2.749986 -0.698943 0.343588
С Н Н С Н С Н Н С Н	0.940151 2.902337 2.775809 4.254460 4.318654 5.089215 4.414056 2.932912	1.232879 2.967650 1.867486 3.243352 2.787290 2.839140 4.335456 3.540644	0.506862 0.591926 -0.181672 -1.186841 0.426842 -0.295974 1.932108 1.934126 2.533440	Si Si P Co Conform Multip Charge E (B97- E (M06/e	-0.205973 -1.233710 1.636939 -0.745807 mation 14. licity: 4: 0: 3c) = -4478.40583 def2-TZVP) = -447	0.634180 -2.174440 -2.525314 0.023505	3.325519 2.749986 -0.698943 0.343588
C H H H C H H H H H H H H H H H H H	0.940151 2.902337 2.775809 4.254460 4.318654 5.089215 4.414056 2.932912 3.197074	1.232879 2.967650 1.867486 3.243352 2.787290 2.839140 4.335456 3.540644 4.618079	0.506862 0.591926 -0.181672 -1.186841 0.426842 -0.295974 1.932108 1.934126	Si Si P Co Conform Multip Charge E (B97- E (M06/e	-0.205973 -1.233710 1.636939 -0.745807 mation 14. licity: 4: 0: 3c) = -4478.40583 def2-TZVP) = -447	0.634180 -2.174440 -2.525314 0.023505	3.325519 2.749986 -0.698943 0.343588
C H H H C H H H C H H H H H H H H H H H H H	0.940151 2.902337 2.775809 4.254460 4.318654 5.089215 4.414056 2.932912 3.197074 3.702703 1.962317	1.232879 2.967650 1.867486 3.243352 2.787290 2.839140 4.335456 3.540644 4.618079 3.016978 3.423284	0.506862 0.591926 -0.181672 -1.186841 0.426842 -0.295974 1.932108 1.934126 2.533440 2.445660	Si Si P Co Conform Multip Charge E (B97- E (M06/ E (PBE	-0.205973 -1.233710 1.636939 -0.745807 mation 14. licity: 4: 0: 3c) = -4478.40583 def2-TZVP) = -447 - D3(BJ)/def2-TZV	0.634180 -2.174440 -2.525314 0.023505 88585287 Hartree 8.396031220862 Ha	3.325519 2.749986 -0.698943 0.343588
C H H H H C H C H H H H C C H H H C C H C C H C C C C C C C C C C C C C C C C C C C C	0.940151 2.902337 2.775809 4.254460 4.318654 5.089215 4.414056 2.932912 3.197074 3.702703 1.962317 3.104887	1.232879 2.967650 1.867486 3.243352 2.787290 2.839140 4.335456 3.540644 4.618079 3.016978 3.423284 -2.625191	0.506862 0.591926 -0.181672 -1.186841 0.426842 -0.295974 1.932108 1.934126 2.533440 2.445660 0.525321	Si Si P Co Conform Multip Charge E (B97- E (M06/ E (PBE )	-0.205973 -1.233710 1.636939 -0.745807 mation 14. licity: 4: 0: 3c) = -4478.40583 def2-TZVP) = -447 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV	0.634180 -2.174440 -2.525314 0.023505 88585287 Hartree 88.396031220862 Ha PP) = -4476.710650	3.325519 2.749986 -0.698943 0.343588
СННННСНННСНННС	0.940151 2.902337 2.775809 4.254460 4.318654 5.089215 4.414056 2.932912 3.197074 3.702703 1.962317 3.104887 2.737363	1.232879 2.967650 1.867486 3.243352 2.787290 2.839140 4.335456 3.540644 4.618079 3.016978 3.423284 -2.625191 -1.575878	0.506862 0.591926 -0.181672 -1.186841 0.426842 -0.295974 1.932108 1.934126 2.533440 2.445660 0.525321 1.588576	Si PCo Conform Multip Charge E(B97- E(M06/ E(PBE) E(PBE0) E(PBE0)	-0.205973 -1.233710 1.636939 -0.745807 mation 14. licity: 4 : 0 3c) = -4478.40583 def2-TZVP) = -447 - D3(BJ)/def2-TZ - D3(BJ)/def2-TZ -3c) = -4473.0060	0.634180 -2.174440 -2.525314 0.023505 0.8585287 Hartree 8.396031220862 Ha PP) = -4476.710650 0.000000000000000000000000000000000	3.325519 2.749986 -0.698943 0.343588
СННННСНННСНННССН	0.940151 2.902337 2.775809 4.254460 4.318654 5.089215 4.414056 2.932912 3.197074 3.702703 1.962317 3.104887 2.737363 1.666392	1.232879 2.967650 1.867486 3.243352 2.787290 2.839140 4.335456 3.540644 4.618079 3.016978 3.423284 -2.625191 -1.575878 -1.596454	0.506862 0.591926 -0.181672 -1.186841 0.426842 -0.295974 1.932108 1.934126 2.533440 2.445660 0.525321 1.588576 1.873824	Si Si P Co Conform Multip Charge E (B97- E (M06/ E (PBE E (PBE E (PBE) E (PBE)	-0.205973 -1.233710 1.636939 -0.745807 mation 14. licity: 4: : 0 3c) = -4478.40583 def2-TZVP) = -447 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV -3c) = -4473.0060 = -138.89991 Kca	0.634180 -2.174440 -2.525314 0.023505 88585287 Hartree 8.396031220862 Ha PP) = -4476.710650 WP) = -4477.08631 122444982 Hartree	3.325519 2.749986 -0.698943 0.343588
СНННСНСНННСНННССН	0.940151 2.902337 2.775809 4.254460 4.318654 5.089215 4.414056 2.932912 3.197074 3.702703 1.962317 3.104887 2.737363	1.232879 2.967650 1.867486 3.243352 2.787290 2.839140 4.335456 3.540644 4.618079 3.016978 3.423284 -2.625191 -1.575878	0.506862 0.591926 -0.181672 -1.186841 0.426842 -0.295974 1.932108 1.934126 2.533440 2.445660 0.525321 1.588576	Si Si P Co Conform Multip Charge E (B97- E (M06/ E (PBE E (PBE E (PBE) E (PBE)	-0.205973 -1.233710 1.636939 -0.745807 mation 14. licity: 4 : 0 3c) = -4478.40583 def2-TZVP) = -447 - D3(BJ)/def2-TZ - D3(BJ)/def2-TZ -3c) = -4473.0060	0.634180 -2.174440 -2.525314 0.023505 88585287 Hartree 8.396031220862 Ha PP) = -4476.710650 WP) = -4477.08631 122444982 Hartree	3.325519 2.749986 -0.698943 0.343588
СННННСННННСННН	0.940151 2.902337 2.775809 4.254460 4.318654 5.089215 4.414056 2.932912 3.197074 3.702703 1.962317 3.104887 2.737363 1.666392	1.232879 2.967650 1.867486 3.243352 2.787290 2.839140 4.335456 3.540644 4.618079 3.016978 3.423284 -2.625191 -1.575878 -1.596454	0.506862 0.591926 -0.181672 -1.186841 0.426842 -0.295974 1.932108 1.934126 2.533440 2.445660 0.525321 1.588576 1.873824	Si Si P Co Conform Multip Charge E (B97- E (M06/ E (PBE0 E (PBE0 E (PBE0 E (PM6) E (PM7)	-0.205973 -1.233710 1.636939 -0.745807 mation 14. licity: 4: 0: 3c) = -4478.40583 def2-TZVP) = -447 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV	0.634180 -2.174440 -2.525314 0.023505 88585287 Hartree 8.396031220862 Ha PP) = -4476.710650 WP) = -4477.08631 122444982 Hartree	3.325519 2.749986 -0.698943 0.343588 artree 425274 Hartree 7034547 Hartree
СННННСНСННННССННН	0.940151 2.902337 2.775809 4.254460 4.318654 5.089215 4.414056 2.932912 3.197074 3.702703 1.962317 3.104887 2.737363 1.666392 2.949094 3.349939	1.232879 2.967650 1.867486 3.243352 2.787290 2.839140 4.335456 3.540644 4.618079 3.016978 3.423284 -2.625191 -1.575878 -1.596454 -0.551654 -1.736979	0.506862 0.591926 -0.181672 -1.186841 0.426842 -0.295974 1.932108 1.934126 2.533440 2.445660 0.525321 1.588576 1.873824 1.222519 2.500155	Si Si P Co Conform Multip Charge E(B97- E(M96/ E(PBE) E(PBE) E(PBE) E(PBE) E(PBE) E(PM6) E(PM6) E(PM6) E(PM6)	-0.205973 -1.233710 1.636939 -0.745807 mation 14. licity: 4: 0 3c) = -4478.40583 def2-TZVP) = -447 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - 3c) = -4473.0060 = -194.58364 Kca X-V/def2-TZVP) =	0.634180 -2.174440 -2.525314 0.023505 88585287 Hartree 8.396031220862 Ha PP) = -4476.710650 NPP) = -4477.08631 222444982 Hartree 11/mol 11/mol -4480.43415970233	3.325519 2.749986 -0.698943 0.343588 artree 425274 Hartree 7034547 Hartree
СНННСНСНННССНННССН	0.940151 2.902337 2.775809 4.254460 4.318654 5.089215 4.414056 2.932912 3.197074 3.702703 1.962317 3.104887 2.737363 1.666392 2.949094 3.349939 4.531219	1.232879 2.967650 1.867486 3.243352 2.787290 2.839140 4.335456 3.540644 4.618079 3.016978 3.423284 -2.625191 -1.575878 -1.596454 -0.551654 -1.736979 -2.333884	0.506862 0.591926 -0.181672 -1.186841 0.426842 -0.295974 1.932108 1.934126 2.533440 2.445660 0.525321 1.588576 1.873824 1.222519 2.500155 0.037795	Si P Co Conform Multip Charge E(M96/ E(PBE) E(PBE) E(PBE) E(PM6) E(PM6) E(PM7) E(M97) E(M97) E(M97)	-0.205973 -1.233710 1.636939 -0.745807 mation 14. licity: 4: 0 3c) = -4478.40583 def2-TZVP) = -447 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - 3c) = -4473.0060 = -138.89991 Kca = -194.58364 Kca X-V/def2-TZVP) = -xTB) = -139.7672	0.634180 -2.174440 -2.525314 0.023505 88585287 Hartree 8.396031220862 Ha PP) = -4476.710650 EVP) = -4477.08631 122444982 Hartree 11/mol 11/mol 1-4480.43415970233 173729267 Hartree	3.325519 2.749986 -0.698943 0.343588 artree 425274 Hartree 7034547 Hartree
СНННСНСНННССНННССН	0.940151 2.902337 2.775809 4.254460 4.318654 5.089215 4.414056 2.932912 3.197074 3.702703 1.962317 3.104887 2.737363 1.666392 2.949094 3.349939 4.531219 5.203552	1.232879 2.967650 1.867486 3.243352 2.787290 2.839140 4.335456 3.540644 4.618079 3.016978 3.423284 -2.625191 -1.575878 -1.596454 -0.551654 -1.736979 -2.333884 -2.294915	0.506862 0.591926 -0.181672 -1.186841 0.426842 -0.295974 1.932108 1.934126 2.533440 2.445660 0.525321 1.588576 1.873824 1.222519 2.500155 0.037795 0.922222	Si Si P Co Conform Multip Charge E (B97- E (M06/ E (PBE) E (PBE) E (PBE) E (PBE) E (PM6) E (PM7) E (B97: E (B97: E (GFN1) E (GFN2	-0.205973 -1.233710 1.636939 -0.745807 mation 14. licity: 4: : 0 3c) = -4478.40583 def2-TZVP) = -447 - D3 (BJ) / def2-TZV - D3 (BJ) / def2-TZV -3c) = -4473.0060 = -138.89991 Kca = -194.58364 Kca X-V/def2-TZVP) = -xTB) = -139.7672 -xTB) = -136.9590	0.634180 -2.174440 -2.525314 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.02	3.325519 2.749986 -0.698943 0.343588 artree 425274 Hartree 7034547 Hartree
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СНИНСИСИННИСИННИСИННИСИННИ	0.940151 2.902337 2.775809 4.254460 4.318654 5.089215 4.414056 2.932912 3.197074 3.702703 1.962317 3.104887 2.737363 1.666392 2.949094 3.349939 4.531219 5.203552 4.605588 4.932112	1.232879 2.967650 1.867486 3.243352 2.787290 2.839140 4.335456 3.540644 4.618079 3.016978 3.423284 -2.625191 -1.575878 -1.596454 -0.551654 -1.736979 -2.333884 -2.294915 -1.346375 -3.105193	0.506862 0.591926 -0.181672 -1.186841 0.426842 -0.295974 1.932108 1.934126 2.533440 2.445660 0.525321 1.588576 1.873824 1.222519 2.500155 0.037795 0.922222 -0.458650 -0.642312	Si Si P Co Conform Multip Charge E (B97- E (PBE) E (PBE) E (PBE) E (PM7) E (GFN1- E (GFN1- E (GFN2- E (GFN1-	-0.205973 -1.233710 1.636939 -0.745807  mation 14. licity: 4: 0 3c) = -4478.40583 def2-TZVP) = -447 - D3(BJ)/def2-TZV - T3(BJ) = -1473.0060 = -138.89991 Kca = -194.58364 Kca X-V/def2-TZVP) = -xTB) = -139.7672 -xTB) = -136.9590 FFF) = -18.0674520	0.634180 -2.174440 -2.525314 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.02	3.325519 2.749986 -0.698943 0.343588 artree 425274 Hartree 7034547 Hartree
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СНННСНСНННССНННССНННС	0.940151 2.902337 2.775809 4.254460 4.318654 5.089215 4.414056 2.932912 3.197074 3.702703 1.962317 3.104887 2.737363 1.666392 2.949094 3.349939 4.531219 5.203552 4.605588 4.932112 3.020922 3.717671	1.232879 2.967650 1.867486 3.243352 2.787290 2.839140 4.335456 3.540644 4.618079 3.016978 3.423284 -2.625191 -1.575878 -1.596454 -0.551654 -1.736979 -2.333884 -2.294915 -1.346375 -3.105193 -4.037190 -4.108811	0.506862 0.591926 -0.181672 -1.186841 0.426842 -0.295974 1.932108 1.934126 2.533440 2.445660 0.525321 1.588576 1.873824 1.222519 2.500155 0.037795 0.922222 -0.458650 -0.642312 1.137210 1.999224	Si Si P Co Conform Multipe E(B97- E(M06/ E(PBE) E(PBE) E(PBE) E(PBE) E(PBE) E(PM6) E(B97: E(GFN1- E(GFN2- E(GFN1- Coordi	-0.205973 -1.233710 1.636939 -0.745807  mation 14. licity: 4: 0: 3c) = -4478.40583 def2-TZVP) = -447 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV -3c) = -4473.0060 = -138.89991 Kca = -194.58364 Kca X-V/def2-TZVP) = -XTB) = -139.7672 -XTB) = -136.9590 FF) = -18.0674520  nates: 1.087327	0.634180 -2.174440 -2.525314 0.023505 0.8585287 Hartree (8.396031220862 Ha (P) = -4476.710650 (NP) = -4477.08631 (122444982 Hartree (1/mol) -4480.43415970233 (73729267 Hartree (105112215 Hartree (178324 Hartree (178324 Hartree	3.325519 2.749986 -0.698943 0.343588 artree 425274 Hartree 425274 Hartree 7034547 Hartree
СНННСНСНННССННННСНННСНН	0.940151 2.902337 2.775809 4.254460 4.318654 5.089215 4.414056 2.932912 3.197074 3.702703 1.962317 3.104887 2.737363 1.666392 2.949094 3.349939 4.531219 5.203552 4.605588 4.932112 3.020922 3.717671 3.308540	1.232879 2.967650 1.867486 3.243352 2.787290 2.839140 4.335456 3.540644 4.618079 3.016978 3.423284 -2.625191 -1.575878 -1.596454 -0.551654 -1.736979 -2.333884 -2.294915 -1.346375 -3.105193 -4.037190 -4.108811 -4.826964	0.506862 0.591926 -0.181672 -1.186841 0.426842 -0.295974 1.932108 1.934126 2.533440 2.445660 0.525321 1.588576 1.873824 1.222519 2.500155 0.037795 0.922222 -0.458650 -0.642312 1.137210 1.999224 0.413911	Si Si P Co Conform Multip Charge E (B97- E (M06/ E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (E) E	-0.205973 -1.233710 1.636939 -0.745807  mation 14. licity: 4:0 3c) = -4478.40583 def2-TZVP) = -447 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - T38.89991 Kca = -194.58364 Kca X-V/def2-TZVP) = -139.7672 -xTB) = -139.7672 -xTB) = -136.9590 FF) = -18.0674520  nates: 1.087327 3.173120	0.634180 -2.174440 -2.525314 0.023505 0.8585287 Hartree 18.396031220862 Ha 19. = -4476.710650 10.79 = -4477.08631 122444982 Hartree 11/mo1 -4480.43415970233 173729267 Hartree 173729267 Hartree 178324 Hartree 178324 Hartree	3.325519 2.749986 -0.698943 0.343588 Artree 425274 Hartree 425274 Hartree 41 Hartree
СНННСНСНННССННННСННННСНН	0.940151 2.902337 2.775809 4.254460 4.318654 5.089215 4.414056 2.932912 3.197074 3.702703 1.962317 3.104887 2.737363 1.666392 2.949094 3.349939 4.531219 5.203552 4.605588 4.932112 3.020922 3.717671	1.232879 2.967650 1.867486 3.243352 2.787290 2.839140 4.335456 3.540644 4.618079 3.016978 3.423284 -2.625191 -1.575878 -1.596454 -0.551654 -1.736979 -2.333884 -2.294915 -1.346375 -3.105193 -4.037190 -4.108811	0.506862 0.591926 -0.181672 -1.186841 0.426842 -0.295974 1.932108 1.934126 2.533440 2.445660 0.525321 1.588576 1.873824 1.222519 2.500155 0.037795 0.922222 -0.458650 -0.642312 1.137210 1.999224	Si Si P Co Conform Multipe E(B97- E(M06/ E(PBE) E(PBE) E(PBE) E(PBE) E(PBE) E(PM6) E(B97: E(GFN1- E(GFN2- E(GFN1- Coordi	-0.205973 -1.233710 1.636939 -0.745807  mation 14. licity: 4: 0: 3c) = -4478.40583 def2-TZVP) = -447 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV -3c) = -4473.0060 = -138.89991 Kca = -194.58364 Kca X-V/def2-TZVP) = -XTB) = -139.7672 -XTB) = -136.9590 FF) = -18.0674520  nates: 1.087327	0.634180 -2.174440 -2.525314 0.023505 0.8585287 Hartree (8.396031220862 Ha (P) = -4476.710650 (NP) = -4477.08631 (122444982 Hartree (1/mol) -4480.43415970233 (73729267 Hartree (105112215 Hartree (178324 Hartree (178324 Hartree	3.325519 2.749986 -0.698943 0.343588 artree 425274 Hartree 425274 Hartree 7034547 Hartree
Снннснснннснннснннснннсннн	0.940151 2.902337 2.775809 4.254460 4.318654 5.089215 4.414056 2.932912 3.197074 3.702703 1.962317 3.104887 2.737363 1.666392 2.949094 3.349939 4.531219 5.203552 4.605588 4.932112 3.020922 3.717671 3.308540	1.232879 2.967650 1.867486 3.243352 2.787290 2.839140 4.335456 3.540644 4.618079 3.016978 3.423284 -2.625191 -1.575878 -1.596454 -0.551654 -1.736979 -2.333884 -2.294915 -1.346375 -3.105193 -4.037190 -4.108811 -4.826964	0.506862 0.591926 -0.181672 -1.186841 0.426842 -0.295974 1.932108 1.934126 2.533440 2.445660 0.525321 1.588576 1.873824 1.222519 2.500155 0.037795 0.922222 -0.458650 -0.642312 1.137210 1.999224 0.413911	Si Si P Co Conform Multip Charge E (B97- E (M06/ E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (E) E	-0.205973 -1.233710 1.636939 -0.745807  mation 14. licity: 4:0 3c) = -4478.40583 def2-TZVP) = -447 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - T38.89991 Kca = -194.58364 Kca X-V/def2-TZVP) = -139.7672 -xTB) = -139.7672 -xTB) = -136.9590 FF) = -18.0674520  nates: 1.087327 3.173120	0.634180 -2.174440 -2.525314 0.023505 0.8585287 Hartree 18.396031220862 Ha 19. = -4476.710650 10.79 = -4477.08631 122444982 Hartree 11/mo1 -4480.43415970233 173729267 Hartree 173729267 Hartree 178324 Hartree 178324 Hartree	3.325519 2.749986 -0.698943 0.343588 Artree 425274 Hartree 425274 Hartree 41 Hartree
СНННСНСНННССНННССНННСНННС	0.940151 2.902337 2.775809 4.254460 4.318654 5.089215 4.414056 2.932912 3.197074 3.702703 1.962317 3.104887 2.737363 1.666392 2.949094 3.349939 4.531219 5.203552 4.605588 4.932112 3.020922 3.717671 3.308540 2.001425 2.001425 2.003317	1.232879 2.967650 1.867486 3.243352 2.787290 2.839140 4.335456 3.540644 4.618079 3.016978 3.423284 -2.625191 -1.575878 -1.596454 -0.551654 -1.736979 -2.333884 -2.294915 -1.346375 -3.105193 -4.037190 -4.108811 -4.826964 -4.262236 -3.557839	0.506862 0.591926 -0.181672 -1.186841 0.426842 -0.295974 1.932108 1.934126 2.533440 2.445660 0.525321 1.588576 1.873824 1.222519 2.500155 0.037795 0.92222 -0.458650 -0.642312 1.137210 1.999224 0.413911 1.512043 -2.286237	Si Si P Co Conform Multip Charge E (B97- E (PBE) E (PBE) E (PMT) E (GFN1- E (GFN1- C (GFN2- C C C C C C C C C C C C C C C C C C C	-0.205973 -1.233710 1.636939 -0.745807  mation 14. licity: 4: 0 3c) = -4478.40583 def2-TZVP) = -447 - D3(BJ)/def2-TZV - T3(BJ)/def2-TZV - T3(BJ)/def2-TZV - T3(BJ)/def2-TZV - T3(BJ)/def2-TZVP) = -136.9590 FF) = -18.0674520  nates:  1.087327 3.173120 4.249539 2.305829	0.634180 -2.174440 -2.525314 0.023505 88585287 Hartree 8.396031220862 Ha PP) = -4476.710650 PP) = -4477.08631 122444982 Hartree 11/mol -4480.43415970233 173729267 Hartree 105112215 Hartree 178324 Hartree 0.362499 0.871323 0.736986 1.793180	3.325519 2.749986 -0.698943 0.343588 artree 425274 Hartree 7034547 Hartree 1 Hartree 0.462283 1.273038 1.410510 1.789036
СНННСНСННННССННННСНННСНННСС	0.940151 2.902337 2.775809 4.254460 4.318654 5.089215 4.414056 2.932912 3.197074 3.702703 1.962317 3.104887 2.737363 1.666392 2.949094 3.349939 4.531219 5.203552 4.605588 4.932112 3.020922 3.717671 3.308540 2.001425 2.003317 3.464639	1.232879 2.967650 1.867486 3.243352 2.787290 2.839140 4.335456 3.540644 4.618079 3.016978 3.423284 -2.625191 -1.575878 -1.596454 -0.551654 -1.736979 -2.333884 -2.294915 -1.346375 -3.105193 -4.037190 -4.108811 -4.826964 -4.262236 -3.557839 -3.866442	0.506862 0.591926 -0.181672 -1.186841 0.426842 -0.295974 1.932108 1.934126 2.533440 2.445660 0.525321 1.588576 1.873824 1.222519 2.500155 0.037795 0.922222 -0.458650 -0.642312 1.137210 1.999224 0.413911 1.512043 -2.286237 -2.639702	Si Si P Co Conform Multip Charge E(B97- E(M06/ E(PBE) E(PBE) E(PBE) E(PBE) E(PBE) E(GFN1) E(GFN2- CGOTdi: C C H	-0.205973 -1.233710 1.636939 -0.745807  mation 14. licity: 4: 0: 3c) = -4478.40583 def2-TZVP) = -447 - D3(BJ)/def2-TZV-3c) = -4473.0060 = -138.89991 Kca = -194.58364 Kca X-V/def2-TZVP) = -473.0060 = -138.89991 FCa = -194.58364 Kca X-V/def2-TZVP) = -3787879 -xTB) = -136.9590 FF) = -18.0674520  nates: 1.087327 3.173120 4.249539 2.305829 2.484308	0.634180 -2.174440 -2.525314 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023606 0.023606 0.023606 0.023606 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499 0.0362499	3.325519 2.749986 -0.698943 0.343588 artree 425274 Hartree 7034547 Hartree 425274 Hartree 11 Hartree 0.462283 1.273038 1.410510 1.789036 2.471304
Сннно ноннно ннноснннноннносн	0.940151 2.902337 2.775809 4.254460 4.318654 5.089215 4.414056 2.932912 3.197074 3.702703 1.962317 3.104887 2.737363 1.666392 2.949094 3.349939 4.531219 5.203552 4.605588 4.932112 3.020922 3.717671 3.308540 2.001425 2.003317 3.464639 3.488049	1.232879 2.967650 1.867486 3.243352 2.787290 2.839140 4.335456 3.540644 4.618079 3.016978 3.423284 -2.625191 -1.575878 -1.596454 -0.551654 -1.736979 -2.333884 -2.294915 -1.346375 -3.105193 -4.037190 -4.108811 -4.826964 -4.262236 -3.557839 -3.866442 -4.470432	0.506862 0.591926 -0.181672 -1.186841 0.426842 -0.295974 1.932108 1.934126 2.533440 2.445660 0.525321 1.588576 1.873824 1.222519 2.500155 0.037795 0.922222 -0.458650 -0.642312 1.137210 1.999224 0.413911 1.512043 -2.286237 -2.6639702 -3.572660	Si Si P Co Conform Multip Charge E (B97- E (M06/ E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (E) E (GFN- COORDI C C C H C C H	-0.205973 -1.233710 1.636939 -0.745807  mation 14. licity: 4: 0 3c) = -4478.40583 def2-TZVP) = -447 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV -3c) = -4473.0060 = -138.89991 Kca = -194.58364 Kca X-V/def2-TZVP) = -32.7672 -xTB) = -139.7672 -xTB) = -139.7672 -xTB) = -136.9590 FF) = -18.0674520  nates: 1.087327 3.173120 4.249539 2.305829 2.484308 3.091062	0.634180 -2.174440 -2.525314 0.023505 0.8585287 Hartree 0.8396031220862 Hartree 0.92444982 Hartree 0.1/mol -4480.43415970233 1.73729267 Hartree 1.73729267 Hartree 0.362499 0.871323 0.736986 1.793180 2.627119 -0.887147	3.325519 2.749986 -0.698943 0.343588 0.343588 0.45274 Hartree 425274 Hartree 425274 Hartree 41 Hartree 0.462283 1.273038 1.410510 1.789036 2.471304 -0.452860
	0.940151 2.902337 2.775809 4.254460 4.318654 5.089215 4.414056 2.932912 3.197074 3.702703 1.962317 3.104887 2.737363 1.666392 2.949094 3.349939 4.531219 5.203552 4.605588 4.932112 3.020922 3.717671 3.308540 2.001425 2.003317 3.464639 3.488049 3.971584	1.232879 2.967650 1.867486 3.243352 2.787290 2.839140 4.335456 3.540644 4.618079 3.016978 3.423284 -2.625191 -1.575878 -1.596454 -0.551654 -1.736979 -2.333884 -2.294915 -1.346375 -3.105193 -4.037190 -4.108811 -4.826964 -4.262236 -3.557839 -3.866442 -4.470432 -4.460650	0.506862 0.591926 -0.181672 -1.186841 0.426842 -0.295974 1.932108 1.934126 2.533440 2.445660 0.525321 1.588576 1.873824 1.222519 2.500155 0.037795 0.922222 -0.458650 -0.642312 1.137210 1.999224 0.413911 1.512043 -2.286237 -2.639702 -3.572660 -1.855734	Si Si P Co Conform Multip Charge E (B97- E (M06/ E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (GFN2- E (GFN2- C C C H C C	-0.205973 -1.233710 1.636939 -0.745807  mation 14. licity: 4: 0 3c) = -4478.40583 def2-TZVP) = -447 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZVP) = -134.58364 Kca X-V/def2-TZVP) = -139.7672 -xTB) = -139.7672 -xTB) = -136.9590 FF) = -18.0674520  nates:	0.634180 -2.174440 -2.525314 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023505 0.023606 0.022044982 Hartree 0.1/mol -4480.43415970233 0.17369267 Hartree 0.362499 0.871323 0.736986 1.793180 2.627119 -0.887147 -2.279277	3.325519 2.749986 -0.698943 0.343588 artree 425274 Hartree 7034547 Hartree 11 Hartree 0.462283 1.273038 1.410510 1.789036 2.471304 -0.452860 -0.200288
СНННСНСНННСННННСННННСННН	0.940151 2.902337 2.775809 4.254460 4.318654 5.089215 4.414056 2.932912 3.197074 3.702703 1.962317 3.104887 2.737363 1.666392 2.949094 3.349939 4.531219 5.203552 4.605588 4.932112 3.020922 3.717671 3.308540 2.001425 2.003317 3.464639 3.488049	1.232879 2.967650 1.867486 3.243352 2.787290 2.839140 4.335456 3.540644 4.618079 3.016978 3.423284 -2.625191 -1.575878 -1.596454 -0.551654 -1.736979 -2.333884 -2.294915 -1.346375 -3.105193 -4.037190 -4.108811 -4.826964 -4.262236 -3.557839 -3.866442 -4.470432	0.506862 0.591926 -0.181672 -1.186841 0.426842 -0.295974 1.932108 1.934126 2.533440 2.445660 0.525321 1.588576 1.873824 1.222519 2.500155 0.037795 0.922222 -0.458650 -0.642312 1.137210 1.999224 0.413911 1.512043 -2.286237 -2.6639702 -3.572660	Si Si P Co Conform Multip Charge E (B97- E (M06/ E (PBE) E (PBE) E (PBE) E (PBE) E (PBE) E (E) E (GFN- COORDI C C C H C C H	-0.205973 -1.233710 1.636939 -0.745807  mation 14. licity: 4: 0 3c) = -4478.40583 def2-TZVP) = -447 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV -3c) = -4473.0060 = -138.89991 Kca = -194.58364 Kca X-V/def2-TZVP) = -32.7672 -xTB) = -139.7672 -xTB) = -139.7672 -xTB) = -136.9590 FF) = -18.0674520  nates: 1.087327 3.173120 4.249539 2.305829 2.484308 3.091062	0.634180 -2.174440 -2.525314 0.023505 0.8585287 Hartree 0.8396031220862 Hartree 0.92444982 Hartree 0.1/mol -4480.43415970233 1.73729267 Hartree 1.73729267 Hartree 0.362499 0.871323 0.736986 1.793180 2.627119 -0.887147	3.325519 2.749986 -0.698943 0.343588 0.343588 0.45274 Hartree 425274 Hartree 425274 Hartree 41 Hartree 0.462283 1.273038 1.410510 1.789036 2.471304 -0.452860

С	4.449163	-2.594240	-2.190222	С	-1.780140	-5.113677	0.937818
H	4.978487	-3.270569	-2.878395	H	-0.721614	-5.394807	0.774011
C	4.478302	-1.213692	-2.407334	H	-2.406250	-5.830687	0.364906
Н	5.025743	-0.808966	-3.271096	H	-2.012468	-5.250069	2.009760
C			-1.554249	C		-3.077253	0.593394
	3.791961	-0.329368			-4.014226		
C	2.383233	-2.842513	1.036949	H	-4.254072	-3.167761	1.672791
H	1.485292	-2.222164	1.233310	H	-4.632898	-3.823264	0.051745
С	1.886186	-4.279503	0.861599	H	-4.331867	-2.068451	0.265075
Н	1.263353	-4.382537	-0.048473	N	2.429132	0.030140	0.448328
H	1.259224	-4.565138	1.728667	N	1.046708	1.481135	1.283346
H	2.719289	-5.010529	0.801120	N	-1.572242	-0.074906	-1.782031
С	3.345254	-2.740481	2.236459	N	-1.197651	-2.056844	0.972337
Н	4.282068	-3.298927	2.030765	Si	-0.767433	-0.361382	-3.324986
						0.523704	
H	2.885398	-3.171755	3.148457	Si	-3.230163		-1.764293
H	3.615392	-1.690362	2.464607	Si	-1.335502	-1.761995	2.702408
C	3.812526	1.166921	-1.850168	Si	-2.158923	-3.367741	0.274024
H	3.011480	1.638756	-1.245219	P	-0.487044	2.415471	1.357640
C	5.152560	1.803888	-1.438829	Co	-0.611193	-0.602940	-0.184923
				CO	0.011195	0.002340	0.104323
H	5.375160	1.654909	-0.364408				
H	5.143135	2.895452	-1.636487	Confo	ormation 17.		
H	5.989850	1.361856	-2.017593	Multi	plicity: 4		
С	3.507251	1.470581	-3.326515	Charo			
Н	4.345813	1.171641	-3.988241		(7-3c) = -4478.40465	7727001 1125+500	
H	3.349739	2.558755	-3.469557		S/def2-TZVP) = -4478		
H	2.597810	0.944811	-3.670559	E(PBE	E - D3(BJ)/def2-TZVI	?) = -4476.711087	665895 Hartree
С	-0.081243	3.782873	0.074665	E (PBE	0 - D3(BJ)/def2-TZV	JP) = -4477.08491	8833831 Hartree
Ċ	1.212597	4.589319	0.255970		(2h-3c) = -4473.00195	,	
H	2.099980	3.930626	0.339896		5) = -145.17434  Kcal		
H	1.193725	5.268867	1.125542		7) = -217.64925  Kcal		
Н	1.365890	5.217604	-0.648061	E(ωB9	97X-V/def2-TZVP) = -	-4480.43155409420	0 Hartree
С	-1.308523	4.714011	0.048670		11-xTB) = $-139.77418$		
Н	-1.229690	5.400403	-0.820891		(12-xTB) = -136.95962		
H	-1.382977	5.343661	0.957702	E (GFN	I-FF) = -18.05990871	17412 Hartree	
H	-2.255088	4.146009	-0.062909				
C	0.011391	3.026261	-1.261588	Coord	linates:		
H	-0.005054	3.755119	-2.099122	С	-0.207602	-0.900670	-0.728243
H	-0.805386	2.294339	-1.412934	С	-1.153471	-2.584555	-1.969549
Н	0.957608	2.454872	-1.335422	Н	-1.914534	-3.050961	-2.601454
C							
	-0.509066	3.171956	3.126313	C	0.023504	-3.064460	-1.471157
C	0.333011	4.424980	3.407346	Н	0.494433	-4.041098	-1.596098
H	0.208562	4.704311	4.475885	C	-2.323705	-0.413657	-2.022173
H	0.008889	5.295260	2.805659	С	-3.637134	-0.606592	-1.533217
Н	1.416429	4.272850	3.236500	С	-4.659439	0.194362	-2.078274
С	-2.002857	3.515176	3.336976	Н	-5.689362	0.074576	-1.710410
Н				C			
	-2.149096	3.890026	4.372344		-4.383395	1.142748	-3.065571
H	-2.649207	2.625588	3.203163	H	-5.192835	1.771182	-3.466530
H	-2.357935	4.303544	2.645047	C	-3.078998	1.290633	-3.555938
C	-0.125127	2.061789	4.118789	H	-2.880922	2.027259	-4.345880
H	0.951062	1.807048	4.082820	С	-2.020363	0.505262	-3.065361
Н	-0.697519	1.135146	3.941008	Č	-3.979101	-1.682361	-0.510368
H	-0.354203	2.407046	5.149473	H	-3.028781	-2.094646	-0.121374
C	0.747814	-1.470760	-3.084774	C	-4.750495	-1.133817	0.698030
H	1.497536	-1.011705	-2.414423	H	-4.139825	-0.393950	1.247135
Н	1.242828	-1.645473	-4.063008	H	-5.003850	-1.957032	1.396329
H	0.477829	-2.457858	-2.663365	H	-5.703513	-0.650272	0.400840
C	-0.157964	1.238124	-4.161400	C	-4.752264	-2.832477	-1.183119
H	-0.994505	1.932927	-4.372206	H	-5.737052	-2.486882	-1.560343
H	0.324671	0.987142	-5.129770	H	-4.935613	-3.653089	-0.459916
H	0.582510	1.780971	-3.545936	H	-4.199730	-3.254961	-2.046739
С	-1.868084	-1.190371	-4.640430	C	-0.621956	0.597480	-3.676267
Н	-2.317918	-2.136080	-4.279670	Н	0.098939	0.567677	-2.830820
H	-1.246502	-1.425031	-5.530306	C	-0.323546	-0.612473	-4.585575
H	-2.689280	-0.524898	-4.976426	H	-0.414628	-1.578377	-4.055029
C	-3.450443	2.070514	-2.858353	H	0.710234	-0.545356	-4.982122
H	-2.772551	2.895198	-2.557945	H	-1.019420	-0.630827	-5.449718
H	-4.494569	2.439586	-2.777207	С	-0.366936	1.888760	-4.461788
Н	-3.259425	1.847819	-3.928041	Н	-0.975976	1.928646	-5.388517
C	-3.779384	0.999856	-0.019438	H	0.696232	1.936595	-4.768923
H	-3.780854	0.118869	0.649463	H	-0.582781	2.791937	-3.862543
H	-4.810109	1.410045	-0.050151	C	3.291293	-1.655689	-1.513934
H	-3.107357	1.756375	0.431363	C	2.989729	-2.515423	-2.748763
С	-4.494322	-0.746180	-2.405425	H	1.944969	-2.381855	-3.091775
H	-4.414465	-0.895002	-3.499638	H	3.172445	-3.593496	-2.588638
Н	-5.522991	-0.389054	-2.186973	Н	3.647349	-2.188970	-3.583328
H	-4.369526		-1.920849		4.762190	-1.805844	-1.083580
		-1.733755		C			
C	0.329786	-1.317765	3.502427	H	5.418540	-1.412666	-1.888518
H	0.967533	-2.222397	3.535375	H	5.050779	-2.861008	-0.909121
H	0.167829	-0.998071	4.552838	H	4.983256	-1.225882	-0.164246
H	0.894455	-0.520612	2.985810	С	3.018889	-0.180434	-1.861357
C	-1.896883	-3.252335	3.749064	Н	3.703088	0.144112	-2.674057
Н	-2.897223	-3.639582	3.472429	H	3.148475		-0.994365
						0.495496	
H	-1.950549	-2.917407	4.806884	H	1.981142	-0.036441	-2.219941
H	-1.173971	-4.091080	3.700553	C	2.487327	-3.744619	0.696421
С	-2.609471	-0.407641	3.086249	C	2.895046	-4.847080	-0.291676
H	-2.415207	0.512985	2.503427	H	3.032464	-5.798087	0.267143
H	-2.617790	-0.154759	4.167164	H	3.852776	-4.628461	-0.801433
H	-3.624751	-0.762285	2.815460	H	2.131607	-5.042335	-1.069339
С							
	-1.886362	-3.531750	-1.588206	C	3.613298	-3.560040	1.741942
H	-2.026537	-2.565719	-2.104559	H	3.796755	-4.526618	2.257500
H	-2.603818	-4.267784	-2.006451	H	3.332109	-2.811373	2.509018
H H			-2.006451 -1.805130	H H	3.332109 4.569151	-2.811373 -3.238278	2.509018 1.285588

С	1.208400	-4.158622	1.447976	Н	2.920131	1.866444	-4.475372
Н	0.354885	-4.357721	0.772677	С	2.452762	0.694406	-2.713606
Н	0.891483	-3.384341	2.170209	C	1.557691	-3.097107	-2.686034
Н	1.411091	-5.089490	2.019258	Н	1.192700	-3.019126	-1.642402
С	-3.492461	2.290662	0.539345	С	0.442146	-3.745830	-3.522727
H	-3.002273	1.976717	-0.399103	H	-0.437017	-3.081941	-3.619593
H	-3.751392	3.365981	0.443193	H	0.111299	-4.691291	-3.048215
H	-4.445481	1.730795	0.614215	H	0.793526	-3.998229	-4.544435
С	-1.469591	3.589981	2.502861	С	2.807316	-3.999128	-2.689548
Н	-1.133755	3.574146	3.559558	Н	3.222405	-4.089861	-3.714721
Н	-2.082028	4.502368	2.348452	Н	2.551064	-5.018761	-2.335784
H	-0.560715	3.653506	1.874948	H	3.611926	-3.608547	-2.036992
С	-3.743020	1.827571	3.481930	С	2.696595	1.833042	-1.728547
H	-4.327180	0.888619	3.394835	Н	1.919041	1.733957	-0.943013
Н	-4.456424	2.672899	3.377798	C	4.085735	1.725533	-1.069103
H	-3.312102	1.874379	4.500167	H	4.227074	0.774298	-0.522210
C	-1.806946	-0.455497	4.805602	H	4.232384	2.552747	-0.344603
H	-1.468259	0.492321	5.271355	H	4.886106	1.799873	-1.834537
H	-1.437947	-1.290539	5.438321	С	2.529733	3.218276	-2.359645
Н	-2.913274	-0.476674	4.830693	Н	3.348756	3.451528	-3.071412
C	0.770487	-0.964634	3.354403	Н	2.554791	3.997710	-1.572218
Н	1.329982	-1.076713	2.403442	H	1.567009	3.301935	-2.895506
H	0.922424	-1.888330	3.951987	C	2.314418	0.527807	3.730533
Н	1.224430	-0.122552	3.911088	С	2.813886	1.541184	2.684215
С	-1.791534	-2.310719	2.392618	Н	1.974568	2.060809	2.181699
H	-2.897278	-2.271255	2.350964	H	3.436713	1.065745	1.901632
H	-1.509648	-3.163156	3.045413	H	3.434427	2.311897	3.188735
H	-1.415201	-2.520996	1.371639	C	3.507703	-0.208804	4.354292
С	1.301490	5.124980	0.044898	H	4.186612	0.534610	4.825830
H	0.883550	5.256124	1.063674	H	4.111378	-0.761336	3.608609
H	0.737565	5.797472	-0.636117	Н	3.199081	-0.915817	5.148263
Н	2.354212	5.466675	0.054381	C	1.562481	1.300334	4.838310
C	-0.696607	3.233548	-1.149796	Н	2.260344	2.007050	5.335631
Н	-1.041389	2.203824	-1.377719	H	1.153730		5.620192
			-2.063184			0.630309	
H	-0.855142	3.843292		H	0.720428	1.889235	4.422611
H	-1.359332	3.642284	-0.365072	С	0.805882	-2.246017	3.635651
С	2.228299	3.198019	-2.119685	С	2.024506	-3.181086	3.605258
H	3.299518	3.218890	-1.831980	Н	1.757836	-4.119692	4.137926
H	2.046006	4.045013	-2.814168	H	2.916084	-2.764265	4.108097
H	2.047784	2.257176	-2.674144	H	2.295854	-3.472055	2.572918
С	3.898013	3.592178	1.490570	С	0.360222	-2.036617	5.096359
H	4.310335	3.546836	0.461326	H	0.020322	-3.005091	5.520267
H	4.747312	3.461965	2.193960	H	-0.485467	-1.325169	5.181679
H	3.483020	4.605048	1.652460	Н	1.187485	-1.668073	5.734981
C	1.826703	2.595582	3.503665	C	-0.326121	-2.908882	2.825574
Н	1.511972	3.658501	3.534450	Н	0.000507	-3.115878	1.787039
H	2.520365	2.415906	4.351004	H	-1.226928	-2.272362	2.763298
H	0.916085	1.982278	3.648194	H	-0.603038	-3.877889	3.293151
С	3.744218	0.674769	2.011038	С	-0.020521	3.149536	0.737770
H	3.191802	-0.264378	2.187471	Н	-0.050806	2.170543	1.267010
H	4.439735	0.837940	2.861128	Н	-0.238921	3.930497	1.494170
H	4.358581	0.543271	1.096190	H	1.015721	3.299059	0.372689
N	-1.267397	-1.266015	-1.533138	C	-3.011357	3.471171	-0.149450
N	0.593847	-2.034100	-0.726779	H	-3.639475	3.808477	-0.998125
N	-1.333345	0.647321	1.938754	H	-3.080550	4.241901	0.646108
N	1.403702	2.054198	0.574614	H	-3.443583	2.528346	0.232042
Si	-2.439161	2.007643	2.105164	С	-0.823640	4.770438	-1.735358
Si	-1.083018	-0.675158	3.061897	Н	0.207845	4.790955	-2.134280
Si	1.110404	3.336862	-0.586631	H	-0.950888	5.650566	-1.069520
Si	2.630870	2.205401	1.827417	H	-1.527295	4.896878	-2.583161
P	2.215001	-1.957113	0.044032	С	-3.410995	2.121479	-3.413294
Со	0.009534	0.701451	0.533429	Н	-4.106085	1.709994	-2.654794
				H	-3.802530	1.854717	-4.417589
Confo	rmation 18.			H	-3.441953	3.227615	-3.329425
Multi	plicity: 4			C	-1.569847	-0.321771	-3.800204
Charg	e: 0			H	-0.544463	-0.728461	-3.701433
	-3c) = -4478.40857	1759936 Hartree		Н	-1.842570	-0.357429	-4.875484
	/def2-TZVP) = -4478		rtree	Н	-2.268115	-0.981252	-3.251554
	- D3(BJ)/def2-TZV			C	-0.612157	2.456257	-4.490508
	0 - D3(BJ)/def2-TZV			Н	-0.547586	3.533532	-4.242757
	h-3c) = -4473.00094	,	1333112 11010100	Н	-1.095257	2.367497	-5.486598
	) = -146.03076  Kca			H	0.415177	2.054112	-4.577440
	) = -212.78351  Kca			C	-2.264638	1.944481	3.012547
			6 Hartree	Н			
	7X-V/def2-TZVP) = -		о нагитее		-1.211556	1.740397	3.290202
	1-xTB) = $-139.77428$			H	-2.816705	2.216855	3.936285
	(2-xTB) = -136.9625			H	-2.288463	2.813537	2.332234
E (GFN	-FF) = $-18.04870513$	38171 Hartree		С	-3.172060	-0.787256	3.795515
				H	-3.549432	-1.797050	3.546092
	inates:			H	-3.866584	-0.341075	4.538503
С	1.120977	-0.474054	0.087169	H	-2.187703	-0.898875	4.289708
С	3.169215	-1.455202	-0.250811	C	-4.883461	0.768358	1.875873
H	4.026360	-1.794648	-0.838117	H	-4.999549	1.391993	0.967630
С	2.936485	-1.463208	1.091541	Н	-5.358738	1.308132	2.722046
Н	3.561207	-1.821921	1.909420	Н	-5.459022	-0.167139	1.716348
C	2.081782	-0.602292	-2.270789	C	-4.253860	-1.048239	-1.207385
C	1.896528	-1.688369	-3.161072	Н	-5.167470	-0.720367	-0.672159
C	2.078096	-1.442138	-4.536702	H	-4.541573	-1.861039	-1.906763
Н	1.929339	-2.263356	-5.252705	H	-3.891589	-0.189727	-1.803442
C	2.445217	-0.176732	-5.000862	C	-1.519574	-2.466237	-0.937459
Н	2.585563	-0.176732	-6.078644	Н	-0.911916	-1.740966	-1.519525
н С							
C	2.629466	0.877255	-4.096731	Н	-1.910820	-3.212274	-1.658651

H	-0.837417	-2.985006	-0.234237	H	-0.791796	-3.721130	3.309934
C	-3.746167	-2.985028	1.071809	С	0.556736	3.308502	1.174440
H	-3.046454	-3.429495	1.807099	H	0.535124	2.295291	1.625717
Н	-4.095768	-3.796690	0.399088	H	0.487290	4.049501	1.997041
Н	-4.631879	-2.607915	1.622047	Н	1.542745	3.433818	0.682646
N	2.060866	-0.857227	-0.849539	C	-2.450473	4.021401	0.775247
		-0.868669	1.289338	Н	-3.218215	4.284760	0.019643
N	1.689490						
N	-1.026958	1.667699	-1.570719	H	-2.275872	4.921252	1.402434
N	-2.202897	-0.305404	0.920965	H	-2.877864	3.233170	1.418815
Si	-1.226470	3.201670	-0.736659	C	-0.430712	5.075877	-1.117924
Si	-1.626923	1.477044	-3.211683	H	0.460753	4.975821	-1.764702
Si	-3.061158	0.383040	2.291406	H	-0.241464	5.906435	-0.404721
Si	-2.928147	-1.625560	0.020251	H	-1.287673	5.379865	-1.752607
P	0.921404	-0.489597	2.870652	С	-3.638451	2.434259	-2.349167
Co	-0.733281	0.342398	-0.180458	Н	-4.110797	1.887248	-1.508510
				Н	-4.216954	2.218356	-3.271756
Confor	mation 19.			Н	-3.736787	3.519426	-2.139242
	licity: 4			C	-1.727204	0.207054	-3.300481
_							
Charge				H	-0.683300	-0.060792	-3.549804
	-3c) = -4478.40842			H	-2.311927	0.194541	-4.244035
	def2-TZVP) = -447			H	-2.144611	-0.580298	-2.647006
E (PBE	- D3(BJ)/def2-TZV	P) = -4476.714887	455842 Hartree	C	-1.086483	3.078032	-3.892693
E(PBEC	- D3(BJ)/def2-TZ	VP) = -4477.08937	7533198 Hartree	H	-1.111874	4.150009	-3.619739
E (PBEh	1-3c) = -4473.0069	10938894 Hartree		H	-1.679282	2.951039	-4.823287
E(PM6)	= -144.35197 Kca	1/mol		H	-0.038895	2.801475	-4.125703
E (PM7)	= -214.56319 Kca	1/mo1		С	-1.870364	1.488787	3.241712
	X-V/def2-TZVP) =		9 Hartree	Н	-1.064726	0.942707	3.771042
	-xTB) = $-139.7734$			H	-2.478081	2.032557	3.994827
				н Н			
	2-xTB) = $-136.9628$				-1.388525	2.241073	2.594108
E (GFN-	-FF) = -18.0642497	o∠40/ Hartree		C	-3.515363	-0.953687	3.687508
				H	-4.329055	-1.636221	3.377495
Coordi	.nates:			H	-3.887233	-0.358887	4.548837
C	1.080817	-0.624478	-0.110882	H	-2.672482	-1.575429	4.050599
C	2.912550	-1.867421	-0.712386	С	-4.580413	1.121223	1.745020
Н	3.647162	-2.291812	-1.401995	Н	-4.406609	1.737022	0.840760
С	2.804687	-1.942045	0.646643	H	-5.005661	1.774319	2.535462
Н	3.435770	-2.451754	1.377361	Н	-5.348319	0.362096	1.488837
C	1.795303	-0.644619	-2.541570	C	-4.327446	-1.271331	-1.078777
C	1.466094	-1.594920	-3.540038	Н	-5.214900	-0.974083	-0.483549
C	1.490949	-1.167769	-4.882844	H	-4.634226	-2.107144	-1.742572
Н	1.230959	-1.882922		п Н	-4.056592	-0.409356	
			-5.676648				-1.716665
C	1.823588	0.146230	-5.218392	C	-1.576131	-2.702054	-0.925883
H	1.823160	0.463566	-6.272044	H	-1.017453	-2.000745	-1.572825
C	2.162057	1.061030	-4.213462	Н	-2.010142	-3.492350	-1.571237
H	2.439161	2.086890	-4.490444	H	-0.844696	-3.175177	-0.240090
C	2.172683	0.688647	-2.857437	С	-3.711383	-3.174212	1.160439
C	1.112117	-3.044194	-3.228305	H	-3.048584	-3.529997	1.973097
Н	0.903682	-3.114975	-2.142336	Н	-3.944803	-4.041223	0.506400
С	-0.153754	-3.501343	-3.973752	H	-4.664797	-2.840350	1.615812
H	-0.984250	-2.782007	-3.844065	N	1.864284	-1.063084	-1.160755
Н	-0.488310	-4.487101	-3.592967	N	1.693861	-1.178443	1.001639
Н	0.032115	-3.615422	-5.061478	N	-0.956575	2.016125	-1.011146
C	2.288094	-3.984792	-3.553622	N	-2.160850	-0.496653	0.953992
H	2.537958	-3.943340	-4.633985	Si	-0.840602	3.516380	-0.102120
H	2.027499	-5.034161	-3.306113	Si	-1.811186	1.943224	-2.546985
H	3.206997	-3.723202	-2.992394	Si	-2.981703	0.261211	2.314782
C	2.659245	1.658322	-1.786579	Si	-2.920373	-1.818470	0.079671
H	2.008665	1.509218	-0.900260	P	1.166675	-0.633121	2.627899
C	4.117254	1.341732	-1.399282	Co	-0.706530	0.372553	-0.012773
Н	4.241581	0.303828	-1.035548				
H	4.462019	2.023906	-0.595805	Confor	mation 26.		
Н	4.787086	1.478245	-2.273512		olicity: 4		
С	2.531336	3.126805	-2.195460	Charge			
Н	3.244310	3.400624	-3.000681		-3c) = -4478.408297	694679 Hartree	
Н	2.754408	3.781820	-1.330228		def2-TZVP) = -4478		rtree
H	1.505369	3.353491	-2.537925		- D3(BJ)/def2-TZVP		
C	2.761164	0.212952	3.306174		- D3(BJ)/def2-TZV		
		0.996080	2.139705		(-3c) = -4472.99978		0343492 Hartree
					= -144.64162 Kcal		
C	3.387407					/ MOT	
H	2.634507	1.582217	1.578916			/ -	
H H	2.634507 3.907749	0.329351	1.425867		= -214.11234 Kcal		
H H H	2.634507 3.907749 4.136597	0.329351 1.712073	1.425867 2.539884	Ε(ωΒ97	= -214.11234 Kcal  X-V/def2-TZVP) = -	4480.43514378355	4 Hartree
H H H C	2.634507 3.907749 4.136597 3.834792	0.329351 1.712073 -0.660638	1.425867 2.539884 3.966302	E(ωB97 E(GFN1	= -214.11234 Kcal X-V/def2-TZVP) = - -xTB) = -139.77453	4480.43514378355 4268981 Hartree	4 Hartree
H H H C	2.634507 3.907749 4.136597 3.834792 4.682537	0.329351 1.712073 -0.660638 -0.014623	1.425867 2.539884 3.966302 4.283097	E (ωB97 E (GFN1 E (GFN2	= -214.11234 Kcal X-V/def2-TZVP) = - -xTB) = -139.77453 -xTB) = -136.96276	4480.43514378355 4268981 Hartree 3915174 Hartree	4 Hartree
Н Н Н С Н	2.634507 3.907749 4.136597 3.834792 4.682537 4.248699	0.329351 1.712073 -0.660638 -0.014623 -1.423846	1.425867 2.539884 3.966302 4.283097 3.278549	E (ωB97 E (GFN1 E (GFN2	= -214.11234 Kcal X-V/def2-TZVP) = - -xTB) = -139.77453	4480.43514378355 4268981 Hartree 3915174 Hartree	4 Hartree
H H H C	2.634507 3.907749 4.136597 3.834792 4.682537	0.329351 1.712073 -0.660638 -0.014623	1.425867 2.539884 3.966302 4.283097	E (ωB97 E (GFN1 E (GFN2	= -214.11234 Kcal X-V/def2-TZVP) = - -xTB) = -139.77453 -xTB) = -136.96276	4480.43514378355 4268981 Hartree 3915174 Hartree	4 Hartree
Н Н Н С Н	2.634507 3.907749 4.136597 3.834792 4.682537 4.248699	0.329351 1.712073 -0.660638 -0.014623 -1.423846	1.425867 2.539884 3.966302 4.283097 3.278549	E (ωB97 E (GFN1 E (GFN2 E (GFN-	= -214.11234 Kcal X-V/def2-TZVP) = - -xTB) = -139.77453 -xTB) = -136.96276	4480.43514378355 4268981 Hartree 3915174 Hartree	4 Hartree
Н Н С Н Н	2.634507 3.907749 4.136597 3.834792 4.682537 4.248699 3.461107	0.329351 1.712073 -0.660638 -0.014623 -1.423846 -1.171975	1.425867 2.539884 3.966302 4.283097 3.278549 4.874238	E (ωB97 E (GFN1 E (GFN2 E (GFN-	= -214.11234 Kcal X-V/def2-TZVP) = - -xTB) = -139.77453 -xTB) = -136.96276 FFF) = -18.05670184	4480.43514378355 4268981 Hartree 3915174 Hartree	4 Hartree -0.484431
H H C H H C	2.634507 3.907749 4.136597 3.834792 4.682537 4.248699 3.461107 2.206158 3.042841	0.329351 1.712073 -0.660638 -0.014623 -1.423846 -1.171975 1.216569 1.809187	1.425867 2.539884 3.966302 4.283097 3.278549 4.874238 4.342180 4.769848	E (ωB97 E (GFN1 E (GFN2 E (GFN-	= -214.11234 Kcal X-V/def2-TZVP) = - -xTB) = -139.77453 -xTB) = -136.96276 FF) = -18.05670184 .nates: 0.659939	4480.43514378355 4268981 Hartree 3915174 Hartree 9400 Hartree 0.921753	-0.484431
Н Н С Н Н С Н Н	2.634507 3.907749 4.136597 3.834792 4.682537 4.248699 3.461107 2.206158 3.042841 1.691413	0.329351 1.712073 -0.660638 -0.014623 -1.423846 -1.171975 1.216569 1.809187 0.711123	1.425867 2.539884 3.966302 4.283097 3.278549 4.874238 4.342180 4.769848 5.183868	E (ωB97 E (GFN1 E (GFN2 E (GFN- Coordi C	= -214.11234 Kcal X-V/def2-TZVP) = - -xTB) = -139.77453 -xTB) = -136.96276 -FF) = -18.05670184 .nates: 0.659939 1.671749	4480.43514378355 4268981 Hartree 3915174 Hartree 9400 Hartree 0.921753 2.912631	-0.484431 -1.018752
Н Н С Н Н С Н Н Н	2.634507 3.907749 4.136597 3.834792 4.682537 4.248699 3.461107 2.206158 3.042841 1.691413 1.487321	0.329351 1.712073 -0.660638 -0.014623 -1.423846 -1.171975 1.216569 1.809187 0.711123 1.920712	1.425867 2.539884 3.966302 4.283097 3.278549 4.874238 4.342180 4.769848 5.183868 3.878654	E (\omega B97 E (GFN1 E (GFN2 E (GFN- Coordi C C H	= -214.11234 Kcal X-V/def2-TZVP) = - -xTB) = -139.77453 -xTB) = -136.96276 FF) = -18.05670184 .nates: 0.659939 1.671749 1.787752	4480.43514378355 4268981 Hartree 3915174 Hartree 9400 Hartree 0.921753 2.912631 3.999510	-0.484431 -1.018752 -1.028365
Н Н С Н Н С Н Н С Н С Н С С Н С С С Н С С С С С С С С С С С С С С С С С С С С	2.634507 3.907749 4.136597 3.834792 4.682537 4.248699 3.461107 2.206158 3.042841 1.691413 1.487321 0.845813	0.329351 1.712073 -0.660638 -0.014623 -1.423846 -1.171975 1.216569 1.809187 0.711123 1.920712 -2.295312	1.425867 2.539884 3.966302 4.283097 3.278549 4.874238 4.342180 4.769848 5.183868 3.878654 3.515143	E(\omega B97 E(GFN1 E(GFN2 E(GFN- Coordi C C H C	= -214.11234 Kcal X-V/def2-TZVP) = - -xTB) = -139.77453 -xTB) = -136.96276 FF) = -18.05670184 .nates: 0.659939 1.671749 1.787752 2.380919	4480.43514378355 4268981 Hartree 3915174 Hartree 9400 Hartree 0.921753 2.912631 3.999510 1.924740	-0.484431 -1.018752 -1.028365 -1.633733
Н Н С Н Н С С Н Н С С С С	2.634507 3.907749 4.136597 3.834792 4.682537 4.248699 3.461107 2.206158 3.042841 1.691413 1.487321 0.845813 1.956003	0.329351 1.712073 -0.660638 -0.014623 -1.423846 -1.171975 1.216569 1.809187 0.711123 1.920712 -2.295312 -3.352654	1.425867 2.539884 3.966302 4.283097 3.278549 4.874238 4.342180 4.769848 5.183868 3.878654 3.515143 3.618599	E (\omega B97 E (GFN1 E (GFN2 E (GFN2 Coordi C C H C H	= -214.11234 Kcal X-V/def2-TZVP) = - -xTB) = -139.77453 -xTB) = -136.96276 FF) = -18.05670184 .nates: 0.659939 1.671749 1.787752 2.380919 3.252862	4480.43514378355 4268981 Hartree 3915174 Hartree 9400 Hartree 0.921753 2.912631 3.999510 1.924740 1.985613	-0.484431 -1.018752 -1.028365 -1.633733 -2.285473
Н Н С Н Н С Н Н С Н Н С С Н Н Н С С Н Н Н С С Н Н С С С Н Н С С С С С С С С С С С С С С С С С С С С	2.634507 3.907749 4.136597 3.834792 4.682537 4.248699 3.461107 2.206158 3.042841 1.691413 1.487321 0.845813 1.956003 1.544794	0.329351 1.712073 -0.660638 -0.014623 -1.423846 -1.171975 1.216569 1.809187 0.711123 1.920712 -2.295312 -3.352654 -4.238325	1.425867 2.539884 3.966302 4.283097 3.278549 4.874238 4.342180 4.769848 5.183868 3.878654 3.515143 3.618599 4.149886	E (\omega B97 E (GFN1 E (GFN2 E (GFN- Coordi C C H C	= -214.11234 Kcal X-V/def2-TZVP) = - -xTB) = -139.77453 -xTB) = -136.96276 FF) = -18.05670184 .nates: 0.659939 1.671749 1.787752 2.380919 3.252862 -0.371021	4480.43514378355 4268981 Hartree 3915174 Hartree 9400 Hartree 0.921753 2.912631 3.999510 1.924740 1.985613 3.111034	-0.484431 -1.018752 -1.028365 -1.633733 -2.285473 0.314100
H H C H H C C H H H H C H H H H H H H H	2.634507 3.907749 4.136597 3.834792 4.682537 4.248699 3.461107 2.206158 3.042841 1.691413 1.487321 0.845813 1.956003 1.544794 2.840495	0.329351 1.712073 -0.660638 -0.014623 -1.423846 -1.171975 1.216569 1.809187 0.711123 1.920712 -2.295312 -3.352654 -4.238325 -3.012851	1.425867 2.539884 3.966302 4.283097 3.278549 4.874238 4.342180 4.769848 5.183868 3.878654 3.515143 3.618599 4.149886 4.184318	E (\omega B97 E (GFN1 E (GFN2 E (GFN- Coordi C C H C C H C	= -214.11234 Kcal X-V/def2-TZVP) = - -xTB) = -139.77453 -xTB) = -136.96276 FF) = -18.05670184 .nates: 0.659939 1.671749 1.787752 2.380919 3.252862 -0.371021 -1.574289	4480.43514378355 4268981 Hartree 3915174 Hartree 9400 Hartree 0.921753 2.912631 3.999510 1.924740 1.985613 3.111034 3.361716	-0.484431 -1.018752 -1.028365 -1.633733 -2.285473 0.314100 -0.395822
H H C H H C H H C H H H C H H H H H H H	2.634507 3.907749 4.136597 3.834792 4.682537 4.248699 3.461107 2.206158 3.042841 1.691413 1.487321 0.845813 1.956003 1.544794 2.840495 2.282009	0.329351 1.712073 -0.660638 -0.014623 -1.423846 -1.171975 1.216569 1.809187 0.711123 1.920712 -2.295312 -3.352654 -4.238325 -3.012851 -3.711361	1.425867 2.539884 3.966302 4.283097 3.278549 4.874238 4.342180 4.769848 5.183868 3.878654 3.515143 3.618599 4.149886 4.184318 2.623335	E (WB97 E (GFN1 E (GFN2 E (GFN- COORDI C C H C H C C	= -214.11234 Kcal X-V/def2-TZVP) = - -xTB) = -139.77453 -xTB) = -136.96276 -FF) = -18.05670184 .nates: 0.659939 1.671749 1.787752 2.380919 3.252862 -0.371021 -1.574289 -2.468775	4480.43514378355 4268981 Hartree 3915174 Hartree 9400 Hartree 0.921753 2.912631 3.999510 1.924740 1.985613 3.111034 3.361716 4.293860	-0.484431 -1.018752 -1.028365 -1.633733 -2.285473 0.314100 -0.395822 0.159472
H H C H H C H H C C H H C C H C C H	2.634507 3.907749 4.136597 3.834792 4.682537 4.248699 3.461107 2.206158 3.042841 1.691413 1.487321 0.845813 1.956003 1.544794 2.840495 2.282009 0.373084	0.329351 1.712073 -0.660638 -0.014623 -1.423846 -1.171975 1.216569 1.809187 0.711123 1.920712 -2.295312 -3.352654 -4.238325 -3.012851 -3.711361 -1.893092	1.425867 2.539884 3.966302 4.283097 3.278549 4.874238 4.342180 4.769848 5.183868 3.878654 3.515143 3.618599 4.149886 4.184318 2.623335 4.927172	E(GFN1 E(GFN2 E(GFN- COORDIC C C H C C H C C	= -214.11234 Kcal X-V/def2-TZVP) = - -xTB) = -139.77453 (-xTB) = -136.96276 (-FF) = -18.05670184 .nates: 0.659939 1.671749 1.787752 2.380919 3.252862 -0.371021 -1.574289 -2.468775 -3.407763	4480.43514378355 4268981 Hartree 3915174 Hartree 9400 Hartree  0.921753 2.912631 3.999510 1.924740 1.985613 3.111034 3.361716 4.293860 4.516492	-0.484431 -1.018752 -1.028365 -1.633733 -2.285473 0.314100 -0.395822 0.159472 -0.365313
H H C H H C H H C H H H C H H H H H H H	2.634507 3.907749 4.136597 3.834792 4.682537 4.248699 3.461107 2.206158 3.042841 1.691413 1.487321 0.845813 1.956003 1.544794 2.840495 2.282009	0.329351 1.712073 -0.660638 -0.014623 -1.423846 -1.171975 1.216569 1.809187 0.711123 1.920712 -2.295312 -3.352654 -4.238325 -3.012851 -3.711361 -1.893092 -2.781999	1.425867 2.539884 3.966302 4.283097 3.278549 4.874238 4.342180 4.769848 5.183868 3.878654 3.515143 3.618599 4.149886 4.184318 2.623335	E (WB97 E (GFN1 E (GFN2 E (GFN- COORDI C C H C H C C	= -214.11234 Kcal X-V/def2-TZVP) = - -xTB) = -139.77453 -xTB) = -136.96276 -FF) = -18.05670184 .nates: 0.659939 1.671749 1.787752 2.380919 3.252862 -0.371021 -1.574289 -2.468775	4480.43514378355 4268981 Hartree 3915174 Hartree 9400 Hartree 0.921753 2.912631 3.999510 1.924740 1.985613 3.111034 3.361716 4.293860	-0.484431 -1.018752 -1.028365 -1.633733 -2.285473 0.314100 -0.395822 0.159472
H H C H H C H H C C H H C C H C C H	2.634507 3.907749 4.136597 3.834792 4.682537 4.248699 3.461107 2.206158 3.042841 1.691413 1.487321 0.845813 1.956003 1.544794 2.840495 2.282009 0.373084	0.329351 1.712073 -0.660638 -0.014623 -1.423846 -1.171975 1.216569 1.809187 0.711123 1.920712 -2.295312 -3.352654 -4.238325 -3.012851 -3.711361 -1.893092	1.425867 2.539884 3.966302 4.283097 3.278549 4.874238 4.342180 4.769848 5.183868 3.878654 3.515143 3.618599 4.149886 4.184318 2.623335 4.927172	E(GFN1 E(GFN2 E(GFN- COORDIC C C H C C H C C	= -214.11234 Kcal X-V/def2-TZVP) = - -xTB) = -139.77453 (-xTB) = -136.96276 (-FF) = -18.05670184 .nates: 0.659939 1.671749 1.787752 2.380919 3.252862 -0.371021 -1.574289 -2.468775 -3.407763	4480.43514378355 4268981 Hartree 3915174 Hartree 9400 Hartree  0.921753 2.912631 3.999510 1.924740 1.985613 3.111034 3.361716 4.293860 4.516492	-0.484431 -1.018752 -1.028365 -1.633733 -2.285473 0.314100 -0.395822 0.159472 -0.365313
H H C H H C H H H C H H H C H H H H H H	2.634507 3.907749 4.136597 3.834792 4.682537 4.248699 3.461107 2.206158 3.042841 1.691413 1.487321 0.845813 1.956003 1.544794 2.840495 2.282009 0.3733084 -0.046949	0.329351 1.712073 -0.660638 -0.014623 -1.423846 -1.171975 1.216569 1.809187 0.711123 1.920712 -2.295312 -3.352654 -4.238325 -3.012851 -3.711361 -1.893092 -2.781999	1.425867 2.539884 3.966302 4.283097 3.278549 4.874238 4.342180 4.769848 5.183868 3.878654 3.515143 3.618599 4.149886 4.184318 2.623335 4.927172 5.443619	E(WB97 E(GFN1) E(GFN2) E(GFN- Coordi C C H C C H C C	= -214.11234 Kcal X-V/def2-TZVP) = - -xTB) = -139.77453 -xTB) = -136.96276 FF) = -18.05670184 nates: 0.659939 1.671749 1.787752 2.380919 3.252862 -0.371021 -1.574289 -2.468775 -3.407763 -2.183986	4480.43514378355 4268981 Hartree 3915174 Hartree 9400 Hartree  0.921753 2.912631 3.999510 1.924740 1.985613 3.111034 3.361716 4.293860 4.516492 4.945806	-0.484431 -1.018752 -1.028365 -1.633733 -2.285473 0.314100 -0.395822 0.159472 -0.365313 1.366371
H H C H H C H H C H H H C H H H H C H H H H H H H H H H H H H H H H H H H H	2.634507 3.907749 4.136597 3.834792 4.682537 4.248699 3.461107 2.206158 3.042841 1.691413 1.487321 0.845813 1.956003 1.544794 2.840495 2.282009 0.373084 -0.046949 -0.4421990	0.329351 1.712073 -0.660638 -0.014623 -1.423846 -1.171975 1.216569 1.809187 0.711123 1.920712 -2.295312 -3.352654 -4.238325 -3.012851 -3.711361 -1.893092 -2.781999 -1.120822	1.425867 2.539884 3.966302 4.283097 3.278549 4.874238 4.342180 4.769848 5.183868 3.878654 3.515143 3.618599 4.149886 4.184318 2.623335 4.927172 5.443619 4.892506	E(GFN1 E(GFN2 E(GFN2 E(GFN- Coordi C C C H C C C C H C C H	= -214.11234 Kcal X-V/def2-TZVP) = - -xTB) = -139.77453 -xTB) = -136.96276 FF) = -18.05670184 .nates: 0.659939 1.671749 1.787752 2.380919 3.252862 -0.371021 -1.574289 -2.468775 -3.407763 -2.183986 -2.902860	4480.43514378355 4268981 Hartree 3915174 Hartree 9400 Hartree  0.921753 2.912631 3.999510 1.924740 1.985613 3.111034 3.361716 4.293860 4.516492 4.945806 5.668242	-0.484431 -1.018752 -1.028365 -1.633733 -2.285473 0.314100 -0.395822 0.159472 -0.365313 1.366371 1.781469
H H C H H C H H C C H H H C H H H H H H	2.634507 3.907749 4.136597 3.834792 4.682537 4.248699 3.461107 2.206158 3.042841 1.691413 1.487321 0.845813 1.956003 1.544794 2.840495 2.282009 0.373084 -0.046949 -0.421990 1.203539	0.329351 1.712073 -0.660638 -0.014623 -1.423846 -1.171975 1.216569 1.809187 0.711123 1.920712 -2.295312 -3.352654 -4.238325 -3.012851 -3.711361 -1.893092 -2.781999 -1.120822 -1.508596	1.425867 2.539884 3.966302 4.283097 3.278549 4.874238 4.342180 4.769848 5.183868 3.878654 3.515143 3.618599 4.149886 4.184318 2.623335 4.927172 5.443619 4.892506 5.553242	E(WB97 E(GFN) E(GFN- Coordi C C C H C C C H C C H C C	= -214.11234 Kcal X-V/def2-TZVP) = - -xTB) = -139.77453 -xTB) = -136.96276 FF) = -18.05670184 .nates:	4480.43514378355 4268981 Hartree 3915174 Hartree 9400 Hartree  0.921753 2.912631 3.999510 1.924740 1.985613 3.111034 3.361716 4.293860 4.516492 4.945806 5.668242 4.675756	-0.484431 -1.018752 -1.028365 -1.633733 -2.285473 0.314100 -0.395822 0.159472 -0.365313 1.366371 1.781469 2.046256
H H H C H H H C C H H H C H H H C H H H H C H H H H H H H H H H H H H H H H H H H H	2.634507 3.907749 4.136597 3.834792 4.682537 4.248699 3.461107 2.206158 3.042841 1.691413 1.487321 0.845813 1.956003 1.544794 2.840495 2.282009 0.373084 -0.046949 -0.421990 1.203539 -0.328156 0.021012	0.329351 1.712073 -0.660638 -0.014623 -1.423846 -1.171975 1.216569 1.809187 0.711123 1.920712 -2.295312 -3.352654 -4.238325 -3.012851 -3.711361 -1.893092 -2.781999 -1.120822 -1.508596 -2.899906 -3.327177	1.425867 2.539884 3.966302 4.283097 3.278549 4.874238 4.342180 4.769848 5.183868 3.878654 3.515143 3.618599 4.149886 4.184318 2.623335 4.927172 5.443619 4.892506 5.553242 2.723106 1.762325	E(WB97 E(GFN1 E(GFN2 E(GFN- Coordi C C H C C C H C C C H C C C H C C H C C H C C H C C C C H C C C C C C C C C C C C C C C C C C C C	= -214.11234 Kcal X-V/def2-TZVP) = - -xTB) = -139.77453 -xTB) = -136.96276 FF) = -18.05670184 .nates: 0.659939 1.671749 1.787752 2.380919 3.252862 -0.371021 -1.574289 -2.468775 -3.407763 -2.183986 -2.902860 -0.993662 -0.781650 -0.054356	4480.43514378355 4268981 Hartree 3915174 Hartree 9400 Hartree  0.921753 2.912631 3.999510 1.924740 1.985613 3.111034 3.361716 4.293860 4.516492 4.945806 5.668242 4.675756 5.188257 3.758964	-0.484431 -1.018752 -1.028365 -1.633733 -2.285473 0.314100 -0.395822 0.159472 -0.365313 1.366371 1.781469 2.046256 2.995867 1.533313
H H H C H H H C C H H H C H H C H H C H H C H H C H C H C H C H C H C H C H C H C H C H C H C H C H H C H H H C H H H H H H H H H H H H H H H H H H H H	2.634507 3.907749 4.136597 3.834792 4.682537 4.248699 3.461107 2.206158 3.042841 1.691413 1.487321 0.845813 1.956003 1.544794 2.840495 2.282009 0.373084 -0.046949 -0.421990 1.203539 -0.328156	0.329351 1.712073 -0.660638 -0.014623 -1.423846 -1.171975 1.216569 1.809187 0.711123 1.920712 -2.295312 -3.352654 -4.238325 -3.012851 -3.711361 -1.893092 -2.781999 -1.120822 -1.508596 -2.899906	1.425867 2.539884 3.966302 4.283097 3.278549 4.874238 4.342180 4.769848 5.183868 3.878654 3.515143 3.618599 4.149886 4.184318 2.623335 4.927172 5.443619 4.892506 5.553242 2.723106	E ( WB97 E ( GFN ) E ( GFN ) E ( GFN ) Coordi C C H C H C H C H C H C H C H C H C H	= -214.11234 Kcal X-V/def2-TZVP) = - (-xTB) = -139.77453 (-xTB) = -136.96276 (-xTB) = -18.05670184  .nates:	4480.43514378355 4268981 Hartree 3915174 Hartree 9400 Hartree  0.921753 2.912631 3.999510 1.924740 1.985613 3.111034 3.361716 4.293860 4.516492 4.945806 5.668242 4.675756 5.188257	-0.484431 -1.018752 -1.028365 -1.633733 -2.285473 0.314100 -0.395822 0.159472 -0.365313 1.366371 1.781469 2.046256 2.995867

H	-1.474308	1.650641	-1.646385	H	-0.044097	-5.101575	-1.641328
С	-3.361915	2.580807	-2.040130	Н	0.298379	-3.381819	-2.026833
Н	-3.916905	2.135672	-1.194718	N	0.634111	2.293325	-0.322688
Н	-3.518446	1.940507	-2.931086	N	1.760575	0.719342	-1.303563
H	-3.808284	3.570305	-2.271648	N	-2.403504	-0.236998	0.608933
C	-1.141429	3.393071	-2.893703	N	0.331836	-2.171421	1.024942
H	-1.499570	4.438659	-2.995996	Si	-3.174586	-1.272942	-0.582418
Н	-1.348167	2.869421	-3.849545	Si	-3.331697	0.369915	1.971221
Н				Si		-1.842832	2.712382
	-0.043490	3.421266	-2.759098		0.687086		
С	1.263682	3.531752	2.265920	Si	0.407500	-3.825239	0.434195
H	1.703347	2.593282	1.873138	P	2.170506	-0.911820	-1.933917
С	2.255723	4.678891	1.991937	Co	-0.497198	-0.532839	0.363749
Н	2.482302	4.792595	0.914298				
H	3.214047			0			
		4.498251	2.520511		ormation 31.		
H	1.845742	5.645180	2.352005		plicity: 4		
C	1.071547	3.359021	3.781749	Charg	ge: O		
H	0.776368	4.312356	4.266350	E(B97	7-3c) = -4478.404808	017763 Hartree	
H	2.021794	3.034839	4.251500	E (M06	5/def2-TZVP) = -4478	3.393357518231 Ha	rtree
Н	0.297625	2.603959	4.014467		E - D3(BJ)/def2-TZVF		
С	3.974641	-1.080059	-1.306636		EO - D3(BJ)/def2-TZV		5220489 Hartree
C	4.981389	0.058024	-1.535788		Eh-3c) = -4473.00152		
H	4.698699	0.977081	-0.988127	E(PM6	5) = -143.91038 Kcal	./mol	
H	5.133050	0.307332	-2.601756	E (PM7	7) = -201.53475  Kcal	/mol	
Н	5.966806	-0.259620	-1.131003		7X-V/def2-TZVP) = -		O Hartree
							O Hartree
С	4.516190	-2.375067	-1.943249		11-xTB) = $-139.76916$		
H	5.435969	-2.692340	-1.408369		12-xTB) = -136.95841		
H	4.783591	-2.232684	-3.009375	E (GFN	I-FF) = -18.05709242	6330 Hartree	
H	3.791215	-3.210908	-1.878215				
С	3.794731	-1.261889	0.214602	Coord	dinates:		
						0 305100	0 407151
H	4.759913	-1.565525	0.673236	С	1.067720	-0.395109	0.487151
H	3.026622	-2.017433	0.460970	C	3.246323	-1.113370	0.623948
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C	2.137675	-0.608462	-3.837230	C	3.056249	-0.215377	1.630519
C	3.336993	0.072367	-4.510207	Н	3.754672	0.155352	2.380361
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H	4.275511	-0.499620	-4.378120	C	1.147076	-3.318152	-0.975006
H	3.503099	1.106322	-4.150658	C	1.145656	-4.248448	-2.029679
С	1.969927	-2.030574	-4.419464	Н	0.564302	-5.173853	-1.928505
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Н	-1.326312	-3.867967	-1.434631	H	-1.369830	-1.606679	2.631749
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C	-1.684673	-2.709155	-3.125396	H	4.811148	0.454882	2.651479
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H	-2.999500	3.595128	1.978025	Н	-3.666206	1.651064	0.073612
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Si	-3.215362	-1.385991	0.995248	С	3.061814	-2.387107	-3.703460
Si	-2.924608	-1.815910	-1.995048	H	3.799440	-1.703840	-4.170203
Si	-0.387872	2.007942	-2.572501	H	2.776895	-3.139187	-4.469795
Si	-2.132750	2.996166	-0.272284	H	3.559897	-2.921706	-2.870073
P	0.930702	1.373471	2.666975	C	3.586402	1.573051	-3.277877
Co	-0.813575	-0.012358	-0.274470	H	3.718836	0.903786	-4.153134
				H	4.536737	2.131120	-3.139182
Conform	mation 4.			H	2.796284	2.306868	-3.533289
Multip	licity: 4			С	4.694724	-0.567107	-1.462920
Charge				Н	4.462222	-1.429233	-0.806883
	3c) = -4478.40374	7200211 Hartree		H	5.536773	0.000941	-1.014466
		8.391927752165 Ha	rtree	Н	5.049703	-0.969955	-2.430763
		P) = -4476.710135			3.073040	1.760280	-0.246260
		VP) = -4477.08467			2.388015	2.600912	-0.468206
	-3c) = -4473.0035		101/03/ Hartree	H	4.066443	2.184533	0.005967
	= -144.87756 Kca			H	2.686175	1.228880	0.644176
	= -201.17456 Kca			C		3.463155	
			7		-2.773890		-1.777983 -1.900279
		-4480.43591801443	/ Hartree	H	-3.817363	3.114973	
	-xTB) = $-139.7651$			H	-2.682106	4.446937	-2.285050
	-xTB) = $-136.9539$			H	-2.577832	3.620540	-0.699268
E (GFN-1	FF) = -18.0608430	84280 Hartree		С	-1.700233	2.329473	-4.383290
				H	-0.916951	1.748962	-4.909650
Coordi				H	-1.642927	3.380806	-4.735683
C	-0.091032	-0.264198	1.148057	H	-2.686195	1.927591	-4.694758
C	-0.034918	-1.169120	3.257753	С	0.191595	3.054327	-2.076473
H	0.230557	-1.901072	4.024065	H	0.316060	3.114628	-0.975573
C	-0.747401	-0.009131	3.337379	H	0.252533	4.085286	-2.482645
Н	-1.217726	0.466616	4.197902	H	1.027338	2.462983	-2.493537
C	1.264391	-2.366098	1.528146	C	-2.657585	-1.321526	-3.948190
Č	0.733551	-3.582349	1.030197	Н	-2.604089	-0.594134	-4.782971
C	1.652091	-4.569517	0.624830	H	-3.538264	-1.974907	-4.126018
Н	1.276779	-5.516378	0.212402	H	-1.750560	-1.952102	-3.993018
C	3.032256	-4.365658	0.740842	C	-3.097479	-1.802199	-0.973341
Н	3.731720	-5.143885	0.399913	Н	-2.350235	-2.607896	-1.100224
С	3.524846	-3.143885	1.321256		-4.099736	-2.265705	-1.100224
				H			
H	4.608710	-3.064483	1.455504	H	-3.007439	-1.413734	0.060113
C	2.653331	-2.172308	1.749800	C	-4.537385	0.458780	-2.452839
C H	-0.766537	-3.857896	1.036795 0.822187	H	-4.879219	0.951623 -0.290681	-1.522566 -2.740134
	1 070000			H	-5.304686	-n 290681	
	-1.279662	-2.898448					
С	-1.228172	-4.884256	-0.006217	H	-4.510198	1.223976	-3.254857

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N	-0.777679	0.535043	2.054178	C	1.965744	-2.848547	2.037087	
N	1.682324	-0.344506	-1.829911	H	1.036462	-3.268773	2.470141	
N	-1.535731	0.633796	-1.839492	H	2.798207	-3.551919	2.244332	
Si	1.474917	-1.499304	-3.139695	H	1.833582	-2.789900	0.940456	
Si	3.176185	0.563474	-1.714077	С	2.186025	-1.440157	4.675052	
Si	-1.475584					-0.545732		
		2.267075	-2.494906	H	2.454268		5.272061	
Si	-2.861003	-0.436287	-2.276212	H	2.919320	-2.236427	4.924805	
P	-1.355424	2.176735	1.593128	H	1.183427	-1.787595	4.995405	
Co	0.045973	0.046738	-0.871347	С	2.037467	2.436696	3.764383	
				H	2.731170	1.846925	4.398580	
				Н	1.656717	3.278162	4.381310	
0	nation 7.			Н	2.626980	2.866807	2.930566	
	icity: 4			С	-0.280867	0.790365	4.761249	
Charge:				Н	-0.980770	-0.047683	4.576807	
E(B97-3	(c) = -4478.40384	9343878 Hartree		H	-0.846027	1.631837	5.213401	
E(M06/d	lef2-TZVP) = -447	8.392241751249 Has	rtree	H	0.459707	0.454318	5.511225	
		P) = -4476.7101000		С	-0.593802	2.483240	2.195599	
		VP) = -4477.08418			-0.045334	3.011114	1.391837	
			/301/0/ Hartree					
		84774375 Hartree		H	-1.034055	3.252806	2.862934	
	= -143.67055 Kca			H	-1.418315	1.911555	1.726640	
E(PM7)	= -196.38174 Kca	1/mol		С	2.349056	2.629412	-0.086797	
E(ωB97X	I-V/def2-TZVP) =	-4480.43218219903	7 Hartree	H	1.274968	2.772519	-0.323727	
E(GFN1-	$\times XTB) = -139.7669$	08000021 Hartree		H	2.857618	3.608553	-0.207501	
		92775997 Hartree		Н	2.432013	2.316034	0.970546	
	F) = -18.0646645			C	2.985356	2.055083	-2.994513	
E (GrN-r	r) = -10.0040043	J4300 Haltiee						
				H	3.278111	1.335863	-3.782942	
Coordin				Н	3.650153	2.940899	-3.076777	
С	-1.177992	-0.050136	-0.283416	H	1.949478	2.390244	-3.192457	
С	-3.462870	-0.265390	-0.381536	C	4.979908	1.278923	-0.862202	
Н	-4.445241	-0.631592	-0.074660	Н	5.191488	0.927783	0.166740	
C	-3.088648	0.522230	-1.429373	Н	5.401388	2.301087	-0.966385	
				п Н				
H	-3.693089	0.995780	-2.204446		5.530391	0.622183	-1.566406	
C	-2.336702	-1.429499	1.487919	C	4.481258	-2.350660	-0.662656	
C	-1.780314	-2.736360	1.435398	H	5.282110	-1.593506	-0.549582	
C	-1.800976	-3.488224	2.624954	H	4.918227	-3.227147	-1.187094	
H	-1.364638	-4.495086	2.633569	H	4.182063	-2.675815	0.351558	
С	-2.377934	-2.986954	3.798550	С	1.789506	-3.102275	-1.875115	
Н	-2.367801	-3.593751	4.716472	Н	1.546009	-3.566341	-0.901246	
C	-3.000135	-1.736578	3.792943	Н	2.256744	-3.889305	-2.503286	
H	-3.499136	-1.372044	4.702851	H	0.842961	-2.797067	-2.359938	
C	-3.009571	-0.933141	2.636055	С	3.760410	-1.357792	-3.414669	
С	-1.238137	-3.336606	0.136700	H	3.004303	-1.017004	-4.150192	
Н	-0.448015	-2.646112	-0.234156	Н	4.190998	-2.309889	-3.790122	
C	-0.609743	-4.724096	0.312872	Н	4.577834	-0.609352	-3.395426	
H	0.211349	-4.730709	1.053434	N	-2.298767	-0.604301	0.306542	
H	-0.190336	-5.065557	-0.652986	N	-1.702398	0.649047	-1.361261	
H	-1.368525	-5.471560	0.625271	N	1.091379	0.001874	2.161547	
С	-2.315196	-3.434742	-0.964555	N	2.290445	-0.211113	-0.992314	
Н	-3.144915	-4.096519	-0.639846	Si	2,271249	-1.141618	2.797070	
H	-1.870026	-3.875185	-1.879677	Si	0.588662	1.353794	3.160746	
H	-2.748114	-2.458255	-1.247336	Si	3.112725	1.332708	-1.235422	
С							-1.676208	
	-3.852320	0.342697	2.627544	Si	3.021268	-1.665689		
H	-3.852320 -3.578628	0.342697 0.936031	2.627544 1.731645	Si P	3.021268 -0.638560	-1.665689 1.611033	-2.439333	
H C								
С	-3.578628 -5.344353	0.936031 -0.036878	1.731645 2.513001	P	-0.638560	1.611033	-2.439333	
C H	-3.578628 -5.344353 -5.549106	0.936031 -0.036878 -0.716631	1.731645 2.513001 1.661777	P Co	-0.638560 0.798664	1.611033	-2.439333	
C H H	-3.578628 -5.344353 -5.549106 -5.973599	0.936031 -0.036878 -0.716631 0.868733	1.731645 2.513001 1.661777 2.392657	P Co Confor	-0.638560 0.798664 mation 9.	1.611033	-2.439333	
C H H H	-3.578628 -5.344353 -5.549106 -5.973599 -5.680003	0.936031 -0.036878 -0.716631 0.868733 -0.564191	1.731645 2.513001 1.661777 2.392657 3.429597	P Co Confor Multip	-0.638560 0.798664 mation 9. dicity: 4	1.611033	-2.439333	
С Н Н С	-3.578628 -5.344353 -5.549106 -5.973599 -5.680003 -3.649198	0.936031 -0.036878 -0.716631 0.868733 -0.564191 1.255718	1.731645 2.513001 1.661777 2.392657 3.429597 3.844253	P Co Confor Multip Charge	-0.638560 0.798664 mation 9. clicity: 4	1.611033 -0.118704	-2.439333	
С Н Н Н С	-3.578628 -5.344353 -5.549106 -5.973599 -5.680003 -3.649198 -3.922939	0.936031 -0.036878 -0.716631 0.868733 -0.564191 1.255718 0.751497	1.731645 2.513001 1.661777 2.392657 3.429597 3.844253 4.793448	P Co Confor Multip Charge E(B97-	-0.638560 0.798664 mation 9. dicity: 4 :: 0 3c) = -4478.40821	1.611033 -0.118704 8852044 Hartree	-2.439333 0.253529	
С Н Н С	-3.578628 -5.344353 -5.549106 -5.973599 -5.680003 -3.649198	0.936031 -0.036878 -0.716631 0.868733 -0.564191 1.255718	1.731645 2.513001 1.661777 2.392657 3.429597 3.844253	P Co Confor Multip Charge E(B97-	-0.638560 0.798664 mation 9. clicity: 4	1.611033 -0.118704 8852044 Hartree	-2.439333 0.253529	
С Н Н Н С	-3.578628 -5.344353 -5.549106 -5.973599 -5.680003 -3.649198 -3.922939	0.936031 -0.036878 -0.716631 0.868733 -0.564191 1.255718 0.751497	1.731645 2.513001 1.661777 2.392657 3.429597 3.844253 4.793448	P Co Confor Multip Charge E(B97- E(M06/	-0.638560 0.798664 mation 9. dicity: 4 :: 0 3c) = -4478.40821	1.611033 -0.118704 8852044 Hartree 8.397373388160 Ha	-2.439333 0.253529	
C H H C H H	-3.578628 -5.344353 -5.549106 -5.973599 -5.680003 -3.649198 -3.922939 -4.297051 -2.604154	0.936031 -0.036878 -0.716631 0.868733 -0.564191 1.255718 0.751497 2.150794 1.596035	1.731645 2.513001 1.661777 2.392657 3.429597 3.844253 4.793448 3.751574 3.928694	P Co Confor Multip Charge E(B97- E(M06/ E(PBE	-0.638560 0.798664 mation 9. licity: 4::0 3c) = -4478.40821 def2-TZVP) = -447 - D3(BJ)/def2-TZV	1.611033 -0.118704 8852044 Hartree 8.397373388160 Ha P) = -4476.714735	-2.439333 0.253529 artree 5189170 Hartree	
C H H C H H H	-3.578628 -5.344353 -5.549106 -5.973599 -5.680003 -3.649198 -3.922939 -4.297051 -2.604154 -1.562987	0.936031 -0.036878 -0.716631 0.868733 -0.564191 1.255718 0.751497 2.150794 1.596035 3.294863	1.731645 2.513001 1.661777 2.392657 3.429597 3.844253 4.793448 3.751574 3.928694 -2.542264	P Co Confor Multip Charge E(B97- E(M06/ E(PBE E(PBE0	-0.638560 0.798664 mation 9. licity: 4 :: 0 3c) = -4478.40821 def2-TZVP) = -447 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV	1.611033 -0.118704 8852044 Hartree 8.397373388160 Ha P) = -4476.714733 VP) = -4477.08869	-2.439333 0.253529 artree 5189170 Hartree	
C H H C H H C C	-3.578628 -5.344353 -5.549106 -5.973599 -5.680003 -3.649198 -3.922939 -4.297051 -2.604154 -1.562987 -1.966430	0.936031 -0.036878 -0.716631 0.868733 -0.564191 1.255718 0.751497 2.150794 1.596035 3.294863 3.668018	1.731645 2.513001 1.661777 2.392657 3.429597 3.844253 4.793448 3.751574 3.928694 -2.542264 -1.104673	P Co Confor Multip Charge E(B97- E(M06/ E(PBE E(PBE0)	-0.638560 0.798664 mation 9. dicity: 4 : 0 3c) = -4478.40821 def2-TZVP) = -447 - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZ-3c) = -4473.0060	1.611033 -0.118704 8852044 Hartree 8.397373388160 Ha P) = -4476.714735 VP) = -4477.08866 23753136 Hartree	-2.439333 0.253529 artree 5189170 Hartree	
C H H C H H C C C	-3.578628 -5.344353 -5.549106 -5.973599 -5.680003 -3.649198 -3.922939 -4.297051 -2.604154 -1.562987 -1.966430 -1.124938	0.936031 -0.036878 -0.716631 0.868733 -0.564191 1.255718 0.751497 2.150794 1.596035 3.294863 3.668018 3.556821	1.731645 2.513001 1.661777 2.392657 3.429597 3.844253 4.793448 3.751574 3.928694 -2.542264 -1.104673 -0.393021	P Co Confor Multip Charge E (B97- E (M06/ E (PBE E (PBE0 E (PBEh E (PM6))	-0.638560 0.798664 mation 9. dicity: 4 :: 0 3c) = -4478.40821 def2-TZVP) = -447 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV-03c) = -4473.0060 = -146.48849 Kca	1.611033 -0.118704 8852044 Hartree 8.397373388160 Ha P) = -4476.714735 VP) = -4477.08869 23753136 Hartree 1/mol	-2.439333 0.253529 artree 5189170 Hartree	
C H H C H H C C H H	-3.578628 -5.344353 -5.549106 -5.973599 -5.680003 -3.649198 -3.922939 -4.297051 -2.604154 -1.562987 -1.966430 -1.124938 -2.807129	0.936031 -0.036878 -0.716631 0.868733 -0.564191 1.255718 0.751497 2.150794 1.596035 3.294863 3.668018 3.556821 3.052943	1.731645 2.513001 1.661777 2.392657 3.429597 3.844253 4.793448 3.751574 3.928694 -2.542264 -1.104673 -0.393021 -0.727915	P Co Confor Multip Charge E(B97- E(M06/ E(PBE E(PBE0 E(PBE0 E(PBE0) E(PM6) E(PM7)	-0.638560 0.798664 mation 9. licity: 4::0 3c) = -4478.40821 def2-TZVP) = -447 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZ -3c) = -4473.0060 = -146.48849 Kca = -214.72955 Kca	1.611033 -0.118704 8852044 Hartree 8.397373388160 Ha P) = -4476.714735 VP) = -4477.08869 23753136 Hartree 1/mol 1/mol	-2.439333 0.253529 artree 5189170 Hartree 99543199 Hartree	
C H H C H H C C H H H	-3.578628 -5.344353 -5.549106 -5.973599 -5.680003 -3.649198 -3.922939 -4.297051 -2.604154 -1.562987 -1.966430 -1.124938 -2.807129 -2.287057	0.936031 -0.036878 -0.716631 0.868733 -0.564191 1.255718 0.751497 2.150794 1.596035 3.294863 3.668018 3.556821 3.052943 4.731228	1.731645 2.513001 1.661777 2.392657 3.429597 3.844253 4.793448 3.751574 3.928694 -2.542264 -1.104673 -0.393021 -0.727915 -1.079856	P Co Confor Multip Charge E(B97- E(M06/ E(PBE) E(PBE) E(PBE) E(PM6) E(PM7) E(WB97	-0.638560 0.798664 mation 9. dicity: 4::0 3c) = -4478.40821 def2-TZVP) = -447 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - 3c) = -4473.0060 = -146.48849 Kca = -214.72955 Kca X-V/def2-TZVP) =	1.611033 -0.118704 8852044 Hartree 8.397373388160 Ha P) = -4476.71473 VP) = -4477.08869 23753136 Hartree 1/mol 1/mol -4480.43663619669	-2.439333 0.253529 artree 5189170 Hartree 99543199 Hartree	
C H H C H H C C H H C C H	-3.578628 -5.344353 -5.549106 -5.973599 -5.680003 -3.649198 -3.922939 -4.297051 -2.604154 -1.562987 -1.966430 -1.124938 -2.807129 -2.287057 -2.772846	0.936031 -0.036878 -0.716631 0.868733 -0.564191 1.255718 0.751497 2.150794 1.596035 3.294863 3.668018 3.556821 3.052943 4.731228 3.431739	1.731645 2.513001 1.661777 2.392657 3.429597 3.844253 4.793448 3.751574 3.928694 -2.542264 -1.104673 -0.393021 -0.727915 -1.079856 -3.476364	P Co Confor Multip Charge E(B97- E(PBE) E(PBE) E(PBE) E(PM6) E(PM7) E(WB97 E(GFN1	-0.638560 0.798664 mation 9. licity: 4 :: 0 3c) = -4478.40821 def2-TZVP) = -447 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZ -3c) = -4473.0060 = -146.48849 Kca = -214.72955 Kca X-V/def2-TZVP) = -xTB) = -139.7728	1.611033 -0.118704 8852044 Hartree 8.397373388160 Ha P) = -4476.71473; VP) = -4477.0886; 23753136 Hartree 1/mo1 1/mo1 -4480.4366361966; 90041799 Hartree	-2.439333 0.253529 artree 5189170 Hartree 99543199 Hartree	
C H H C H H C C H H H C H	-3.578628 -5.344353 -5.549106 -5.973599 -5.680003 -3.649198 -3.922939 -4.297051 -2.604154 -1.562987 -1.966430 -1.124938 -2.807129 -2.287057 -2.772846 -3.153360	0.936031 -0.036878 -0.716631 0.868733 -0.564191 1.255718 0.751497 2.150794 1.596035 3.294863 3.668018 3.556821 3.052943 4.731228 3.431739 4.475060	1.731645 2.513001 1.661777 2.392657 3.429597 3.844253 4.793448 3.751574 3.928694 -2.542264 -1.104673 -0.393021 -0.727915 -1.079856 -3.476364 -3.424068	P Co Confor Multip Charge E(B97- E(PBE E(PBE0 E(PBE0 E(PM6) E(PM7) E(DM7) E(DM7) E(GFN1)	-0.638560 0.798664 mation 9. dicity: 4 : 0 3c) = -4478.40821 def2-TZVP) = -447 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - 3c) = -4473.0060 = -146.48849 Kca = -214.72955 Kca X-V/def2-TZVP) = -xTB) = -139.7728 -xTB) = -136.9626	1.611033 -0.118704 8852044 Hartree 8.397373388160 Ha P) = -4476.714735 VP) = -4477.08866 23753136 Hartree 1/mol 1/mol -4480.43663619665 90041799 Hartree 22835129 Hartree	-2.439333 0.253529 artree 5189170 Hartree 99543199 Hartree	
C H H C H H C C H H C C H	-3.578628 -5.344353 -5.549106 -5.973599 -5.680003 -3.649198 -3.922939 -4.297051 -2.604154 -1.562987 -1.966430 -1.124938 -2.807129 -2.287057 -2.772846	0.936031 -0.036878 -0.716631 0.868733 -0.564191 1.255718 0.751497 2.150794 1.596035 3.294863 3.668018 3.556821 3.052943 4.731228 3.431739	1.731645 2.513001 1.661777 2.392657 3.429597 3.844253 4.793448 3.751574 3.928694 -2.542264 -1.104673 -0.393021 -0.727915 -1.079856 -3.476364	P Co Confor Multip Charge E(B97- E(PBE E(PBE0 E(PBE0 E(PM6) E(PM7) E(DM7) E(DM7) E(GFN1)	-0.638560 0.798664 mation 9. licity: 4 :: 0 3c) = -4478.40821 def2-TZVP) = -447 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZ -3c) = -4473.0060 = -146.48849 Kca = -214.72955 Kca X-V/def2-TZVP) = -xTB) = -139.7728	1.611033 -0.118704 8852044 Hartree 8.397373388160 Ha P) = -4476.714735 VP) = -4477.08866 23753136 Hartree 1/mol 1/mol -4480.43663619665 90041799 Hartree 22835129 Hartree	-2.439333 0.253529 artree 5189170 Hartree 99543199 Hartree	
C H H C H H C C H H H C H	-3.578628 -5.344353 -5.549106 -5.973599 -5.680003 -3.649198 -3.922939 -4.297051 -2.604154 -1.562987 -1.966430 -1.124938 -2.807129 -2.287057 -2.772846 -3.153360	0.936031 -0.036878 -0.716631 0.868733 -0.564191 1.255718 0.751497 2.150794 1.596035 3.294863 3.668018 3.556821 3.052943 4.731228 3.431739 4.475060	1.731645 2.513001 1.661777 2.392657 3.429597 3.844253 4.793448 3.751574 3.928694 -2.542264 -1.104673 -0.393021 -0.727915 -1.079856 -3.476364 -3.424068	P Co Confor Multip Charge E(B97- E(PBE E(PBE0 E(PBE0 E(PM6) E(PM7) E(DM7) E(DM7) E(GFN1)	-0.638560 0.798664 mation 9. dicity: 4 : 0 3c) = -4478.40821 def2-TZVP) = -447 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - 3c) = -4473.0060 = -146.48849 Kca = -214.72955 Kca X-V/def2-TZVP) = -xTB) = -139.7728 -xTB) = -136.9626	1.611033 -0.118704 8852044 Hartree 8.397373388160 Ha P) = -4476.714735 VP) = -4477.08866 23753136 Hartree 1/mol 1/mol -4480.43663619665 90041799 Hartree 22835129 Hartree	-2.439333 0.253529 artree 5189170 Hartree 99543199 Hartree	
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СНННСНННСНННССНННССНННСНН	-3.578628 -5.344353 -5.549106 -5.973599 -5.680003 -3.649198 -3.922939 -4.297051 -2.604154 -1.562987 -1.966430 -1.124938 -2.807129 -2.287057 -2.772846 -3.153360 -3.615923 -2.516065 -0.454230 -0.857596 -0.078996 0.411079 -0.855195 -2.274063 -2.205034 -2.922704 -2.773069 -0.146573 -0.064001 0.880391 -0.707497 -0.070354 -0.592714 0.940127 0.025942	0.936031 -0.036878 -0.716631 0.868733 -0.564191 1.255718 0.751497 2.150794 1.596035 3.294863 3.668018 3.556821 3.052943 4.731228 3.431739 4.475060 2.772359 3.233187 4.268428 5.303147 4.031192 4.255845 0.623879 0.246950 -0.315607 1.122654 -0.422469 1.424685 0.790826 1.720859 2.336668 -0.668950 -1.292405 -0.456731 -1.269492	1.731645 2.513001 1.661777 2.392657 3.429597 3.844253 4.793448 3.751574 3.928694 -2.542264 -1.104673 -0.393021 -0.727915 -1.079856 -3.476364 -3.424068 -3.193143 -4.534407 -3.005319 -3.031129 -4.020293 -2.312911 -4.071386 -4.521905 -5.478180 -4.703895 -3.794803 -5.180041 -6.088435 -4.889278 -5.466024 -3.785673 -3.032663 -3.388023 -4.715290	P Co Confor Multip Charge E(B97- E(M06/ E(PBE) E(PBE) E(PBE) E(PM7) E(GFN1- E(GFN2- Coordi C C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C C H C C H C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C C H C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C C H C C C C C H C C C C C C C C C C C C C C C C C C C C	-0.638560 0.798664 mation 9. licity: 4 :0 3c) = -4478.40821 def2-TZVP) = -447 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - 146.48849 Kca = -214.72955 Kca X-V/def2-TZVP) = -xTB) = -139.7728 -xTB) = -139.7728 -xTB) = -136.9626 FF) = -18.0658131 nates: 0.590487 1.632658 1.721547 2.502234 3.516464 -0.723471 -0.712957 -1.866834 -1.884970 -2.984118 -3.880375 -2.961312 -3.838813 -1.834657 0.477707 1.191906	1.611033 -0.118704 8852044 Hartree 8.397373388160 Hartree 8.397373388160 Hartree 1/mol 1/mol -4477.08863 23753136 Hartree 1/mol -4480.43663619663 90041799 Hartree 22835129 Hartree 91970 Hartree 0.170859 -0.256072 -0.648984 0.468866 0.805874 -0.977680 -2.324019 -2.809224 -3.852392 -1.996804 -2.398428 -0.664823 -0.029657 -0.116461 -3.262780 -2.790214	-2.439333 0.253529 artree 5189170 Hartree 99543199 Hartree 99543199 Hartree 58 Hartree -1.041947 -3.040777 -4.056752 -2.279578 -2.479410 -2.880672 -3.328865 -3.976906 -4.324622 -4.172479 -4.668649 -3.741228 -3.918931 -3.103072 -3.164002 -2.461803	
СНННСНННССНННСНННССНННСНННС	-3.578628 -5.344353 -5.549106 -5.973599 -5.680003 -3.649198 -3.922939 -4.297051 -2.604154 -1.562987 -1.966430 -1.124938 -2.807129 -2.287057 -2.772846 -3.153360 -3.615923 -2.516065 -0.454230 -0.857596 -0.078996 0.411079 -0.855195 -2.274063 -2.205034 -2.205034 -2.2705034 -2.773069 -0.146573 -0.064001 0.880391 -0.707497 -0.070354 -0.592714 0.940127 0.025942 4.029183	0.936031 -0.036878 -0.716631 0.868733 -0.564191 1.255718 0.751497 2.150794 1.596035 3.294863 3.668018 3.556821 3.052943 4.731228 3.431739 4.475060 2.772359 3.233187 4.268428 5.303147 4.031192 4.255845 0.623879 0.246950 -0.315607 1.122654 -0.422469 1.422468 1.720859 2.336668 -0.668950 -1.292405 -0.456731 -1.269492 -0.548405	1.731645 2.513001 1.661777 2.392657 3.429597 3.844253 4.793448 3.751574 3.928694 -2.542264 -1.104673 -0.393021 -0.727915 -1.079856 -3.476364 -3.424068 -3.193143 -4.534407 -3.005319 -3.031129 -4.020293 -2.312911 -4.071386 -4.521905 -5.478180 -4.703895 -3.794803 -5.180041 -6.088435 -4.889278 -5.466024 -3.785673 -3.032663 -3.388023 -4.715290 2.421841	P Co Confor Multip Charge E(B97- E(M06/ E(PBE) E(PBE0) E(PEE) E(PMT) E(GFN1 E(GFN1 C C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C C H C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C C H C C C C H C C C C H C C C C H C C C C C H C C C C C H C C C C C C C C C C C C C C C C C C C C	-0.638560 0.798664 mation 9. dicity: 4: 0 3c) = -4478.40821 def2-TZVP) = -447 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - T3(BJ)/def2-TZV - T46.48849 Kca - 214.72955 Kca X-V/def2-TZVP) = -xTB) = -139.7728 -xTB) = -136.9626 FF) = -18.0658131 nates: 0.590487 1.632658 1.721547 2.502234 3.516464 -0.723471 -0.712957 -1.866834 -1.884970 -2.964118 -3.880375 -2.961312 -3.838813 -1.834657 0.477707 1.191906 0.063975	1.611033 -0.118704 8852044 Hartree 8.397373388160 Ha P) = -4476.714733 VP) = -4477.08863 23753136 Hartree 1/mol 1/mol -4480.43663619663 90041799 Hartree 22835129 Hartree 91970 Hartree 0.170859 -0.256072 -0.648984 0.468866 0.805874 -0.977680 -2.324019 -2.809224 -3.852392 -1.996804 -2.398428 -0.664823 -0.029657 -0.116461 -3.262780 -2.790214 -4.615798	-2.439333 0.253529 artree 5189170 Hartree 99543199 Hartree 99543199 Hartree 68 Hartree -1.041947 -3.040777 -4.056752 -2.279578 -2.497410 -2.880672 -3.328865 -3.976906 -4.324622 -4.172479 -4.668649 -3.741228 -3.918931 -3.103072 -3.164002 -2.461803 -2.557358	
СНННСНННСНННССНННССНННСНН	-3.578628 -5.344353 -5.549106 -5.973599 -5.680003 -3.649198 -3.922939 -4.297051 -2.604154 -1.562987 -1.966430 -1.124938 -2.807129 -2.287057 -2.772846 -3.153360 -3.615923 -2.516065 -0.454230 -0.857596 -0.078996 0.411079 -0.855195 -2.274063 -2.205034 -2.922704 -2.773069 -0.146573 -0.064001 0.880391 -0.707497 -0.070354 -0.592714 0.940127 0.025942	0.936031 -0.036878 -0.716631 0.868733 -0.564191 1.255718 0.751497 2.150794 1.596035 3.294863 3.668018 3.556821 3.052943 4.731228 3.431739 4.475060 2.772359 3.233187 4.268428 5.303147 4.031192 4.255845 0.623879 0.246950 -0.315607 1.122654 -0.422469 1.424685 0.790826 1.720859 2.336668 -0.668950 -1.292405 -0.456731 -1.269492	1.731645 2.513001 1.661777 2.392657 3.429597 3.844253 4.793448 3.751574 3.928694 -2.542264 -1.104673 -0.393021 -0.727915 -1.079856 -3.476364 -3.424068 -3.193143 -4.534407 -3.005319 -3.031129 -4.020293 -2.312911 -4.071386 -4.521905 -5.478180 -4.703895 -3.794803 -5.180041 -6.088435 -4.889278 -5.466024 -3.785673 -3.032663 -3.388023 -4.715290	P Co Confor Multip Charge E(B97- E(M06/ E(PBE) E(PBE) E(PBE) E(PM7) E(GFN1- E(GFN2- Coordi C C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C C H C C H C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C C H C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C C H C C C C C H C C C C C C C C C C C C C C C C C C C C	-0.638560 0.798664 mation 9. licity: 4 :0 3c) = -4478.40821 def2-TZVP) = -447 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - 146.48849 Kca = -214.72955 Kca X-V/def2-TZVP) = -xTB) = -139.7728 -xTB) = -139.7728 -xTB) = -136.9626 FF) = -18.0658131 nates: 0.590487 1.632658 1.721547 2.502234 3.516464 -0.723471 -0.712957 -1.866834 -1.884970 -2.984118 -3.880375 -2.961312 -3.838813 -1.834657 0.477707 1.191906	1.611033 -0.118704 8852044 Hartree 8.397373388160 Hartree 8.397373388160 Hartree 1/mol 1/mol -4477.08863 23753136 Hartree 1/mol -4480.43663619663 90041799 Hartree 22835129 Hartree 91970 Hartree 0.170859 -0.256072 -0.648984 0.468866 0.805874 -0.977680 -2.324019 -2.809224 -3.852392 -1.996804 -2.398428 -0.664823 -0.029657 -0.116461 -3.262780 -2.790214	-2.439333 0.253529 artree 5189170 Hartree 99543199 Hartree 99543199 Hartree 58 Hartree -1.041947 -3.040777 -4.056752 -2.279578 -2.479410 -2.880672 -3.328865 -3.976906 -4.324622 -4.172479 -4.668649 -3.741228 -3.918931 -3.103072 -3.164002 -2.461803	
СНННСНННССНННССНННССНННССН	-3.578628 -5.344353 -5.549106 -5.973599 -5.680003 -3.649198 -3.922939 -4.297051 -2.604154 -1.562987 -1.966430 -1.124938 -2.807129 -2.287057 -2.772846 -3.153360 -3.615923 -2.516065 -0.454230 -0.857596 -0.078996 0.411079 -0.855195 -2.274063 -2.205034 -2.922704 -2.773069 -0.146573 -0.064001 0.880391 -0.707497 -0.070354 -0.592714 0.940127 0.025942 4.029183 4.131867	0.936031 -0.036878 -0.716631 0.868733 -0.564191 1.255718 0.751497 2.150794 1.596035 3.294863 3.668018 3.556821 3.052943 4.731228 3.431739 4.475060 2.772359 3.233187 4.268428 5.303147 4.031192 4.255845 0.623879 0.246950 -0.315607 1.122654 -0.422469 1.424685 0.790826 1.720859 2.336668 -0.668950 -1.292405 -0.456731 -1.269492 -0.548405 -0.372372	1.731645 2.513001 1.661777 2.392657 3.429597 3.844253 4.793448 3.751574 3.928694 -2.542264 -1.104673 -0.393021 -0.727915 -1.079856 -3.476364 -3.424068 -3.193143 -4.534407 -3.005319 -3.031129 -4.020293 -2.312911 -4.071386 -4.521905 -5.478180 -4.703895 -3.794803 -5.180041 -6.088435 -4.889278 -5.466024 -3.785673 -3.032663 -3.388023 -4.715290 2.421841 1.335553	P Co Confor Multip Charge E(B97- E(M06/ E(PBE E(PBE0 E(PE0H E(PM6)) E(GFN1 E(GFN2 E(GFN- Coordi C C C H C H C C H C C H C H C H C H C	-0.638560 0.798664  mation 9. licity: 4 :: 0 3c) = -4478.40821 def2-TZVP) = -447 - D3(BJ)/def2-TZV - T46.9626 X-V/def2-TZVP) = -146.9626 FF) = -18.0658131  nates:	1.611033 -0.118704 8852044 Hartree 8.397373388160 Ha P) = -4476.714733 VP) = -4477.08869 23753136 Hartree 1/mol 1/mol -4480.43663619669 90041799 Hartree 22835129 Hartree 91970 Hartree 0.170859 -0.256072 -0.648984 0.468866 0.805874 -0.977680 -2.324019 -2.809224 -3.852392 -1.996804 -2.398428 -0.664823 -0.029657 -0.116461 -3.262780 -2.790214 -4.615798 -4.483412	-2.439333 0.253529 artree 5189170 Hartree 99543199 Hartree 99543199 Hartree 58 Hartree -1.041947 -3.040777 -4.056752 -2.279578 -2.497410 -2.880672 -3.328865 -3.976906 -4.324622 -4.172479 -4.668649 -3.741228 -3.918931 -3.103072 -3.164002 -2.461803 -2.557358 -1.642954	
СНННСНННССНННСНННССНННСНННС	-3.578628 -5.344353 -5.549106 -5.973599 -5.680003 -3.649198 -3.922939 -4.297051 -2.604154 -1.562987 -1.966430 -1.124938 -2.807129 -2.287057 -2.772846 -3.153360 -3.615923 -2.516065 -0.454230 -0.857596 -0.078996 0.411079 -0.855195 -2.274063 -2.205034 -2.205034 -2.2705034 -2.773069 -0.146573 -0.064001 0.880391 -0.707497 -0.070354 -0.592714 0.940127 0.025942 4.029183	0.936031 -0.036878 -0.716631 0.868733 -0.564191 1.255718 0.751497 2.150794 1.596035 3.294863 3.668018 3.556821 3.052943 4.731228 3.431739 4.475060 2.772359 3.233187 4.268428 5.303147 4.031192 4.255845 0.623879 0.246950 -0.315607 1.122654 -0.422469 1.422468 1.720859 2.336668 -0.668950 -1.292405 -0.456731 -1.269492 -0.548405	1.731645 2.513001 1.661777 2.392657 3.429597 3.844253 4.793448 3.751574 3.928694 -2.542264 -1.104673 -0.393021 -0.727915 -1.079856 -3.476364 -3.424068 -3.193143 -4.534407 -3.005319 -3.031129 -4.020293 -2.312911 -4.071386 -4.521905 -5.478180 -4.703895 -3.794803 -5.180041 -6.088435 -4.889278 -5.466024 -3.785673 -3.032663 -3.388023 -4.715290 2.421841	P Co Confor Multip Charge E(B97- E(M06/ E(PBE) E(PBE0) E(PEE) E(PMT) E(GFN1 E(GFN1 C C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C C H C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C C H C C C C H C C C C H C C C C H C C C C C H C C C C C H C C C C C C C C C C C C C C C C C C C C	-0.638560 0.798664 mation 9. dicity: 4: 0 3c) = -4478.40821 def2-TZVP) = -447 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - T3(BJ)/def2-TZV - T46.48849 Kca - 214.72955 Kca X-V/def2-TZVP) = -xTB) = -139.7728 -xTB) = -136.9626 FF) = -18.0658131 nates: 0.590487 1.632658 1.721547 2.502234 3.516464 -0.723471 -0.712957 -1.866834 -1.884970 -2.964118 -3.880375 -2.961312 -3.838813 -1.834657 0.477707 1.191906 0.063975	1.611033 -0.118704 8852044 Hartree 8.397373388160 Ha P) = -4476.714733 VP) = -4477.08863 23753136 Hartree 1/mol 1/mol -4480.43663619663 90041799 Hartree 22835129 Hartree 91970 Hartree 0.170859 -0.256072 -0.648984 0.468866 0.805874 -0.977680 -2.324019 -2.809224 -3.852392 -1.996804 -2.398428 -0.664823 -0.029657 -0.116461 -3.262780 -2.790214 -4.615798	-2.439333 0.253529 artree 5189170 Hartree 99543199 Hartree 99543199 Hartree 68 Hartree -1.041947 -3.040777 -4.056752 -2.279578 -2.497410 -2.880672 -3.328865 -3.976906 -4.324622 -4.172479 -4.668649 -3.741228 -3.918931 -3.103072 -3.164002 -2.461803 -2.557358	

С	1.200347	-3.487306	-4.506157	N	0.554342	-0.810111	2.175115
H	0.527314	-3.975723	-5.240809	Si	-3.434043	-1.295206	0.615864
H	2.082739	-4.144840	-4.367401	Si	-3.006102	1.646299	1.370026
H	1.550998	-2.541195	-4.965097	Si	0.571162	0.027299	3.723224
С	-1.792747	1.366777	-2.746923	Si	0.895470	-2.533468	2.101775
H	-1.365222	1.437274	-1.724614	P	2.363446	1.861000	0.240825
С	-0.879831	2.135203	-3.723567	Co	-0.472380	-0.096766	0.681245
H	0.163024	1.763752	-3.717076				
H	-0.855340	3.212442	-3.461628				
Н	-1.263020	2.049321	-4.761618	AQI	NUK		
C	-3.174759	2.023120	-2.706773	_			
Н	-3.628888	2.097680	-3.716746	Confor	mation 13.		
		3.054985					
H	-3.092151		-2.311506		licity: 2		
H	-3.868566	1.466165	-2.050075	Charge		00065100	
С	2.568156	3.516804	-0.715273		3c) = -14780.0953		
С	3.305130	3.520221	-2.062219	, ,	def2-TZVP) = -147		
Н	2.744846	2.959002	-2.834405		- D3(BJ)/def2-TZV		
H	4.331914	3.115700	-2.003420		- D3(BJ)/def2-TZ		
H	3.384927	4.568678	-2.423105	•	-3c) = -14765.504		
С	3.256028	4.480193	0.271401		= 117.70812 Kcal		
H	3.164737	5.519679	-0.109034	E(PM7)	= 60.57875 Kcal/	mol	
H	4.336079	4.264678	0.389420	E(ωB97	X-V/def2-TZVP) =	-14776.3336733396	06 Hartree
H	2.781485	4.452063	1.274528	E(GFN1	-xTB) = $-208.6945$	66201214 Hartree	
С	1.123619	3.996974	-0.949531	E (GFN2	-xTB) = $-205.3314$	27868363 Hartree	
H	1.137339	4.968140	-1.489452	E(GFN-	FF) = -24.5802822	18097 Hartree	
H	0.576118	4.140451	0.000556				
Н	0.547364	3.279059	-1.565530	Coordi	nates:		
C	4.085944	1.156451	0.704138	C	1.788253	2.709541	0.888428
C	5.281295	1.432736	-0.217223	C	2.277646	3.934097	0.273004
Н	6.180820	0.933430	0.217223	C	1.622811	4.064619	-0.940796
Н	5.516903	2.511565	-0.299271	C	0.732941	2.920224	-1.067260
н Н	5.140867	1.025677	-1.237535	C	-0.247300	2.710609	-2.067635
	4.376987				-0.24/300		-2.06/635
С		1.742292	2.103716	C		1.449927	
H	5.292550	1.267729	2.516660	C	-1.945794	1.216881	-3.204714
H	3.547754	1.541562	2.808893	H	-2.494404	1.997843	-3.740570
H	4.552007	2.834984	2.079389	С	-2.155122	-0.139544	-3.237092
С	3.861641	-0.359696	0.842753	H	-2.909266	-0.693048	-3.805452
H	3.803803	-0.859658	-0.144348	C	-1.180980	-0.735799	-2.344472
H	2.922136	-0.578932	1.391673	С	-0.988998	-2.126448	-2.187769
H	4.710352	-0.809245	1.400453	С	-0.113131	-2.666604	-1.214507
С	-4.127534	-1.819949	2.307480	С	0.407085	-4.024634	-1.162970
H	-3.317875	-1.927422	3.057609	С	1.074650	-4.154925	0.044013
H	-4.665239	-2.788624	2.237181	С	0.959318	-2.877249	0.731529
H	-4.844543	-1.067227	2.695684	C	1.342092	-2.588981	2.064515
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H	-3.205931	-3.623617	-0.225841	Н	1.757932	-1.628497	4.760546
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C	-4.925541	-1.046148	-0.540224		2.156022	1.063914	4.835787
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H	-5.472356	-2.008437	-0.632768	C	2.057041	2.250282	2.200677
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C	-3.190793	1.725708	3.260785	С	-1.635212	6.073141	-4.402161
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			5.229019				-6.760570 -6.827746
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H	-0.994777	0.107695	5.714228	C	-1.784051	-3.044568	-3.041074
Н	-0.644973	-1.579036	5.222399	С	-1.722467	-2.993738	-4.454059
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H	-1.495052	-3.252374	2.585207	C	-3.311582	-4.830399	-4.632635
С	1.152426	-2.992246	0.280818	С	-3.401471	-4.880148	-3.225130
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H	-7.244040	-8.076672	-5.065933	С	-1.140913	-2.798293	0.237383
C	-5.785292	-9.670279	-4.815464	C	-0.760670	-3.381882	-0.991565
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H	-4.946548	-10.149656	-5.362621	C	0.483283	-2.030154	-4.151304
C	1.550123	-3.707625	3.016310	C	0.785608	-0.990631	-3.178668
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H	-0.435481	-4.525435	2.713091	С	1.592894	1.249322	-2.485875
C	0.696436	-5.732704	4.105672	C	2.508140	2.370557	-2.567590
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H	3.913289	-5.115172	5.097893	C	0.958645	2.706777	-0.947908
C	2.767929	-3.878197	3.715802	C	0.179195	3.384761	0.015122
H	3.588026	-3.164620	3.547509	С	-3.001889	-0.217233	3.625946
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Н	1.599142	-8.545868	6.664956	C	-4.880030	-1.029290	4.978341
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H	1.222764	-8.408829	3.600893	С	-4.360803	-0.368983	6.112210
H	2.430697	-9.360204	4.490009	С	-3.152523	0.355237	5.999481
C	0.397006	-10.144864	4.620639	H	-2.757933	0.854070	6.896321
H	0.523491	-10.673622	5.592200	C	-2.492381	0.432831	4.775505
H	0.667915	-10.887935	3.841262	H	-1.557435	1.007316	4.694270
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Н	5.210514	3.719712	5.375915		-6.536039	0.451421	11.467353
С	3.783048	2.972727	3.908423	Н	-8.250951	0.224566	11.016690
H	4.373479	2.075339	3.671340	С	-0.817381	-4.860410	-1.111964
C	3.392108	7.098329	6.396209	C	0.344835	-5.590484	-1.432252
H	2.380578	6.864268	6.802238	H	1.288958	-5.047640	-1.590371
H	3.246943	7.706342	5.471727	С	0.326281	-6.985684	-1.554151
С	4.208280	7.873348	7.421704	Н	1.255664	-7.515442	-1.799951
Н	3.545053	8.673871	7.813944	C	-0.883563	-7.686206	-1.363011
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С	5.509337	8.508465	6.907842		-2.990673	-7.531157	-0.899157
H	5.877920	9.209814	7.687544	С	-2.017987	-5.580847	-0.905750
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C	6.627767	7.526803	6.548119	C	0.118147	-9.818221	-1.826418
H	7.550933	8.066830	6.255172	H	0.935456	-9.662915	-1.082320
H	6.338560	6.860427	5.713154	H	0.502021	-9.481161	-2.817184
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N	0.309272	-1.981977	-0.093398	C	-0.550904	-11.964049	-0.530267
N	1.479706	-0.126813	1.765696	H	0.332836	-11.811595	0.129772
0	-2.091068	7.181429	-5.041652	Н	-0.606515	-13.060964	-0.701445
0	-3.992164	-5.647487	-5.477737	C	-1.820053	-11.505044	0.192936
0	2.216661	-6.929401	5.622331	H	-1.975806	-12.082826	1.126539
0	4.066763	5.882514	6.074328	H	-2.716599	-11.649959	-0.445281
Cu	0.563389	0.059091	-0.010550	H	-1.778633	-10.430407	0.454372
Br	3.682255	5.044376	0.835616	С	2.526363	0.202181	-4.533213
Br	2.031334	5.374041	-2.221258	C	3.513611	-0.790462	-4.696116
Br	0.419119	-5.322204	-2.518822	Н	3.581468	-1.603117	-3.957055
Br	2.108715	-5.648911	0.518500	С	4.410786	-0.765009	-5.770862
DI	2.100/13	-2.040311	0.310300				
0	15			H	5.169152	-1.554503	-5.853379
	mation 15.			C	4.324923	0.266716	-6.730312
	licity: 2			С	3.344055	1.271948	-6.574796
Charge				H	3.288183	2.064291	-7.335178
E(B97-	3c) = -14780.0949	958319898 Hartree		С	2.467738	1.241892	-5.490627
E(M06/	def2-TZVP) = -14	775.724403138262 Ha	artree	H	1.696852	2.020253	-5.390536
E (PBE	- D3(BJ)/def2-TZV	IP) = -14773.096372	2453192 Hartree	С	6.193431	-0.537951	-8.033030
		ZVP) = -14773.63350			6.428962	-0.451486	-9.112574
		1187436916 Hartree		Н	5.857407	-1.583833	-7.855793
	= 120.01410 Kcal			C	7.424633	-0.202758	-7.188751
	= 62.93994 Kcal,		27	H	7.214688	-0.417559	-6.119826
		-14776.3336071071	9/ Hartree	H	8.231245	-0.907043	-7.492650
		170886094 Hartree		C	7.910489	1.247625	-7.324453
		612273747 Hartree		H	8.776460	1.387301	-6.642939
E (GFN-	FF) = -24.5813606	634561 Hartree		H	7.115685	1.926847	-6.948711
				C	8.302540	1.658995	-8.744895
Coordi	nates:			Н	8.721323	2.685146	-8.763183
C	-0.878497	2.754524	0.715242	Н	7.431395	1.653193	-9.431576
C	-1.939705	3.407405	1.466949	H	9.070795	0.978614	-9.170014
_	±•>>>/UJ	2.409031	2.119449	н С	0.526358	4.792001	
C	-2 644333	∠ . 4∪⊅UJI					0.335550 1.655457
С	-2.644332	1 1 4 6 4 0 0		C	0.863906	5.152888	1 655/157
С	-2.010044	1.146430	1.771374	**			
C C	-2.010044 -2.279482	-0.125497	2.331870	H	0.865025	4.377739	2.436607
C C C	-2.010044 -2.279482 -1.832803	-0.125497 -1.326374	2.331870 1.736663	С	0.865025 1.196554	4.377739 6.470383	2.436607 1.994710
C C C	-2.010044 -2.279482 -1.832803 -1.954004	-0.125497 -1.326374 -2.635709	2.331870 1.736663 2.347012	C H	0.865025 1.196554 1.458991	4.377739 6.470383 6.707648	2.436607 1.994710 3.033748
C C C H	-2.010044 -2.279482 -1.832803	-0.125497 -1.326374 -2.635709 -2.825079	2.331870 1.736663 2.347012 3.363869	С	0.865025 1.196554 1.458991 1.185090	4.377739 6.470383 6.707648 7.470646	2.436607 1.994710 3.033748 0.999447
C C C	-2.010044 -2.279482 -1.832803 -1.954004	-0.125497 -1.326374 -2.635709	2.331870 1.736663 2.347012	C H	0.865025 1.196554 1.458991	4.377739 6.470383 6.707648	2.436607 1.994710 3.033748

H	0.846526	7.916880	-1.090120	H	8.817677	4.718483	9.359053
C	0.539463	5.803808	-0.653877	H	9.463215	3.238755	10.126235
H	0.263187	5.546844	-1.687145	С	3.526806	-2.086917	-2.710965
C	1.789386	9.205812	2.544549	C	4.604860	-2.907094	-2.304356
H	2.699040	8.667516	2.898807	H	4.678558	-3.212232	-1.250022
H	0.954492	8.939645	3.235479	С	5.537608	-3.377822	-3.228233
С	2.027032	10.709797	2.549500	Н	6.359110	-4.043247	-2.925832
H	2.496442	10.952765	3.526801	C	5.431429	-3.027154	-4.592532
H	2.787931	10.946443	1.773598	C	4.388346	-2.170646	-5.004886
С	0.781589	11.589420	2.360063	Н	4.293425	-1.859622	-6.053683
Н	1.064339	12.637758	2.598089	C	3.450988	-1.718410	-4.069871
H	0.025259	11.305019	3.126142	H	2.627708	-1.067836	-4.401412
C	0.146994	11.545308	0.967349	С	6.189125	-3.495589	-6.833249
Н	-0.701217	12.255936	0.894973	Н	7.169608	-3.801787	-7.248484
H	-0.227706	10.534297	0.717841	H	6.007900	-2.449453	-7.168483
H	0.884242	11.821098	0.184731	C	5.080481	-4.430382	-7.323805
N	-1.002256	1.387978	0.859287	H	5.122149	-4.427582	-8.435990
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N	-1.293314	-1.446796	0.472289		4.087709	-4.015366	-7.050997
N	0.234386	-1.341405	-1.962308	C	5.181366	-5.867487	-6.792208
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0	-4.941380	-0.374412	7.340125	Н	5.018845	-5.854680	-5.692993
0	-1.019666	-9.034129	-1.469106	C	6.501610	-6.574386	-7.104172
0	5.113412	0.376637	-7.833281	H	6.476510	-7.632823	-6.775896
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Cu	-0.335792	0.011865	-0.518641	H	6.720971	-6.569370	-8.193173
Br	-2.460607	5.209874	1.425872	C	-3.348071	-1.147213	-3.091461
Br	-4.237666	2.693479	3.068911	С	-3.035380	-0.799436	-4.427605
Br	-0.964392	-4.527780	-4.300325	Н	-2.031786	-0.411587	-4.658222
Br	0.704978	-1.988249	-6.014120	C	-3.974193	-0.937456	-5.447154
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Conform	nation 17.			С	-5.262765	-1.444249	-5.164778
Multipl	icity: 2			C	-5.593940	-1.791800	-3.837786
Charge:	0			H	-6.585247	-2.192486	-3.588819
E (B97-3	3c) = -14780.0975	72059831 Hartree		С	-4.642396	-1.633670	-2.820640
	•			Н			
		75.727575084500 Ha			-4.899746	-1.925044	-1.791537
E(PBE -	<ul> <li>D3(BJ)/def2-TZV:</li> </ul>	P) = -14773.09853	5778976 Hartree	С	-7.416750	-2.079110	-6.014883
E (PBEO	- D3(BJ)/def2-TZ	VP) = -14773.63588	30265881 Hartree	H	-7.978288	-1.426690	-5.306959
		170753935 Hartree		Н	-7.350247	-3.090436	-5.550629
E(PM6)	= 117.13815 Kcal	/mol		C	-8.123274	-2.141054	-7.362222
E(PM7)	= 59.28318  Kcal/i	mol		H	-9.155245	-2.513175	-7.178767
		-14776.3358951985	22 Hartree	Н	-8.226253	-1.105901	-7.751340
			2 narciee				
	-xTB) = $-208.6970$			C	-7.423234	-3.017790	-8.410952
E (GFN2-	-xTB) = $-205.3325$	57611256 Hartree		H	-6.409982	-2.602822	-8.596027
E (GFN-F	$^{\circ}F) = -24.5835202^{\circ}$	75293 Hartree		H	-7.975315	-2.921343	-9.370013
2 (011, 1	1, 21.0000202	,0230 Hardroo		C			
					-7.312884	-4.495478	-8.029765
Coordin	nates:			H	-6.856973	-5.088380	-8.847771
C	-1.029405	0.768935	2.972256	H	-8.309155	-4.936352	-7.813611
С	-0.669987	0.742495	4.382054	Н	-6.679964	-4.645837	-7.130975
C	0.705755	0.591574	4.444354	C	-3.310387	1.771733	3.251495
C	1.186573	0.520605	3.072703	C	-3.011539	3.015876	3.843014
С	2.536642	0.513926	2.643388	Н	-2.015298	3.456482	3.686723
C		0.113798	1.342244	C	-3.951535		4.617543
	2.914560					3.706400	
C	4.263475	0.199189	0.817368	H	-3.676769	4.676652	5.051374
H	5.107575	0.674898	1.326467	C	-5.230276	3.147121	4.830580
С	4.250294	-0.408757	-0.413569	С	-5.543478	1.901636	4.241111
Н	5.081181	-0.531923	-1.115632	Н	-6.541027	1.477282	4.425101
C	2.892528	-0.860892	-0.643144	C	-4.601460	1.232436	3.460949
C	2.487242	-1.630296	-1.755845	H	-4.851018	0.255288	3.021769
Ċ	1.128789	-1.931692	-2.019060	C	-6.027917	5.007289	6.147671
C	0.616554	-2.937293	-2.938431	H	-5.030454	5.080131	6.635593
C	-0.753597	-2.748401	-3.018678	H	-6.792521	5.072781	6.948710
C	-1.079227	-1.630857	-2.145393	С	-6.236156	6.129975	5.131885
C	-2.333254	-0.984418	-2.020528	Н	-6.062308	7.096494	5.655397
C	-2.642682	-0.138567	-0.932190	H	-5.457412	6.067394	4.341110
C	-3.860277	0.639950	-0.820037	C	-7.624795	6.122107	4.485235
Н	-4.616461	0.741696	-1.604769	H	-8.397315	6.219141	5.280535
C	-3.852559	1.211921	0.428057	H	-7.795478	5.127451	4.021291
H	-4.602062	1.875597	0.870621	C	-7.807985	7.224291	3.442397
C	-2.628635	0.785965	1.077563	H	-8.818870	7.194156	2.988636
C	-2.298110	1.072045	2.421507	H	-7.069583	7.125228	2.619494
С	3.596309	0.997093	3.563602	H	-7.671190	8.232222	3.887576
C	4.701389	0.195998	3.913550	N	0.104961	0.549367	2.216640
Н	4.768687	-0.827063	3.514692	N	2.089404	-0.492314	0.416583
C	5.693866	0.658094	4.789043	N	0.067951	-1.218264	-1.499278
H	6.528568	-0.004638	5.052244	N	-1.887791	0.004856	0.214591
С	5.601343	1.959619	5.326641	0	6.504792	2.505514	6.181320
С	4.507457	2.780157	4.969909	0	6.380771	-3.546533	-5.416954
H	4.457464	3.794635	5.390866	0	-6.105985	-1.557380	-6.223619
C	3.522590	2.301376	4.109425	0	-6.213856	3.705674	5.586555
H	2.670248	2.944539	3.843521	Cu	0.094572	-0.281471	0.333179
C	7.629240	1.729320	6.591365	Br	-1.805650	0.682185	5.875081
H	8.239925	1.448930	5.702128	Br	1.662994	0.310826	6.033731
H	7.280078	0.784101	7.070524	Br	1.525476	-4.386552	-3.713764
С	8.445810	2.556773	7.571720	Br	-1.924943	-3.901236	-3.925051
					1.721747	0.701230	0.720001
H	8.768443	3.491041	7.062066				
H	9.374972	1.991062	7.802574		mation 20.		
C	7.700854	2.899681	8.865593	Multip:	licity: 2		
Н	6.757658	3.422936	8.601904	Charge			
H	7.393721	1.955138	9.367953		3c) = -14780.09135	3752483 =+	
	1.3331∠⊥	T.200T20					
	0 = 0 = 0 : -	0					
C	8.526718	3.754459	9.826325			5.721276112887 H	
C H	8.526718 7.963838	3.754459 3.989343	9.826325 10.751863		def2-TZVP) = -1471 - D3(BJ)/def2-TZVI		

E(PBE0 - D3(BJ)/def2-TZVP) = -14773.629674476910 Hartree E(PBEh-3c) = -14765.499354599709 Hartree E(PM6) = 120.46322 Kcal/mol E(PM7) = 62.59465 Kcal/mol E(WB97X-V/def2-TZVP) = -14776.329552213820 Hartree E(GFN1-xTB) = -208.694121062031 Hartree E(GFN2-xTB) = -205.328599452042 Hartree E(GFN-FF) = -24.579821293631 Hartree				Н Н С Н Н С Н	1.744054 2.458870 0.457785 -0.044299 -0.155325 0.452717 -0.577055 1.096429 0.882907	-0.731855 0.480148 0.987927 0.363290 0.882758 2.455643 2.701201 2.560918 3.469141	-9.824127 -10.926776 -10.239253 -11.010211 -9.317945 -10.692439 -11.030842 -11.594839 -9.627174
Coordi	nates:			Н	0.726723	4.508750	-9.979420
С	2.359114	0.733360	1.773633	H	1.950704	3.354544	-9.359852
C	2.536246	1.215545	3.135302	H	0.297852	3.338653	-8.692493
C	1.314750	1.077448	3.773856	С	4.787859	0.445595	1.231717
C	0.390958	0.510593	2.802857	C	5.179636	-0.523962	2.176585
C	-0.925381	0.050007	3.047678	H C	4.420515	-1.207422	2.586042 2.605845
C C	-1.848514 -3.153475	-0.195317 -0.797417	2.006695 2.196164	Н	6.508035 6.772090	-0.636615 -1.408498	3.340192
Н	-3.522439	-1.214840	3.138321	C	7.483474	0.244888	2.093317
C	-3.793725	-0.748899	0.982776	C	7.106988	1.217064	1.139140
H	-4.792785	-1.119092	0.731716	H	7.880864	1.897185	0.754942
С	-2.881089	-0.114770	0.051791	С	5.783076	1.307559	0.712530
C	-3.210281	0.231451	-1.277682	Н	5.495346	2.080843	-0.014912
C C	-2.249946 -2.511530	0.731860 1.405753	-2.190717 -3.453649	C H	9.239216 9.057074	-0.699701 -1.736119	3.431619 3.063512
C	-1.290668	1.555846	-4.091156	Н	8.651064	-0.572248	4.371410
C	-0.282914	0.972227	-3.217761	C	10.723045	-0.484159	3.697431
С	1.083053	0.751937	-3.519772	H	11.078176	-1.374785	4.258755
C	2.045689	0.476858	-2.524219	H	11.257679	-0.499585	2.722336
С	3.423518	0.119616	-2.797380	С	11.088837	0.782847	4.485594
H C	3.838681	-0.068949 0.057304	-3.792575 -1.585273	H H	12.158809 10.520205	0.706487	4.777052 5.442908
Н	4.065153 5.112088	-0.193606	-1.387667	С	10.862701	0.783440 2.106926	3.750845
C	3.079433	0.378705	-0.571765	Н	11.217437	2.963670	4.358960
C	3.370374	0.539397	0.801229	H	9.793604	2.270758	3.515893
С	-1.350246	-0.247657	4.438849	H	11.413460	2.127191	2.787396
С	-2.472203	0.375669	5.019852	N	1.034636	0.393426	1.587401
H	-3.032905	1.120820	4.436157	N	-1.687667	0.168864	0.685203
C H	-2.865636 -3.733541	0.097170 0.619578	6.336196 6.759272	N N	-0.888258 1.849331	0.560739 0.584392	-2.047863 -1.162650
C	-2.137771	-0.840004	7.099883	0	-2.432046	-1.183855	8.380597
C	-1.022024	-1.487108	6.522329	0	-8.556663	-0.636504	-2.994825
H	-0.473289	-2.221510	7.129275	0	2.608541	0.978949	-8.982326
С	-0.635005	-1.188342	5.218061	0	8.794246	0.236881	2.450900
H	0.240177	-1.690804	4.779369	Cu	0.077876	0.418277	-0.235148
C H	-3.534419 -4.475975	-0.554755 -0.770485	9.031547 8.475390	Br Br	4.022101 0.945913	2.085880 1.733645	3.881806 5.492843
H	-3.390819	0.551798	9.031429	Br	-4.117560	2.165740	-4.059117
С	-3.612000	-1.084040	10.455054	Br	-1.044428	2.549266	-5.666908
H	-3.753603	-2.186365	10.415468				
H	-4.531935	-0.668659	10.921834		rmation 22.		
C H	-2.387020	-0.746294 -1.133487	11.310657 10.798519	Multi	plicity: 2		
п Н	-1.481118 -2.265096	0.359385	11.348456	_	-3c) = -14780.09394	8277321 Hartree	
C	-2.470959	-1.308925	12.729129		def2-TZVP) = -1477		artree
H	-1.571977	-1.052508	13.324705		- D3(BJ)/def2-TZVE		
H	-2.559581	-2.415428	12.718593		0 - D3(BJ)/def2-TZV		
H	-3.355346	-0.913488 0.000301	13.271758		h-3c) = $-14765.5028$		
C C	-4.601806 -5.713155	0.589475	-1.737689 -1.090726		5) = 120.13182 Kcal/ 7) = 62.90533 Kcal/m		
Н	-5.542307	1.261724	-0.236987		7X-V/def2-TZVP) = -		49 Hartree
C	-7.012552	0.364347	-1.543612		(1-xTB) = -208.69559		
H	-7.878313	0.837212	-1.058148		12-xTB) = $-205.32979$		
C	-7.251083	-0.477004	-2.654389	E (GFN	I-FF) = -24.58152502	19679 Hartree	
C H	-6.153131 -6.298257	-1.090760 -1.775989	-3.295336 -4.140700	Coord	linates:		
C	-4.853165	-0.841430	-2.840662	COOLG	-2.818711	0.513739	0.166278
Н	-4.003792	-1.321760	-3.349361	C	-3.747349	1.440949	0.795531
C	-8.949237	-1.341556	-4.176525	С	-2.985126	2.431255	1.393125
H	-8.098873	-1.433278	-4.884966	С	-1.590771	2.111196	1.126792
H	-9.707778	-0.693643	-4.664917	C	-0.463599	2.922350	1.402027
C H	-9.572792 -10.027456	-2.704966 -3.040277	-3.884821 -4.842896	C C	0.855760 2.044847	2.417889 3.235933	1.385240 1.521139
H	-10.027430	-2.557740	-3.181053	Н	2.055207	4.329954	1.552398
C	-8.648855	-3.813225	-3.354253	C	3.113566	2.376506	1.582513
H	-7.737473	-3.869646	-3.991268	H	4.175479	2.625387	1.674952
H	-9.169300	-4.783666	-3.504183	С	2.577591	1.033022	1.485691
С	-8.252662	-3.696405	-1.879435	C	3.346816	-0.143048	1.629136
H H	-7.692419 -9.151327	-4.594266 -3.607027	-1.548937 -1.234215	C C	2.810679 3.394577	-1.434821 -2.704343	1.407757 1.814960
н Н	-7.610846	-2.817249	-1.678795	C	2.623643	-3.703913	1.244616
C	1.518604	0.760707	-4.937818	C	1.570015	-3.045943	0.486146
Ċ	0.922888	-0.116045	-5.867368	С	0.640876	-3.658462	-0.388721
H	0.158154	-0.826145	-5.518104	С	-0.518286	-2.996056	-0.850825
C	1.269797	-0.092876	-7.222705	C	-1.417021	-3.530055	-1.855521
H	0.779155	-0.790831	-7.913741	H	-1.246294	-4.447133	-2.428115
C C	2.226982 2.859908	0.835761 1.692610	-7.684447 -6.756791	C H	-2.476661 -3.348733	-2.661791 -2.724835	-1.942764 -2.601273
Н	3.609962	2.403865	-7.131628	C	-2.227389	-1.598987	-0.989008
С	2.515732	1.647477	-5.406189	C	-3.144789	-0.568709	-0.686877
H	2.990441	2.343136	-4.698480	C	-0.650914	4.372776	1.659887
С	1.835952	0.361412	-10.016691	С	-0.201079	4.977794	2.849996

Н	0.280348	4.354899	3.618467	N	1.208586	1.085281	1.319567
C	-0.388489	6.345742	3.092968	N	1.668212	-1.681731	0.674057
H	-0.042788	6.775146	4.042371	N	-1.009365	-1.799043	-0.371351
C	-1.025835	7.147158	2.121974	0	-1.257422	8.479080	2.253772
С	-1.463283	6.556667	0.914859	0	8.832045	0.408958	3.003127
Н	-1.948286	7.198914	0.165768	0	1.754284	-8.845969	-2.412200
C					-8.270896		
	-1.283217	5.193077	0.695033	0		-0.707036	-3.123930
Н	-1.635046	4.740256	-0.244111	Cu	0.087205	-0.369818	0.512846
С	-0.856424	9.138026	3.453693	Br	-5.605160	1.273786	1.002927
Н	0.246524	9.045928	3.585500	Br	-3.684734	3.769796	2.506752
Н	-1.341622	8.650123	4.332137	Br	4.774309	-3.013785	3.049047
С	-1.271195	10.597805	3.355432	Br	2.837798	-5.533464	1.610992
H	-0.770160	11.048968	2.471011				
H	-0.867073	11.126879	4.246134	Confor	rmation 29.		
С	-2.785706	10.807293	3.259557		olicity: 2		
H	-3.167708	10.229011	2.392128	Charge			
Н	-3.270553	10.363727	4.157937		-3c) = -14780.09355		
C	-3.182701	12.277318	3.127986	E (M06)	/def2-TZVP) = -1477	75.722412020570 H	artree
Н	-4.282543	12.399230	3.063702	E (PBE	- D3(BJ)/def2-TZVI	P = -14773.09468	0285094 Hartree
Н	-2.742872	12.733337	2.216406		0 - D3(BJ)/def2-TZ\		
H	-2.830397	12.872894	3.996396		h-3c) = -14765.5016		
С	4.783928	0.002240	1.972885	E(PM6)	) = 115.56808 Kcal,	/mol	
C	5.205534	0.653271	3.155789	E(PM7)	= 58.46810  Kcal/r	nol	
Н	4.448399	1.041195	3.853109		7X-V/def2-TZVP) = -		81 Hartree
							or marcice
С	6.559318	0.773541	3.467437		1-xTB) = $-208.69640$		
Н	6.891289	1.256520	4.397772	E (GFN2	2-xTB) = $-205.33211$	14814830 Hartree	
С	7.543365	0.256879	2.594747	E (GFN-	-FF) = $-24.58159039$	97895 Hartree	
С	7.139099	-0.375879	1.399272				
Н	7.876070	-0.776104	0.690947	Coord	inates:		
						1 050005	1 465040
С	5.775455	-0.502628	1.107669	С	2.194569	1.058225	-1.465942
H	5.467961	-1.005325	0.178256	C	2.571554	2.042119	-2.469382
С	9.902650	0.013642	2.141111	С	1.560997	2.988848	-2.505240
Н	9.708032	-1.005137	1.737237	Ċ	0.567520	2.585448	-1.521455
			2.812197				
H	10.782926	-0.063199		С	-0.557107	3.331114	-1.092877
C	10.194018	1.001636	1.009446	C	-1.617358	2.751198	-0.361138
H	9.279929	1.137432	0.391328	С	-2.713049	3.500239	0.222765
Н	10.939111	0.509570	0.346621	H	-2.789536	4.591991	0.239112
C	10.733616	2.371540	1.447010	C	-3.588360	2.581393	0.746385
H	11.093163	2.903285	0.539621	H	-4.527330	2.767276	1.277498
H	11.636689	2.217157	2.079821	C	-3.029732	1.271021	0.478746
С	9.730439	3.262155	2.186299	С	-3.689598	0.053668	0.752740
Н	10.162566	4.262023	2.393790	C	-3.068697	-1.206138	0.570385
H	9.418609	2.814019	3.149180	С	-3.727388	-2.501849	0.497552
H	8.811120	3.412910	1.582331	С	-2.728197	-3.461429	0.486137
С	0.902534	-5.028572	-0.899532	C	-1.459610	-2.752337	0.558149
С	2.080818	-5.307988	-1.632017	С	-0.175687	-3.319527	0.743596
Н						-2.592309	
	2.805190	-4.499227	-1.811327	C	1.013638		0.512882
С	2.333376	-6.583917	-2.131064	С	2.341941	-3.075467	0.834671
H	3.244897	-6.804600	-2.704994	H	2.559909	-4.004066	1.371546
С	1.415720	-7.633582	-1.899809	C	3.230310	-2.143831	0.357709
C	0.233817	-7.372516	-1.174768	Н	4.322736	-2.156956	0.424936
H	-0.495266	-8.168278	-0.973882	C	2.445081	-1.093393	-0.260031
C	-0.012849	-6.079252	-0.692853	C	2.991108	-0.006927	-0.979266
H	-0.928221	-5.884736	-0.114409	С	-0.611163	4.791956	-1.354419
С	0.869985	-9.949380	-2.220198	С	-1.675518	5.378420	-2.067058
Н	-0.132835	-9.709718	-2.647530	Н	-2.473974	4.733793	-2.463739
Н	0.732179	-10.127606	-1.128425	C	-1.719803	6.757529	-2.315194
C	1.451699	-11.187335	-2.889359	H	-2.556361	7.172513	-2.892400
H	2.487281	-11.335515	-2.511841	C	-0.688073	7.588730	-1.829499
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C	1.438723	-11.193081	-4.425685	Н	1.164579	7.680398	-0.716294
H	0.398732	-11.000298	-4.773746	C	0.412221	5.641687	-0.870563
H	1.678297	-12.223935	-4.765620	H	1.248417	5.203711	-0.305007
C	2.399226	-10.208456	-5.098241	C	-1.664839	9.576322	-2.756963
Н	2.376673	-10.322771	-6.201042	H	-2.648529	9.416489	-2.257821
Н	3.443668	-10.380328	-4.764000	Н	-1.728956	9.127234	-3.776449
Н	2.149799	-9.158141	-4.854600	C	-1.335465	11.058377	-2.845802
С	-4.478291	-0.603759	-1.338772	H	-1.279246	11.471229	-1.814693
C	-4.895046	0.468320	-2.153182	H	-2.192307	11.567699	-3.338810
Н	-4.217064	1.323003	-2.297541	С	-0.036446	11.360802	-3.599379
C	-6.147995	0.471723	-2.779169	Н	0.791434	10.803360	-3.112844
H	-6.431422	1.324441	-3.409620	H	-0.112574	10.951220	-4.631543
С	-7.026901	-0.614981	-2.585171	С	0.294064	12.851868	-3.654581
C	-6.618650	-1.701741	-1.779101	H	1.238051	13.041277	-4.203811
Н	-7.318801	-2.537747	-1.637693	H	0.410018	13.276483	-2.635468
C	-5.362348	-1.696531	-1.175038	H	-0.508667	13.428104	-4.161147
H	-5.062405	-2.537189	-0.532104	С	-5.067861	0.104278	1.300352
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Н	-8.101353	0.487953	-4.820594	Н	-5.930693	1.156416	-0.389282
Н	-8.718053	1.321071	-3.352095	C	-7.437318	0.697500	1.093876
С	-10.188139	0.065085	-4.358201	H	-8.239507	1.144885	0.492881
H	-10.434793	0.786855	-5.166130	С	-7.711144	0.091800	2.338872
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C	-11.255827	0.161946	-3.257556	Н	-6.875282	-0.929261	4.050207
Н	-12.253969	0.124414	-3.745294	C	-5.353274	-0.477350	2.557565
H	-11.192347	1.169653	-2.788229	H	-4.537271	-0.944547	3.129183
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Н	-10.241345	-0.863634	-1.599947	Н	-10.840783	0.693526	2.943226
H	-11.240521	-1.932524	-2.617467	C	-10.720061	-0.976740	1.562565
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Н	-10.898261	-1.717264	2.373240	Н	-2.065066	-4.582666	-0.270564
C	-9.878271	-1.623912	0.456805	C	-1.588636	-3.214474	
							-1.955255
H	-8.873186	-1.876538	0.856354	H	-1.617707	-3.840452	-2.852707
H	-9.698523	-0.883230	-0.353433	С	-1.278530	-1.798648	-1.936703
C	-10.527936	-2.879869	-0.124761	C	-1.100604	-1.007035	-3.092911
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H	-10.684768	-3.651104	0.658147	С	-0.087899	2.458649	-3.652576
C	-0.053929	-4.704807	1.263017	C	0.413558	2.154346	-2.320563
C	0.655587	-5.699789	0.561057	C	1.301421	2.939274	-1.545840
H	1.106526	-5.450376	-0.410939	С	1.498313	2.720646	-0.164180
С	0.770210	-7.005904	1.055605	С	2.496991	3.400935	0.636426
H	1.317971	-7.753561	0.466653	H	3.260971	4.080532	0.245624
C	0.176569	-7.342910	2.291372	C	2.297449	3.009773	1.937131
C	-0.522443	-6.349034	3.012866	H	2.865079	3.304279	2.825367
H	-0.970841	-6.626722	3.977532	С	1.173720	2.093748	1.932180
C	-0.639091	-5.058083	2.502142	Č	0.573589	1.561079	3.094719
Н	-1.192090	-4.294745	3.069897	C	-2.466294	-3.549153	2.201476
C	0.947146	-9.626220	2.240571	C	-3.697059	-4.099998	1.793062
H	0.741261	-9.655259	1.145992	H	-4.261786	-3.608602	0.986944
H	0.532393	-10.560641	2.671089	С	-4.234988	-5.234999	2.415631
C	2.446783	-9.540972	2.517979	H	-5.206861	-5.621401	2.081759
H	2.840616	-8.570344	2.146235	С	-3.527422	-5.856953	3.466308
H	2.598585	-9.532472	3.619011	C	-2.281943	-5.326529	3.872088
С	3.230323	-10.694109	1.883979	H	-1.740152	-5.830822	4.685094
Н	3.065041	-10.689362	0.783266	С	-1.767897	-4.189685	3.253031
H	2.816182	-11.662557	2.243662	Н	-0.801332	-3.778912	3.581414
C	4.729796	-10.635020	2.177320	C	-5.210480	-7.538923	3.790486
Н	5.273031	-11.477580	1.704540	Н	-5.191336	-7.874132	2.727656
H	4.928251	-10.677634	3.268405	H	-6.019283	-6.776298	3.887387
H	5.176917	-9.692554	1.798227	С	-5.466039	-8.710256	4.726143
С	4.462405	0.036450	-1.170458	H	-4.639446	-9.444711	4.607253
C	5.206582	1.132860	-0.688998	H	-6.391101	-9.223656	4.383772
Н	4.678905	1.954306	-0.181258	С	-5.598266	-8.308407	6.198427
С	6.597603	1.197608	-0.833324	Н	-4.684022	-7.752873	6.495716
H	7.136078	2.066639	-0.433466	Н	-6.439416	-7.586960	6.303003
C	7.283080	0.151710	-1.488385	C	-5.816048	-9.499239	7.131021
C	6.549203	-0.952929	-1.976336	Н	-5.908956	-9.178761	8.188044
H	7.097319	-1.753580	-2.493577	H	-4.970315	-10.216055	7.073295
С	5.165524	-1.009515	-1.812903	H	-6.738921	-10.058518	6.869111
H	4.603182	-1.866020	-2.213029	С	-1.311160	-1.646025	-4.416660
С	9.467184	1.122659	-1.145555	С	-0.261251	-1.692817	-5.355584
H	9.045849	2.130891	-1.357898	H	0.711055	-1.250004	-5.091739
H	10.415875	1.038712	-1.714769	С	-0.426235	-2.287323	-6.613042
С	9.738787	0.949923	0.350277	Н	0.418622	-2.307045	-7.313621
Н	10.281958	1.862930	0.678876	С	-1.674207	-2.845650	-6.962382
Н	8.775138	0.954321	0.904681	C	-2.734056	-2.811670	-6.028405
C	10.555378	-0.291738	0.738341	Н	-3.700673	-3.246262	-6.321485
							-4.775459
H	10.858119	-0.182978	1.802292	С	-2.549563	-2.229018	
H	11.505406	-0.294556	0.157511	H	-3.386820	-2.190178	-4.063056
C	9.833826	-1.630317	0.556233	С	-0.924228	-3.502735	-9.146603
H	10.452225	-2.470964	0.930961	H	-0.044313	-4.050789	-8.736605
H	9.595576	-1.824414	-0.507178	H	-0.579857	-2.477369	-9.414621
H	8.874121	-1.645260	1.114352	С	-1.492638	-4.213469	-10.367486
N	0.944542	1.375036	-0.974657	Н	-0.692860	-4.236706	-11.140076
N	-1.810432	1.400601	-0.155092	H	-2.313399	-3.591344	-10.783179
N	-1.702945	-1.393859	0.523261	C	-2.010578	-5.633678	-10.097159
N	1.099859	-1.364538	-0.111299	Н	-2.472690	-6.019717	-11.030600
0	-0.632705	8.933834	-2.011162	H	-2.830319	-5.571670	-9.350655
0	-8.936251	0.013273	2.925984	C	-0.944304	-6.616344	-9.609107
0	0.205882	-8.577514	2.861861	H	-1.363806	-7.634968	-9.486334
0	8.624925	0.113444	-1.709441	H	-0.525710	-6.319279	-8.625475
Cu	-0.365691	0.006870	-0.173384	H	-0.097313	-6.689252	-10.323977
Br	4.004753	1.984888	-3.679851	С	2.111407	3.993395	-2.207443
Br	1.460276	4.373838	-3.767716	C	2.057261	5.345158	-1.792587
Br	-5.547937	-2.877744	0.228046	Н	1.381626	5.627055	-0.971537
Br	-3.027637	-5.291639	0.199322	С	2.813266	6.325294	-2.433887
	3.02/00/	3.232003		Н	2.758397	7.380931	-2.131053
Confor	mation 32.			C	3.665953	5.980052	-3.506563
_	licity: 2			С	3.749667	4.632651	-3.917581
Charge		0001016011		H	4.412832	4.331521	-4.738878
		8371216211 Hartree		C	2.972484	3.662226	-3.272634
		4775.728183140178 Hai		H	3.033649	2.614515	-3.603690
		ZVP) = -14773.0997149		С	5.216046	6.729021	-5.179533
E(PBE0	- D3(BJ)/def2-	TZVP) = -14773.637249	0647230 Hartree	H	4.632666	6.240123	-5.995341
E (PBEh	-3c) = -14765.5	07380490557 Hartree		H	6.019372	6.020789	-4.870788
	= 120.04579 Kc			С	5.807179	8.045456	-5.659321
	= 62.51227 Kca			Н	6.371588	8.506737	-4.819445
		= -14776.337313630278	Hartree	H	6.556019	7.814449	-6.448233
		= -14770.337313030270 5118121392 Hartree		C	4.766112	9.034474	-6.192926
				Н			
		0908527077 Hartree			4.007641	9.210563	-5.401271
E (GFN-	rr; = -24.58146	9969634 Hartree		H	4.218065	8.562215	-7.038775
				С	5.372786	10.362669	-6.644084
Coordi		_	_	H	4.597152	11.058982	-7.021183
C	-0.445202	0.578585	3.041472	H	6.114103	10.216225	-7.457739
C	-1.344836	0.193517	4.118420	H	5.898257	10.869961	-5.808091
С	-2.051787	-0.913082	3.676807	С	1.080634	2.013802	4.414497
C	-1.581086	-1.206746	2.331692	C	1.607866	1.074454	5.333130
C	-1.897542	-2.343089	1.548287	H	1.631845	0.010109	5.054942
C	-1.640932	-2.401632	0.160212	С	2.095543	1.475437	6.574401
C	-1.814537	-3.588553	-0.653855	Н	2.513212	0.750314	7.287569
					-		

C C							
	2.059938	2.838309	6.946705	С	-0.636929	-9.340382	-9.301269
	1.540995	3.789584	6.042933	H	-1.327916	-9.031781	-10.111121
H	1.492641	4.854055	6.306990	H	-1.177143	-10.068876	-8.661122
С	1.067672	3.371363	4.791211	H	0.210332	-9.881760	-9.772427
H	0.645684	4.114661	4.098638	С	4.385609	-1.404111	1.982482
C	2.530436	4.486283	8.629487	C	5.507521	-1.925427	1.308343
H	1.487276	4.882594	8.608336	H	5.552345	-1.856042	0.211320
H	3.137723	5.111808	7.934659	С	6.582854	-2.494439	2.005062
C	3.098808	4.555920	10.040519	H	7.447880	-2.870272	1.443374
H	4.089491	4.050446	10.041906	C	6.542439	-2.566467	3.413621
H	3.298830	5.628548	10.250071	C	5.415504	-2.062518	4.101673
C	2.208276	3.985481	11.154906	H	5.398890	-2.134056	5.198707
H	1.216432	4.489811	11.111752	C	4.361876	-1.486859	3.395492
H	2.649265	4.284179	12.130600	H	3.491336	-1.090978	3.939759
С	2.016209	2.466642	11.135442	C	8.686784	-3.636611	3.556741
H	1.421997	2.130501	12.009239	H	9.195826	-2.834861	2.972820
H	2.993402	1.941471	11.170775	H	8.390595	-4.435830	2.836235
H	1.500128	2.128316	10.216699	С	9.625642	-4.196884	4.616375
N	-0.673705	-0.237830	1.952833	H	9.821308	-3.401003	5.368207
N	-1.270145	-1.337256	-0.635950	H	10.595644	-4.386980	4.108893
N	-0.034541	0.902982	-1.948362	C	9.163683	-5.485886	5.313177
N	0.735254	1.897188	0.638176	H	10.027953	-5.898147	5.877660
0	-3.955048	-6.957498	4.137530	H	8.927946	-6.246654	4.534954
0	-1.949439	-3.429336	-8.157703	С	7.972367	-5.332997	6.262783
0	4.359544	7.002080	-4.071848	H	7.744506	-6.291829	6.771164
0	2.543800	3.131351	8.181970	H	7.061634	-4.999458	5.729790
Cu	-0.303969	0.302555	0.001652	Н	8.183952	-4.578419	7.048908
Br	-1.702900	1.099403	5.722250	C	0.125260	3.980799	3.112257
Br	-3.486735	-1.685179	4.607027	C	0.315807	3.602076	4.456588
Br	-1.766810	1.264511	-5.680514	Н	0.573600	2.556815	4.684530
Br	-0.066702	4.100124	-4.561774	C	0.185666	4.521882	5.504617
				H	0.338536	4.184492	6.537972
Confor	mation 6.			С	-0.133720	5.866078	5.217353
Multip.	licity: 2			C	-0.331165	6.259462	3.874442
Charge	: 0			H	-0.571224	7.312920	3.670303
F/B97-	3c) = -14780.0962	69367965 Hartree		С	-0.210996	5.328902	2.843471
	•						
		775.725834511941 H		H	-0.347113	5.650276	1.800288
E (PBE -	<ul> <li>D3(BJ)/def2-TZV</li> </ul>	(P) = -14773.09775	8140699 Hartree	C	-0.093574	6.514118	7.528827
F (DBF)	- D3 (B.T) /def2-T7	(VP) = -14773.6349	55911630 Hartree	H	0.939609	6.133315	7.700201
		•					
		086378176 Hartree		H	-0.798728	5.699617	7.814928
E(PM6)	= 121.47409 Kcal	./mol		C	-0.345132	7.770347	8.351801
E. (PM7)	= 64.17224 Kcal/	mol		H	-0.171848	7.508005	9.418703
			E C 11	Н			
		-14776.3349851689	об нагитее		0.425433	8.524025	8.084015
E (GFN1-	-xTB) = $-208.6945$	35215524 Hartree		C	-1.743510	8.380315	8.176631
E (GFN2-	-xTB) = $-205.3291$	51590731 Hartree		H	-1.872639	8.662827	7.110513
				Н			
E (GFN-1	FF) = -24.5806495	002302 Hartree			-1.784293	9.328528	8.753811
				C	-2.892599	7.467676	8.609955
Coordin	nates:			H	-3.870406	7.980976	8.514853
C	-1.662008	0.684668	-2.522059	Н	-2.784500	7.150136	9.668783
C	-1.782150	0.321324	-3.926048	H	-2.948876	6.548995	7.990337
C	-0.951901	-0.768176	-4.132726	C	-3.743242	2.072672	-2.384854
C	-0.322142	-1.069150	-2.855944	C	-4.741708	1.125967	-2.689913
C	0.487802	-2.189858	-2.549108	H	-4.542102	0.060354	-2.501109
C	1.311791	-2.236329	-1.402325	C	-5.978051	1.508906	-3.225337
С	2.061084	-3.402581	-0.977781	H	-6.730810	0.740166	-3.442565
H	1.988372	-4.396333	-1.430712	С	-6.234805	2.872698	-3.480644
C	2.838383	-3.010660	0.083883	C	-5.245825	3.834180	-3.172689
H	3.530475	-3.618532	0.675140	H	-5.462275	4.890991	-3.385687
						3.438099	
C	2.561665	-1.605810	0.310648	С			
C	3.246025	-0.799387	1.247500		-4.025862		-2.626820
С				H	-3.254814	4.191815	
	2.846363	0.526237			-3.254814	4.191815	-2.626820 -2.409137
C	2.846363	0.526237	1.543928	С	-3.254814 -8.422270	4.191815 2.437228	-2.626820 -2.409137 -4.369917
C	3.619816	1.537083	1.543928 2.249188	C H	-3.254814 -8.422270 -8.742786	4.191815 2.437228 1.857799	-2.626820 -2.409137 -4.369917 -3.471370
C C			1.543928	С	-3.254814 -8.422270	4.191815 2.437228	-2.626820 -2.409137 -4.369917
C	3.619816	1.537083	1.543928 2.249188	C H	-3.254814 -8.422270 -8.742786	4.191815 2.437228 1.857799	-2.626820 -2.409137 -4.369917 -3.471370
C C	3.619816 2.771575 1.480388	1.537083 2.608622 2.254216	1.543928 2.249188 2.475434 1.905398	C H H C	-3.254814 -8.422270 -8.742786 -8.027410 -9.598463	4.191815 2.437228 1.857799 1.706259 3.205604	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075
C C C	3.619816 2.771575 1.480388 0.268554	1.537083 2.608622 2.254216 2.977194	1.543928 2.249188 2.475434 1.905398 2.028039	C H H C	-3.254814 -8.422270 -8.742786 -8.027410 -9.598463 -9.218192	4.191815 2.437228 1.857799 1.706259 3.205604 3.848603	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075 -5.781016
С С С	3.619816 2.771575 1.480388 0.268554 -0.841422	1.537083 2.608622 2.254216 2.977194 2.742808	1.543928 2.249188 2.475434 1.905398 2.028039 1.186208	C H H C H	-3.254814 -8.422270 -8.742786 -8.027410 -9.598463 -9.218192 -10.262028	4.191815 2.437228 1.857799 1.706259 3.205604 3.848603 2.452637	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075 -5.781016 -5.433700
C C C	3.619816 2.771575 1.480388 0.268554	1.537083 2.608622 2.254216 2.977194	1.543928 2.249188 2.475434 1.905398 2.028039	C H H C	-3.254814 -8.422270 -8.742786 -8.027410 -9.598463 -9.218192	4.191815 2.437228 1.857799 1.706259 3.205604 3.848603	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075 -5.781016
C C C C	3.619816 2.771575 1.480388 0.268554 -0.841422 -2.138865	1.537083 2.608622 2.254216 2.977194 2.742808 3.369157	1.543928 2.249188 2.475434 1.905398 2.028039 1.186208 1.347919	C H H C H H	-3.254814 -8.422270 -8.742786 -8.027410 -9.598463 -9.218192 -10.262028 -10.422323	4.191815 2.437228 1.857799 1.706259 3.205604 3.848603 2.452637 4.042119	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075 -5.781016 -5.433700 -3.966513
C C C H	3.619816 2.771575 1.480388 0.268554 -0.841422 -2.138865 -2.430315	1.537083 2.608622 2.254216 2.977194 2.742808 3.369157 4.005812	1.543928 2.249188 2.475434 1.905398 2.028039 1.186208 1.347919 2.189221	C H H C H C H	-3.254814 -8.422270 -8.742786 -8.027410 -9.598463 -9.218192 -10.262028 -10.422323 -10.766203	4.191815 2.437228 1.857799 1.706259 3.205604 3.848603 2.452637 4.042119 3.380120	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075 -5.781016 -5.433700 -3.966513 -3.139752
С С С С Н С	3.619816 2.771575 1.480388 0.268554 -0.841422 -2.138865 -2.430315 -2.898039	1.537083 2.608622 2.254216 2.977194 2.742808 3.369157 4.005812 2.995202	1.543928 2.249188 2.475434 1.905398 2.028039 1.186208 1.347919 2.189221 0.266922	С Н С Н С Н Н С	-3.254814 -8.422270 -8.742786 -8.027410 -9.598463 -9.218192 -10.262028 -10.422323 -10.766203 -11.348201	4.191815 2.437228 1.857799 1.706259 3.205604 3.848603 2.452637 4.042119 3.380120 4.371205	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075 -5.781016 -5.433700 -3.966513 -3.139752 -4.486168
С С С С Н С Н	3.619816 2.771575 1.480388 0.268554 -0.841422 -2.138865 -2.430315 -2.898039 -3.935760	1.537083 2.608622 2.254216 2.977194 2.742808 3.369157 4.005812 2.995202 3.264074	1.543928 2.249188 2.475434 1.905398 2.028039 1.186208 1.347919 2.189221 0.266922 0.045499	С Н С Н С Н С Н	-3.254814 -8.422270 -8.742786 -8.027410 -9.598463 -9.218192 -10.262028 -10.422323 -10.766203 -11.348201 -9.712509	4.191815 2.437228 1.857799 1.706259 3.205604 3.848603 2.452637 4.042119 3.380120 4.371205 5.267621	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075 -5.781016 -5.433700 -3.966513 -3.139752 -4.486168 -3.384350
С С С С Н С Н	3.619816 2.771575 1.480388 0.268554 -0.841422 -2.138865 -2.430315 -2.898039	1.537083 2.608622 2.254216 2.977194 2.742808 3.369157 4.005812 2.995202	1.543928 2.249188 2.475434 1.905398 2.028039 1.186208 1.347919 2.189221 0.266922	С Н С Н С Н Н С	-3.254814 -8.422270 -8.742786 -8.027410 -9.598463 -9.218192 -10.262028 -10.422323 -10.766203 -11.348201	4.191815 2.437228 1.857799 1.706259 3.205604 3.848603 2.452637 4.042119 3.380120 4.371205	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075 -5.781016 -5.433700 -3.966513 -3.139752 -4.486168
С С С С Н С Н С	3.619816 2.771575 1.480388 0.268554 -0.841422 -2.138865 -2.430315 -2.898039 -3.935760 -2.065711	1.537083 2.608622 2.254216 2.977194 2.742808 3.369157 4.005812 2.995202 3.264074 2.137844	1.543928 2.249188 2.475434 1.905398 2.028039 1.186208 1.347919 2.189221 0.266922 0.045499 -0.553907	С Н С Н С Н С Н С	-3.254814 -8.422270 -8.742786 -8.027410 -9.598463 -9.218192 -10.262028 -10.422323 -10.766203 -11.348201 -9.712509 -10.397995	4.191815 2.437228 1.857799 1.706259 3.205604 3.848603 2.452637 4.042119 3.380120 4.371205 5.267621 5.853045	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075 -5.781016 -5.433700 -3.966513 -3.139752 -4.486168 -3.384350 -2.738485
C C C C H C H C	3.619816 2.771575 1.480388 0.268554 -0.841422 -2.138865 -2.430315 -2.898039 -3.935760 -2.065711 -2.444187	1.537083 2.608622 2.254216 2.977194 2.742808 3.369157 4.005812 2.995202 3.264074 2.137844 1.631827	1.543928 2.249188 2.475434 1.905398 2.028039 1.186208 1.347919 2.189221 0.266922 0.045499 -0.553907 -1.817421	С Н С Н С Н С Н Н С Н	-3.254814 -8.422270 -8.742786 -8.027410 -9.598463 -9.218192 -10.262028 -10.422323 -10.766203 -11.348201 -9.712509 -10.397995 -9.353453	4.191815 2.437228 1.857799 1.706259 3.205604 3.848603 2.452637 4.042119 3.380120 4.371205 5.267621 5.853045 5.940723	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075 -5.781016 -5.433700 -3.966513 -3.139752 -4.486168 -3.384350 -2.738485 -4.190587
C C C C H C H C C	3.619816 2.771575 1.480388 0.268554 -0.841422 -2.138865 -2.430315 -2.898039 -3.935760 -2.065711 -2.444187 0.438023	1.537083 2.608622 2.254216 2.977194 2.742808 3.369157 4.005812 2.995202 3.264074 2.137844 1.631827 -3.388470	1.543928 2.249188 2.475434 1.905398 2.028039 1.186208 1.347919 2.189221 0.266922 0.045499 -0.553907 -1.817421 -3.423296	С Н С Н С Н Н С Н Н С Н Н Н С Н Н Н С Н Н Н С Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н	-3.254814 -8.422270 -8.742786 -8.027410 -9.598463 -9.218192 -10.262028 -10.422323 -10.766203 -11.348201 -9.712509 -10.397995 -9.353453 -8.828572	4.191815 2.437228 1.857799 1.706259 3.205604 3.848603 2.452637 4.042119 3.380120 4.371205 5.267621 5.853045 5.940723 4.984343	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075 -5.781016 -5.433700 -3.966513 -3.139752 -4.486168 -3.384350 -2.78485 -4.190587 -2.781537
C C C C H C H C	3.619816 2.771575 1.480388 0.268554 -0.841422 -2.138865 -2.430315 -2.898039 -3.935760 -2.065711 -2.444187	1.537083 2.608622 2.254216 2.977194 2.742808 3.369157 4.005812 2.995202 3.264074 2.137844 1.631827	1.543928 2.249188 2.475434 1.905398 2.028039 1.186208 1.347919 2.189221 0.266922 0.045499 -0.553907 -1.817421	С Н С Н С Н С Н Н С Н	-3.254814 -8.422270 -8.742786 -8.027410 -9.598463 -9.218192 -10.262028 -10.422323 -10.766203 -11.348201 -9.712509 -10.397995 -9.353453	4.191815 2.437228 1.857799 1.706259 3.205604 3.848603 2.452637 4.042119 3.380120 4.371205 5.267621 5.853045 5.940723	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075 -5.781016 -5.433700 -3.966513 -3.139752 -4.486168 -3.384350 -2.738485 -4.190587
C C C H C C C C	3.619816 2.771575 1.480388 0.268554 -0.841422 -2.138865 -2.430315 -2.898039 -3.935760 -2.065711 -2.444187 0.438023 1.596893	1.537083 2.608622 2.254216 2.977194 2.742808 3.369157 4.005812 2.995202 3.264074 2.137844 1.631827 -3.388470 -3.918125	1.543928 2.249188 2.475434 1.905398 2.028039 1.186208 1.347919 2.189221 0.266922 0.045499 -0.553907 -1.817421 -3.423296 -4.024837	C H H C H H C H H H H N	-3.254814 -8.422270 -8.742786 -8.027410 -9.598463 -9.218192 -10.262028 -10.422323 -10.766203 -11.348201 -9.712509 -10.3977995 -9.353453 -8.828572 -0.712512	4.191815 2.437228 1.857799 1.706259 3.205604 3.848603 2.452637 4.042119 3.380120 4.371205 5.267621 5.853045 5.940723 4.984343 -0.123430	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075 -5.781016 -5.433700 -3.966513 -3.139752 -4.486168 -3.384350 -2.738485 -4.190587 -2.781537 -1.930022
C C C C H C H C C C H	3.619816 2.771575 1.480388 0.268554 -0.841422 -2.138865 -2.430315 -2.898039 -3.935760 -2.065711 -2.444187 0.438023 1.596893 2.561231	1.537083 2.608622 2.254216 2.977194 2.742808 3.369157 4.005812 2.995202 3.264074 2.137844 1.631827 -3.388470 -3.918125 -3.413916	1.543928 2.249188 2.475434 1.905398 2.028039 1.186208 1.347919 2.189221 0.266922 0.045499 -0.553907 -1.817421 -3.423296 -4.024837 -3.863514	C H C H H C H H H N N	-3.254814 -8.422270 -8.742786 -8.027410 -9.598463 -9.218192 -10.262028 -10.422323 -10.766203 -11.348201 -9.712509 -10.397995 -9.355453 -8.828572 -0.712512	4.191815 2.437228 1.857799 1.706259 3.205604 3.848603 2.452637 4.042119 3.380120 4.371205 5.267621 5.853045 5.940723 4.984343 -0.123430 -1.169744	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075 -5.781016 -5.433700 -3.966513 -3.139752 -4.486168 -3.384350 -2.738485 -4.190587 -2.781537 -1.930022 -0.573796
C C C C H C C C C H C C C C H C	3.619816 2.771575 1.480388 0.268554 -0.841422 -2.138865 -2.430315 -2.898039 -3.935760 -2.065711 -2.444187 0.438023 1.596893 2.561231 1.542062	1.537083 2.608622 2.254216 2.977194 2.742808 3.369157 4.005812 2.995202 3.264074 2.137844 1.631827 -3.388470 -3.918125 -3.413916 -5.047062	1.543928 2.249188 2.475434 1.905398 2.028039 1.186208 1.347919 2.189221 0.266922 0.045499 -0.553907 -1.817421 -3.423296 -4.024837 -3.863514 -4.854086	C H C H H C H H H N N	-3.254814 -8.42270 -8.742786 -8.027410 -9.598463 -9.218192 -10.262028 -10.422323 -10.766203 -11.348201 -9.712509 -10.397995 -9.353453 -8.828572 -0.712512 1.596338 1.586896	4.191815 2.437228 1.857799 1.706259 3.205604 3.848603 2.452637 4.042119 3.380120 4.371205 5.267621 5.853045 5.940723 4.984343 -0.123430 -1.169744 1.027379	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075 -5.781016 -5.433700 -3.966513 -3.139752 -4.486168 -3.384350 -2.738485 -4.190587 -2.781537 -1.930022 -0.573796 1.282986
C C C C H C H C C C H	3.619816 2.771575 1.480388 0.268554 -0.841422 -2.138865 -2.430315 -2.898039 -3.935760 -2.065711 -2.444187 0.438023 1.596893 2.561231	1.537083 2.608622 2.254216 2.977194 2.742808 3.369157 4.005812 2.995202 3.264074 2.137844 1.631827 -3.388470 -3.918125 -3.413916	1.543928 2.249188 2.475434 1.905398 2.028039 1.186208 1.347919 2.189221 0.266922 0.045499 -0.553907 -1.817421 -3.423296 -4.024837 -3.863514	C H C H H C H H H N N	-3.254814 -8.422270 -8.742786 -8.027410 -9.598463 -9.218192 -10.262028 -10.422323 -10.766203 -11.348201 -9.712509 -10.397995 -9.355453 -8.828572 -0.712512	4.191815 2.437228 1.857799 1.706259 3.205604 3.848603 2.452637 4.042119 3.380120 4.371205 5.267621 5.853045 5.940723 4.984343 -0.123430 -1.169744	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075 -5.781016 -5.433700 -3.966513 -3.139752 -4.486168 -3.384350 -2.738485 -4.190587 -2.781537 -1.930022 -0.573796
С С С С С С Н С С С С С Н С Н С С С Н С Н С С С Н С С С С С С С С С С С С С С С С С С С С	3.619816 2.771575 1.480388 0.268554 -0.841422 -2.138865 -2.430315 -2.898039 -3.935760 -2.065711 -2.444187 0.438023 1.596893 2.561231 1.542062 2.464709	1.537083 2.608622 2.254216 2.977194 2.742808 3.369157 4.005812 2.995202 3.264074 2.137844 1.631827 -3.388470 -3.918125 -3.413916 -5.047062 -5.416703	1.543928 2.249188 2.475434 1.905398 2.028039 1.186208 1.347919 2.189221 0.266922 0.045499 -0.553907 -1.817421 -3.423296 -4.024837 -3.863514 -4.854086 -5.320190	С Н С Н С Н Н С Н Н Н П П Н Н П П Н Н П П П П П П П П П П П П П	-3.254814 -8.422270 -8.742786 -8.027410 -9.598463 -9.218192 -10.262028 -10.422323 -10.766203 -11.348201 -9.712509 -10.397995 -9.353453 -8.828572 -0.712512 1.596338 1.586896 -0.836521	4.191815 2.437228 1.857799 1.706259 3.205604 3.848603 2.452637 4.042119 3.380120 4.371205 5.267621 5.853045 5.940723 4.984343 -0.123430 -1.169744 1.027379 1.962124	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075 -5.781016 -5.433700 -3.966513 -3.139752 -4.486168 -3.384350 -2.738485 -4.190587 -2.781537 -1.930022 -0.573796 1.282986 0.048131
С С С С С С С С С С С С С С С С С С С	3.619816 2.771575 1.480388 0.268554 -0.841422 -2.138865 -2.430315 -2.898039 -3.935760 -2.065711 -2.444187 0.438023 1.596893 2.561231 1.542062 2.464709 0.304463	1.537083 2.608622 2.254216 2.977194 2.742808 3.369157 4.005812 2.995202 3.264074 2.137844 1.631827 -3.388470 -3.918125 -3.413916 -5.047062 -5.416703 -5.683983	1.543928 2.249188 2.475434 1.905398 2.028039 1.186208 1.347919 2.189221 0.266922 0.045499 -0.553907 -1.817421 -3.423296 -4.024837 -3.863514 -4.854086 -5.320190 -5.086578	С Н С Н С Н Н С Н Н Н П П П П П П П П П П П П П	-3.254814 -8.422270 -8.742786 -8.027410 -9.598463 -9.218192 -10.262028 -10.422323 -10.766203 -11.348201 -9.712509 -10.397995 -9.353453 -8.828572 -0.712512 1.596338 1.586896 -0.836521 0.138143	4.191815 2.437228 1.857799 1.706259 3.205604 3.848603 2.452637 4.042119 3.380120 4.371205 5.267621 5.853045 5.940723 4.984343 -0.123430 -1.169744 1.027379 1.962124 -6.781010	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075 -5.781016 -5.433700 -3.966513 -3.139752 -4.486168 -3.384350 -2.78457 -4.190587 -2.781537 -1.930022 -0.573796 1.282986 0.048131 -5.870231
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С С С С С С С С С С С С С С С С С С С	3.619816 2.771575 1.480388 0.268554 -0.841422 -2.138865 -2.430315 -2.898039 -3.935760 -2.065711 -2.444187 0.438023 1.596893 2.561231 1.542062 2.464709 0.304463	1.537083 2.608622 2.254216 2.977194 2.742808 3.369157 4.005812 2.995202 3.264074 2.137844 1.631827 -3.388470 -3.918125 -3.413916 -5.047062 -5.416703 -5.683983	1.543928 2.249188 2.475434 1.905398 2.028039 1.186208 1.347919 2.189221 0.266922 0.045499 -0.553907 -1.817421 -3.423296 -4.024837 -3.863514 -4.854086 -5.320190 -5.086578	С Н С Н С Н Н С Н Н Н П П П П П П П П П П П П П	-3.254814 -8.422270 -8.742786 -8.027410 -9.598463 -9.218192 -10.262028 -10.422323 -10.766203 -11.348201 -9.712509 -10.397995 -9.353453 -8.828572 -0.712512 1.596338 1.586896 -0.836521 0.138143	4.191815 2.437228 1.857799 1.706259 3.205604 3.848603 2.452637 4.042119 3.380120 4.371205 5.267621 5.853045 5.940723 4.984343 -0.123430 -1.169744 1.027379 1.962124 -6.781010	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075 -5.781016 -5.433700 -3.966513 -3.139752 -4.486168 -3.384350 -2.78457 -4.190587 -2.781537 -1.930022 -0.573796 1.282986 0.048131 -5.870231
С С С С С Н С Н С С С Н С Н С С Н	3.619816 2.771575 1.480388 0.268554 -0.841422 -2.138865 -2.430315 -2.898039 -3.935760 -2.065711 -2.444187 0.438023 1.596893 2.561231 1.542062 2.464709 0.304463 -0.863002 -1.816315	1.537083 2.608622 2.254216 2.977194 2.742808 3.369157 4.005812 2.995202 3.264074 2.137844 1.631827 -3.388470 -3.918125 -3.413916 -5.047062 -5.416703 -5.683983 -5.173662 -5.689322	1.543928 2.249188 2.475434 1.905398 2.028039 1.186208 1.347919 2.189221 0.266922 0.045499 -0.553907 -1.817421 -3.423296 -4.024837 -3.863514 -4.854086 -5.320190 -5.086578 -4.475207 -4.659977	C H C H H C H H H N N N O O	-3.254814 -8.42270 -8.742786 -8.027410 -9.598463 -9.218192 -10.262028 -10.422323 -10.766203 -11.348201 -9.712509 -10.397995 -9.353453 -8.828572 -0.712512 1.596338 1.586896 -0.836521 0.138143 7.525064 -0.270047	4.191815 2.437228 1.857799 1.706259 3.205604 3.848603 2.452637 4.042119 3.380120 4.371205 5.267621 5.853045 5.940723 4.984343 -0.123430 -1.169744 1.027379 1.962124 -6.781010 -3.098757 6.842226	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075 -5.781016 -5.433700 -3.966513 -3.139752 -4.486168 -3.384350 -2.738485 -4.190587 -2.781537 -1.930022 -0.573796 1.282986 0.048131 -5.870231 4.187077 6.151904
С С С С Н С Н С С С Н С Н С С Н С С Н С	3.619816 2.771575 1.480388 0.268554 -0.841422 -2.138865 -2.430315 -2.998039 -3.935760 -2.065711 -2.444187 0.438023 1.596893 2.561231 1.542062 2.464709 0.304463 -0.863002 -1.816315 -0.793888	1.537083 2.608622 2.254216 2.977194 2.742808 3.369157 4.005812 2.995202 3.264074 2.137844 1.631827 -3.388470 -3.918125 -3.413916 -5.047062 -5.416703 -5.683983 -5.173662 -5.689322 -4.043065	1.543928 2.249188 2.475434 1.905398 2.028039 1.186208 1.347919 2.189221 0.266922 0.045499 -0.553907 -1.817421 -3.423296 -4.024837 -3.863514 -4.854086 -5.320190 -5.086578 -4.475207 -4.659977 -3.664702	С Н С Н Н С Н Н Н Н Н Н Н Н Н Н Н Н Н	-3.254814 -8.422270 -8.742786 -8.027410 -9.598463 -9.218192 -10.262028 -10.422323 -10.766203 -11.348201 -9.712509 -10.397995 -9.353453 -8.828572 -0.712512 1.596338 1.586896 -0.836521 0.138143 7.525064 -0.270047 -7.388768	4.191815 2.437228 1.857799 1.706259 3.205604 3.848603 2.452637 4.042119 3.380120 4.371205 5.267621 5.853045 5.940723 4.984343 -0.123430 -1.169744 1.027379 1.962124 -6.781010 -3.098757 6.842226 3.354217	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075 -5.781016 -5.433700 -3.966513 -3.139752 -4.486168 -3.384350 -2.738485 -4.190587 -2.781537 -1.930022 -0.5773796 1.282986 0.048131 -5.870231 4.18707 6.151904
С С С С Н С С С Н С С Н С Н С Н С Н С Н	3.619816 2.771575 1.480388 0.268554 -0.841422 -2.138865 -2.430315 -2.898039 -3.935760 -2.065711 -2.444187 0.438023 1.596893 2.561231 1.542062 2.464709 0.304463 -0.863002 -1.816315 -0.793888 -1.709185	1.537083 2.608622 2.254216 2.977194 2.742808 3.369157 4.005812 2.995202 3.264074 2.137844 1.631827 -3.388470 -3.918125 -3.413916 -5.047062 -5.416703 -5.683983 -5.173662 -5.689322 -4.043065 -3.648463	1.543928 2.249188 2.475434 1.905398 2.028039 1.186208 1.347919 2.189221 0.266922 0.045499 -0.5553907 -1.817421 -3.423296 -4.024837 -3.863514 -4.854086 -5.320190 -5.086578 -4.475207 -4.659977 -3.664702 -3.198524	С Н Н С Н Н С Н Н Н П П П П П П П П П П П П П	-3.254814 -8.422270 -8.742786 -8.027410 -9.598463 -9.218192 -10.262028 -10.422323 -10.766203 -11.348201 -9.712509 -10.397995 -9.353453 -8.828572 -0.712512 1.596338 1.586896 -0.836521 0.138143 7.525064 -0.270047 -7.388768 0.404257	4.191815 2.437228 1.857799 1.706259 3.205604 3.848603 2.452637 4.042119 3.380120 4.371205 5.267621 5.853045 5.940723 4.984343 -0.123430 -1.169744 1.027379 1.962124 -6.781010 -3.098757 6.842226 3.354217 0.420273	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075 -5.781016 -5.433700 -3.966513 -3.139752 -4.486168 -3.384350 -2.738485 -4.190587 -1.930022 -0.573786 0.048131 -5.870231 4.187077 6.151904 -4.012507 -0.289044
С С С С Н С Н С С С Н С Н С С Н С С Н С	3.619816 2.771575 1.480388 0.268554 -0.841422 -2.138865 -2.430315 -2.998039 -3.935760 -2.065711 -2.444187 0.438023 1.596893 2.561231 1.542062 2.464709 0.304463 -0.863002 -1.816315 -0.793888	1.537083 2.608622 2.254216 2.977194 2.742808 3.369157 4.005812 2.995202 3.264074 2.137844 1.631827 -3.388470 -3.918125 -3.413916 -5.047062 -5.416703 -5.683983 -5.173662 -5.689322 -4.043065	1.543928 2.249188 2.475434 1.905398 2.028039 1.186208 1.347919 2.189221 0.266922 0.045499 -0.553907 -1.817421 -3.423296 -4.024837 -3.863514 -4.854086 -5.320190 -5.086578 -4.475207 -4.659977 -3.664702	С Н С Н Н С Н Н Н Н Н Н Н Н Н Н Н Н Н	-3.254814 -8.422270 -8.742786 -8.027410 -9.598463 -9.218192 -10.262028 -10.422323 -10.766203 -11.348201 -9.712509 -10.397995 -9.353453 -8.828572 -0.712512 1.596338 1.586896 -0.836521 0.138143 7.525064 -0.270047 -7.388768	4.191815 2.437228 1.857799 1.706259 3.205604 3.848603 2.452637 4.042119 3.380120 4.371205 5.267621 5.853045 5.940723 4.984343 -0.123430 -1.169744 1.027379 1.962124 -6.781010 -3.098757 6.842226 3.354217	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075 -5.781016 -5.433700 -3.966513 -3.139752 -4.486168 -3.384350 -2.738485 -4.190587 -2.781537 -1.930022 -0.5773796 1.282986 0.048131 -5.870231 4.18707 6.151904
С С С С Н С Н С С Н С Н С Н С Н С Н С С	3.619816 2.771575 1.480388 0.268554 -0.841422 -2.138865 -2.430315 -2.898039 -3.935760 -2.065711 -2.444187 0.438023 1.596893 2.561231 1.542062 2.464709 0.304463 -0.863002 -1.816315 -0.793888 -1.709185 1.275111	1.537083 2.608622 2.254216 2.977194 2.742808 3.369157 4.005812 2.995202 3.264074 2.137844 1.631827 -3.388470 -3.918125 -3.413916 -5.047062 -5.416703 -5.683983 -5.173662 -5.689322 -4.043065 -3.648463 -7.350037	1.543928 2.249188 2.475434 1.905398 2.028039 1.186208 1.347919 2.189221 0.266922 0.045499 -0.553907 -1.817421 -3.423296 -4.024837 -3.863514 -4.854086 -5.320190 -5.086578 -4.475207 -4.659977 -3.664702 -3.198524 -6.517077	С Н С Н Н С Н Н Н Н П П П П П П П П П П П П П	-3.254814 -8.422270 -8.742786 -8.027410 -9.598463 -9.218192 -10.262028 -10.422323 -10.766203 -11.348201 -9.712509 -10.3977995 -9.353453 -8.828572 -0.712512 1.596338 1.586896 -0.836521 0.138143 7.525064 -0.270047 -7.388768 0.404257 -2.677865	4.191815 2.437228 1.857799 1.706259 3.205604 3.848603 2.452637 4.042119 3.380120 4.371205 5.267621 5.853045 5.940723 4.984343 -0.123430 -1.169744 1.027379 1.962124 -6.781010 -3.098757 6.842226 3.354217 0.420273 1.238429	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075 -5.781016 -5.433700 -3.966513 -3.139752 -4.486168 -3.384350 -2.78485 -4.190587 -2.781537 -1.930022 -0.573796 1.282986 0.048131 -5.870231 4.187077 6.151904 -4.012507 -0.289044 -5.296803
С С С С Н С Н С С С С Н С Н С С С Н С Н	3.619816 2.771575 1.480388 0.268554 -0.841422 -2.138865 -2.430315 -2.898039 -3.935760 -2.065711 -2.444187 0.438023 1.596893 2.561231 1.542062 2.464709 0.304463 -0.863002 -1.816315 -0.793888 -1.709185 1.275111 2.020415	1.537083 2.608622 2.254216 2.9777194 2.772808 3.369157 4.005812 2.995202 3.264074 2.137844 1.631827 -3.388470 -3.918125 -3.413916 -5.047062 -5.416703 -5.683983 -5.173662 -5.689322 -4.043065 -3.648463 -7.350037 -7.674028	1.543928 2.249188 2.475434 1.905398 2.028039 1.186208 1.347919 2.189221 0.266922 0.045499 -0.553907 -1.817421 -3.423296 -4.024837 -3.863514 -4.854086 -5.320190 -5.086578 -4.475207 -4.659977 -3.664702 -3.198524 -6.517077 -5.754352	C H H C H H C H H H N N N N O O O O C B B B B B	-3.254814 -8.422270 -8.742786 -8.027410 -9.598463 -9.218192 -10.262028 -10.422323 -10.766203 -11.348201 -9.712509 -10.3977995 -9.353453 -8.828572 -0.712512 1.596338 1.586896 -0.836521 0.138143 7.525064 -0.270047 -7.388768 0.404257 -2.677865 -0.587671	4.191815 2.437228 1.857799 1.706259 3.205604 3.848603 2.452637 4.042119 3.380120 4.371205 5.267621 5.853045 5.940723 4.984343 -0.123430 -1.169744 1.027379 1.962124 -6.781010 -3.098757 6.842226 3.354217 0.420273 1.238429 -1.510278	-2.626820 -2.409137 -4.369917 -3.471370 -5.113175 -4.957075 -5.781016 -5.433700 -3.966513 -3.139752 -4.486168 -3.384350 -2.738485 -4.190587 -2.781537 -1.930022 -0.573796 1.282986 0.048131 -5.870231 4.187077 6.151904 -4.012507 -0.289043 -5.296803 -5.817484
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E (PBE E (PBE0 E (PBEh E (PM6) E (PM7) E (ωB97 E (GFN1 E (GFN2	- D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI -3c) = -14765.5033 = 116.39312 Kcal/r = 59.57135 Kcal/r	/mol mol -14776.33262525986 66177722 Hartree 01832048 Hartree	625714 Hartree 5561653 Hartree	H C H H C H	-3.044196 -7.739585 -8.121930 -7.350868 -8.859335 -9.210577 -8.445729 -10.036101 -10.867109 -10.426804	-0.687522 -4.074244 -4.565332 -4.880355 -3.278220 -2.512765 -2.718058 -4.148618 -3.478499 -4.731072	4.662384 5.036579 5.954951 4.375469 4.364925 5.088275 3.498320 3.902417 3.596589 4.766950
Coordi	na+aa.			C H	-9.705306 -10.602825	-5.098391 -5.656771	2.746616 2.412960
C	1.157856	-1.896711	-1.785289	Н	-8.940295	-5.851570	3.026360
C	1.830735	-1.862423	-3.075233	H	-9.315621	-4.539985	1.869481
C	2.444267	-0.624691	-3.176948	C	0.856819	-4.381491	-1.663040
С	2.144159	0.098794	-1.950537	С	2.196369	-4.839381	-1.670728
C	2.684027	1.343076	-1.543414	H	2.992748	-4.168862	-1.314378
С	2.109609	2.116906	-0.510696	С	2.518676	-6.118139	-2.118865
С	2.694011	3.331862	0.022953	H	3.557281	-6.478893	-2.123801
H C	3.681465 1.784209	3.723252 3.855078	-0.240947 0.907738	C C	1.505504 0.163577	-6.983310 -6.547016	-2.590185 -2.582602
Н	1.875360	4.761430	1.514659	Н	-0.644390	-7.195306	-2.945934
C	0.645089	2.958544	0.917267	C	-0.145747	-5.261970	-2.115117
С	-0.553852	3.203408	1.622323	Н	-1.191149	-4.919653	-2.130282
C	-1.590887	2.243936	1.715973	C	0.947227	-9.126738	-3.516865
С	-2.963371	2.478442	2.138962	H	0.404711	-8.670847	-4.377466
С	-3.569034	1.237433	2.248379	H	0.192016	-9.341570	-2.723508
C C	-2.566385 -2.682741	0.244020 -1.162494	1.893724 2.010352	C H	1.643681 0.898025	-10.408913 -10.989968	-3.952756 -4.536705
C	-1.798876	-2.052390	1.360220	Н	2.453454	-10.140455	-4.666282
C	-1.798633	-3.489373	1.551267	С	2.198118	-11.294446	-2.826689
H	-2.405204	-4.025478	2.287960	H	2.474389	-12.276046	-3.269172
C	-0.896761	-4.009026	0.656065	H	1.376537	-11.514432	-2.107902
H	-0.615665	-5.056895	0.511290	C	3.404657	-10.727510	-2.073586
C C	-0.345147 0.536064	-2.889598 -3.014938	-0.081655 -1.178819	H H	3.782197 3.156248	-11.453253 -9.786187	-1.324900 -1.547195
C	3.935794	1.835488	-2.172071	Н	4.238007	-10.499741	-2.770480
C	4.006532	3.090734	-2.807911	N	1.300916	-0.668090	-1.172775
Н	3.101518	3.713611	-2.865926	N	0.884545	1.886373	0.081866
C	5.191998	3.545815	-3.402052	N	-1.413111	0.892457	1.501172
H	5.200510	4.521304	-3.905657	N	-0.873402	-1.707505	0.396157
C C	6.351115	2.742344	-3.354693	0	7.549218	3.085931	-3.894710
Н	6.298543 7.213904	1.488590 0.880560	-2.704888 -2.669147	0	-1.141975 -6.668258	8.065969 -3.243688	4.500438 5.482957
C	5.109421	1.044793	-2.131343	0	1.917388	-8.203320	-3.024896
Н	5.076509	0.063918	-1.633706	Cu	-0.020900	0.098997	0.207915
С	7.674248	4.336936	-4.567960	Br	1.741337	-3.110327	-4.474067
H	7.448516	5.170370	-3.863047	Br	3.290800	0.006797	-4.728301
H C	6.935095	4.393563	-5.402062	Br	-3.874081	4.111608	2.302181
Н	9.093274 9.800564	4.448896 4.386432	-5.103516 -4.247628	Br	-5.400617	0.985946	2.572868
H	9.214248	5.467038	-5.534141	Confo	ormation 9.		
С	9.446952	3.387622	-6.150197		iplicity: 2		
H	9.269009	2.384190	-5.709461		ge: 0		
H	8.740637	3.473472	-7.006115		7-3c) = -14780.09586		
C H	10.886713 11.115752	3.494313 2.715244	-6.651710 -7.406172		6/def2-TZVP) = -1477 E - D3(BJ)/def2-TZVI		
Н	11.612230	3.376631	-5.819796		E0 - D3(BJ)/def2-TZ\		
Н	11.081845	4.481663	-7.120823	E (PBI	Eh-3c) = -14765.5045	541605114 Hartree	
C	-0.692299	4.497245	2.337359		6) = 119.33705 Kcal,		
С	-0.891728	4.518492	3.738058		7) = 61.75105 Kcal/r		00
H C	-0.936981 -1.031396	3.565344 5.720514	4.286014 4.428485		97X-V/def2-TZVP) = -0.01		U9 Hartree
Н	-1.181370	5.742523	5.517390		N2-xTB) = $-205.33125$		
C	-0.991286	6.951020	3.735272		N-FF) = $-24.58290418$		
C	-0.785778	6.947557	2.338386				
H	-0.756700	7.885318	1.767727		dinates:	0 501000	1 (0005
C	-0.628059	5.731374	1.660424	C	2.482075	-0.501899	1.638654
H C	-0.488520 -1.244176	5.736864 9.343512	0.569172 3.874038	C C	3.911871 4.212143	-0.656653 0.014906	1.416126 0.242367
Н	-0.443388	9.471469	3.109784	C	2.965653	0.014906	-0.253902
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H	-2.855642	8.822143	2.517884	H	2.063843	3.441270	-3.320453
C H	-2.744455 -1.978122	10.990684 11.096060	2.640375 1.839901	C H	0.027835 -0.510521	2.553930 3.131144	-3.396893 -4.155347
Н	-2.493199	11.765988	3.398394	C	-0.534954	1.464275	-2.624042
C	-4.131838	11.268426	2.060300	C	-1.818410	0.915191	-2.839124
H	-4.189515	12.275280	1.600463	C	-2.381807	-0.059833	-1.980575
H	-4.914479	11.212474	2.845143	С	-3.533999	-0.906103	-2.253451
H	-4.396000	10.526225	1.278616	C	-3.837684	-1.565988	-1.073902
C C	-3.733532 -4.695806	-1.737218 -2.642426	2.887333 2.396756	C C	-2.869702 -2.880041	-1.125277	-0.080791 1.305126
Н	-4.678882	-2.642426	1.331345	C	-2.880041	-1.415020 -1.218566	2.129128
C	-5.700452	-3.163443	3.222935	C	-1.749836	-1.381318	3.569641
H	-6.447247	-3.843202	2.791694	H	-2.637191	-1.573027	4.181208
C	-5.748969	-2.796343	4.585600	C	-0.450300	-1.233131	3.986359
C	-4.774406	-1.908775	5.094669	H	-0.059178	-1.278498	5.007621
H C	-4.820340 -3.791317	-1.642856 -1.386351	6.160450 4.257072	C C	0.344356 1.753750	-0.979220 -0.884225	2.800635 2.791325
J	0./9101/	1.500551	1.20/0/2	C	1.155150	J. 00 122J	2,1020

С	3.984916	2.224899	-1.845056	Н	7.086339	-1.454882	7.589959
C	4.398353	2.144651	-3.189520	N	1.933662	0.178713	0.570536
Н	3.850642	1.485026	-3.878872	N	0.397158	1.002122	-1.717270
С	5.513767	2.853625	-3.656879	N	-1.960727	-0.281061	-0.685181
H	5.816274	2.747787	-4.706889	N	-0.473634	-0.928584	1.690266
C	6.235403	3.683229	-2.772297	0	7.325915	4.414793	-3.119554
С	5.819966	3.787210	-1.425553	0	-5.043906	2.832891	-7.103535
Н	6.388781	4.446002	-0.753763	0	-7.669400	-3.244699	3.746806
С	4.718692	3.064353	-0.972974	0	4.610513	-1.747564	7.621086
Н	4.407454	3.144914	0.079388	Cu	-0.028373	0.000508	-0.031470
C	7.811554	4.344459	-4.458706	Br	5.132280	-1.729198	2.355350
H	7.019398	4.680388	-5.167191	Br	5.889316	-0.034702	-0.597969
Н	8.063664	3.287773	-4.713766	Br	-4.355431	-1.269497	-3.902164
C	9.043447	5.230074	-4.564500	Br		-2.927785	-0.929391
					-5.121276		
Н	8.752529	6.271992	-4.306478	C	-1.106074	-2.961684	-6.098957
H	9.356924	5.249562	-5.631312	H	-1.052378	-4.026746	-6.366573
С	10.209884	4.780650	-3.679158	С	-1.591143	-2.051473	-7.064837
H	9.853973	4.722423	-2.629033	С	-1.682599	-0.681315	-6.739978
Н	10.499712	3.743206	-3.959590	Н	-2.053773	0.049427	-7.470358
С	11.425121	5.702829	-3.771963	С	-1.285672	-0.241086	-5.469579
H	12.252681	5.355125	-3.121679	H	-1.340419	0.830903	-5.228636
H	11.169487	6.737623	-3.461884	C	-2.395089	-1.716155	-9.302162
H	11.816041	5.757753	-4.809839	H	-1.629397	-0.928639	-9.491966
С	-2.618340	1.428285	-3.979414	H	-3.330511	-1.198381	-8.987283
C			-5.308031	C			-10.549297
	-2.156352	1.343848			-2.640517	-2.554614	
H	-1.179242	0.878934	-5.506713	H	-3.013826	-1.868804	-11.341376
C	-2.934054	1.792552	-6.383800	H	-3.464884	-3.267632	-10.335856
H	-2.546393	1.683147	-7.405239	С	-1.411050	-3.325549	-11.051810
С	-4.203285	2.361526	-6.142837	Н	-1.722163	-3.953195	-11.913890
C						-4.031430	
	-4.662050	2.483310	-4.812142	Н	-1.090588		-10.256835
H	-5.646262	2.942957	-4.642195	C	-0.231524	-2.440970	-11.460867
С	-3.884402	2.018308	-3.753846	H	0.600083	-3.046364	-11.873672
Н	-4.258760	2.103103	-2.722583	Н	0.179057	-1.873335	-10.600542
C	-4.756546	2.582169	-8.481212	Н	-0.524885	-1.703586	-12.237956
Н	-3.708255	2.870936	-8.719552	C	4.405825	-2.838690	-0.193184
H	-5.421884	3.279545	-9.030160	C	4.210362	-4.109938	-0.769675
С	-5.045194	1.140554	-8.897856	H	3.220188	-4.365086	-1.176469
Н	-4.355429	0.451205	-8.364019	С	5.243474	-5.052968	-0.836282
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		1.044837			5.047153		
С	-6.492980	0.705906	-8.650358	С	6.519173	-4.728056	-0.327551
H	-7.177093	1.375562	-9.218077	С	6.726981	-3.460714	0.262342
H	-6.736614	0.866540	-7.578638	H	7.729151	-3.224682	0.648239
С	-6.753633	-0.751179	-9.031223	С	5.684485	-2.538039	0.333679
Н	-7.806888	-1.041170	-8.843520	Н	5.863377	-1.546270	0.774605
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H	-6.542376	-0.935010	-10.105652	H	7.120516	-6.699472	-2.034251
C	-4.135964	-1.885513	1.942134	H	6.692644	-7.441009	-0.455977
С	-5.306439	-1.104954	1.860006	С	8.819498	-7.522797	-0.924905
Н	-5.273701	-0.149076	1.315602	Н	9.560119	-6.894240	-1.465592
C	-6.506583	-1.515513	2.453938	Н	9.145397	-7.545600	0.136213
H	-7.393710	-0.874478	2.370693	C	8.811343	-8.944899	-1.501027
C	-6.558090	-2.744479	3.145405	H	8.078753	-9.565206	-0.937527
С	-5.391097	-3.535957	3.239658	H	9.802866	-9.404210	-1.303326
H	-5.451941	-4.492907	3.777902	С	8.508726	-9.025482	-3.000315
C	-4.200905	-3.106651	2.654260	Н	8.585804	-10.067231	-3.370982
		-3.738814					-3.587094
Н	-3.302948		2.717577	H	9.221076	-8.408379	
С	-8.885788	-2.501515	3.677587	H	7.486712	-8.668614	-3.242542
H	-9.165052	-2.331086	2.610557	C	1.567906	1.157904	4.790236
H	-8.735373	-1.500863	4.145537	С	0.508312	1.114747	5.719502
С	-9.987698	-3.262316	4.402122	Н	-0.508576	0.896486	5.360004
Н	-9.633590	-3.498411	5.429698	C	0.717489	1.351620	7.082583
Н	-10.833677	-2.552156	4.522706	Н	-0.137701	1.309978	7.769925
С	-10.498163	-4.535413	3.709764	C	2.015338	1.650545	7.550721
Н	-10.801121	-4.278538	2.669561	C	3.089400	1.676317	6.633145
H	-11.433596	-4.850118	4.221158	H	4.092703	1.913079	7.015575
С	-9.519581	-5.712611	3.687000	С	2.867856	1.426587	5.279325
Н	-9.986807	-6.608734	3.230519	Н	3.707843	1.477944	4.570946
	-9.202205	-5.986192	4.714921	C	1.294727	2.082557	9.807493
H							
Н	-8.601294	-5.473930	3.117080	H	1.798281	1.984671	10.790753
С	2.478460	-1.144247	4.060894	H	0.554950	1.252047	9.739405
C	3.300361	-0.142928	4.631640	C	0.607685	3.442385	9.697636
H	3.392853	0.827625	4.121447	H	1.381659	4.234125	9.794939
C	3.988321	-0.366697	5.821871	Н	0.174007	3.559859	8.680873
Н	4.622836	0.410344	6.271831	C	-0.485839	3.638418	10.751750
С	3.886907	-1.613983	6.478578	Н	-0.048602	3.504438	11.766490
С	3.065518	-2.621158	5.928871	H	-1.246944	2.833176	10.645466
Н	2.970642	-3.601259	6.414109	C	-1.168401	5.003765	10.661312
С	2.368080	-2.374736	4.737979	Н	-1.957935	5.118663	11.430697
Н	1.745101	-3.170617	4.303509	Н	-1.642341	5.150799	9.668645
С	4.569857	-2.988523	8.324117	H	-0.438918	5.828017	10.803013
Н	4.880710	-3.818479	7.645767	N	-0.309755	1.374584	1.531900
Н	3.523174	-3.197691	8.646442	N	-1.025237	0.608741	-1.146089
С	5.492644	-2.918206	9.533172	N	1.359163	-0.978071	-1.402926
Н	5.217445	-2.023802	10.134262	N	1.968448	-0.370867	1.341645
	5.251941	-3.800392	10.164329	0	-7.251755	4.859204	1.054649
H							
С	6.999233	-2.914055	9.231496	0	-1.943864	-2.583615	-8.263996
Н	7.235868	-3.791074	8.587558	0	7.594456	-5.557260	-0.357362
Н	7.539411	-3.093735	10.186257	0	2.336216	1.908478	8.847152
С	7.539563	-1.636673	8.583166	Cu	0.493741	0.151973	0.084214
Н	8.639888	-1.690723	8.456341	Br	0.517849	4.172629	4.455350
Н	7.317570	-0.747567	9.209631	Br	-2.087846	5.022538	2.294425
11	1.311310	0.141301	J.∠∪೨UJ⊥	DŢ	-2.00/040	J.U22J30	4.4.444.3

Br	2.296770	-1.170526	-5.420259	N	-0.805330	8.125453	2.947203
Br	4.902346	-2.009659	-3.255614	H	-1.729269	8.273518	3.362926
				N	-2.251139	7.718748	0.399413
3 TTT32	T ^			H	-2.702668	7.184816	1.153555
AVIX:	TO			N	2.116388	1.343958	-7.339521
						1.038393	-7.817393
				H	1.265654		
Conformat	cion 1.			N	0.475011	3.768150	-7.800294
Multiplic	city: 2			H	0.307585	3.956612	-8.798451
Charge: C				S	-1.363824	6.643085	-0.558924
		.3542538888 Hartree		S	-0.636075	4.749561	-6.948087
•		552543788501 Hartree		F	-2.238332	3.550741	2.886601
E (GFN2-xT	$^{\circ}$ B) = $-362.1$	.72746393175 Hartree		F	-2.775602	6.191461	3.142251
E (GFN-FF)	= -35.1927	734101492 Hartree		F	2.346028	4.587982	2.134293
		-9172.854485914644 Har	tree	F	1.810933	7.206597	2.450451
,	,	-TZVP) = $-9169.2706735$		F	3.731804	1.629743	-2.790377
		2-TZVP) = -9169.509589	829700 Hartree	F	3.995909	2.313944	-5.351141
E(PBEh-3c	c) = -9158.8	325362182719 Hartree		F	-0.134131	-0.940551	-3.826407
E(PM6) =	-561.13899	Kcal/mol		F	0.120869	-0.248327	-6.425719
	-673.07934			0	-1.934304	5.311252	-0.235426
				0	0.094727	6.901246	-0.439209
E (WD9/A-V	//deiz=12vP)	= -9174.414034021638	пагстее				
				0	0.024920	5.981452	-6.451876
Coordinat	es:			0	-1.803507	4.838470	-7.857360
Cu	0.773103	-0.820359	1.498124	С	1.334233	-4.165770	0.810130
C	0.356433	2.532813	2.234563	C	0.815029	-3.828235	2.075232
C	0.707611	2.188497	0.915103	С	0.467749	-4.803202	3.089341
C	0.807459	3.143396	-0.171716	H	0.575433	-5.887579	2.982378
H	0.610731	4.217319	-0.095994	С	-0.012089	-4.101183	4.164206
С	1.142574	2.427847	-1.290356	H	-0.360178	-4.490772	5.126627
Н	1.280923	2.805254	-2.307541	C	0.045684	-2.698442	3.805622
C	1.251429	1.039835	-0.887644	C	-0.326499	-1.654034	4.672535
C	1.587196	-0.012038	-1.762578	С	-0.184844	-0.285958	4.363348
С	1.684298	-1.361394	-1.371813	С	-0.475540	0.793310	5.285326
C	2.176974	-2.417817	-2.233432	Н	-0.826896	0.676266	6.314181
H	2.538641	-2.275885	-3.257430	С	-0.230516	1.962779	4.614720
C	2.136908	-3.578966	-1.506630	H	-0.320993	2.987312	4.990579
H	2.461196	-4.580005	-1.814136	C	0.160994	1.599168	3.269570
C	1.595561	-3.229282	-0.206981	C	1.596333	-5.603045	0.524890
C	0.085377	3.967795	2.521362	C	2.635317	-6.308609	1.165702
C	-1.214558	4.420067	2.816796	C	2.878630	-7.655243	0.899089
C	-1.489462	5.777826	2.985717	С	2.113431	-8.396101	-0.039999
C	-0.496156	6.768226	2.843416	С	1.063586	-7.686486	-0.663770
С	0.816564	6.314737	2.582755	С	0.832938	-6.329913	-0.402999
C	1.087351	4.952613	2.407884	C	2.086513	-10.532495	-1.378434
C	-0.539457	8.995526	1.801057	H	2.232230	-11.598619	-1.103110
H	0.389441	8.646546	1.316635	H	1.007097	-10.408770	-1.585381
H	-0.361409	10.034037	2.153663	С	2.899296	-10.257558	-2.660583
С	-1.693491	9.016095	0.771659	H	2.569120	-10.966093	-3.452980
H	-2.544706	9.609796	1.170466	Н	3.972909	-10.462697	-2.472742
H	-1.364127	9.539963	-0.151087	С	5.020539	-7.682992	-4.214115
C	-1.837999	7.081917	-2.225628	C	6.295820	-8.260638	-4.168256
C	-0.924753	7.755934	-3.050022	H	6.643558	-8.730553	-3.237330
H	0.064258	8.027313	-2.654200	С	7.107682	-8.202489	-5.309906
C	-1.284831	8.030389	-4.376451	Н	8.114389	-8.647885	-5.278882
H	-0.564245	8.530436	-5.039855	С	6.665174	-7.573840	-6.491404
C	-2.536814	7.634504	-4.892050	C	5.379153	-6.987609	-6.496959
C	-3.433734	6.963719	-4.029435	H	5.023189	-6.475204	-7.404549
H	-4.411547	6.639015	-4.417896	C	4.554645	-7.033990	-5.368692
C	-3.096703	6.681769	-2.702216	Н	3.562285	-6.560302	-5.369080
H	-3.785767	6.134299	-2.043363	С	7.530174	-7.539106	-7.724612
C	-2.888007	7.860600	-6.336477	H	8.602095	-7.662971	-7.476861
H	-2.674220	6.944393	-6.928109	H	7.255286	-8.360218	-8.421318
H	-2.290473	8.680934	-6.777770	Н	7.408172	-6.588752	-8.280878
H	-3.963631	8.094490	-6.462901	С	-0.980806	-2.008933	5.961633
			-3.199253				7.218702
C	1.794326	0.313953		C	-0.430644	-1.700713	
С	2.830815	1.148087	-3.656769	С	-1.121192	-1.928598	8.418277
C	2.967849	1.506346	-5.006333	C	-2.423926	-2.480702	8.426026
C	2.059364	1.046225	-5.988610	С	-2.953320	-2.832423	7.159781
C	1.033425	0.186205	-5.524872	С	-2.258899	-2.603901	5.972636
C	0.905317	-0.166509	-4.182463	C	-3.147888	-1.842723	10.720648
C	2.643581	2.600548	-7.853644	H	-3.791220	-2.306406	11.497636
H	2.615965	2.533532	-8.961347	H	-2.124621	-1.803997	11.137364
H	3.706600	2.709540	-7.568865	C	-3.627784	-0.412844	10.432635
C	1.876279	3.844919	-7.386476	Н	-2.973261	0.042592	9.659984
Н	1.901231	3.890623	-6.277878	Н	-3.523075	0.218194	11.344355
H	2.385074	4.767045	-7.747821	C	-4.936657	0.743944	7.452280
C	-1.034208	3.724439	-5.538894	С	-4.184565	1.764392	6.854486
C	-0.986127	4.292550	-4.259575	H	-3.944591	2.666164	7.436005
Н	-0.644648	5.329380	-4.136511	C	-3.752278	1.602659	5.529975
C	-1.377976	3.519992	-3.157297	Н	-3.162479	2.393817	5.044594
H	-1.361705	3.962891	-2.150784	С	-4.050222	0.431842	4.802552
C	-1.794464	2.182699	-3.315488	С	-4.825149	-0.569707	5.432055
C	-1.838189	1.642355	-4.622216	H	-5.056930	-1.496044	4.885771
Н	-2.142617	0.594592	-4.765050	С	-5.280395	-0.419112	6.744752
C	-1.476078	2.405104	-5.736344	H	-5.870318	-1.207507	7.231991
H	-1.501530	1.975323	-6.747206	С	-3.545375	0.236040	3.397259
C	-2.154712	1.339041	-2.121808	H	-3.007211	-0.729126	3.308195
H	-3.195321	0.960468	-2.196564	Н	-4.386969	0.204377	2.673596
H	-2.052556	1.907692	-1.178439	Н	-2.858270	1.046593	3.092246
H	-1.493060	0.450502	-2.061272	N	0.549921	-2.554428	2.530466
N	0.976383	0.914106	0.458271	N	0.216163	0.226638	3.146479
N	1.349015	-1.872813	-0.137507	N	2.446626	-9.723324	-0.230817

H	3.364405	-9.934383	0.168193	С	-3.786373	-7.889520	-2.700696
N	2.796585	-8.894509	-3.161366	C	-3.603681	-7.444876	-1.384564
H	1.865278	-8.460581	-3.136077	H	-4.256679	-7.829632	-0.587833
N	-3.181115	-2.725016	9.559518	С	-2.569460	-6.536402	-1.113182
H	-4.134678	-2.991805	9.301193	H	-2.405814	-6.199351	-0.078000
N	-4.990333	-0.437828	9.903671	С	-1.721338	-6.063560	-2.136116
H	-5.714864	-0.667663	10.598633	C	-1.935639	-6.535146	-3.451789
	3.970356		-2.762513	Н			
S		-7.742541			-1.291859	-6.168489	-4.265894
S	-5.553645	0.981182	9.117777	С	-2.951602	-7.450200	-3.740875
F	3.415783	-5.680751	2.055405	H	-3.099624	-7.827751	-4.762705
F	3.906078	-8.287360	1.503423	С	-0.619897	-5.076145	-1.855299
F	-0.160145	-5.726995	-1.071437	Н	-0.869663	-4.081826	-2.280464
F	0.304903	-8.278700		Н	0.331561	-5.395741	
			-1.630027				-2.326275
F	0.794202	-1.160705	7.297923	H	-0.449561	-4.939422	-0.771507
F	-0.512347	-1.597953	9.577932	N	-1.206897	-0.984011	0.430064
F	-2.863627	-2.914375	4.812545	N	-1.513010	0.593104	-1.948999
F	-4.203908	-3.346774	7.118765	N	1.236940	-4.356329	7.220862
0	3.236538	-6.459293	-2.690050	Н	2.237222	-4.601926	7.228317
0	4.804190	-8.255231	-1.649233	N	2.357622	-2.047067	8.556483
0	-4.891685	2.182979	9.676443	Н	2.424998	-1.968833	7.531096
0	-7.023382	0.832766	9.136101	N	-6.258796	-5.571221	-3.520180
				Н	-5.790836	-6.090615	-4.273557
Conforma	ation 10.			N	-6.149190	-8.296956	-4.079087
Multipli				Н	-6.338274	-8.952945	-4.847979
Charge:				S	3.719982	-2.928536	9.108882
E(B97-3c	= -9171.808	552998102 Hartree		S	-5.037476	-9.128274	-3.048679
E(GFN1->	(TB) = -378.64	4547962878 Hartree		F	-1.912521	-1.756505	4.649304
		2721674580 Hartree		F	-1.364920	-3.211180	6.830880
•				F		-2.372848	3.077403
		8258495 Hartree			2.533218		
		172.848934895033 Hai		F	3.102771	-3.828976	5.279567
		ZVP) = -9169.265357		F	-2.296145	-2.970391	-3.926363
E(PBE0 -	- D3(BJ)/def2-	TZVP) = -9169.502476	6600435 Hartree	F	-4.028227	-4.812602	-4.883112
		9719304962 Hartree		F	-5.151957	-2.274988	-0.181918
				F			
	= -563.75709 K				-6.833374	-4.142198	-1.093280
E(PM7) =	= -672.86791 K	cal/mol		0	3.886449	-4.201783	8.348538
E(ωB97X-	-V/def2-TZVP) :	= -9174.404364332700	) Hartree	0	3.596776	-2.970587	10.579587
				0	-5.713822	-9.461812	-1.774037
Coordina	+00.			0	-4.444864	-10.159189	-3.925082
		0 775007	0 240701	C			
Cu	-0.436716	0.775907	-0.240791		-0.773970	2.652141	-3.125581
С	0.001333	-1.160341	2.589038	С	0.132372	3.104330	-2.146861
C	-0.853360	-1.649642	1.585809	C	0.939336	4.300321	-2.285268
C	-1.512295	-2.938378	1.642163	H	0.966288	4.943310	-3.171153
H	-1.396539	-3.671360	2.447671	С	1.628014	4.450400	-1.110166
C	-2.282247	-3.035104	0.512117	Н	2.322234	5.249921	-0.831237
H	-2.925148	-3.864416	0.201321	С	1.259681	3.332154	-0.264978
C	-2.082632	-1.811403	-0.239236	C	1.754021	3.136235	1.037627
C	-2.704510	-1.534029	-1.474826	С	1.415461	2.038310	1.851646
С	-2.447913	-0.378605	-2.238825	С	1.922342	1.838897	3.194199
C	-3.135605	-0.054833	-3.473641	Н	2.582339	2.525464	3.732923
H	-3.950861	-0.639852	-3.912020	С	1.431736	0.633589	3.624547
C	-2.589742	1.110136	-3.943684	H	1.586876	0.148218	4.594039
H	-2.869544	1.671387	-4.842745	С	0.633613	0.096215	2.542189
С	-1.570633	1.499654	-2.987647	С	-0.915986	3.450153	-4.374456
C	0.281426	-2.014182	3.775792	C	-1.496584	4.735258	-4.378038
С	-0.679496	-2.265200	4.773201	С	-1.633738	5.473934	-5.552641
C	-0.390849	-3.025955	5.915134	C	-1.219563	4.978054	-6.817392
C	0.890888	-3.593504	6.125317	С	-0.628801	3.694812	-6.803163
С	1.855869	-3.331674	5.115765	С	-0.506030	2.952037	-5.622233
Ċ	1.555408	-2.581340	3.977289	Č	-1.433502	5.357682	-9.300287
С	0.777971	-4.039509	8.570925	Н	-1.295646	6.252959	-9.943019
H	1.329429	-4.721615	9.246499	H	-0.564338	4.700489	-9.488615
H	-0.302116	-4.255421	8.688325	С	-2.730402	4.647282	-9.742538
C	1.054899	-2.573778	8.985311	H	-2.648199	4.389377	-10.822192
Н	0.291609	-1.898578	8.547378	Н	-3.589534	5.341563	-9.643227
H	0.985007	-2.474032	10.087154		-5.658350	2.896981	-8.334738
				C			
С	5.041820	-1.839871	8.604449	С	-5.808399	1.515454	-8.539322
С	5.519497	-0.882456	9.511668	H	-4.988128	0.830654	-8.279553
H	5.063932	-0.805844	10.509524	С	-7.015930	1.036260	-9.054928
C	6.581916	-0.060422	9.121181	Н	-7.143112	-0.046372	-9.212997
Н	6.969687	0.693705	9.823564	C	-8.081262	1.912445	-9.365605
C	7.173800	-0.179896	7.843132	C	-7.901780	3.290761	-9.133805
С	6.651361	-1.140767	6.949845	H	-8.726263	3.987316	-9.352456
H	7.090705	-1.236431	5.944910	С	-6.697753	3.791915	-8.617565
C	5.594589	-1.982482	7.322260	H	-6.560687	4.863535	-8.414157
Н	5.201959	-2.747582	6.636211	С	-9.369154	1.376557	-9.935086
C	8.349348	0.679967	7.469394	Н	-9.232250	1.055977	-10.989929
H	9.283155	0.273359	7.913868	H	-9.720607	0.487793	-9.372971
H	8.227891	1.713730	7.843731	H	-10.173173	2.136981	-9.918835
H	8.499945	0.731469	6.374559	C	2.736517	4.114994	1.579203
С	-3.658840	-2.538268	-2.014792	C	2.433682	4.961934	2.660062
C	-3.422091	-3.213480	-3.231098	C	3.373514	5.847539	3.207352
C	-4.302166	-4.176624	-3.722501	С	4.690605	5.932872	2.696802
С	-5.461435	-4.570625	-3.009363	C	4.984233	5.084537	1.599970
С	-5.717812	-3.875089	-1.803944	C	4.043951	4.205178	1.064088
C	-4.838276	-2.892554	-1.329872	C	5.775633	7.207631	4.551704
C	-7.020214	-6.473503	-2.665272	Н	6.607948	7.940167	4.606746
H	-7.959793	-6.001191	-2.315134	H	4.858091	7.746829	4.852044
H	-6.443853	-6.752190	-1.753563	C	6.028000	6.061399	5.541417
С	-7.354613	-7.740304	-3.451580	Н	5.191468	5.334228	5.481642
Н	-7.856083	-8.465152	-2.774567	Н	6.031475	6.449635	6.585002
H	-8.051811	-7.496925	-4.280054	C	6.596807	2.780230	4.621714
п	-0.031811	-/.490923	-4.280034	C	0.390807	2.100230	4.021/14

С	5.695397	1.811041	5.083540	С	-9.281069	-4.405333	7.691941
Н	5.483799	1.732351	6.159423	Н	-8.753144	-4.676740	8.624476
С	5.082142	0.959992	4.152015	H	-9.194797	-5.268519	7.001490
H	4.375101	0.192475	4.501235	H	-10.359004	-4.270262	7.921624
C	5.340512	1.075504	2.770271	С	1.462238	4.129694	-2.281791
С	6.257161	2.063870	2.341984	С	1.581963	3.963313	-3.679857
Н	6.454968	2.187393	1.266594	C		4.941289	-4.494727
					2.149158		
C	6.896985	2.906033	3.255265	С	2.625534	6.179233	-3.984466
H	7.599528	3.678595	2.914133	C	2.466573	6.359602	-2.587108
С	4.648044	0.194939	1.765019	C	1.909726	5.361121	-1.771674
Н	4.055060	0.808001	1.054642	Č	4.030053	8.183492	-4.498761
H	5.385737	-0.372372	1.160316	H	3.548095	8.777917	-3.701346
Н	3.962737	-0.524456	2.249064	H	4.127410	8.850351	-5.381170
N	0.353331	2.522161	-0.916956	С	5.441113	7.776026	-4.017204
N	0.617336	0.975988	1.481998	H	5.856401	8.589403	-3.385386
N	-1.408931	5.792190	-7.917098	H	5.368408	6.886825	-3.354980
Н	-2.045659	6.563236	-7.701821	С	6.682661	4.829913	-4.845423
N	-3.049010	3.446774	-8.984247	С	5.775549	3.764830	-4.760590
H	-2.270321	2.811182	-8.770647	H	4.867040	3.766879	-5.379722
N	5.676762	6.783495	3.162473	C	6.064552	2.704624	-3.893843
H	6.581894	6.566488	2.739667	H	5.380627	1.846764	-3.863499
N	7.259672	5.356840	5.189045	C	7.223427	2.703085	-3.086380
				C			
H	8.129113	5.865826	5.400474		8.112950	3.795132	-3.200459
S	-4.113052	3.516076	-7.671197	H	9.025569	3.811727	-2.584519
S	7.479294	3.783127	5.814476	C	7.862567	4.851082	-4.083754
F	-1.936691	5.270290	-3.231040	H	8.563913	5.692473	-4.179117
F	-2.225304		-5.520827	C	7.503027	1.559670	-2.150192
		6.685793					
F	0.026424	1.725218	-5.710430	H	6.636522	1.352173	-1.490267
F	-0.263243	3.086894	-7.967546	H	8.384575	1.759181	-1.511936
F	1.209606	4.933822	3.204118	H	7.695249	0.631790	-2.726609
F	2.990803	6.622884	4.246092	N	-0.529507	1.981772	0.167806
F	4.425734	3.393440	0.062330	N	1.759555	0.631526	-0.897792
F	6.245855	5.103709	1.108555	N	-7.335871	3.942253	3.814408
0	-3.606775	2.507175	-6.713487	H	-8.073748	3.714402	3.144641
0	-4.338553	4.933450	-7.300308	N	-7.084107	1.852699	6.115722
0	6.795260	3.635861	7.123481	H	-6.168272	2.273735	6.321512
0	8.934183	3.547873	5.686998	N	3.154107	7.088211	-4.876710
				H	3.427901	6.645722	-5.764397
Conform	mation 13.			N	6.452271	7.502111	-5.036333
	licity: 2			H	6.741926	8.296845	-5.620598
Charge:	: 0			S	-6.842960	0.540555	5.084183
E(B97-3	3c) = -9171.8203	68251789 Hartree		S	6.397297	6.130515	-6.031306
E (GFN1-	-xTB) = $-378.662$	387022279 Hartree		F	-2.666848	2.780849	4.415241
		403200733 Hartree		F	-4.909112	3.777024	5.455506
				F		2.021707	
						2 021707	0.266381
	FF) = -35.202469				-4.845679		
	,	72.860170840058 Ha	irtree	F	-7.141441	3.018686	1.306963
E(M06/c	def2-TZVP) = -91	72.860170840058 Ha		F	-7.141441		
E(M06/c E(PBE -	def2-TZVP) = -91 - D3(BJ)/def2-TZ	72.860170840058 Ha VP) = $-9169.278208$	466691 Hartree	F F	-7.141441 1.188531	3.018686 2.817152	-4.253094
E (M06/c E (PBE - E (PBE0	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-T	72.860170840058 Ha $VP) = -9169.278208$ $ZVP) = -9169.51651$	466691 Hartree	F F	-7.141441 1.188531 2.293015	3.018686 2.817152 4.704224	-4.253094 -5.817046
E (M06/c E (PBE - E (PBE0 E (PBEh-	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-T -3c) = -9158.829	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree	466691 Hartree	F F F	-7.141441 1.188531 2.293015 1.857753	3.018686 2.817152 4.704224 5.595045	-4.253094 -5.817046 -0.451625
E (M06/c E (PBE - E (PBE0 E (PBEh-	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-T	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree	466691 Hartree	F F F F	-7.141441 1.188531 2.293015	3.018686 2.817152 4.704224	-4.253094 -5.817046
E (M06/c E (PBE - E (PBE0 E (PBEh- E (PM6)	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-T -3c) = -9158.829	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol	466691 Hartree	F F F	-7.141441 1.188531 2.293015 1.857753	3.018686 2.817152 4.704224 5.595045	-4.253094 -5.817046 -0.451625
E (M06/c E (PBE - E (PBE0 E (PBEh- E (PM6) E (PM7)	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-T -3c) = -9158.829 = -570.47663 Kc = -683.23308 Kc	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol	466691 Hartree 6938764 Hartree	F F F F	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483	-4.253094 -5.817046 -0.451625 -1.986983 5.137364
E (M06/c E (PBE - E (PBE0 E (PBEh- E (PM6) E (PM7)	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-T -3c) = -9158.829 = -570.47663 Kc = -683.23308 Kc	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol	466691 Hartree 6938764 Hartree	F F F F O	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148
E (M06/c E (PBE - E (PBE0 E (PBEh- E (PM6) E (PM7) E (ωB97)	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-T -3c) = -9158.829 = -570.47663 Kc = -683.23308 Kc K-V/def2-TZVP) =	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol	466691 Hartree 6938764 Hartree	F F F F O	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401
E (M06/α E (PBE - E (PBE0 E (PBEh- E (PM6) E (PM7) E (ωB97)	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-TZ - D3(BJ)/def2-TZ - 3c) = -9158.829 = -570.47663 Kc = -683.23308 Kc K-V/def2-TZVP) =	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858	4466691 Hartree 6938764 Hartree 31 Hartree	F F F F O O	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972
E (M06/c E (PBE - E (PBE0 E (PBEh- E (PM6) E (PM7) E (ωB97)	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-T -3c) = -9158.829 = -570.47663 Kc = -683.23308 Kc K-V/def2-TZVP) =	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol	466691 Hartree 6938764 Hartree	F F F F O	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203
E (M06/c E (PBE - E (PBE0 E (PBEh- E (PM6) E (PM7) E (\omega B97) Coordin Cu	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-TZ - D3(BJ)/def2-T - 9158.829 = -570.47663 Kc = -683.23308 Kc K-V/def2-TZVP) =  nates: 0.235209	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532	8466691 Hartree .6938764 Hartree 81 Hartree 0.290195	F F F O O O	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203
E M06/c E (PBE - E (PBE0 E (PBEh- E (PM6) E (PM7) E (\omega B97) Coordir Cu	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-T - D3(BJ)/def2-T -3c) = -9158.829 = -570.47663 Kc = -683.23308 Kc K-V/def2-TZVP) =  nates: 0.235209 -2.438601	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589	0.290195 1.728977	F F F F O O O C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423
E M06/c E (PBE - E (PBE0 E (PBEh- E (PM6) E (PM7) E (\omega B97) Coordir Cu C	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-T - D3(BJ)/def2-T -3c) = -9158.829 = -570.47663 Kc = -683.23308 Kc K-V/def2-TZVP) =  nates:	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266	0.290195 1.728977 0.794573	F F F O O O C C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278
E M06/c E (PBE - E (PBE0 E (PBEh- E (PMT) E (\omega B97) Coordir Cu C C	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-TZ - D3(BJ)/def2-TZ - D3(BJ)/def2-TZ - D3(BJ)/def2-TZ = -570.47663 KC = -683.23308 KC K-V/def2-TZVP) =  nates: 0.235209 -2.438601 -1.663302 -1.952139	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395	0.290195 1.728977 0.794573 0.358241	F F F O O C C C H	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343
E M06/c E (PBE - E (PBE0 E (PBEh- E (PM6) E (PM7) E (\omega B97) Coordir Cu C	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-T - D3(BJ)/def2-T -3c) = -9158.829 = -570.47663 Kc = -683.23308 Kc K-V/def2-TZVP) =  nates:	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266	0.290195 1.728977 0.794573 0.358241 0.710075	F F F O O O C C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PM6)) E (PM7) E (wB97) Coordir Cu C C C	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-TZ - D3(BJ)/def2-TZ - D3(BJ)/def2-TZ - D3(BJ)/def2-TZ = -570.47663 KC = -683.23308 KC K-V/def2-TZVP) =  nates: 0.235209 -2.438601 -1.663302 -1.952139	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395	0.290195 1.728977 0.794573 0.358241	F F F O O C C C H	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PM6) E (PM7) E (wB97) Coordir Cu C C C C	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-TZ - D3(BJ)/def2-TZ - D3(BJ)/def2-TZ - = -9158.829 = -570.47663 Kc = -683.23308 Kc K-V/def2-TZVP) =  nates: 0.235209 -2.438601 -1.663302 -1.952139 -2.794531 -0.981111	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113	F F F F O O O C C C H C H	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635
E (M06/c E (PBE - E (PBE0 - E (PBEh- E (PM6) E (PM7) E (ωB97) Coordir Cu C C C C H	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-T - D3(BJ)/def2-TZVP) =   nates:	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680	F F F F O O O C C C H C H C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.312423 -0.513343 0.647361 0.995635 0.940353
E (M06/c E (PBE - E (PBE0 - E (PBE0 - E (PM6)) E (PM7) E (wB97) Coordin Cu C C C C H C	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-T - D3(BJ)/def2-TZVP) =   nates:	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407	F F F F O O O C C C H C H C C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.312423 -0.513343 0.647361 0.995635 0.940353 1.774880
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PM6)) E (PM7) E (wB97) Coordir Cu C C C C H C C	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-TZVP) = 0.235209 - 2.438601 - 1.663302 - 1.952139 - 2.794531 - 0.981111 - 0.862699 - 0.088006 1.085503	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006	F F F F O O O O C C C H C H C C C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PM6)) E (PM7) E (wB97) Coordir Cu C C C C H C C H	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-T - D3(BJ)/def2-TZVP) =   nates:	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407	F F F F O O O C C C H C H C C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.312423 -0.513343 0.647361 0.995635 0.940353 1.774880
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PM6)) E (PM7) E (wB97) Coordir Cu C C C C H C C	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-TZVP) = 0.235209 - 2.438601 - 1.663302 - 1.952139 - 2.794531 - 0.981111 - 0.862699 - 0.088006 1.085503	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006	F F F F O O O O C C C H C H C C C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PM6) E (PM7) E (wB97) Coordir Cu C C C C H C C C C	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-TZ - D3(BJ)/def2-TZ - D3(BJ)/def2-TZ - D3(BJ)/def2-TZ - D3(BJ)/def2-TZ = -570.47663 Kc - C483.23308 Kc - C483.2300 Kc -	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038	F F F F O O O O C C C H C H C C C C H	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.99380 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.550389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442
E M06/c E (PBE - E (PBE0 - E (PBEh- E (PM6)) E (PM7) E (wB97X Coordin C C C C C C C C C H C C C C	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-TZ - D3(BJ)/def2-T3 - D3(BJ)/def2-T3 - D3(BJ)/def2-T3 - D3(BJ)/def2-T3 = -570.47663 Kc = -683.23308 Kc K-V/def2-TZVP) =  nates:	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735	F F F F F O O O O C C C H C H C C C C H C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750
E M06/c E(PBE - E(PBE0 - E(PBE0 - E(PM6)) E(PM7)) E(wB97) Coordin Cu C C C C C C C C C C H C C C C C H C C C C C C C C C C C C C C C C C C C C	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-TZVP) = 0.235209 - 2.438601 - 1.663302 - 1.952139 - 2.794531 - 0.981111 - 0.862699 - 0.088006 1.085503 1.966057 3.221034 3.642115 3.743490	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100	F F F F O O O O C C C H C H C C C H C H	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PM6)) E (PM7) E (wB97) Coordir Cu C C C C C C C C C C C C C H C C C C	def2-TZVP) = -91 - D3 (BJ) /def2-TZ - D4 (B3	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691	F F F F O O O O C C C H C H C C C H C H C H C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110
E M06/c E(PBE - E(PBE0 - E(PBE0 - E(PM6)) E(PM7)) E(wB97) Coordin Cu C C C C C C C C C C H C C C C C H C C C C C C C C C C C C C C C C C C C C	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-TZVP) = 0.235209 - 2.438601 - 1.663302 - 1.952139 - 2.794531 - 0.981111 - 0.862699 - 0.088006 1.085503 1.966057 3.221034 3.642115 3.743490	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100	F F F F O O O O C C C H C H C C C H C H	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PM6)) E (PM7) E (wB97) Coordir Cu C C C C H C C C C H C C C C C H C C C C C C C C C C C C C C C C C C C C	def2-TZVP) = -91 - D3 (BJ) /def2-TZ - D3 (BJ) /def2-TZVP) = 0.235209 - 2.438601 - 1.663302 - 1.952139 - 2.794531 - 0.981111 - 0.862699 - 0.088006 1.085503 1.966057 3.221034 3.642115 3.743490 4.640368 2.821971	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019	F F F F F O O O O C C C H C H C C C C H C H C C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110 -1.703077
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PM6)) E (PM7) E (wB97) Coordir Cu C C C C H C C C C H C C C C C C C C	def2-TZVP) = -91 - D3 (BJ) / def2-TZ - D3 (BJ) / def2-TZVP) = D3 (BJ) / def2-TZVP) / def2-TZVP) = D3 (BJ) / def2-TZVP) / def2-TZVP) = D3 (BJ) / def2-TZVP) / def2-TZVP) / def2-TZVP) = D3 (BJ) / def2-TZVP) / def	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348	F F F F F O O O O C C C H C H C C C C H C H C C C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.99380 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.550389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110 -1.703077 -1.353619
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PM6)) E (PM7)) E (wB97) Coordin Cu C C C C C C C C C C C C C C C C C C	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-TZVP) = 0.235209 - 2.438601 - 1.663302 - 1.952139 - 2.794531 - 0.981111 - 0.862699 - 0.088006 1.085503 1.966057 3.221034 3.642115 3.743490 4.640368 2.821971 - 3.656934 - 3.736725	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660 2.858366	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348 3.613433	F F F F O O O O C C C H C H C C C C H C H C C C C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851 6.580343	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617 -2.284138	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110 -1.703077 -1.353619 -2.098089
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PM6)) E (PM7) E (wB97) Coordir Cu C C C C C C C C C C C C C C C C C C	def2-TZVP) = -91 - D3 (BJ) /def2-TZ = -9158.829 = -570.47663 Kc K-V/def2-TZVP) =  nates:  0.235209 -2.438601 -1.663302 -1.952139 -2.794531 -0.981111 -0.862699 -0.088006 1.085503 1.966057 3.221034 3.642115 3.743490 4.640368 2.821971 -3.656934 -3.736725 -4.917296	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660 2.858366 3.399607	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348 3.613433 4.144988	F F F F F O O O O C C C H C H C C C C H C H C C C C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851 6.580343 6.439434	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617 -2.284138 -3.075286	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110 -1.703077 -1.353619 -2.098089 -3.268564
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PM6)) E (PM7)) E (wB97) Coordin Cu C C C C C C C C C C C C C C C C C C	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-TZVP) = 0.235209 - 2.438601 - 1.663302 - 1.952139 - 2.794531 - 0.981111 - 0.862699 - 0.088006 1.085503 1.966057 3.221034 3.642115 3.743490 4.640368 2.821971 - 3.656934 - 3.736725	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660 2.858366	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348 3.613433	F F F F O O O O C C C H C H C C C C H C H C C C C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851 6.580343	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617 -2.284138	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110 -1.703077 -1.353619 -2.098089
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PM6)) E (PM7) E (wB97) Coordir Cu C C C C C C C C C C C C C C C C C C	def2-TZVP) = -91 - D3 (BJ) / def2-TZ - D3 (BJ) / def2-TZVP) = 0.235209 - 2.438601 - 1.663302 - 1.952139 - 2.794531 - 0.981111 - 0.862699 - 0.088006 1.085503 1.966057 3.221034 3.64215 3.743490 4.640368 2.821971 - 3.656934 - 3.736725 - 4.917296 - 6.111887	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660 2.858366 3.399607 3.457235	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348 3.613433 4.144988 3.394813	F F F F F O O O O C C C H C H C C C C H C H C C C C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851 6.580343 6.439434 5.112980	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617 -2.284138 -3.075286 -3.442005	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110 -1.703077 -1.353619 -2.098089 -3.268564 -3.590688
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PBE0 - E (PM6)) E (PM7) E (WB97)  Coordir Cu C C C C C H C C C C C C C C C C C C	def2-TZVP) = -91 - D3 (BJ) / def2-TZ - D3 (BJ) / def2-TZVP) = 0.235209 - 2.438601 - 1.663302 - 1.952139 - 2.794531 - 0.981111 - 0.862699 - 0.088066 - 1.085503 1.966057 - 3.221034 - 3.642115 - 3.743490 - 4.640368 - 2.821971 - 3.656934 - 3.736725 - 4.917296 - 6.111887 - 6.016932	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660 2.858366 3.399607 3.457235 2.998434	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348 3.613433 4.144988 3.394813 2.054962	F F F F F O O O O C C C H C H C C C C C H C H C H	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851 6.580343 6.439434 5.112980 4.018552	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617 -2.284138 -3.075286 -3.442005 -2.991100	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.055203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.63735 2.096110 -1.703077 -1.353619 -2.098089 -3.268564 -3.590688
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PM6)) E (PM7)) E (wB97) Coordin Cu C C C C C C C C C C C C C C C C C C	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-TZVP) = 0.235209 - 2.438601 - 1.663302 - 1.952139 - 2.794531 - 0.981111 - 0.862699 - 0.088006 1.085503 1.966057 3.221034 3.642115 3.743490 4.640368 2.821971 - 3.656934 - 3.736725 - 4.917296 - 6.111887 - 6.016932 - 4.839223	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660 2.858366 3.399607 3.457235 2.998434 2.472475	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348 3.613433 4.144988 3.394813 2.054962 1.528341	F F F F F O O O O C C C H C H C C C C H C H C C C C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851 6.580343 6.439434 5.112980 4.018552 7.657456	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617 -2.284138 -3.075286 -3.442005 -2.991100 -3.895719	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110 -1.703077 -1.353619 -2.098089 -3.268564 -3.590688 -2.840509 -5.323560
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PM6)) E (PM7)) E (wB97) Coordin Cu C C C C C C C C C C C C C C C C C C	def2-TZVP) = -91 - D3 (BJ) / def2-TZ - D3 (BJ) / def2-TZVP) = defa  nates:  0.235209 -2.438601 -1.663302 -1.952139 -2.794531 -0.981111 -0.862699 -0.088006 1.085503 1.966057 3.221034 3.642115 3.743490 4.640368 2.821971 -3.656934 -3.736725 -4.917296 -6.111887 -6.016932 -4.839223 -7.86858	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660 2.858366 3.399607 3.457235 2.998434 2.472475 4.085174	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348 3.613433 4.144988 3.394813 2.054962 1.528341 5.184139	F F F F F O O O O C C C H C H C C C C H C H C H C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851 6.580343 6.439434 5.112980 4.018552 7.657456 8.617423	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617 -2.284138 -3.075286 -3.442005 -2.991100 -3.8895719 -4.440165	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110 -1.703077 -1.353619 -2.098089 -3.268564 -3.590688 -2.840509 -5.323560 -5.452315
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PM6)) E (PM7)) E (wB97) Coordin Cu C C C C C C C C C C C C C C C C C C	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-TZVP) = 0.235209 - 2.438601 - 1.663302 - 1.952139 - 2.794531 - 0.981111 - 0.862699 - 0.088006 1.085503 1.966057 3.221034 3.642115 3.743490 4.640368 2.821971 - 3.656934 - 3.736725 - 4.917296 - 6.111887 - 6.016932 - 4.839223	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660 2.858366 3.399607 3.457235 2.998434 2.472475	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348 3.613433 4.144988 3.394813 2.054962 1.528341	F F F F F O O O O C C C H C H C C C C H C H C C C C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851 6.580343 6.439434 5.112980 4.018552 7.657456	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617 -2.284138 -3.075286 -3.442005 -2.991100 -3.895719	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110 -1.703077 -1.353619 -2.098089 -3.268564 -3.590688 -2.840509 -5.323560
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PM6)) E (PM7)) E (wB97) Coordin Cu C C C C C C C C C C C C C C C C C C	def2-TZVP) = -91 - D3 (BJ) / def2-TZ - D3 (BJ) / def2-TZVP) = defa  nates:  0.235209 -2.438601 -1.663302 -1.952139 -2.794531 -0.981111 -0.862699 -0.088006 1.085503 1.966057 3.221034 3.642115 3.743490 4.640368 2.821971 -3.656934 -3.736725 -4.917296 -6.111887 -6.016932 -4.839223 -7.86858	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660 2.858366 3.399607 3.457235 2.998434 2.472475 4.085174	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348 3.613433 4.144988 3.394813 2.054962 1.528341 5.184139	F F F F F O O O O C C C H C H C C C C H C H C H C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851 6.580343 6.439434 5.112980 4.018552 7.657456 8.617423	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617 -2.284138 -3.075286 -3.442005 -2.991100 -3.8895719 -4.440165	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110 -1.703077 -1.353619 -2.098089 -3.268564 -3.590688 -2.840509 -5.323560 -5.452315
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PBE0 - E (PM6)) E (PM7) E (WB97)  Coordir Cu C C C C C C C C C C C C C C C C C C	def2-TZVP) = -91 - D3 (BJ) / def2-TZ - D3 (BJ) / def2-TZVP) =   nates:	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660 2.858366 3.399607 3.457235 2.998434 2.472475 4.085174 4.754879 4.607123	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348 3.613433 4.144988 3.394813 2.054962 1.528341 5.184139 5.177938 5.773300	F F F F F O O O O C C C H C H C C C C H C H C H C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851 6.580343 6.439434 5.112980 4.018552 7.657456 8.617423 6.854614 7.592138	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617 -2.284138 -3.075286 -3.442005 -2.991100 -3.895719 -4.440165 -4.636401 -2.795096	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.055203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110 -1.703077 -1.353619 -2.098089 -3.268564 -3.590688 -2.840509 -5.323560 -5.452315 -5.490816 -6.405700
E M06/c E (PBE - E (PBE) - E (PBE) - E (PM6) E (PM7) E (	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-TZVP) = 0.235209 - 2.438601 - 1.663302 - 1.952139 - 2.794531 - 0.981111 - 0.862699 - 0.088006 1.085503 1.966057 3.221034 3.642115 3.743490 4.640368 2.821971 - 3.656934 - 3.736725 - 4.917296 - 6.111887 - 6.016932 - 4.839223 - 7.786858 - 8.672791 - 7.008451 - 8.188133	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660 2.858366 3.399607 3.457235 2.998434 2.472475 4.085174 4.754879 4.607123 2.779746	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348 3.613433 4.144988 3.394813 2.054962 1.528341 5.184139 5.177938 5.773300 5.899305	F F F F F O O O O C C C H C H C C C C C H C H C C C C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851 6.580343 6.439434 5.112980 4.018552 7.657456 8.617423 6.854614 7.592138 7.646757	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617 -2.284138 -3.075286 -3.442005 -2.991100 -3.895719 -4.440165 -4.636401 -2.795096 -3.274715	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110 -1.703077 -1.353619 -2.098089 -3.268564 -3.590688 -2.840509 -5.323560 -5.452315 -5.490816 -6.405700 -7.407977
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PM6)) E (PM7)) E (wB97) Coordin Cu C C C C C C C C C C C C C C C C C C	def2-TZVP) = -91 - D3 (BJ) / def2-TZ - D3 (BJ) / def2-TZVP) = 0.235209 - 2.438601 - 1.663302 - 1.952139 - 2.794531 - 0.981111 - 0.862699 - 0.088006 1.085503 1.966057 3.221034 3.642115 3.743490 4.640368 2.821971 - 3.656934 - 3.736725 - 4.917296 - 6.111887 - 6.016932 - 4.839223 - 7.786858 - 8.672791 - 7.008451 - 8.188133 - 8.646513	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660 2.858366 3.399607 3.457235 2.998434 2.472475 4.085174 4.754879 4.607123 2.779746 3.037589	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348 3.613433 4.144988 3.394813 2.054962 1.528341 5.184139 5.177938 5.773300 5.899305 6.880255	F F F F F O O O O C C C H C H C C C C C H C H C H	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851 6.580343 6.439434 5.112980 4.018552 7.657456 8.617423 6.854614 7.592138 7.646757 8.473928	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617 -2.284138 -3.075286 -3.442005 -2.991100 -3.895719 -4.440165 -4.636401 -2.795096 -3.274715 -2.129327	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110 -1.703077 -1.353619 -2.098089 -3.268564 -3.590688 -2.840509 -5.323560 -5.452315 -5.490816 -6.405700 -7.407977 -6.318167
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PBE0 - E (PM6)) E (PM7) E (\omega B97) Coordir Cu C C C C C C C C C C C C C C C C C C	def2-TZVP) = -91 - D3 (BJ) / def2-TZ - D4 (B3	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660 2.858366 3.399607 3.457235 2.998434 2.472475 4.085174 4.754879 4.607123 2.779746 3.037589 2.251286	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348 3.613433 4.144988 3.394813 2.054962 1.528341 5.1773300 5.899305 6.880255 5.309851	F F F F F O O O O O C C C H C H C C C C H C H C C C C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851 6.580343 6.439434 5.112980 4.018552 7.657456 8.617423 6.854614 7.592138 7.646757 8.473928 6.379510	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617 -2.284138 -3.075286 -3.442005 -2.991100 -3.895719 -4.440165 -4.636401 -2.795096 -3.274715 -2.129327 0.826454	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110 -1.703077 -1.353619 -2.098089 -3.268564 -3.590688 -2.840509 -5.323560 -5.452315 -5.490816 -6.405700 -7.407977 -6.318167 -6.638769
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PM6)) E (PM7)) E (wB97) Coordin Cu C C C C C C C C C C C C C C C C C C	def2-TZVP) = -91 - D3 (BJ) / def2-TZ - D3 (BJ) / def2-TZVP) = 0.235209 - 2.438601 - 1.663302 - 1.952139 - 2.794531 - 0.981111 - 0.862699 - 0.088006 1.085503 1.966057 3.221034 3.642115 3.743490 4.640368 2.821971 - 3.656934 - 3.736725 - 4.917296 - 6.111887 - 6.016932 - 4.839223 - 7.786858 - 8.672791 - 7.008451 - 8.188133 - 8.646513	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660 2.858366 3.399607 3.457235 2.998434 2.472475 4.085174 4.754879 4.607123 2.779746 3.037589	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348 3.613433 4.144988 3.394813 2.054962 1.528341 5.184139 5.177938 5.773300 5.899305 6.880255	F F F F F O O O O C C C H C H C C C C C H C H C H	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851 6.580343 6.439434 5.112980 4.018552 7.657456 8.617423 6.854614 7.592138 7.646757 8.473928	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617 -2.284138 -3.075286 -3.442005 -2.991100 -3.895719 -4.440165 -4.636401 -2.795096 -3.274715 -2.129327	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110 -1.703077 -1.353619 -2.098089 -3.268564 -3.590688 -2.840509 -5.323560 -5.452315 -5.490816 -6.405700 -7.407977 -6.318167
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PBE0 - E (PMG)) E (WB97) Coordir Cu C C C C C C C C C C C C C C C C C C	def2-TZVP) = -91 - D3 (BJ) / def2-TZ - D4 (B3	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660 2.858366 3.399607 3.457235 2.998434 2.472475 4.085174 4.754879 4.607123 2.779746 3.037589 2.251286	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348 3.613433 4.144988 3.394813 2.054962 1.528341 5.1773300 5.899305 6.880255 5.309851	F F F F F O O O O O C C C H C H C C C C H C H C C C C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851 6.580343 6.439434 5.112980 4.018552 7.657456 8.617423 6.854614 7.592138 7.646757 8.473928 6.379510	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617 -2.284138 -3.075286 -3.442005 -2.991100 -3.895719 -4.440165 -4.636401 -2.795096 -3.274715 -2.129327 0.826454	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110 -1.703077 -1.353619 -2.098089 -3.268564 -3.590688 -2.840509 -5.323560 -5.452315 -5.490816 -6.405700 -7.407977 -6.318167 -6.638769
E (M06/c E (PBE - E (PBE) - E (PBE) - E (PM6) E (PM7) E (wB97) Coordin Cu C C C C C C C C C C C C C C C C C C	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-TZVP) = -9158.829 = -570.47663 Kc - V/def2-TZVP) = -9148.829 - 0.235209 - 2.438601 - 1.663302 - 1.952139 - 2.794531 - 0.981111 - 0.862699 - 0.088006 - 1.085503 - 1.966057 - 3.221034 - 3.642115 - 3.743490 - 4.640368 - 2.821971 - 3.656934 - 3.736725 - 4.917296 - 6.111887 - 6.016932 - 4.839223 - 7.786888 - 8.672791 - 7.008451 - 8.188133 - 8.646513 - 8.965505 - 7.633357 - 7.165343	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660 2.858366 3.399607 3.457235 2.998434 2.472475 4.085174 4.754879 4.607123 2.779746 3.037589 2.251286 -0.840440 -1.254750	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348 3.613433 4.144988 3.394813 2.054962 1.528341 5.184139 5.177938 5.773300 5.899305 6.880255 5.309851 5.900773 7.157383	F F F F F O O O O C C C H C H C C C C C H C H C C C C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851 6.580343 6.439434 5.112980 4.018552 7.657456 8.617423 6.854614 7.592138 7.646757 8.473928 6.379510 5.140272 4.239442	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617 -2.284138 -3.075286 -3.442005 -2.991100 -3.895719 -4.440165 -4.636401 -2.795096 -3.274715 -2.129327 0.826454 1.167466 0.590212	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.63735 2.096110 -1.703077 -1.353619 -2.098089 -3.268564 -3.590688 -2.840509 -5.323560 -5.452315 -5.490816 -6.405700 -7.407977 -6.318167 -6.638769 -7.203709 -6.950225
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PM6)) E (PM7)) E (wB97) Coordin Cu C C C H C C C C H C C C C H C C C C	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-TZVP) = -683.23308 Kc K-V/def2-TZVP) = -0.235209 - 2.438601 - 1.663302 - 1.952139 - 2.794531 - 0.981111 - 0.862699 - 0.088006 1.085503 1.966057 3.221034 3.642115 3.743490 4.640368 2.821971 - 3.656934 - 3.736725 - 4.917296 - 6.111887 - 6.016932 - 4.839223 - 7.786858 - 8.672791 - 7.008451 - 8.188133 - 8.646513 - 8.965505 - 7.633357 - 7.165343 - 6.375906	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660 2.858366 3.399607 3.457235 2.998434 2.472475 4.085174 4.754879 4.607123 2.779746 3.037589 2.251286 -0.840440 -1.254750 -0.685361	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348 3.613433 4.144988 3.394813 2.054962 1.528341 5.184139 5.177938 5.773300 5.899305 6.880255 5.309851 5.900773 7.157383 7.669213	F F F F F O O O O C C C H C H C C C C C H C H C C C C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851 6.580343 6.439434 5.112980 4.018552 7.657456 8.617423 6.854614 7.592138 7.646757 8.473928 6.379510 5.140272 4.239442 5.068917	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617 -2.284138 -3.075286 -3.442005 -2.991100 -3.895719 -4.440165 -4.636401 -2.795096 -3.274715 -2.129327 0.826454 1.167466 0.590212 2.275132	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110 -1.703077 -1.353619 -2.098089 -3.268564 -3.590688 -2.840509 -5.323560 -5.452315 -5.490816 -6.405700 -7.407977 -6.318167 -6.638769 -7.203709 -6.950225 -8.055829
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PM6)) E (PM7)) E (WB97) Coordin Cu C C C H C C C C H C C C C H C C C C	def2-TZVP) = -91 - D3 (BJ) / def2-TZ - D3 (BJ) / def2-TZVP) = defa  nates:  0.235209 -2.438601 -1.663302 -1.952139 -2.794531 -0.981111 -0.862699 -0.088006 1.085503 1.966057 3.221034 3.642115 3.743490 4.640368 2.821971 -3.656934 -3.736725 -4.917296 -6.111887 -6.016932 -4.839223 -7.786858 -8.672791 -7.008451 -8.188133 -8.646513 -8.965505 -7.633357 -7.165343 -6.375906 -7.707510	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660 2.858366 3.399607 3.457235 2.998434 2.472475 4.085174 4.754879 4.607123 2.779746 3.037589 2.251286 -0.840440 -1.254750 -0.685361 -2.408830	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348 3.613433 4.144988 3.394813 2.054962 1.528341 5.177938 5.7773300 5.899305 6.880255 5.309851 5.900773 7.157383 7.669213 7.733151	F F F F F O O O O C C C H C H C C C C C H C H C H	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851 6.580343 6.439434 5.112980 4.018552 7.657456 8.617423 6.854614 7.592138 7.646757 8.473928 6.379510 5.140272 4.239442 5.068917 4.098253	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617 -2.284138 -3.075286 -3.442005 -2.991100 -3.895719 -4.440165 -4.636401 -2.795096 -3.274715 -2.129327 0.826454 1.167466 0.590212 2.275132 2.558346	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110 -1.703077 -1.355619 -2.098089 -2.2098089 -3.268564 -3.590688 -2.840509 -5.323560 -5.452315 -5.490816 -6.405700 -7.407977 -6.318167 -6.638769 -7.203709 -6.950225 -8.055829 -8.491071
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PBE0 - E (PMG)) E (PM7) E (WB97) Coordir Cu C C C C C C C C C C C C C C C C C C	def2-TZVP) = -91 - D3 (BJ) / def2-TZ - D4 (B3	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660 2.858366 3.399607 3.457235 2.998434 2.472475 4.085174 4.754879 4.607123 2.779746 3.037589 2.251286 -0.840440 -1.254750 -0.685361 -2.408830 -2.754525	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348 3.613433 4.144988 3.394813 2.054962 1.528341 5.177938 5.773300 5.899305 6.880255 5.309851 5.900773 7.157383 7.669213 7.733151 8.709560	F F F F F O O O O C C C H C H C C C C H C H C H C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851 6.580343 6.439434 5.112980 4.018552 7.657456 8.617423 6.854614 7.592138 7.646757 8.473928 6.379510 5.140272 4.239442 5.068917 4.098253 6.208983	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617 -2.284138 -3.075286 -3.442005 -2.991100 -3.895719 -4.440165 -4.636401 -2.795096 -3.274715 -2.129327 0.826454 1.167466 0.590212 2.275132 2.558346 3.057374	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110 -1.703077 -1.353619 -2.098089 -3.268564 -3.590688 -2.840509 -5.323560 -5.452315 -5.490816 -6.405700 -7.407977 -6.318167 -6.638769 -7.203709 -6.950225 -8.055829 -8.491071 -8.344627
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PM6)) E (PM7)) E (WB97) Coordin Cu C C C H C C C C H C C C C H C C C C	def2-TZVP) = -91 - D3 (BJ) / def2-TZ - D3 (BJ) / def2-TZVP) = defa  nates:  0.235209 -2.438601 -1.663302 -1.952139 -2.794531 -0.981111 -0.862699 -0.088006 1.085503 1.966057 3.221034 3.642115 3.743490 4.640368 2.821971 -3.656934 -3.736725 -4.917296 -6.111887 -6.016932 -4.839223 -7.786858 -8.672791 -7.008451 -8.188133 -8.646513 -8.965505 -7.633357 -7.165343 -6.375906 -7.707510	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660 2.858366 3.399607 3.457235 2.998434 2.472475 4.085174 4.754879 4.607123 2.779746 3.037589 2.251286 -0.840440 -1.254750 -0.685361 -2.408830	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348 3.613433 4.144988 3.394813 2.054962 1.528341 5.177938 5.7773300 5.899305 6.880255 5.309851 5.900773 7.157383 7.669213 7.733151	F F F F F O O O O C C C H C H C C C C C H C H C H	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851 6.580343 6.439434 5.112980 4.018552 7.657456 8.617423 6.854614 7.592138 7.646757 8.473928 6.379510 5.140272 4.239442 5.068917 4.098253	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617 -2.284138 -3.075286 -3.442005 -2.991100 -3.895719 -4.440165 -4.636401 -2.795096 -3.274715 -2.129327 0.826454 1.167466 0.590212 2.275132 2.558346	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110 -1.703077 -1.355619 -2.098089 -2.2098089 -3.268564 -3.590688 -2.840509 -5.323560 -5.452315 -5.490816 -6.405700 -7.407977 -6.318167 -6.638769 -7.203709 -6.950225 -8.055829 -8.491071
E M06/c E (PBE - E (PBE) - E (PBE) - E (PM6) E (PM7) E (\omega B97) Coordin Cu C C C H C C C H C C C C H C C C H C C C H C C C C C C C C C C C C C C C C C C C C	def2-TZVP) = -91 - D3(BJ)/def2-TZ - D3(BJ)/def2-TZVP) = 0.0235209 - 2.438601 - 1.663302 - 1.952139 - 2.794531 - 0.981111 - 0.862699 - 0.088006 - 1.085503 - 1.966057 - 3.221034 - 3.642115 - 3.743490 - 4.640368 - 2.821971 - 3.656934 - 3.736725 - 4.917296 - 6.111887 - 6.016932 - 4.839223 - 7.786888 - 8.672791 - 7.008451 - 8.188133 - 8.965505 - 7.633357 - 7.165343 - 6.375906 - 7.707510 - 7.336019 - 8.706391	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660 2.858366 3.399607 3.457235 2.998434 2.472475 4.085174 4.754879 4.607123 2.779746 3.037589 2.251286 -0.840440 -1.254750 -0.685361 -2.408830 -2.754525 -3.159744	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348 3.613433 4.144988 3.394813 2.054962 1.528341 5.184139 5.177938 5.773300 5.899305 6.880255 5.309851 5.900773 7.157383 7.669213 7.733151 8.709560 7.074367	F F F F F O O O O C C C H C H C C C C C H C H C C C C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851 6.580343 6.439434 5.112980 4.018552 7.657456 8.617423 6.854614 7.592138 7.646757 8.473928 6.379510 5.140272 4.239442 5.068917 4.098253 6.208983 7.433373	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617 -2.284138 -3.075286 -3.442005 -2.991100 -3.895719 -4.440165 -4.636401 -2.795096 -3.274715 -2.129327 0.826454 1.167466 0.590212 2.275132 2.558346 3.057374 2.699391	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.055203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110 -1.703077 -1.353619 -2.098089 -3.268564 -3.590688 -2.840509 -5.323560 -5.452315 -5.490816 -6.405700 -7.407977 -6.318167 -6.638769 -7.203709 -6.950225 -8.055829 -8.491071 -8.344627 -7.738532
E (M06/c E (PBE - E (PBE) - E (PBE) - E (PM6) E (PM7) E (wB97) Coordin Cu C C C C C C C C C C C C C C C C C C	def2-TZVP) = -91 - D3 (BJ)/def2-TZ - D3 (BJ)/def2-TZVP) = D3 (BJ)/def2-TZ	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660 2.858366 3.399607 3.457235 2.998434 2.472475 4.085174 4.754879 4.607123 2.779746 3.037589 2.251286 -0.840440 -1.254750 -0.685361 -2.408830 -2.754525 -3.159744 -2.716097	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348 3.613433 4.144988 3.394813 2.054962 1.528341 5.184139 5.177938 5.773300 5.899305 6.880255 5.309851 5.900773 7.157383 7.669213 7.733151 8.709560 7.074367 5.809688	F F F F F O O O O C C C H C H C C C C C H C H C C C C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851 6.580343 6.439434 5.112980 4.018552 7.657456 8.617423 6.854614 7.592138 7.646757 8.473928 6.379510 5.140272 4.239442 5.068917 4.098253 6.208983 7.433373 8.321725	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617 -2.284138 -3.075286 -3.442005 -2.991100 -3.895719 -4.440165 -4.636401 -2.795096 -3.274715 -2.129327 0.826454 1.167466 0.590212 2.275132 2.558346 3.057374 2.699391 3.325371	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110 -1.703077 -1.353619 -2.098089 -3.268564 -3.590688 -2.840509 -5.323560 -5.452315 -5.490816 -6.405700 -7.407977 -6.318167 -6.638769 -7.203709 -6.950225 -8.055829 -8.491071 -8.344627 -7.738532 -7.913151
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PBE0 - E (PM6)) E (PM7)) E (WB97)  Coordir Cu C C C H C C C C C H C C C C H C C C C	def2-TZVP) = -91 - D3 (BJ) / def2-TZ - D3 (BJ) / def2-TZVP) = def3 - D3 (B3 (B) / def3-TZ - C3 (B)	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660 2.858366 3.399607 3.457235 2.998434 2.472475 4.085174 4.754879 4.607123 2.779746 3.037589 2.251286 -0.840440 -1.254750 -0.685361 -2.408830 -2.754525 -3.159744 -2.716097 -3.297527	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348 3.613433 4.144988 3.394813 2.054962 1.528341 5.184139 5.177938 5.773300 5.899305 6.880255 5.309851 5.900773 7.157383 7.669213 7.733151 8.709560 7.074367 5.809688 5.271273	F F F F F O O O O C C C H C H C C C C C H C H C C C C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851 6.580343 6.439434 5.112980 4.018552 7.657456 8.617423 6.854614 7.592138 7.646757 8.473928 6.379510 5.140272 4.239442 5.068917 4.098253 6.208983 7.433373 8.321725 7.529912	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.7747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617 -2.284138 -3.075286 -3.442005 -2.991100 -3.895719 -4.440165 -4.636401 -2.775096 -3.274715 -2.129327 0.826454 1.167466 0.590212 2.275132 2.558346 3.057374 2.699391 3.325371 1.588322	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110 -1.703077 -1.353619 -2.098089 -2.2098089 -3.268564 -3.590688 -2.240509 -5.323560 -5.452315 -5.490816 -6.405700 -7.407977 -6.318167 -6.638769 -7.203709 -6.950225 -8.055829 -8.491071 -8.344627 -7.738532 -7.913151 -6.891435
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PBE0 - E (PM6)) E (PM7)) E (WB97) Coordir Cu C C C H C C C C H C C C C H C C C C	def2-TZVP) = -91 - D3 (BJ) / def2-TZ - C438601 - 1.663302 - 1.952139 - 2.794531 - 0.981111 - 0.862699 - 0.088006 1.085503 1.966057 3.221034 3.642115 3.743490 4.640368 2.821971 - 3.656934 - 3.736725 - 4.917296 - 6.111887 - 6.016932 - 4.839223 - 7.786858 - 8.672791 - 7.008451 - 8.188133 - 8.646513 - 8.965505 - 7.633357 - 7.165343 - 6.375906 - 7.707510 - 7.336019 - 8.706391 - 9.148508 - 9.912976 - 8.619804	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660 2.858366 3.399607 3.457235 2.998434 2.472475 4.085174 4.754879 4.607123 2.779746 3.037589 2.251286 -0.840440 -1.254750 -0.685361 -2.408830 -2.754525 -3.159744 -2.716097 -3.297527 -1.564057	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348 3.613433 4.144988 3.394813 2.054962 1.528341 5.1773300 5.899305 6.880255 5.309851 5.900773 7.157383 7.669213 7.733151 8.709560 7.074367 5.809688 5.271273 5.215379	F F F F F O O O O C C C H C H C C C C C H C H C H	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851 6.580343 6.439434 5.112980 4.018552 7.657456 8.617423 6.854614 7.592138 7.646757 8.473928 6.379510 5.140272 4.239442 5.068917 4.098253 6.208983 7.433373 8.321725 7.529912 8.473488	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617 -2.284138 -3.075286 -3.442005 -2.991100 -3.895719 -4.440165 -4.636401 -2.795096 -3.274715 -2.129327 0.826454 1.167466 0.590212 2.275132 2.558346 3.057374 2.699391 3.325371 1.588322 1.588322	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110 -1.703077 -1.353619 -2.098089 -3.268564 -3.590688 -2.840509 -5.32356 -5.452315 -5.452315 -5.490816 -6.405700 -7.407977 -6.318167 -6.638769 -7.203709 -6.638769 -7.203709 -6.638769 -7.738532 -7.913151 -6.891435 -6.891435 -6.891435 -6.891974
E M06/c E (PBE - E (PBE0 - E (PBE0 - E (PBE0 - E (PM6)) E (PM7)) E (WB97)  Coordir Cu C C C H C C C C C H C C C C H C C C C	def2-TZVP) = -91 - D3 (BJ) / def2-TZ - D3 (BJ) / def2-TZVP) = def3 - D3 (B3 (B) / def3-TZ - C3 (B)	72.860170840058 Ha VP) = -9169.278208 ZVP) = -9169.51651 396510075 Hartree al/mol al/mol -9174.41877847858  0.090532 1.740589 2.451266 3.803395 4.408733 4.140983 5.079672 3.004248 2.974422 1.873717 1.890278 2.761589 0.628262 0.235859 -0.152258 2.392660 2.858366 3.399607 3.457235 2.998434 2.472475 4.085174 4.754879 4.607123 2.779746 3.037589 2.251286 -0.840440 -1.254750 -0.685361 -2.408830 -2.754525 -3.159744 -2.716097 -3.297527	0.290195 1.728977 0.794573 0.358241 0.710075 -0.550113 -1.101680 -0.645407 -1.420006 -1.457667 -2.178038 -2.686735 -2.096100 -2.581691 -1.298019 2.292348 3.613433 4.144988 3.394813 2.054962 1.528341 5.184139 5.177938 5.773300 5.899305 6.880255 5.309851 5.900773 7.157383 7.669213 7.733151 8.709560 7.074367 5.809688 5.271273	F F F F F O O O O C C C H C H C C C C C H C H C C C C	-7.141441 1.188531 2.293015 1.857753 2.893011 -5.373341 -7.552107 5.056693 7.565166 2.985939 2.074496 2.188568 2.993880 1.113048 0.852351 0.362762 -0.770280 -1.455788 -2.545023 -2.903550 -3.012368 -3.834523 -2.198413 4.162746 5.486851 6.580343 6.439434 5.112980 4.018552 7.657456 8.617423 6.854614 7.592138 7.646757 8.473928 6.379510 5.140272 4.239442 5.068917 4.098253 6.208983 7.433373 8.321725 7.529912	3.018686 2.817152 4.704224 5.595045 7.497457 0.323483 0.7747910 5.909919 6.295741 -1.530389 -2.304046 -3.734538 -4.360499 -4.114594 -5.119558 -2.909003 -2.859845 -1.673196 -1.614068 -2.458809 -0.325210 0.096036 0.402941 -2.177915 -1.842617 -2.284138 -3.075286 -3.442005 -2.991100 -3.895719 -4.440165 -4.636401 -2.775096 -3.274715 -2.129327 0.826454 1.167466 0.590212 2.275132 2.558346 3.057374 2.699391 3.325371 1.588322	-4.253094 -5.817046 -0.451625 -1.986983 5.137364 3.795148 -6.645401 -6.927972 -1.053203 -0.312423 -0.114278 -0.513343 0.647361 0.995635 0.940353 1.774880 2.100646 3.053639 3.650442 3.048750 3.637335 2.096110 -1.703077 -1.353619 -2.098089 -2.2098089 -3.268564 -3.590688 -2.240509 -5.323560 -5.452315 -5.490816 -6.405700 -7.407977 -6.318167 -6.638769 -7.203709 -6.950225 -8.055829 -8.491071 -8.344627 -7.738532 -7.913151 -6.891435

H	5.085279	4.568145	-9.422003	С	-4.109590	6.852407	3.876268
Н	6.707746	5.093580	-8.869847	Н	-4.794136	5.984009	3.873459
Н	6.556182	3.980469	-10.265961	Н	-4.745757	7.758197	3.831087
С	-1.308010	-4.125339	2.348475	С	-3.339264	6.859902	5.212677
C	-0.629459	-4.860893	3.336796	H	-2.669715	5.970441	5.270094
C	-1.164165	-6.026617	3.906038	H	-2.681720	7.752489	5.259151
C	-2.441108	-6.511161	3.533744	С	-3.706326	4.543236	7.704885
C	-3.112767	-5.774470	2.525916	С	-3.039137	3.553557	6.964585
C	-2.571379	-4.618731	1.960035	Н	-3.319221	3.365632	5.919358
C	-2.965006	-8.033253	5.433507	C	-2.039382	2.796455	7.591808
Н	-3.196584	-9.117174	5.517456	Н	-1.524447	2.007857	7.021160
H	-1.937300	-7.897898	5.813775	С	-1.692639	3.007147	8.943973
С	-3.946953	-7.230307	6.297431	С	-2.390025	4.006093	9.660097
H	-3.722349	-6.148391	6.188436	H	-2.151166	4.171379	10.722527
H	-3.819184	-7.476943	7.375697	C	-3.393472	4.770760	9.055823
C	-6.339265	-5.077503	4.962962	H	-3.960881	5.521323	9.625511
С	-5.686016	-3.869155	5.246371	С	-0.608592	2.200627	9.604403
H	-5.283426	-3.690480	6.252953	Н	-0.484755	1.204751	9.138950
С	-5.605926	-2.893720	4.246851	Н	-0.807323	2.051610	10.683668
Н	-5.139032	-1.926335	4.479701	Н	0.375749	2.709961	9.526477
C	-6.164817	-3.107556	2.966712	C	-2.414468	-0.378765	-4.088282
С	-6.813477	-4.336553	2.717904	С	-3.602490	-0.768714	-3.438366
H	-7.256104	-4.519172	1.726595	С	-4.841838	-0.670502	-4.066396
C	-6.911279	-5.322971	3.705851	С	-4.990528	-0.128831	-5.364647
H	-7.433893	-6.271707	3.518062	C	-3.792540	0.191222	-6.042537
C	-6.067827	-2.042134	1.909306	C	-2.543990	0.082519	-5.409348
H	-5.017174	-1.934293	1.568409	С	-6.648501	1.148696	-6.732924
H	-6.692319	-2.281507	1.027680	Н	-7.755658	1.127332	-6.795634
H	-6.380440	-1.055479	2.307485	H	-6.271157	0.989161	-7.764605
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N	-1.237113	-0.426854	1.555653	Н	-5.056258	2.574200	-6.376885
	7.587391	-3.424802		н Н			
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H	8.387363	-2.861953	-3.654267	С	-5.445104	3.319002	-2.370649
N	6.407212	-1.949273	-6.346216	С	-5.585004	1.967209	-2.026959
H	5.512811	-2.428465	-6.181451	H	-5.784952	1.220538	-2.802957
N	-3.025878	-7.669930	4.023055	C	-5.482162	1.592164	-0.683490
H	-3.977090	-7.779776	3.655631	H	-5.579103	0.527237	-0.421880
N	-5.311590	-7.456645	5.818246	C	-5.236001	2.545384	0.328738
H	-5.706513	-8.375078	6.065630	C	-5.117883	3.901656	-0.047536
S	6.445406	-0.511497	-5.453498	H	-4.939001	4.663824	0.727656
S	-6.503789	-6.305204	6.247917	С	-5.218402	4.297203	-1.388419
F	5.720023	-1.036490	-0.305482	Н	-5.123594	5.351577	-1.685758
F	7.827537	-1.890459	-1.752947	С	-5.079632	2.120522	1.764029
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F	4.845380	-4.127107	-4.737670	Н	-5.342162	2.930702	2.470722
F	0.575144	-4.453651	3.761375	H	-4.026192	1.840364	1.975324
F		-6.679732		n N		0.990159	
	-0.427996		4.832254		-0.220538		-1.358864
F	-3.292649	-3.964453	1.036608	N	0.943069	-1.341890	-2.556968
F	-4.327015	-6.213526	2.127688	N	-3.261267	6.851412	2.697268
0	5.165425	-0.480625	-4.702358	H	-3.009754	7.758954	2.305468
0	7.764591	-0.431748	-4.771736	N	-4.259922	6.933526	6.342895
0	-6.159036	-5.663425	7.539832	H	-3.985014	7.545192	7.117312
0	-7.778061	-7.041205	6.069530	N	-6.267701	0.035901	-5.872258
				H	-6.968117	-0.185584	-5.163111
Confor	mation 14.			N	-6.471365	2.833634	-4.879584
Multip	olicity: 2			H	-7.395702	3.261501	-4.736386
Charge				S	-5.003062	5.528638	6.945434
	-3c) = -9171.79657	1575876 Hartree		S	-5.311274	3.825911	-4.082451
	-xTB) = $-378.6327$			F	0.085318	5.417862	-0.359689
	2-xTB) = $-362.15138$			F	-1.477611	7.351787	0.734642
•	FF) = $-35.17525538$			F	-1.727801	2.269288	2.707928
	def2-TZVP) = -9172		x+x00	F	-3.330235	4.129917	3.723346
	- D3(BJ)/def2-TZV						-2.161538
					-3.567568	-1.178322	
	- D3(BJ)/def2-TZV		שטענים: Hartree	F	-5.971706	-0.982519	-3.380259
	1-3c) = -9158.80613			F	-1.456035	0.467877	-6.087475
	= -554.04840 Kcal			F	-3.843165	0.677326	-7.302255
	= -663.36746 Kca			0	-5.496156	4.789544	5.764484
E(ωB97	'X-V/def2-TZVP) = -	-9174.39610272123	35 Hartree	0	-5.888074	6.014397	8.019891
				0	-3.997116	3.377173	-4.607401
Coordi	.nates:			0	-5.694864	5.252305	-4.164755
Cu	1.349602	-0.201096	-0.923741	C	2.863466	-2.905148	-2.457838
С	-0.031197	2.646208	0.474123	C	3.405091	-2.438396	-1.242827
Č	-0.616008	2.132758	-0.695849	C	4.534684	-3.055178	-0.575913
Č	-1.782513	2.706783	-1.336634	Н	5.100626	-3.909725	-0.961174
Н	-2.291804	3.625305	-1.029798	С	4.720122	-2.374842	0.600079
C	-2.104383	1.883136	-2.382257	Н	5.481629	-2.545293	1.368744
Н	-2.896851	2.028060	-3.122918	C	3.712285	-1.335015	0.644076
C	-1.134887	0.804508	-2.371419	C	3.594762	-0.402796	1.692426
C							
	-1.166163	-0.271553	-3.278629	C	2.693965	0.682299	1.688410
C	-0.151995	-1.236458	-3.387540	C	2.615032	1.686713	2.730901
C	-0.084915	-2.234237	-4.435910	H	3.228810	1.718383	3.635570
H	-0.826255	-2.355680	-5.233246	C	1.626114	2.562370	2.362721
С	1.083052	-2.928236	-4.250259	H	1.280906	3.458645	2.889463
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С	-0.747803	3.771494	1.139089	С	4.789085	-3.908312	-3.757204
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С	-0.718496	0.030000					
	-0.718496 -1.539274	6.086082	1.205698	C	4.852786	-6.282517	-4.423012
С			1.205698 2.259119	C C	4.852786 3.610246	-6.282517 -6.423615	-4.423012 -3.766341
C C	-1.539274	6.086082					
C C	-1.539274 -2.457236	6.086082 5.825799	2.259119	С	3.610246	-6.423615	-3.766341

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			-6.880897			-1.384956	0.737937
C	4.207877	-8.403921		C	0.754227		
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C	1.208045	-5.888178	-11.458866	C	1.930601	2.276101	2.965632
С	0.420352	-5.941758	-10.287173	C	1.970098	2.460743	4.363237
H	-0.676906	-5.975968	-10.375457	C	3.083541	3.015518	4.996011
C	1.006121	-5.944541	-9.017171	C	4.242507	3.428415	4.283710
H	0.390869	-5.969622	-8.106228	C	4.193056	3.253630	2.878377
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H	6.930433	-0.367455	8.591828	H	8.940419	-0.451738	8.083030
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Н	0.777142	-1.292350	2.880935	C	5.396364	-6.338587	-1.607755
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				н С			
N	2.925691	-1.389519	-0.487293		6.599877	-6.648545	-2.495766
N	1.753653	0.939790	0.712889	H	7.477702	-6.868155	-1.850486
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H	2.487670	-7.585365	-5.939425	H	6.632818	-2.814415	-0.436920
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H	5.700757	-1.828409	7.280512	H	4.865715	-1.040917	-0.118676
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F	5.392992	-2.712561	-3.769176	H	5.710972	-2.956824	-4.667678
F	6.603477	-4.798392	-5.006337	C	3.204611	0.034218	-2.032267
F	1.771530	-5.552920	-2.597233	H	2.195020	-0.422383	-2.099190
F	2.935023	-7.607940	-3.806315	H	3.265204	0.794928	-2.836328
F	5.687552	1.361934	2.642946	H	3.275062	0.545733	-1.054464
F	6.860673	1.117705	5.024003	N	0.093325	-0.263856	0.840191
F	3.204926	-2.621329	3.406668	N	-2.021180	-1.345222	-0.768039
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Ö	2.777364	2.349113	8.801878	Н	9.180262	2.822775	2.984703
Ö	2.049294	0.122695	9.879173	N	4.266272	-5.957625	-2.448930
-				Н	4.593107	-5.626526	-3.365400
Confo	rmation 18.			N	6.852304	-5.549148	-3.436274
				Н	7.426065	-5.813805	-4.247228
	plicity 2						7.47/440
	plicity: 2			S	9 973262		5 056132
_	re: 0	2722034 Hartree		S	9.973262	3.317397	5.056132
E(B97	re: 0 '-3c) = -9171.79621			S	7.608879	-4.128833	-2.806738
E(B97 E(GFN	re: 0 7-3c) = -9171.79621 11-xTB) = -378.6289	62929520 Hartree		S F	7.608879 0.928373	-4.128833 2.084172	-2.806738 5.116866
E (B97 E (GFN E (GFN	re: 0 -3c) = -9171.79621 (1-xtb) = -378.6289 (2-xtb) = -362.1481	62929520 Hartree 74375241 Hartree		S F F	7.608879 0.928373 3.097217	-4.128833 2.084172 3.156112	-2.806738 5.116866 6.340716
E (B97 E (GFN E (GFN E (GFN	Te: 0 (-3c) = -9171.79621 (1-xTB) = -378.6289 (2-xTB) = -362.1481 (-FF) = -35.1582653	62929520 Hartree 74375241 Hartree 36237 Hartree	*******	S F F	7.608879 0.928373 3.097217 3.111518	-4.128833 2.084172 3.156112 2.553534	-2.806738 5.116866 6.340716 0.916949
E (B97 E (GFN E (GFN E (GFN	e: 0 -3c) = -9171.79621 11-xTB) = -378.6289 12-xTB) = -362.1481 1-FF) = -35.1582653 5/def2-TZVP) = -917	62929520 Hartree 74375241 Hartree 36237 Hartree 2.842458827785 Ha		S F F F	7.608879 0.928373 3.097217 3.111518 5.241433	-4.128833 2.084172 3.156112 2.553534 3.615271	-2.806738 5.116866 6.340716 0.916949 2.102069
E (B97 E (GFN E (GFN E (GFN E (M06 E (PBE	e: 0 -3c) = -9171.79621 11-xTB) = -378.6289 12-xTB) = -362.1481 1-FF) = -35.1582653 //def2-TZVP) = -917 5 - D3(BJ)/def2-TZV	62929520 Hartree 74375241 Hartree 36237 Hartree 2.842458827785 Ha P) = -9169.254649	370218 Hartree	S F F F	7.608879 0.928373 3.097217 3.111518 5.241433 1.379860	-4.128833 2.084172 3.156112 2.553534 3.615271 -4.420997	-2.806738 5.116866 6.340716 0.916949 2.102069 1.091617
E (B97 E (GFN E (GFN E (M06 E (PBE E (PBE	ne: 0 1-3c) = -9171.79621 11-xTB) = -378.6289 12-xTB) = -362.1481 1-FF) = -35.1582653 3/def2-TZVP) = -917 1 - D3(BJ)/def2-TZV 10 - D3(BJ)/def2-TZ	62929520 Hartree 74375241 Hartree 36237 Hartree 2.842458827785 Ha P) = -9169.254649 VP) = -9169.49238	370218 Hartree	S	7.608879 0.928373 3.097217 3.111518 5.241433 1.379860 3.274555	-4.128833 2.084172 3.156112 2.553534 3.615271 -4.420997 -6.108376	-2.806738 5.116866 6.340716 0.916949 2.102069 1.091617 0.239832
E (B97 E (GFN E (GFN E (M06 E (PBE E (PBE	Te: 0  -3c) = -9171.79621  (1-xTB) = -378.6289  (2-xTB) = -362.1481  (-FF) = -35.1582653  (/def2-TZVP) = -917  (0 - D3(BJ)/def2-TZV  (th-3c) = -9158.8085	62929520 Hartree 74375241 Hartree 36237 Hartree 2.842458827785 Ha P) = -9169.254649 VP) = -9169.49238 50530821 Hartree	370218 Hartree	S F F F F F F F	7.608879 0.928373 3.097217 3.111518 5.241433 1.379860 3.274555 1.135519	-4.128833 2.084172 3.156112 2.553534 3.615271 -4.420997 -6.108376 -2.461052	-2.806738 5.116866 6.340716 0.916949 2.102069 1.091617 0.239832 -3.237942
E (B97 E (GFN E (GFN E (M06 E (PBE E (PBE E (PBE	Te: 0  -3c) = -9171.79621  11-xTB) = -378.6289  12-xTB) = -362.1481  1-FF) = -35.1582653  12-472VP) = -917  13-472VP) = -917  14-30 = -9158.8085  15 = -558.81527 Kca	62929520 Hartree 74375241 Hartree 36237 Hartree 2.842458827785 Ha P) = -9169.254649 VP) = -9169.49238 50530821 Hartree 1/mol	370218 Hartree	S F F F F F F F F	7.608879 0.928373 3.097217 3.111518 5.241433 1.379860 3.274555 1.135519 3.008408	-4.128833 2.084172 3.156112 2.553534 3.615271 -4.420997 -6.108376 -2.461052 -4.204267	-2.806738 5.116866 6.340716 0.916949 2.102069 1.091617 0.239832 -3.237942 -4.115953
E (B97 E (GFN E (GFN E (M06 E (PBE E (PBE E (PM6 E (PM7	Te: 0  1-3c) = -9171.79621  11-xTB) = -378.6289  12-xTB) = -362.1481  1-FF) = -35.1582653  1/def2-TZVP) = -917  1- D3(BJ)/def2-TZV  10- D3(BJ)/def2-TZV  10- D3(BJ)/def2-TZV  10- D3(BJ)/def2-TZV  10- C558.81527 Kca  10) = -663.66912 Kca	62929520 Hartree 74375241 Hartree 36237 Hartree 2.842458827785 Ha P) = -9169.254649 VP) = -9169.49238 50530821 Hartree 1/mo1	370218 Hartree 5560572 Hartree	S	7.608879 0.928373 3.097217 3.111518 5.241433 1.379860 3.274555 1.135519 3.008408 9.371496	-4.128833 2.084172 3.156112 2.553534 3.615271 -4.420997 -6.108376 -2.461052 -4.204267 4.112554	-2.806738 5.116866 6.340716 0.916949 2.102069 1.091617 0.239832 -3.237942 -4.115953 6.147913
E (B97 E (GFN E (GFN E (M06 E (PBE E (PBE E (PM6 E (PM7	Te: 0  -3c) = -9171.79621  11-xTB) = -378.6289  12-xTB) = -362.1481  1-FF) = -35.1582653  12-472VP) = -917  13-472VP) = -917  14-30 = -9158.8085  15 = -558.81527 Kca	62929520 Hartree 74375241 Hartree 36237 Hartree 2.842458827785 Ha P) = -9169.254649 VP) = -9169.49238 50530821 Hartree 1/mo1	370218 Hartree 5560572 Hartree	S	7.608879 0.928373 3.097217 3.111518 5.241433 1.379860 3.274555 1.135519 3.008408 9.371496 11.224473	-4.128833 2.084172 3.156112 2.553534 3.615271 -4.420997 -6.108376 -2.461052 -4.204267 4.112554 3.687085	-2.806738 5.116866 6.340716 0.916949 2.102069 1.091617 0.239832 -3.237942 -4.115953 6.147913 4.372299
E (B97 E (GFN E (GFN E (M06 E (PBE E (PBE E (PM6 E (PM7 E (ωB9	Te: 0  -3c) = -9171.79621  11-xTB) = -378.6289  12-xTB) = -362.1481  1-FF) = -35.1582653  1/def2-TZVP) = -917  1 - D3(BJ)/def2-TZV  10 - D3(BJ)/def2-TZV  10 - D3(BJ)/def2-TZV  10 - D3(BJ)/def2-TZV  10 - 558.81527 Kca  10 = -663.66912 Kca  17X-V/def2-TZVP) =	62929520 Hartree 74375241 Hartree 36237 Hartree 2.842458827785 Ha P) = -9169.254649 VP) = -9169.49238 50530821 Hartree 1/mo1	370218 Hartree 5560572 Hartree	S F F F F F O O O	7.608879 0.928373 3.097217 3.111518 5.241433 1.379860 3.274555 1.135519 3.008408 9.371496 11.224473 8.189228	-4.128833 2.084172 3.156112 2.553534 3.615271 -4.420997 -6.108376 -2.461052 -4.204267 4.112554 3.687085 -4.436185	-2.806738 5.116866 6.340716 0.916949 2.102069 1.091617 0.239832 -3.237942 -4.115953 6.147913 4.372299 -1.478398
E (B97 E (GFN E (GFN E (M06 E (PBE E (PBE E (PM6 E (PM7 E (ωB9	Te: 0  -3c) = -9171.79621  11-xTB) = -378.6289  12-xTB) = -362.1481  1-FF) = -35.1582653  1/def2-TZVP) = -917  1- D3(BJ)/def2-TZV  10- D3(BJ)/def2-TZ  10- D3(BJ)/def2	62929520 Hartree 74375241 Hartree 36237 Hartree 2.842458827785 Ha P) = -9169.254649 VP) = -9169.49238 50530821 Hartree 1/mo1 1/mo1 -9174.39369489690	370218 Hartree 5560572 Hartree 8 Hartree	S	7.608879 0.928373 3.097217 3.111518 5.241433 1.379860 3.274555 1.135519 3.008408 9.371496 11.224473 8.189228 8.430712	-4.128833 2.084172 3.156112 2.553534 3.615271 -4.420997 -6.108376 -2.461052 -4.204267 4.112554 3.687085 -4.436185 -3.636051	-2.806738 5.116866 6.340716 0.916949 2.102069 1.091617 0.239832 -3.237942 -4.115953 6.147913 4.372299 -1.478398 -3.931205
E (B97 E (GFN E (GFN E (M06 E (PBE E (PBE E (PM7 E (\omega B9) Coord Cu	Te: 0  -3c) = -9171.79621  11-xTB) = -378.6289  12-xTB) = -362.1481  1-FF) = -35.1582653  12-xTB) = -9158.253  12-xTB) = -9178  13-xTB) = -9178  14-xTB) = -9178  15-xTB) = -9158.8085  15-xTB) = -663.66912  17-xTB) = -663.66912  17-xTB) = -663.66912  17-xTB) = -663.66912  18-xTB) = -1822881	62929520 Hartree 74375241 Hartree 36237 Hartree 2.842458827785 Ha P) = -9169.254649 VP) = -9169.49238 50530821 Hartree 1/mo1 1/mo1 -9174.39369489690	370218 Hartree 5560572 Hartree 8 Hartree 0.441420	S F F F F F F F F O O O C	7.608879 0.928373 3.097217 3.111518 5.241433 1.379860 3.274555 1.135519 3.008408 9.371496 11.224473 8.189228 8.430712 -4.399256	-4.128833 2.084172 3.156112 2.553534 3.615271 -4.420997 -6.108376 -2.461052 -4.204267 4.112554 3.687085 -4.436185 -3.636051 -1.080935	-2.806738 5.116866 6.340716 0.916949 2.102069 1.091617 0.239832 -3.237942 -4.115953 6.147913 4.372299 -1.478398 -3.931205 -1.425608
E (B97 E (GFN E (GFN E (M06 E (PBE E (PBE E (PM7 E (ωB9 Coord Cu	Te: 0  1-3c) = -9171.79621  11-xTB) = -378.6289  12-xTB) = -362.1481  1-FF) = -35.1582653  1/def2-TZVP) = -917  1- D3(BJ)/def2-TZV  10 - D3(BJ)/def2-TZV  10 - D3(BJ)/def2-TZV  10 - 9158.8085  10) = -558.81527 Kca  11/X-V/def2-TZVP) =  11inates:  -1.822881  0.771896	62929520 Hartree 74375241 Hartree 36237 Hartree 2.842458827785 Ha P) = -9169.254649 VP) = -9169.49238 50530821 Hartree 1/mol 1/mol -9174.39369489690  0.274865 1.653308	370218 Hartree 5560572 Hartree 8 Hartree 0.441420 2.269916	S F F F F F F F F O O O C C	7.608879 0.928373 3.097217 3.111518 5.241433 1.379860 3.274555 1.135519 3.008408 9.371496 11.224473 8.189228 8.430712 -4.399256 -4.660808	-4.128833 2.084172 3.156112 2.553534 3.615271 -4.420997 -6.108376 -2.461052 -4.204267 4.112554 3.687085 -4.436185 -3.636051 -1.080935 0.088551	-2.806738 5.116866 6.340716 0.916949 2.102069 1.091617 0.239832 -3.237942 -4.115953 6.147913 4.372299 -1.478398 -3.931205 -1.425608 -0.686988
E (B97 E (GFN E (GFN E (M06 E (PBE E (PBE E (PM7 E (\omega B9) Coord Cu C	Te: 0  -3c) = -9171.79621  11-xTB) = -378.6289  12-xTB) = -362.1481  1-FF) = -35.1582653  1/def2-TZVP) = -917  1 - D3(BJ)/def2-TZV  10 - S58.81527 Kca  10 = -663.66912 Kca  17X-V/def2-TZVP) =  1 inates:  -1.822881  0.771896  0.984842	62929520 Hartree 74375241 Hartree 36237 Hartree 2.842458827785 Ha P) = -9169.254649 VP) = -9169.49238 50530821 Hartree 1/mo1 1/mo1 -9174.39369489690  0.274865 1.653308 0.407329	370218 Hartree 5560572 Hartree 8 Hartree 0.441420 2.269916 1.650135	S	7.608879 0.928373 3.097217 3.111518 5.241433 1.379860 3.274555 1.135519 3.008408 9.371496 11.224473 8.189228 8.430712 -4.399256 -4.660808 -5.949573	-4.128833 2.084172 3.156112 2.553534 3.615271 -4.420997 -6.108376 -2.461052 -4.204267 4.112554 3.687085 -4.436185 -3.636051 -1.080935 0.088551 0.750505	-2.806738 5.116866 6.340716 0.916949 2.102069 1.091617 0.239832 -3.237942 -4.115953 6.147913 4.372299 -1.478398 -3.931205 -1.425608 -0.686988 -0.660896
E (B97 E (GFN E (GFN E (GFN E (PBE E (PBE E (PBE E (PM7 E (ωB9 Coord Cu C	The: 0  -3c) = -9171.79621  11-xTB) = -378.6289  12-xTB) = -362.1481  14-FF) = -35.1582653  14-662-TZVP) = -917  15 - D3(BJ)/def2-TZ  16 -3c) = -9158.8085  17 -663.66912 Kca  17 -71896  0.984842  2.225018	62929520 Hartree 74375241 Hartree 36237 Hartree 2.842458827785 Ha P) = -9169.254649 VP) = -9169.49238 50530821 Hartree 1/mo1 1/mo1 -9174.39369489690  0.274865 1.653308 0.407329 -0.334126	370218 Hartree 5560572 Hartree 8 Hartree 0.441420 2.269916 1.650135 1.746630	S	7.608879 0.928373 3.097217 3.111518 5.241433 1.379860 3.274555 1.135519 3.008408 9.371496 11.224473 8.189228 8.430712 -4.399256 -4.660808 -5.949573 -6.844048	-4.128833 2.084172 3.156112 2.553534 3.615271 -4.420997 -6.108376 -2.461052 -4.204267 4.112554 3.687085 -4.436185 -3.636051 -1.080935 0.088551 0.750505 0.406726	-2.806738 5.116866 6.340716 0.916949 2.102069 1.091617 0.239832 -3.237942 -4.115953 6.147913 4.372299 -1.478398 -3.931205 -1.425608 -0.686988 -0.686986 -1.190312
E (B97 E (GFN E (GFN E (M06 E (PBE E (PBE E (PM7 E (\omega B9) Coord Cu C	Te: 0  -3c) = -9171.79621  11-xTB) = -378.6289  12-xTB) = -362.1481  1-FF) = -35.1582653  1/def2-TZVP) = -917  1 - D3(BJ)/def2-TZV  10 - S58.81527 Kca  10 = -663.66912 Kca  17X-V/def2-TZVP) =  1 inates:  -1.822881  0.771896  0.984842	62929520 Hartree 74375241 Hartree 36237 Hartree 2.842458827785 Ha P) = -9169.254649 VP) = -9169.49238 50530821 Hartree 1/mo1 1/mo1 -9174.39369489690  0.274865 1.653308 0.407329	370218 Hartree 5560572 Hartree 8 Hartree 0.441420 2.269916 1.650135	S	7.608879 0.928373 3.097217 3.111518 5.241433 1.379860 3.274555 1.135519 3.008408 9.371496 11.224473 8.189228 8.430712 -4.399256 -4.660808 -5.949573	-4.128833 2.084172 3.156112 2.553534 3.615271 -4.420997 -6.108376 -2.461052 -4.204267 4.112554 3.687085 -4.436185 -3.636051 -1.080935 0.088551 0.750505	-2.806738 5.116866 6.340716 0.916949 2.102069 1.091617 0.239832 -3.237942 -4.115953 6.147913 4.372299 -1.478398 -3.931205 -1.425608 -0.686988 -0.660896

H C C	-6.570875 -4.429999 -3.879929 -2.549406	2.594177 1.878441 2.902293 2.907463	0.407385 0.581119 1.376229 1.843011	E(GFN-F E(M06/d	F) = -35.1592548 ef2-TZVP) = -917	72108256 Hartree 23016 Hartree 2.839297263821 Ha P) = -9169.257329	
C	-1.966116	3.986593	2.614028			VP) = -9169.49423	37510464 Hartr
H C	-2.483393 -0.661480	4.903427	2.911428 2.854719		3c) = -9158.8112 = -563.74922 Kca	05236058 Hartree	
H	0.098418	3.641680 4.213587	3.397520		= -563.74922 KCa = -664.41659 Kca	, -	
C	-0.450418	2.350125	2.235291			-9174.39370794487	70 Hartree
C	-5.503855	-1.649349	-2.248051				
C	-6.606157	-2.307264	-1.667539 -2.445889	Coordin		0 014547	0 616745
C C	-7.639323 -7.640961	-2.828233 -2.745256	-2.445889	Cu C	0.012696 2.282062	-0.014547 -2.498786	0.616745 1.419456
C	-6.538479	-2.071798	-4.435096	C	1.768209	-2.476909	0.110257
С	-5.495528	-1.566087	-3.649267	С	2.179953	-3.387531	-0.938670
С	-8.737327	-3.671761	-5.935469	H	2.952330	-4.156922	-0.838546
H	-9.798660	-3.792037	-6.239909	C	1.425686	-3.083984	-2.041820
H C	-8.331676 -7.992708	-2.839918 -4.979053	-6.540824 -6.276495	H C	1.457199 0.567543	-3.549778 -1.976466	-3.032155 -1.670317
Н	-8.109413	-5.186064	-7.363865	C	-0.343399	-1.360449	-2.551519
H	-8.460892	-5.826122	-5.735177	C	-1.088836	-0.208786	-2.231930
C	-5.401779	-7.240874	-4.939903	C	-2.043715	0.413895	-3.128298
C	-4.139012	-7.321598	-5.548396	H	-2.319912	0.032354	-4.116419
H C	-3.549718 -3.646303	-6.407530 -8.576635	-5.710735 -5.918724	C H	-2.524254 -3.266111	1.528406 2.247260	-2.493110 -2.859788
Н	-2.653720	-8.648321	-6.390609	C	-1.871716	1.573241	-1.198135
C	-4.391533	-9.755163	-5.688718	Ċ	3.349494	-3.478819	1.760378
С	-5.647697	-9.639081	-5.059535	C	4.657106	-3.046858	2.061065
H	-6.234607	-10.547653	-4.852678	C	5.659606	-3.938842	2.444257
C	-6.159456	-8.390158	-4.680003	C	5.439450	-5.340442	2.511412
H	-7.128242	-8.296516	-4.168993	C	4.122566	-5.771471	2.213270
C H	-3.859007 -4.039869	-11.096598 -11.260569	-6.120956 -7.205170	C C	3.117747 6.312743	-4.865036 -7.332471	1.845162 3.723754
Н	-2.765031	-11.171767	-5.961603	Н	7.329679	-7.732933	3.900264
I	-4.348399	-11.926992	-5.576414	H	5.721840	-8.128573	3.230194
	-4.725387	4.089529	1.675022	C	5.662089	-6.982607	5.083688
C	-5.071397	4.469322	2.985491	H	4.563558	-6.875260	4.970718
2	-5.807346	5.630465	3.263684	H	5.838122	-7.805030	5.805911
	-6.241182 -5.910107	6.494462 6.094791	2.230104 0.911273	C C	7.918627 8.012792	-4.182260	6.984154
	-5.178452	4.938686	0.911273	Н	8.023805	-4.344300 -5.357017	8.374155 8.802008
Š	-6.783160	8.539734	3.546463	C	8.109728	-3.203570	9.177254
I	-7.583693	9.307987	3.503053	Н	8.194652	-3.318282	10.269251
H	-6.923672	7.987048	4.493070	С	8.104392	-1.905191	8.617766
2	-5.406828	9.220063	3.552874	C	8.004488	-1.782447	7.214697
H	-4.619452	8.439555	3.618693	H	8.002581	-0.779355	6.760328
H C	-5.293270 -2.994055	9.861220 8.862174	4.456251 1.153220	C H	7.922472 7.873160	-2.911677	6.388233 5.293289
	-1.926060	8.187154	1.757843	C	8.193482	-2.814802 -0.695073	9.506386
H	-1.496452	8.584719	2.688622	Н	8.247310	0.245721	8.927218
С	-1.431196	7.022596	1.152545	Н	9.081108	-0.749686	10.169948
H	-0.594912	6.480648	1.618764	H	7.297429	-0.623065	10.155304
C	-1.991630	6.522551	-0.040642	C	-0.530886	-1.962556	-3.899091
C H	-3.059951	7.238623	-0.629936	C C	-0.178133	-1.288167	-5.083134
п С	-3.517355 -3.559109	6.859781 8.407862	-1.556101 -0.049594	C	-0.380512 -0.967170	-1.841715 -3.119794	-6.355928 -6.520643
Ŧ	-4.390706	8.959324	-0.509741	C	-1.311795	-3.798733	-5.320942
	-1.484379	5.253123	-0.672160	Č	-1.102416	-3.243003	-4.058996
ł	-2.300237	4.506235	-0.752013	C	-1.187802	-3.168846	-9.042359
ł	-1.114778	5.439538	-1.701812	H	-1.343228	-3.989380	-9.767550
I.	-0.665789	4.800225	-0.082253	H	-0.202356	-2.713012	-9.262669
Į T	-3.753733	0.783471	0.084885 1.619597	С	-2.301060	-2.125617	-9.277513
I	-1.609380 -8.715060	1.923069 -3.296131	-4.535426	H H	-3.251306 -2.051830	-2.498751 -1.182392	-8.830040 -8.752892
ł	-9.263365	-3.903704	-3.921974	C	-5.174490	-2.271099	-11.087061
1	-6.577230	-4.973588	-5.936779	C	-5.827827	-1.216536	-11.743364
	-6.053199	-4.114291	-6.144155	H	-5.350973	-0.743201	-12.614008
1	-6.985803	7.647480	2.410521	C	-7.091221	-0.813660	-11.293283
I T	-7.061229	8.163998	1.529570	H	-7.619615	-0.006090	-11.823560
I I	-5.208044 -5.755017	9.946320 10.815177	2.299824 2.215771	C C	-7.709973 -7.038423	-1.435765 -2.509628	-10.186645 -9.564572
! ;	-6.041864	-5.633011	-4.473567	Н	-7.038423 -7.517071	-3.031200	-9.564572 -8.720945
3	-3.596524	10.379132	1.895238	C	-5.781704	-2.938842	-10.010798
?	-6.677576	-2.435960	-0.335645	H	-5.280533	-3.804449	-9.554425
7	-8.663914	-3.479556	-1.857573	C	-9.041956	-0.957356	-9.670106
?	-4.464713	-0.983311	-4.277174	H	-8.900323	-0.255114	-8.819798
7	-6.399144	-1.994974	-5.789342	H	-9.661589	-1.796022	-9.295431
?	-4.698860 -6.099069	3.704694 5.907567	4.021492 4.552902	H N	-9.616030 0.796643	-0.419803 -1.617493	-10.449747 -0.360000
?	-4.864175	4.669039	-0.635399	N N	-1.010405	0.505271	-1.055098
?	-6.286843	6.901426	-0.106144	N	6.481892	-6.178726	2.846065
)	-4.888891	-4.795822	-4.071943	Н	7.340306	-5.662170	3.086975
)	-7.208756	-5.870292	-3.590893	N	6.131238	-5.729540	5.691361
)	-2.803952	10.625422	3.121778	H	5.846257	-4.902426	5.146623
)	-3.758753	11.416037	0.856219	N	-1.202080	-3.755043	-7.716538 -7.615977
on for	mation 20.			H N	-1.715921 -2.457463	-4.630284 -1.827707	-7.615977 -10.697527
	licity: 2			H	-2.446461	-0.846623	-10.989558
narge				S	7.823339	-5.632534	5.949579
		12544761 Hartree		S	-3.525263	-2.748384	-11.626504
		762794353 Hartree					

-	C 00CE33	3 460204	0 762674	Б	1 422004	4 670640	3 030105
F	6.886533	-3.468284	2.763674	F	-1.422094	4.670649	-2.028105
F	1.897454	-5.351218	1.580837	F	-3.041031	6.641870	-2.771888
F	3.817363	-7.084785	2.272662	F	-0.861762	0.084386	6.191880
F	0.381318	-0.071718	-5.015626	F	-0.471687	1.006548	8.662711
F	-0.017762	-1.110657	-7.437424	F	1.775242	3.609205	4.400101
F	-1.473891	-3.948548	-2.982443	F	2.200119	4.545199	6.907216
F	-1.887377	-5.016974	-5.438608	0	-4.529434	3.635058	-4.036859
0	8.539222	-5.313965	4.680141	0	-6.935851	4.397977	-3.410470
Ō	8.179824	-6.850248	6.705775	Ō	4.933995	-0.053413	9.999988
0	-3.350168	-2.278025	-13.011615	0	6.228049	2.175834	9.913537
0	-3.317741	-4.149764	-11.202989				
C	-2.124713	2.565429	-0.233624	Confo	rmation 21.		
C	-1.583951	2.560049	1.065443		plicity: 2		
C		3.573731	2.060332	Charg			
	-1.870478						
H	-2.501018	4.453306	1.893824	, -	-3c) = -9171.80208		
C	-1.215000	3.199325	3.204458	E (GFN	1-xTB) = $-378.6426$	72725431 Hartree	
Н	-1.206689	3.703213	4.176405	E (GFN	2-xTB) = $-362.1714$ :	21278556 Hartree	
С	-0.516527	1.966278	2.900082		-FF) = $-35.1675607$		
C							
	0.263275	1.254329	3.829187		/def2-TZVP) = -917		
С	0.950313	0.060824	3.532875		- D3(BJ)/def2-TZV		
С	1.756298	-0.667415	4.491385	E(PBE	0 - D3(BJ)/def2-TZ	VP) = -9169.498018	3702177 Hartree
H	1.889804	-0.397374	5.543319	E (PBE	h-3c) = -9158.8118	38795891 Hartree	
С	2.321190	-1.716804	3.813766	E(PM6	) = -560.49513 Kca	1/mo1	
Н	2.984013	-2.495549	4.205727		) = -670.89896  Kca		
C			2.441756		7X-V/def2-TZVP) =		1 11
	1.867292	-1.622773		E (MBA	/x-v/delz-lzvP) =	-91/4.40012/5/0/5	a hartree
С	-3.043711	3.676829	-0.608264				
C	-4.365523	3.746269	-0.125185	Coord	inates:		
C	-5.228661	4.774032	-0.504407	Cu	-0.021773	-1.880249	0.667461
C	-4.840382	5.803983	-1.402080	C	-2.905758	-0.100785	-0.052799
C							
	-3.505151	5.740606	-1.858921	С	-1.730496	0.624439	0.214424
C	-2.651645	4.690250	-1.496544	С	-1.634641	2.067697	0.118363
C	-5.727780	7.692533	-2.823025	H	-2.431541	2.731861	-0.234845
H	-6.430879	8.526104	-2.610797	С	-0.357018	2.394856	0.491035
Н	-4.717990	8.140783	-2.873004	Н	0.101414	3.387730	0.532285
С	-6.103181	7.095997	-4.196300	С	0.327326	1.153320	0.796415
H	-6.049199	7.901058	-4.963273	C	1.672923	1.082764	1.209727
Н	-7.153965	6.741622	-4.175640	C	2.378677	-0.117465	1.389259
С	-6.366334	3.838549	-5.928705	C	3.752339	-0.186804	1.844541
С	-5.432086	3.455654	-6.904731	H	4.365904	0.680312	2.111969
H	-4.359073	3.463587	-6.665567	C	4.092656	-1.513748	1.884945
C	-5.893643	3.051931	-8.160637	H	5.041616	-1.959475	2.204424
H	-5.168883	2.744699	-8.931268	С	2.920879	-2.250928	1.447043
C	-7.274821	3.022626	-8.459413	C	-4.121276	0.668288	-0.436527
С	-8.186438	3.391750	-7.450118	C	-4.622206	0.645012	-1.748048
H	-9.267182	3.355902	-7.659175	C	-5.721257	1.411665	-2.151736
C	-7.742942	3.798251	-6.183127	С	-6.388927	2.278443	-1.255946
H	-8.449960	4.069182	-5.386444	С	-5.891726	2.283517	0.073565
C	-7.745726	2.619717	-9.831947	Ċ	-4.788496	1.523769	0.463345
H	-7.571107	3.438453	-10.562633	С	-7.824209	3.558652	-2.872869
H	-7.191952	1.733377	-10.201056	H	-8.884329	3.889622	-2.852832
H	-8.827969	2.386112	-9.844713	H	-7.774379	2.711799	-3.580066
С	0.425581	1.815761	5.198741	С	-6.968975	4.735365	-3.394658
C	-0.117134	1.188949	6.334045	Н	-7.268643	4.967285	-4.440553
C	0.096465	1.672205	7.633161	H	-7.178054	5.640971	-2.791304
С	0.885717	2.822288	7.871196	C	-3.696435	6.431302	-2.554881
C	1.413130	3.459657	6.720470	C	-4.292715	7.701280	-2.548303
С	1.191317	2.974689	5.431451	H	-5.333215	7.822422	-2.214609
C	1.282165	2.556868	10.318705	С	-3.526369	8.807858	-2.934372
Н	1.405266	3.256966	11.171475	Н	-3.982189	9.810382	-2.919568
H	0.347557	1.996124	10.503684	С	-2.172791	8.669052	-3.308533
C	2.453240	1.565512	10.279017	C	-1.602616	7.377469	-3.297928
H	2.315369	0.874694	9.421187	H	-0.536011	7.261073	-3.543131
H	2.451155	0.933087	11.195294	С	-2.354789	6.257793	-2.927979
C	4.833829	1.373039	7.768032	Н	-1.904414	5.255863	-2.887089
C	4.926059	0.167733	7.700032	C	-1.335820	9.858708	-3.695179
H	5.071309	-0.775147	7.604050	H	-1.782754	10.808348	-3.341752
С	4.824172	0.199170	5.658674	H	-1.239378	9.928230	-4.800018
H	4.893441	-0.737489	5.085427	H	-0.308307	9.759676	-3.291088
С	4.612423	1.409357	4.965379	С	2.353967	2.387599	1.437363
C	4.540806	2.606179	5.714851	C	1.945717	3.233215	2.483760
Н	4.365685	3.559515	5.194195	C	2.386344	4.558834	2.584452
C	4.661513	2.600021	7.106849	C	3.226344	5.126344	1.597976
H	4.590309	3.532335	7.683547	C	3.707713	4.249022	0.596572
С	4.420336	1.435805	3.473613	С	3.278334	2.920613	0.516274
Н	3.368636	1.697692	3.231819	C	2.526283	7.429905	1.966773
Н	5.059702	2.207556	2.999261	Н	2.576844	7.624734	3.057831
H	4.638270	0.456681	3.010574	H	1.510693	7.015940	1.781892
N	-0.751422	1.596830	1.592590	С	2.647110	8.772972	1.258204
N	1.015458	-0.549203	2.297302	H	1.800212	9.404668	1.615574
N	-5.782148	6.766467	-1.710134	Н	3.588484	9.278627	1.562604
Н	-6.723435	6.460924	-1.452350	C	0.055542	7.668551	-0.351129
N	-5.272446	5.975987	-4.614113	С	-0.686751	8.845741	-0.182635
H	-4.263095	6.059273	-4.438146	H	-0.272659	9.817284	-0.491609
N	1.144996	3.368957	9.116488	С	-1.974839	8.757351	0.360622
H	1.847460	4.109398	9.051167	H	-2.570202	9.674096	0.491538
N	3.716483	2.275319	10.079425	C	-2.537412	7.515183	0.726189
Н	4.051877	2.802219	10.897903	C	-1.761938	6.347932	0.541828
S	-5.771586	4.385895	-4.327425	H	-2.184535	5.365350	0.803450
S	5.054323	1.354630	9.544276	C	-0.472470	6.417417	0.007600
F	-4.816622	2.807240	0.717096	Н	0.134144	5.516148	-0.159518
F	-6.500672	4.788184	-0.053310	C	-3.933212	7.418529	1.276798
-				-	0.100212		

H	-3.932232	6.938040	2.277049	Н	-1.717396	-2.999323	-4.464020
H	-4.569169	6.788299	0.619842	H	-2.581171	-2.257283	-3.074130
H	-4.406525	8.414274	1.372463	N	0.479694	-3.846118	0.699162
N	-0.522266	0.086436	0.607064	N	-1.934509	-2.374476	0.185718
N	1.886622	-1.385160	1.160247	N	7.645380	-6.629192	2.605759
N	-7.469561	3.090491	-1.546562	H	7.575242	-6.927001	3.581826
H	-7.632920	3.771205	-0.799806	N	9.096521	-3.942048	2.537772
N	-5.530405	4.515643	-3.348615	H	8.699203	-3.774188	1.604777
H	-5.170729	3.632408	-3.728872	N	-4.712793	-9.416826	-1.715835
N	3.554959	6.474198	1.558671	Н	-4.402883	-9.630261	-2.667627
H	3.961546	6.711943	0.646987	N	-6.604085	-8.320485	-3.682032
N	2.694577	8.679409	-0.203986	H	-6.993334	-9.099187	-4.232545
H	2.802415	9.576824	-0.688340	S	8.066106	-3.300122	3.717939
S	-4.628730	5.007463	-2.006917	S	-7.039712	-6.899906	-4.543300
S	1.659485	7.711484	-1.149979	F	3.210898	-5.304855	3.654616
F	-4.028342	-0.121745	-2.682775	F	5.491070	-6.657383	4.208789
F	-6.050588	1.386274	-3.472159	F	5.218588	-3.606281	-0.300683
F	-4.360780	1.623861	1.728831	F	7.462051	-4.921526	0.222129
F	-6.486552	3.107517	0.961172	F	-3.847803	-6.019028	1.610583
F	1.079498	2.784196	3.403516	F	-5.299670	-8.101159	0.794094
F	1.962217	5.304235	3.629051	F	-1.101462	-6.355280	-2.256947
F	3.704704	2.169015	-0.508032	F	-2.574196	-8.460068	-3.101719
F	4.533006	4.748965	-0.341409	0	7.007579	-2.591757	2.964613
0	-3.654877	3.926792	-1.729694	0	7.771987	-4.346456	4.726265
0	-5.596076	5.484946	-0.981806	0	-8.235385	-6.269128	-3.936902
Ō	1.559352	8.466871	-2.423373	Ō	-7.030693	-7.329862	-5.956757
				O	-7.030093	-7.329002	-3.930737
0	2.177990	6.329647	-1.133478				
C	2.872901	-3.653706	1.341886	Confor	mation 29.		
C	1.721474	-4.377894	0.975676	Multip	licity: 2		
С	1.685005	-5.821259	0.848419	Charge			
Н	2.539109	-6.488072	1.005770		(3c) = -9171.80910	1614103 !!	
С	0.401837	-6.155482	0.502328	E(GFN1	-xTB) = $-378.6488$	97551350 Hartree	
H	-0.015797	-7.153636	0.333881	E (GFN2	-xTB) = $-362.1727$	70499308 Hartree	
С	-0.341625	-4.915310	0.407124	E (GFN-	FF) = -35.1849730	18727 Hartree	
C					def2-TZVP) = -917		x+x00
	-1.708910	-4.844921	0.082698		,		
C	-2.445787	-3.644199	0.016242	E(PBE	<ul> <li>D3(BJ)/def2-TZV:</li> </ul>	P) = -9169.266976	840323 Hartree
C	-3.859876	-3.573246	-0.294029	E(PBEC	- D3(BJ)/def2-TZ	JP) = -9169.50443	7265598 Hartree
H	-4.511884	-4.427393	-0.497541		(-3c) = -9158.8205		
C	-4.197664	-2.245029	-0.298160		= -565.65965 Kca		
H	-5.180312	-1.797434	-0.480916		= -678.72587 Kca		
C	-2.984404	-1.505194	-0.027243	E(ωB97	X-V/def2-TZVP) = -	-9174.40728909216	7 Hartree
С	4.114964	-4.419269	1.640493				
C	4.235699	-5.217811	2.795870	Coordi	nates:		
						0 611071	1 600040
C	5.401400	-5.930217	3.075657	Cu	-0.702032	-0.611871	-1.622842
C	6.541665	-5.886314	2.230939	C	1.465364	2.077746	-1.448617
C	6.406743	-5.095205	1.068518	C	0.747292	1.730773	-0.287205
С	5.239298	-4.369172	0.800947	С	0.897217	2.399331	0.990755
			2.132120				
C	9.001075	-6.430510		H	1.573897	3.234501	1.196557
H	9.582230	-7.348434	2.363492	C	0.057473	1.768776	1.872089
H	8.990194	-6.338094	1.030232	H	-0.101198	2.010070	2.929371
С	9.745057	-5.228144	2.750379	С	-0.599122	0.708586	1.128935
Н	10.777116	-5.192355	2.335201	Č	-1.566260	-0.152058	1.684147
H	9.843398	-5.373064	3.845387	С	-2.282641	-1.112133	0.952132
C			4.531039	C	-3.384049	-1.886592	1.488020
	9.066700	-2.055166	4.001000				0 510665
С	9.066700			H	-3.763129	-1.807712	2.51266/
	9.274438	-0.822508	3.890196		-3.763129 -3.847180	-1.807712 -2.678724	2.512667
H	9.274438 8.814038	-0.822508 -0.629643	3.890196 2.910401	С	-3.847180	-2.678724	0.469336
H C	9.274438 8.814038 10.053526	-0.822508 -0.629643 0.147301	3.890196 2.910401 4.526948	C H	-3.847180 -4.694657	-2.678724 -3.373968	0.469336 0.483605
H C H	9.274438 8.814038 10.053526 10.216653	-0.822508 -0.629643 0.147301 1.117708	3.890196 2.910401 4.526948 4.032030	C H C	-3.847180 -4.694657 -2.992027	-2.678724 -3.373968 -2.416532	0.469336 0.483605 -0.675000
H C	9.274438 8.814038 10.053526	-0.822508 -0.629643 0.147301	3.890196 2.910401 4.526948	C H	-3.847180 -4.694657	-2.678724 -3.373968	0.469336 0.483605
H C H C	9.274438 8.814038 10.053526 10.216653	-0.822508 -0.629643 0.147301 1.117708 -0.088692	3.890196 2.910401 4.526948 4.032030 5.798211	C H C C	-3.847180 -4.694657 -2.992027	-2.678724 -3.373968 -2.416532 3.221540	0.469336 0.483605 -0.675000 -1.332598
H C H C	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270	C H C C	-3.847180 -4.694657 -2.992027 2.409886 3.805248	-2.678724 -3.373968 -2.416532 3.221540 3.039227	0.469336 0.483605 -0.675000 -1.332598 -1.281597
H C H C C	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192	С Н С С С	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246
H C H C C H C	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770	С Н С С С С С	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452
H C H C C H C	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469	С н с с с с с с	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806
H C H C C H C	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770	С Н С С С С С	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452
H C H C C H C	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469	С н с с с с с с	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806
H C H C C H C H C	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345	C H C C C C C C C C C	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724
H C H C C H C H C H	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356	С Н С С С С С С С С С С С С С С С С С С	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297
Н С Н С Н С Н С Н Н Н Н Н	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393	С Н С С С С С С С С С С Н Н Н	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542
Н С Н С С Н С Н Н С Н С Н С Н С С Н С С	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393		-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333
Н С Н С Н С Н С Н Н Н Н Н	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393	С Н С С С С С С С С С С Н Н Н	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542
Н С Н С С Н С Н Н С Н С С Н С С С С Н С С С С С С С С С С С С С С С С С С С С	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393 0.288257 0.452425		-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.6554452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967
Н С Н С Н С Н С Н Н С С С С С С С С С С	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937 -4.272195	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393 -0.288257 0.452425 0.018230	С Н С С С С С С С С Н Н С Н Н	-3.847180 -4.694657 -2.99207 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718
Н С Н С С Н С Н С Н С Н С С С Н С С С С	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937 -4.272195 -3.994783	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323 -8.347147	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393 -0.288257 0.452425 0.018230 -1.204980	СНССССССННСННС	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813 5.107196	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254 4.152973	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718 3.302217
Н С С Н С Н С Н С Н С С Н С С С Н С С С С С С С С С С С С С С С С С С С С	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937 -4.2722195 -3.994783 -2.869306	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323 -8.347147 -7.869400	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393 -0.288257 0.452425 0.018230 -1.204980 -1.920641		-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813 5.107196 4.423413	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254 4.152973 3.874592	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718 3.302217 4.495751
Н С Н С С Н С Н Н Н Н Н С С С С С С С С	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937 -4.272195 -3.994783	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323 -8.347147	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393 -0.288257 0.452425 0.018230 -1.204980	СНССССССННСННС	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813 5.107196	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254 4.152973	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718 3.302217
Н С Н С С Н С Н Н Н Н Н С С С С С С С С	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937 -4.272195 -3.994783 -2.869306 -2.111686	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323 -8.347147 -7.869400 -6.784202	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539345 7.484393 -0.288257 0.452425 0.018230 -1.204980 -1.920641 -1.480113	СНСССССССННСННССН	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813 5.107196 4.423413 4.480670	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254 4.152973 3.874592 4.574176	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718 3.302217 4.495751 5.339668
H C H C C H C C C C C C C C C	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937 -4.272195 -3.994783 -2.869306 -2.111686 -6.162764	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323 -8.347147 -7.869400 -6.784202 -9.506538	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393 -0.288257 0.452425 0.018230 -1.204980 -1.920641 -1.480113 -1.576282	СНССССССННСННССНС	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813 5.107196 4.423413 4.480670 3.685572	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254 4.152973 3.874592 4.574176 2.689649	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718 3.302217 4.495751 5.339668 4.590379
Н С Н С С Н С Н С Н С С С С С С С С С С	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937 -4.272195 -3.994783 -2.869306 -2.111686 -6.162764 -6.470202	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323 -8.347147 -7.869400 -6.784202 -9.506538 -10.479853	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393 -0.288257 0.452425 0.018230 -1.204980 -1.920641 -1.480113 -1.576282 -2.013238	СНССССССННСННССНС	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813 5.107196 4.423413 4.480670 3.685572 3.144847	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254 4.152973 3.874592 4.574176 2.689649 2.456647	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718 3.302217 4.495751 5.339668 4.590379 5.520208
Н С Н С С Н С Н С Н С С С С С С С С С С	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937 -4.272195 -3.994783 -2.869306 -2.111686 -6.162764 -6.470202 -6.437936	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323 -8.347147 -7.869400 -6.784202 -9.506538 -10.479853 -9.538209	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393 -0.288257 0.452425 0.018230 -1.204980 -1.920641 -1.480113 -1.576282 -2.013238 -0.506046	СНССССССННСННССНСНС	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813 5.107196 4.423413 4.480670 3.685572 3.144847 3.616174	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254 4.152973 3.874592 4.574176 2.689649 2.456647 1.778826	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718 3.302217 4.495751 5.339668 4.590379 5.520208 3.513154
Н С Н С С Н С Н С Н С С С С С С С С С С	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937 -4.272195 -3.994783 -2.869306 -2.111686 -6.162764 -6.470202	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323 -8.347147 -7.869400 -6.784202 -9.506538 -10.479853	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393 -0.288257 0.452425 0.018230 -1.204980 -1.920641 -1.480113 -1.576282 -2.013238	СНССССССННСННССНС	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813 5.107196 4.423413 4.480670 3.685572 3.144847	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254 4.152973 3.874592 4.574176 2.689649 2.456647	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718 3.302217 4.495751 5.339668 4.590379 5.520208
Н С Н С С Н С Н С Н С С Н С С С С С С С	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937 -4.272195 -3.994783 -2.869306 -2.111686 -6.162764 -6.470202 -6.437936	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323 -8.347147 -7.869400 -6.784202 -9.506538 -10.479853 -9.538209	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393 -0.288257 0.452425 0.018230 -1.204980 -1.920641 -1.480113 -1.576282 -2.013238 -0.506046	СНССССССННСННССНСНС	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813 5.107196 4.423413 4.480670 3.685572 3.144847 3.616174	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254 4.152973 3.874592 4.574176 2.689649 2.456647 1.778826	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718 3.302217 4.495751 5.339668 4.590379 5.520208 3.513154
Н С Н С С Н С Н С Н С С С С С С С С С С	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.7771870 -2.420414 -3.505937 -4.272195 -3.994783 -2.869306 -2.111686 -6.162764 -6.470202 -6.437936 -6.929855 -6.616765	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323 -8.347147 -7.869400 -6.784202 -9.506538 -10.479853 -9.538209 -8.364096 -7.397225	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393 -0.288257 0.452425 0.018230 -1.920491 -1.480113 -1.576282 -2.013238 -0.506046 -2.257685 -1.810056	СНСССССССННСННССНСНССН	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813 5.107196 4.423413 4.480670 3.685572 3.144847 3.616174 4.315053 4.272546	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254 4.152973 3.874592 4.574176 2.689649 2.456647 1.778826 2.090353 1.400154	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718 3.302217 4.495751 5.339668 4.590379 5.520208 3.513154 2.325833 1.468641
Н С Н С С Н С Н Н Н Н С С С С С С С С С	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937 -4.272195 -3.994783 -2.869306 -2.111686 -6.162764 -6.470202 -6.437936 -6.929855 -6.616765 -8.021501	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323 -8.347147 -7.869400 -6.784202 -9.506538 -10.479853 -9.538209 -8.364096 -7.397225 -8.464178	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393 -0.288257 0.452425 0.018230 -1.204980 -1.204980 -1.576282 -2.013238 -0.506046 -2.257685 -1.810056 -2.060590	СНССССССННСННССНСНССНС	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813 5.107196 4.423413 4.480670 3.685572 3.144847 3.616174 4.315053 4.272546 5.072369	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254 4.152973 3.874592 4.574176 2.689649 2.456647 1.778826 2.090353 1.400154 3.263940	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718 3.302217 4.495751 5.339668 4.590379 5.520208 3.513154 2.325833 1.468641 2.217187
Н С Н С С Н С Н Н Н С С С С С С Н Н С Н Н С Н Н С С С С С С С С С С Н Н С С Н Н С С	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937 -4.272195 -3.994783 -2.869306 -2.111686 -6.162764 -6.470202 -6.437936 -6.929855 -6.616765 -8.021501 -5.637759	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323 -8.347147 -7.869400 -6.784202 -9.506538 -10.479853 -9.538209 -8.364096 -7.397225 -8.464178 -5.833221	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393 -0.288257 0.452425 0.018230 -1.204980 -1.920641 -1.480113 -1.576282 -2.013238 -0.506046 -2.257685 -1.810056 -2.060590 -4.218019	СНСССССССННСННССНССНСК	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813 5.107196 4.423413 4.480670 3.685572 3.144847 3.616174 4.315053 4.272546 5.072369 5.648941	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254 4.152973 3.874592 4.574176 2.689649 2.456647 1.778826 2.090353 1.400154 3.263940 3.486766	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718 3.302217 4.495751 5.339668 4.590379 5.520208 3.513154 2.325833 1.468641 2.217187 1.311184
Н С Н С С Н С Н Н Н Н С С С С С С Н Н С Н Н С С	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937 -4.272195 -3.994783 -2.869306 -2.111686 -6.162764 -6.470202 -6.437936 -6.929855 -6.616765 -8.021501 -5.637759 -5.867906	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323 -8.347147 -7.869400 -6.784202 -9.506538 -10.479853 -9.508538 -10.479853 -9.538209 -8.364096 -7.397225 -8.464178 -5.833221 -4.535996	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393 -0.288257 0.452425 0.018230 -1.204980 -1.920641 -1.480113 -1.576282 -2.013238 -0.506046 -2.257685 -1.810056 -2.060590 -4.218019 -3.739435	СНССССССИННСННССНСНССНС	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813 5.107196 4.423413 4.480670 3.685572 3.144847 3.616174 4.315053 4.272546 5.072369 5.648941 2.842029	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254 4.152973 3.874592 4.574176 2.689649 2.456647 1.778826 2.090353 1.400154 3.263940 3.486766 0.497779	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718 3.302217 4.495751 5.339668 4.590379 5.520208 3.513154 2.325833 1.468641 2.217187 1.311184 3.645756
Н С Н С С Н С Н Н Н С С С С С С Н Н С Н Н С Н Н С С С С С С С С С С Н Н С С Н Н С С	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937 -4.272195 -3.994783 -2.869306 -2.111686 -6.162764 -6.470202 -6.437936 -6.929855 -6.616765 -8.021501 -5.637759	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323 -8.347147 -7.869400 -6.784202 -9.506538 -10.479853 -9.538209 -8.364096 -7.397225 -8.464178 -5.833221	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393 -0.288257 0.452425 0.018230 -1.204980 -1.920641 -1.480113 -1.576282 -2.013238 -0.506046 -2.257685 -1.810056 -2.060590 -4.218019	СНСССССССННСННССНССНСК	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813 5.107196 4.423413 4.480670 3.685572 3.144847 3.616174 4.315053 4.272546 5.072369 5.648941	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254 4.152973 3.874592 4.574176 2.689649 2.456647 1.778826 2.090353 1.400154 3.263940 3.486766	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718 3.302217 4.495751 5.339668 4.590379 5.520208 3.513154 2.325833 1.468641 2.217187 1.311184
Н С Н С С Н С Н Н Н Н С С С С С С Н Н С Н Н С С Н	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937 -4.272195 -3.994783 -2.869306 -2.111686 -6.162764 -6.470202 -6.437936 -6.929855 -6.616765 -8.021501 -5.637759 -5.867906 -6.897789	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323 -8.347147 -7.869400 -6.784202 -9.506538 -10.479853 -9.538209 -8.364096 -7.397225 -8.464178 -5.833221 -4.535996 -4.217762	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393 -0.288257 0.452425 0.018230 -1.204980 -1.920641 -1.480113 -1.576282 -2.013238 -0.506046 -2.257685 -1.810056 -2.060590 -4.218019 -3.739435 -3.522775	СНССССССННСННССНСНССНСНС	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813 5.107196 4.423413 4.480670 3.685572 3.144847 3.616174 4.315053 4.272546 5.072369 5.648941 2.842029 2.166775	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254 4.152973 3.874592 4.574176 2.689649 2.456647 1.778826 2.090353 1.400154 3.263940 3.486766 0.497779 0.513503	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718 3.302217 4.495751 5.339668 4.590379 5.520208 3.513154 2.325833 1.468641 2.217187 1.311184 3.645756 4.521497
Н С Н С С Н С Н Н Н С С С С С С Н Н С С Н С С С С С С С С С С С С С С С С С С С С	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937 -4.272195 -3.994783 -2.869306 -2.111686 -6.162764 -6.470202 -6.4377936 -6.929855 -6.616765 -8.021501 -5.637759 -5.867906 -6.897789 -4.773366	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323 -8.347147 -7.869400 -6.784202 -9.506538 -10.479853 -9.538209 -8.364096 -7.397225 -8.464178 -5.833221 -4.535996 -4.217762 -3.681805	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393 -0.288257 0.452425 0.018230 -1.204980 -1.920641 -1.480113 -1.576282 -2.013238 -0.506046 -2.257685 -1.810056 -2.060590 -4.218019 -3.739435 -3.522775 -3.540349	СНССССССННСННССНСНССНСНСН	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813 5.107196 4.423413 4.480670 3.685572 3.144847 3.616174 4.315053 4.272546 5.072369 5.648941 2.842029 2.166775 3.532136	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254 4.152973 3.874592 4.574176 2.689649 2.456647 1.778826 2.090353 1.400154 3.263940 3.486766 0.497779 0.513503 -0.363384	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718 3.302217 4.495751 5.339668 4.590379 5.520208 3.51154 2.325833 1.468641 2.217187 1.311184 3.645756 4.521497 3.774695
Н С Н С С Н С Н Н Н С С С С С С С Н Н С С Н С Н С Н	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937 -4.272195 -3.994783 -2.869306 -2.111686 -6.162764 -6.470202 -6.437936 -6.929855 -6.616765 -8.021501 -5.637759 -5.867906 -6.897789 -4.773366 -4.773366 -4.773366	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323 -8.347147 -7.869400 -6.784202 -9.506538 -10.479853 -9.538209 -8.364096 -7.397225 -8.464178 -5.833221 -4.535996 -4.217762 -3.681805 -2.661054	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393 -0.288257 0.452425 0.018230 -1.204980 -1.920641 -1.480113 -1.576282 -2.013238 -0.506046 -2.257685 -1.810056 -2.060590 -4.218019 -3.739435 -3.522775 -3.540349 -3.163694	СНСОСОССИННОННССНСНСОНСНСН	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813 5.107196 4.423413 4.480670 3.685572 3.144847 3.616174 4.315053 4.272546 5.072369 5.648941 2.842029 2.166775 3.532136 2.234144	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254 4.152973 3.874592 4.574176 2.689649 2.456647 1.778826 2.090353 1.400154 3.263940 3.486766 0.497779 0.513503 -0.363384 0.294431	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718 3.302217 4.495751 5.339668 4.590379 5.520208 3.513154 2.325833 1.468641 2.217187 1.311184 3.645756 4.521497 3.774695 2.743487
н с н с с н с н н н н с с с с с с н н с н н с н с н с н с н с н с н с н с н с н с н с	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937 -4.272195 -3.994783 -2.869306 -2.111686 -6.162764 -6.470202 -6.437936 -6.929855 -6.616765 -8.021501 -5.637759 -5.867906 -6.897789 -4.773366 -4.935037 -3.455430	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323 -8.347147 -7.869400 -6.784202 -9.506538 -10.479853 -9.538209 -8.364096 -7.397225 -8.464178 -5.833221 -4.535996 -4.217762 -3.681805 -2.661054 -4.111381	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393 -0.288257 0.452425 0.018230 -1.204980 -1.920641 -1.480113 -1.576282 -2.013238 -0.506046 -2.257685 -1.810056 -2.060590 -4.218019 -3.739435 -3.522775 -3.540349 -3.163694 -3.799037	СНССССССННСННССНСНССНСНСН	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813 5.107196 4.423413 4.480670 3.685572 3.144847 3.616174 4.315053 4.272546 5.072369 5.648941 2.842029 2.166775 3.532136 2.234144 -1.799134	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254 4.152973 3.874592 4.574176 2.689649 2.456647 1.778826 2.090353 1.400154 3.263940 3.486766 0.497779 0.513503 -0.363384 0.294431 0.004714	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718 3.302217 4.495751 5.339668 4.590379 5.520208 3.513154 2.325833 1.468641 2.217187 1.311184 3.645756 4.521497 3.774695 2.743487 3.147830
Н С Н С С Н С Н Н Н С С С С С С С Н Н С С Н С Н С Н	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937 -4.272195 -3.994783 -2.869306 -2.111686 -6.162764 -6.470202 -6.437936 -6.929855 -6.616765 -8.021501 -5.637759 -5.867906 -6.897789 -4.773366 -4.773366 -4.773366	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323 -8.347147 -7.869400 -6.784202 -9.506538 -10.479853 -9.538209 -8.364096 -7.397225 -8.464178 -5.833221 -4.535996 -4.217762 -3.681805 -2.661054	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393 -0.288257 0.452425 0.018230 -1.204980 -1.920641 -1.480113 -1.576282 -2.013238 -0.506046 -2.257685 -1.810056 -2.060590 -4.218019 -3.739435 -3.522775 -3.540349 -3.163694	СНСОСОССИННОННССНСНСОНСНСН	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813 5.107196 4.423413 4.480670 3.685572 3.144847 3.616174 4.315053 4.272546 5.072369 5.648941 2.842029 2.166775 3.532136 2.234144	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254 4.152973 3.874592 4.574176 2.689649 2.456647 1.778826 2.090353 1.400154 3.263940 3.486766 0.497779 0.513503 -0.363384 0.294431	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718 3.302217 4.495751 5.339668 4.590379 5.520208 3.513154 2.325833 1.468641 2.217187 1.311184 3.645756 4.521497 3.774695 2.743487
н с н с с н с н н н н с с с с с с н н с н н с н с н с н с н с н с н с н с н с н с н с	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937 -4.272195 -3.994783 -2.869306 -2.111686 -6.162764 -6.470202 -6.437936 -6.929855 -6.616765 -8.021501 -5.637759 -5.867906 -6.897789 -4.773366 -4.935037 -3.455430	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323 -8.347147 -7.869400 -6.784202 -9.506538 -10.479853 -9.538209 -8.364096 -7.397225 -8.464178 -5.833221 -4.535996 -4.217762 -3.681805 -2.661054 -4.111381	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393 -0.288257 0.452425 0.018230 -1.204980 -1.920641 -1.480113 -1.576282 -2.013238 -0.506046 -2.257685 -1.810056 -2.060590 -4.218019 -3.739435 -3.522775 -3.540349 -3.163694 -3.799037	СНССССССИНСННССНСНССНСНСН	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813 5.107196 4.423413 4.480670 3.685572 3.144847 3.616174 4.315053 4.272546 5.072369 5.648941 2.842029 2.166775 3.532136 2.234144 -1.799134	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254 4.152973 3.874592 4.574176 2.689649 2.456647 1.778826 2.090353 1.400154 3.263940 3.486766 0.497779 0.513503 -0.363384 0.294431 0.004714	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718 3.302217 4.495751 5.339668 4.590379 5.520208 3.513154 2.325833 1.468641 2.217187 1.311184 3.645756 4.521497 3.774695 2.743487 3.147830
Н С Н С С Н С Н Н Н Н С С С С С С Н Н С Н Н С С Н С С Н	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937 -4.272195 -3.994783 -2.869306 -2.111686 -6.162764 -6.470202 -6.437936 -6.929855 -6.616765 -8.021501 -5.637759 -5.867906 -6.897789 -4.773366 -4.935037 -3.455430 -3.262707 -2.241225	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323 -8.347147 -7.869400 -6.784202 -9.506538 -10.479853 -9.538209 -8.364096 -7.397225 -8.464178 -5.833221 -4.535996 -4.217762 -3.681805 -2.661054 -4.111381 -5.419929 -5.777366	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393 -0.288257 0.452425 0.018230 -1.204980 -1.920641 -1.480113 -1.576282 -2.013238 -0.506046 -2.257685 -1.810056 -2.060590 -4.218019 -3.739435 -3.522775 -3.540349 -3.163694 -3.799037 -4.299669 -4.496906	СНССССССИНКИНССНСНССНСНСНСН	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813 5.107196 4.423413 4.480670 3.685572 3.144847 3.616174 4.315053 4.272546 5.072369 5.648941 2.842029 2.166775 3.532136 2.234144 -1.799134 -2.850285 -2.910386	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254 4.152973 3.874592 4.574176 2.689649 2.456647 1.778826 2.090353 1.400154 3.263940 3.486766 0.497779 0.513503 -0.363384 0.294431 0.004714 0.767620 1.113864	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718 3.302217 4.495751 5.339668 4.590379 5.520208 3.513154 2.325833 1.468641 2.217187 1.311184 3.645756 4.521497 3.774695 2.743487 3.147830 3.677978 5.036472
Н С Н С С Н С Н Н Н С С С С С С Н Н С Н Н С С Н С С Н С С С С С С Н Н С С Н С С Н С С Н С	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937 -4.272195 -3.994783 -2.869306 -2.111686 -6.162764 -6.470202 -6.437936 -6.929855 -6.616765 -8.021501 -5.637759 -5.867906 -6.897789 -4.773366 -4.935037 -3.455430 -3.262707 -2.241225 -4.341757	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323 -8.347147 -7.869400 -6.784202 -9.506538 -10.479853 -9.538209 -8.364096 -7.397225 -8.464178 -5.833221 -4.535996 -4.217762 -3.681805 -2.661054 -4.111381 -5.419929 -5.777366 -6.279730	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 6.539356 7.484393 -0.288257 0.452425 0.018230 -1.204980 -1.920641 -1.480113 -1.576282 -2.013238 -0.506046 -2.257685 -1.810056 -2.060590 -4.218019 -3.739435 -3.522775 -3.540349 -3.799037 -4.299669 -4.496906 -4.496906 -4.496906	СНСОСОСОННОННСОНСНСОНСНСНННСОСО	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813 5.107196 4.423413 4.480670 3.685572 3.144847 3.616174 4.315053 4.272546 5.072369 5.648941 2.842029 2.166775 3.532136 2.234144 -1.799134 -2.850285 -2.910386 -1.885576	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254 4.152973 3.874592 4.574176 2.689649 2.456647 1.778826 2.090353 1.400154 3.263940 3.486766 0.497779 0.513503 -0.363384 0.294431 0.004714 0.767620 1.113864 0.743630	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718 3.302217 4.495751 5.339668 4.590379 5.520208 3.513154 2.325833 1.468641 2.217187 1.311184 3.645756 4.5521497 3.774695 2.743487 3.147830 3.677978 5.036472 5.937456
н с н с с н с н н н с с с с с с с н с н	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937 -4.272195 -3.994783 -2.869306 -2.111686 -6.162764 -6.470202 -6.437936 -6.929855 -6.616765 -8.021501 -5.637759 -5.867906 -6.897789 -4.773366 -4.935037 -3.455430 -3.262707 -2.241225 -4.341757 -4.182789	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323 -8.347147 -7.869400 -6.784202 -9.506538 -10.479853 -9.538209 -8.364096 -7.397225 -8.464178 -5.833221 -4.535996 -4.217762 -3.681805 -2.661054 -4.111381 -5.419929 -5.777366 -6.279730 -7.300889	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393 -0.288257 0.452425 0.018230 -1.204980 -1.920641 -1.480113 -1.576282 -2.013238 -0.506046 -2.257685 -1.810056 -2.060590 -4.218019 -3.739435 -3.522775 -3.540349 -3.163694 -3.799037 -4.299669 -4.496906 -4.521758 -4.894210	СНССССССННСННССНСНССНСНСН	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813 5.107196 4.423413 4.480670 3.685572 3.144847 3.616174 4.315053 4.272546 5.072369 5.648941 2.842029 2.166775 3.532136 2.234144 -1.799134 -2.850285 -2.910386 -1.885576 -0.865263	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254 4.152973 3.874592 4.574176 2.689649 2.456647 1.778826 2.090353 1.400154 3.263940 3.486766 0.497779 0.513503 -0.363384 0.294431 0.004714 0.767620 1.113864 0.743630 -0.087330	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718 3.302217 4.495751 5.339668 4.590379 5.520208 3.513154 2.325833 1.468641 2.217187 1.311184 3.645756 4.521497 3.774695 2.743487 3.147830 3.677978 5.036472 5.937456 5.408750
Н С Н С С Н С Н Н Н Н С С С С С С Н Н С С Н С Н С С Н С С С С С С С С Н Н С С Н С Н С С Н С С Н С	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937 -4.272195 -3.994783 -2.869306 -2.111686 -6.162764 -6.470202 -6.437936 -6.929855 -6.616765 -8.021501 -5.637759 -5.867906 -6.897789 -4.773366 -4.935037 -3.455430 -3.262707 -2.241225 -4.341757 -4.182789 -2.274463	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323 -8.347147 -7.869400 -6.784202 -9.506538 -10.479853 -9.508538 -10.479853 -9.508538 -10.479853 -9.508538 -10.479853 -9.508538 -10.479853 -9.508538 -10.479853 -9.508538 -10.479853 -9.508538 -10.479853 -9.508538 -10.479853 -9.508538 -10.479853 -9.508538 -10.479853 -9.508538 -10.479853 -9.508538 -10.479853 -9.508538 -10.479853 -9.508538 -10.479853 -9.508538 -10.479853 -9.508538 -10.479853 -9.508538 -10.479853 -9.508538 -10.479853 -9.508538 -10.479853 -9.508538 -10.479853 -9.508538 -10.479853 -9.508538 -10.479853 -9.508538 -10.479853 -9.50889 -3.217361	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393 -0.288257 0.452425 0.018230 -1.204980 -1.920641 -1.480113 -1.576282 -2.013238 -0.506046 -2.257685 -1.810056 -2.060590 -4.218019 -3.739435 -3.522775 -3.540349 -3.739435 -3.522775 -3.540349 -3.799037 -4.299669 -4.496906 -4.521758 -4.894210 -3.528899	СНССССССИННСННССНСНССНСННННССССС	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813 5.107196 4.423413 4.480670 3.685572 3.144847 3.616174 4.315053 4.272546 5.072369 5.648941 2.842029 2.166775 3.532136 2.234144 -1.799134 -2.850285 -2.910386 -1.885576 -0.865263 -0.823733	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254 4.152973 3.874592 4.574176 2.689649 2.456647 1.778826 2.090353 1.400154 3.263940 3.486766 0.497779 0.513503 -0.363384 0.294431 0.004714 0.767620 1.113864 0.743630 -0.087330 -0.439037	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718 3.302217 4.495751 5.339668 4.590379 5.520208 3.513154 2.325833 1.468641 2.217187 1.311184 3.645756 4.521497 3.774695 2.743487 3.147830 3.677978 5.036472 5.937456 5.408750 4.061401
н с н с с н с н н н с с с с с с с н с н	9.274438 8.814038 10.053526 10.216653 10.625665 10.385658 10.809919 9.607013 9.398619 11.465362 12.386688 10.914996 11.771870 -2.420414 -3.505937 -4.272195 -3.994783 -2.869306 -2.111686 -6.162764 -6.470202 -6.437936 -6.929855 -6.616765 -8.021501 -5.637759 -5.867906 -6.897789 -4.773366 -4.935037 -3.455430 -3.262707 -2.241225 -4.341757 -4.182789	-0.822508 -0.629643 0.147301 1.117708 -0.088692 -1.330782 -1.527851 -2.317717 -3.279610 0.970177 1.174738 1.930574 0.669790 -6.098975 -6.600964 -7.692323 -8.347147 -7.869400 -6.784202 -9.506538 -10.479853 -9.538209 -8.364096 -7.397225 -8.464178 -5.833221 -4.535996 -4.217762 -3.681805 -2.661054 -4.111381 -5.419929 -5.777366 -6.279730 -7.300889	3.890196 2.910401 4.526948 4.032030 5.798211 6.418270 7.415192 5.795770 6.285469 6.464351 5.879345 6.539356 7.484393 -0.288257 0.452425 0.018230 -1.204980 -1.920641 -1.480113 -1.576282 -2.013238 -0.506046 -2.257685 -1.810056 -2.060590 -4.218019 -3.739435 -3.522775 -3.540349 -3.163694 -3.799037 -4.299669 -4.496906 -4.521758 -4.894210	СНССССССННСННССНСНССНСНСН	-3.847180 -4.694657 -2.992027 2.409886 3.805248 4.676680 4.213969 2.816241 1.951211 4.729697 4.039487 5.645394 4.054669 3.321682 3.457813 5.107196 4.423413 4.480670 3.685572 3.144847 3.616174 4.315053 4.272546 5.072369 5.648941 2.842029 2.166775 3.532136 2.234144 -1.799134 -2.850285 -2.910386 -1.885576 -0.865263	-2.678724 -3.373968 -2.416532 3.221540 3.039227 4.089146 5.388114 5.587567 4.529394 7.453422 8.112195 8.042142 7.058816 7.843665 6.132254 4.152973 3.874592 4.574176 2.689649 2.456647 1.778826 2.090353 1.400154 3.263940 3.486766 0.497779 0.513503 -0.363384 0.294431 0.004714 0.767620 1.113864 0.743630 -0.087330	0.469336 0.483605 -0.675000 -1.332598 -1.281597 -0.991246 -0.654452 -0.784806 -1.092884 0.614724 0.055297 0.822542 1.953333 2.234967 1.811718 3.302217 4.495751 5.339668 4.590379 5.520208 3.513154 2.325833 1.468641 2.217187 1.311184 3.645756 4.521497 3.774695 2.743487 3.147830 3.677978 5.036472 5.937456 5.408750

H	-2.319969	2.194396	8.950466	Н	3.258934	-1.355375	-10.896838
H	-3.610700	2.074283	7.733790	C	5.068798	-1.154683	-9.722951
C	-2.153547	3.614464	7.308289	H	4.587737	-0.553236	-8.923072
	-2.324876						
H		3.651401	6.214312	H	5.503897	-0.427587	-10.445703
H	-2.823251	4.376175	7.761914	C	6.125336	-1.388159	-6.443976
С	1.646018	4.744257	6.582220	С	5.912901	-0.226630	-5.689409
C	2.669548	4.748064	7.542056	H	6.304978	0.732547	-6.056924
Н	2.740137	3.928694	8.271885	С	5.199716	-0.320563	-4.485258
				Н			-3.881212
C	3.611006	5.784547	7.519733		5.024406	0.581888	
H	4.428412	5.786634	8.257326	C	4.688778	-1.554583	-4.033395
C	3.556021	6.805104	6.545235	С	4.931895	-2.708017	-4.814854
C	2.506560	6.772117	5.601349	H	4.527065	-3.677213	-4.487621
H	2.453206	7.553542	4.828814	C	5.654704	-2.637520	-6.008993
C	1.550054	5.750438	5.610018	H	5.829620	-3.535316	-6.617532
H	0.747723	5.708198	4.859645	C	3.886591	-1.650035	-2.762489
С	4.641815	7.843225	6.472154	H	2.892232	-2.097466	-2.964169
H	4.323124	8.730977	5.892156	H	4.390577	-2.304775	-2.021123
H	5.534831	7.405590	5.974444	H	3.729861	-0.657293	-2.301302
Н							
	4.956532	8.178808	7.480179	N	-1.202669	-1.954571	-3.051442
N	-0.165492	0.703773	-0.179375	N	0.638096	0.238443	-2.893247
N	-2.066118	-1.441579	-0.368576	N	-7.146875	-7.134692	-2.547975
N	5.122574	6.337831	-0.237754	H	-7.936280	-6.699374	-3.031115
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H	5.366351	7.720813	3.470857	N	3.330703	-2.954526	-9.519884
N	-1.799105	1.108714	7.268354	H	3.934955	-3.737420	-9.256565
							-9.093388
H	-0.855638	0.956521	7.638742	N	6.071507	-2.011569	
N	-0.776032	4.042026	7.549636	H	6.697870	-2.492830	-9.754373
H	-0.473537	3.974813	8.530949	S	-7.859257	-5.224471	0.360898
S	6.091294	5.641614	3.183716	S	7.110848	-1.283313	-7.937082
S	0.461162	3.404423	6.564403	F	-5.339619	-2.875969	-3.604679
F	4.332681	1.809850	-1.450129	F	-7.238983	-4.793576	-3.858437
F	6.002456	3.843784	-0.885089	F	-3.050569	-5.606240	-0.463530
F	0.637106	4.788008	-1.126439	F	-4.900629	-7.495888	-0.694566
F	2.268840	6.801053	-0.541393	F	0.334151	0.112851	-7.287551
F	-3.814997	1.226821	2.868110	F	1.690647	-0.568331	-9.479721
F	-3.942181	1.891292	5.447151	F	1.971218	-3.733351	-5.021102
F	0.209965	-1.175965	3.623377	F	3.361515	-4.429616	-7.235818
F	0.129211	-0.476786	6.234002	0	-6.557270	-4.592824	0.670666
0	6.792494	5.907777	4.459399	0	-8.614532	-4.940581	-0.882664
0	6.873560	5.572725	1.920049	0	7.307484	0.151995	-8.246337
0	1.108908	2.242253	7.235249	0	8.252403	-2.217070	-7.853423
0	-0.114043	3.273660	5.206317				
				~ .			
С	-3.070076	-3.116849	-1.893540	CONTO.	rmation 6.		
С	-2.195972	-2.907350	-2.978998	Multi	olicity: 2		
С	-2.195972		-2.978998		plicity: 2		
C C	-2.195972 -2.204100	-3.709811	-2.978998 -4.186232	Charge	plicity: 2 e: 0	000406 #	
C C H	-2.195972	-3.709811 -4.538224	-2.978998 -4.186232 -4.384654	Charge E(B97	plicity: 2 e: 0 -3c) = -9171.783331		
C C	-2.195972 -2.204100	-3.709811	-2.978998 -4.186232	Charge E(B97	plicity: 2 e: 0		
C C H C	-2.195972 -2.204100 -2.891995 -1.197019	-3.709811 -4.538224 -3.233461	-2.978998 -4.186232 -4.384654 -4.984993	Charge E(B97- E(GFN	plicity: 2 e: 0 -3c) = -9171.783331 1-xTB) = -378.61969	7312255 Hartree	
C C H C H	-2.195972 -2.204100 -2.891995 -1.197019 -0.901727	-3.709811 -4.538224 -3.233461 -3.578069	-2.978998 -4.186232 -4.384654 -4.984993 -5.981678	Charge E(B97 E(GFN E(GFN	plicity: 2 e: 0 -3c) = -9171.783331 1-xTB) = -378.61969 2-xTB) = -362.13968	97312255 Hartree 81941343 Hartree	
C C H C H	-2.195972 -2.204100 -2.891995 -1.197019	-3.709811 -4.538224 -3.233461	-2.978998 -4.186232 -4.384654 -4.984993 -5.981678 -4.269398	Charge E(B97- E(GFN) E(GFN) E(GFN)	plicity: 2 e: 0 -3c) = -9171.783331 1-xTB) = -378.61969 2-xTB) = -362.13968 -FF) = -35.15684514	97312255 Hartree 31941343 Hartree 31281 Hartree	
C C H C H	-2.195972 -2.204100 -2.891995 -1.197019 -0.901727 -0.581800	-3.709811 -4.538224 -3.233461 -3.578069 -2.133863	-2.978998 -4.186232 -4.384654 -4.984993 -5.981678	Charge E(B97- E(GFN) E(GFN) E(GFN)	plicity: 2 e: 0 -3c) = -9171.783331 1-xTB) = -378.61969 2-xTB) = -362.13968	97312255 Hartree 31941343 Hartree 31281 Hartree	artree
C C H C H C	-2.195972 -2.204100 -2.891995 -1.197019 -0.901727 -0.581800 0.462057	-3.709811 -4.538224 -3.233461 -3.578069 -2.133863 -1.347405	-2.978998 -4.186232 -4.384654 -4.984993 -5.981678 -4.269398 -4.792004	Charge E (B97 E (GFN) E (GFN) E (GFN) E (M06)	plicity: 2 e: 0 -3c) = -9171.783331 1-xTB) = -378.61969 2-xTB) = -362.13968 -FF) = -35.15684514 /def2-TZVP) = -9172	97312255 Hartree 81941343 Hartree 81281 Hartree 2.826593199343 Ha	
C H C H C C	-2.195972 -2.204100 -2.891995 -1.197019 -0.901727 -0.581800 0.462057 0.983590	-3.709811 -4.538224 -3.233461 -3.578069 -2.133863 -1.347405 -0.204082	-2.978998 -4.186232 -4.384654 -4.984993 -5.981678 -4.269398 -4.792004 -4.152868	Charge E (B97: E (GFN: E (GFN: E (M06: E (PBE	plicity: 2 e: 0 -3c) = -9171.783331 1-xTB) = -378.61969 2-xTB) = -362.13968 -FF) = -35.15684514 /def2-TZVP) = -9172 - D3(BJ)/def2-TZVF	07312255 Hartree 81941343 Hartree 81281 Hartree 8.826593199343 Ha P) = -9169.240990	)988814 Hartree
C C H C H C	-2.195972 -2.204100 -2.891995 -1.197019 -0.901727 -0.581800 0.462057	-3.709811 -4.538224 -3.233461 -3.578069 -2.133863 -1.347405	-2.978998 -4.186232 -4.384654 -4.984993 -5.981678 -4.269398 -4.792004	Charge E (B97: E (GFN: E (GFN: E (M06: E (PBE	plicity: 2 e: 0 -3c) = -9171.783331 1-xTB) = -378.61969 2-xTB) = -362.13968 -FF) = -35.15684514 /def2-TZVP) = -9172	07312255 Hartree 81941343 Hartree 81281 Hartree 8.826593199343 Ha P) = -9169.240990	)988814 Hartree
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ССНСНССССНССССССССННСННССНСНСНСНСННССССС	-2.195972 -2.204100 -2.891995 -1.197019 -0.901727 -0.551800 0.462057 0.983590 1.978628 2.446366 2.211167 2.888646 1.399495 -4.109683 -5.210560 -6.180101 -6.130613 -5.014326 -4.052568 -7.507753 -8.138815 -6.593760 -8.285858 -8.541472 -9.245144 -8.963196 -8.436967 -7.358082 -9.302174 -8.896280 -10.685557 -11.176942 -12.248321 -10.325754 -10.699371 -11.606483 -11.821486 -11.152975 -12.576153 1.099953 1.064958 1.780728 2.588566 2.586875	-3.709811 -4.538224 -3.233461 -3.578069 -2.133863 -1.347405 -0.204082 0.676116 0.550888 1.668482 2.524653 1.363910 -4.173154 -4.009003 -5.000047 -6.224129 -6.388189 -5.382316 -8.226607 -8.936488 -8.780455 -7.819563 -8.738555 -7.342814 -4.882630 -4.816132 -4.953361 -4.554695 -4.495124 -4.353244 -4.409561 -4.235248 -4.670841 -4.694128 -4.694128 -4.698162 -5.041610 -3.399754 -3.676751 -1.777597 -1.010566 -1.369597 -2.530880 -3.320558	-2.978998 -4.186232 -4.384654 -4.984993 -5.981678 -4.269398 -4.792004 -4.152868 -4.733009 -5.713524 -3.816577 -3.903108 -2.657808 -2.036523 -2.901565 -3.048389 -2.330961 -1.481635 -1.325256 -1.665233 -2.240946 -1.381025 -0.396542 0.177149 -0.683532 1.731271 3.031488 3.193198 4.097907 5.120012 3.888678 2.568990 2.383519 1.485661 0.452115 5.053479 5.599696 5.785029 4.725779 -6.066267 -7.244318 -8.395821 -8.429918	Charge E (B97): E (GFN): E (GFN): E (GFN): E (M06): E (PBE): E (PBE): E (PBB): Coord: CC CC CC HC CC CC HC CC CC HC CC CC HC CC C	plicity: 2 e: 0 -3c) = -9171.783331 1-xTB) = -378.61965 2-xTB) = -362.13968 -FF) = -35.15684514 /def2-TZVP) = -9172 - D3 (BJ) /def2-TZVP 0 - D3 (BJ) /def2-TZVP 0 - D3 (BJ) /def2-TZVP 0 - 559.99684 Kcal 7X-V/def2-TZVP) = - inates:	27312255 Hartree 281941343 Hartree 281941343 Hartree 281281 Hartree 2819240990 2819240990 2819240990 2819240990 2819240990 2819240990 2819240990 2819240990 2819240990 2819240900 2819240900 281924000000000000000000000000000000000000	0.488472 -2.680941 Hartree 0.488472 -2.680991 -2.095309 -2.708029 -3.667206 -1.850522 -1.964159 -0.712644 0.387906 1.520151 2.610081 2.659464 3.515737 4.453685 2.975990 -4.025262 -5.180579 -6.453810 -6.660633 -5.489551 -4.223325 -9.142993 -9.150737 -9.290403 -10.343141 -11.247303 -10.199470 -10.805023 -10.426258
ССНСНССССНСНСССССССННСННССНСНСНСНСНННСССС	-2.195972 -2.204100 -2.891995 -1.197019 -0.901727 -0.581800 0.462057 0.983590 1.978628 2.446366 2.211167 2.888646 1.399495 -4.109683 -5.210560 -6.180101 -6.130613 -5.014326 -4.052568 -7.507753 -8.138815 -6.593760 -8.285858 -8.541472 -9.245144 -8.963196 -8.46967 -7.358082 -9.302174 -8.896280 -10.685557 -11.176942 -12.248321 -10.325754 -10.699371 -11.606483 -11.821486 -11.152975 -12.576153 1.099953 1.064958 1.780728 2.588566 2.586875 1.869310	-3.709811 -4.538224 -3.233461 -3.578069 -2.133863 -1.347405 -0.204082 0.676116 0.550888 1.668482 2.524653 1.363910 -4.173154 -4.009003 -5.000047 -6.224129 -6.388189 -5.382316 -8.226607 -8.936488 -8.780455 -7.819563 -8.738555 -7.342814 -4.882630 -4.816132 -4.953361 -4.554695 -4.495124 -4.353244 -4.409561 -4.235248 -4.670841 -4.694128 -4.098162 -5.041610 -3.399754 -3.676751 -1.777597 -1.010566 -1.369597 -2.530880 -3.320558 -2.957729	-2.978998 -4.186232 -4.384654 -4.984993 -5.981678 -4.269398 -4.792004 -4.152868 -4.733009 -5.713524 -3.816577 -3.903108 -2.657808 -2.036523 -2.901565 -3.048389 -2.330961 -1.481635 -1.325256 -1.665233 -2.240946 -1.381025 -0.396542 0.177149 -0.683532 1.731271 3.031488 3.193198 4.097907 5.120012 3.888678 2.568990 2.383519 1.485661 0.452115 5.053479 5.599696 5.785029 4.725779 -6.066267 -7.244318 -8.395821 -8.429918 -7.253417 -6.114331	Charge E (B97: E (GFN: E (GFN: E (GFN: E (GFN: E (M06: E (PBE: E (PBE: E (PM6: E (PM7: E (ωB9) C (C (	plicity: 2 e: 0 -3c) = -9171.783331 1-xTB) = -378.61965 2-xTB) = -362.13968 -FF) = -35.15684514 /def2-TZVP) = -9172 - D3(BJ)/def2-TZVP 0 - D3(BJ)/def2-TZVP 0 - D3(BJ)/def2-TZVP 0 - 559.99684 Kcal 1) = -654.20383 Kcal 7X-V/def2-TZVP) = - inates:  1.158085 -0.204117 0.377656 0.378358 -0.087215 1.045146 1.24099 1.445355 2.163357 2.509285 3.325816 3.766982 3.451480 4.019244 2.702932 -0.830376 -0.075286 -0.654099 -2.041426 -2.798920 -2.215452 -2.105797 -1.038130 -2.135980 -2.775604 -2.162450 -2.803920 -6.802136 -7.736042 -7.601908	27312255 Hartree 21941343 Hartree 21281 Hartree 21826593199343 Ha 2) = -9169.240990 2P) = -9169.47740 355561842 Hartree 2.6000000000000000000000000000000000000	0988814 Hartree 01680941 Hartree 54 Hartree  0.488472 -2.680991 -2.095309 -2.708029 -3.667206 -1.850522 -1.964159 -0.712644 0.387906 1.520151 2.610081 2.659464 3.515737 4.453685 2.975990 -4.025262 -5.180579 -6.453810 -6.660633 -5.489551 -4.223325 -9.142993 -9.150737 -9.290403 -10.343141 -11.247303 -10.199470 -10.805023 -10.426258 -9.477789

~	0 000054	0 000727	10 476060	~	0 607026	0 005044	7 041072	
С	-8.998854	0.882737	-12.476069	С	9.627836	-2.935844	7.841073	
C	-8.039548	-0.098153	-12.820765	H	10.698142	-2.773048	8.042502	
H	-8.159211	-0.666646	-13.756187	С	8.775615	-1.828462	7.718015	
C	-6.944608	-0.364305	-11.994966	H	9.151855	-0.799345	7.806214	
H	-6.203060	-1.132746	-12.256583	C	10.054443	-5.441050	7.857630	
С	-10.173433	1.148037	-13.381117	Н	9.808140	-6.013947	8.776807	
			-14.402564					
Н	-9.837502	1.421500		H	9.949634	-6.143841	7.005942	
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H	-10.807332	0.243046	-13.485538	C	-0.572430	5.927140	0.760236	
С	2.607855	-3.426702	0.348323	C	-0.209967	7.020855	-0.046303	
C	3.607473	-3.864275	-0.544815	C	-0.885493	8.249280	0.005685	
C	4.068634	-5.181317	-0.536994	C	-1.980281	8.452316	0.878458	
Č	3.562999	-6.161153	0.359008	Č	-2.315463	7.359671	1.715704	
C	2.537958	-5.726455	1.233833	C	-1.638504	6.142345	1.657175	
C	2.087207	-4.397535	1.223149	С	-3.005386	10.469045	-0.162271	
С	3.724146	-8.584770	1.079761	Н	-3.526911	11.370153	0.223276	
H	3.507981	-8.305476	2.127938	H	-2.068497	10.822076	-0.631586	
H	4.597782	-9.271354	1.107468	C	-3.870023	9.776982	-1.225867	
С	2.511810	-9.331086	0.500172	Н	-3.325924	8.889593	-1.611795	
	1.627130						-2.096797	
H		-8.662340	0.549149	H	-4.023770	10.453625		
H	2.684103	-9.575452	-0.573533	C	-5.249714	6.618679	-1.040173	
С	-0.438365	-10.451465	1.718977	С	-4.785267	5.749710	-2.036683	
Č	-1.311388	-9.673221	0.949620	Н	-4.859028	6.054049	-3.090436	
H	-1.209652	-9.672475	-0.145087	C	-4.237596	4.514574	-1.659941	
C	-2.298892	-8.920252	1.601659	H	-3.872539	3.818381	-2.429732	
H	-2.987993	-8.301184	1.006352	С	-4.138071	4.144590	-0.302844	
C	-2.425704	-8.942546	3.004696	C	-4.630133	5.040132	0.675236	
C	-1.533545	-9.749213	3.748816	H	-4.550837	4.773821	1.739863	
H	-1.623408	-9.781928	4.846226	С	-5.195103	6.267574	0.318319	
C	-0.542022	-10.505515	3.118155	H	-5.566061	6.963364	1.083391	
H	0.150015	-11.138110	3.692336	C	-3.503920	2.841933	0.105508	
С	-3.494540	-8.143717	3.703973	Н	-2.607610	3.026952	0.733040	
H	-3.077438	-7.576453	4.560616	H	-4.202220	2.233344	0.716231	
H	-4.283003	-8.810602	4.113315	H	-3.191331	2.245759	-0.771421	
H	-3.983863	-7.425733	3.018636	N	1.287646	2.803730	1.851885	
N	1.021767	-0.199444	-0.876262	N	0.179570	2.548321	-0.784300	
N	2.147388	0.063828	1.757792	N	5.074688	2.354094	8.769782	
N	-2.694564	0.600135	-7.870747	Н	5.984268	2.795029	8.613508	
H	-3.711288	0.760205	-7.798284	N	5.452690	-0.679342	8.783829	
N	-4.144876	0.738601	-10.647257	H	4.447674	-0.784673	8.596233	
H	-4.270570	1.760477	-10.633068	N	-2.702032	9.629570	0.992170	
N	4.119328	-7.418916	0.318432	H	-3.520656	9.487265	1.589854	
H	4.755292	-7.563414	-0.465467	N	-5.120504	9.308577	-0.631544	
N	2.231462	-10.507039	1.318503	Н	-5.789379	10.055583	-0.396101	
H	3.000861	-11.191589	1.358745	S	6.306406	-0.645648	7.322320	
S	-5.406115	0.025221	-9.741313	S	-6.028120	8.157119	-1.525861	
S	0.836056	-11.409799	0.901627	F	4.875972	3.266674	4.118554	
F	1.249260	0.393211	-5.082467	F	6.015937	3.550206	6.559350	
F	0.156342	0.164625	-7.490835	F	1.664775	0.313768	5.997056	
F	-3.016500	1.306205	-3.175177	F	2.766977	0.574457	8.397668	
F	-4.122672	1.169464	-5.624888	F	0.809369	6.905832	-0.909977	
F	4.151761	-3.001827	-1.412895	F	-0.467255	9.245240	-0.805684	
F	5.040228	-5.566468	-1.396592	F	-2.061349	5.139675	2.446236	
F	1.120766	-4.062826	2.088971	F	-3.365705	7.505436	2.555774	
				0	5.303639			
F	1.952331	-6.594990	2.091687			-0.965150	6.282016	
0	-5.624496	0.770264	-8.468574	0	7.151917	0.571338	7.274961	
0	-5.121667	-1.422840	-9.723486	0	-5.803579	8.335880	-2.979362	
0				0				
	0.586640	-11.339457	-0.556527	O	-7.381350	8.243490	-0.939683	
0	1.014770	-12.701115	1.595753					
C	2.579568	1.639540	3.625524	Confo	rmation 7.			
C	1.896276	2.747004	3.087348		plicity: 2			
C	1.736035	4.009033	3.781703	Charge				
H	2.120974	4.230611	4.782349	E(B97	-3c) = -9171.803486	5829018 Hartree		
C	1.025030	4.831169	2.947564	E (GFN	1-xTB) = $-378.6404$ 0	01965703 Hartree		
Н	0.722730	5.869543	3.118847		2-xTB) = $-362.16308$			
С	0.747753	4.068081	1.747206		-FF) = $-35.17916294$			
C	0.048850	4.579908	0.638560	E(M06	/def2-TZVP) = -9172	2.845246462613 Ha	rtree	
С	-0.168932	3.863657	-0.555562	E(PBF	- D3(BJ)/def2-TZVI	P) = -9169.262780	436151 Hartree	
C		4.413385	-1.722206		0 - D3(BJ)/def2-TZV			
	-0.828303						DOTOGOA MUTICIOS	
H	-1.225747	5.428270	-1.809323	E (PBE)	h-3c) = -9158.81540	02316801 Hartree		
C	-0.857598	3.419745	-2.664476	E(PM6	) = -559.75136  Kcal	l/mol		
Н	-1.258960	3.470531	-3.681775		) = -669.94150  Kcal			
							0 77 - 1	
С	-0.257930	2.249100	-2.058078	Ε(ωB9	7X-V/def2-TZVP) = -	-91/4.40294079999	y martree	
C	3.208878	1.796857	4.965619					
С	4.337561	2.618553	5.160100	Coord	inates:			
C	4.916227	2.781677	6.417844	Cu Cu	-0.243331	0.800155	1.417999	
C	4.421944	2.122268	7.573990	C	1.546945	2.596664	-0.936514	
С	3.284013	1.310146	7.372060	С	1.672841	1.194213	-0.943973	
C	2.716728	1.137365	6.103116	C	2.485377	0.459077	-1.891966	
C	5.005982	1.512936	9.948508	H	3.068480	0.902856	-2.705289	
H	5.376048	2.104444	10.812764	С	2.379680	-0.865287	-1.558025	
Н		1.275806	10.162484	Н	2.873322	-1.720274	-2.031010	
	3.947240							
C	5.827410	0.208746	9.875386	C	1.489825	-0.940172	-0.416518	
H	5.727990	-0.333508	10.842542	C	1.149578	-2.142218	0.235994	
Н	6.902858	0.450850	9.753181	C	0.327809	-2.208927	1.378348	
C	7.417087	-2.046115	7.458388	C	-0.019494	-3.444562	2.049489	
С	6.903262	-3.343267	7.297072	H	0.334335	-4.438688	1.764431	
Н	5.838118	-3.484597	7.063427	C	-0.890232	-3.121626	3.055532	
С	7.768667	-4.433250	7.424002	H	-1.411245	-3.797553	3.740320	
TT				~	1 074140	1 (01(0)	0 00000	
H	7.373420	-5.453460	7.297237	C	-1.074148	-1.684686	2.999620	
н С	7.373420 9.142588	-5.453460 -4.251459	7.297237 7.704559	C	2.281684	-1.684686 3.379343	-1.968910	

С	1.604288	4.101498	-2.971684	С	-2.797964	-3.277252	6.763337
C	2.290099	4.863914	-3.919269	C	-4.183406	-3.542245	6.605291
С	3.705460	4.932811	-3.952134	C	-4.826542	-2.827436	5.571455
C	4.388877	4.183162	-2.964606	C	-4.112958	-1.998364	4.696716
С	3.688083	3.450482	-1.995024	С	-5.974582	-5.206501	7.218497
С	5.561253	6.404844	-4.831436	Н	-6.309815	-5.641640	8.183408
Н	6.125135	6.025660	-3.962345	H	-6.780654	-4.523235	6.889730
Н	5.360785	7.487801	-4.659365	C	-5.826668	-6.360195	6.205222
C	6.423570	6.219820	-6.087423	H	-6.779307	-6.935492	6.181681
Н	5.923983	6.670583	-6.973651	H	-5.035772	-7.059650	6.545297
Н	7.389124	6.747930	-5.959374	C	-3.787479	-7.485930	3.320441
С	9.264426	3.979719	-6.707787	C	-4.475634	-7.549761	2.098298
C	9.185133	3.086315	-7.788479	H	-5.134790	-6.725829	1.789597
Н	8.307247	2.432691	-7.893401	С	-4.280506	-8.660485	1.271578
С	10.238258	3.040436	-8.705894	H	-4.804074	-8.710363	0.304306
Н	10.184549	2.341598	-9.555639	C	-3.398608	-9.702860	1.634700
С	11.376145	3.867487	-8.559255	С	-2.738487	-9.615951	2.878297
C	11.428871	4.742288	-7.456576	H	-2.032200	-10.406853	3.169226
Н	12.312341	5.385270	-7.319292	С	-2.922988	-8.514187	3.723536
С	10.380749	4.804056	-6.525787	Н	-2.381572	-8.423246	4.675709
H	10.420737	5.472421	-5.653813	С	-3.119051	-10.842987	0.694002
C	12.498893	3.802477	-9.562153	H	-3.965505	-11.024110	0.003367
H	12.151191	4.107804	-10.571390	H	-2.223533	-10.620053	0.074398
Н	12.891089	2.768995	-9.658973	H	-2.901862	-11.780230	1.242453
Н	13.340697	4.462825	-9.279303	С	-2.548689	4.949184	2.808319
C	1.654504	-3.415941	-0.348219	C	-1.951704	6.074074	3.405220
C	2.550126	-4.268787	0.323769	C	-2.645502	7.276692	3.602663
С	3.024436	-5.464036	-0.235989	С	-3.994047	7.424551	3.199667
С	2.645558	-5.875978	-1.536635	С	-4.602642	6.273424	2.640919
C	1.733283	-5.016393	-2.201886	C	-3.906203	5.080001	2.452554
С	1.248423	-3.843092	-1.628797	C	-4.162163	9.905486	3.169232
C	3.761478	-8.141382	-1.642518	H	-4.956590	10.643467	3.407864
Н	4.493358	-7.797455	-0.889841	H	-3.352603	10.061870	3.905366
Н	4.345900	-8.636342	-2.446735	С	-3.615698	10.163779	1.757846
C	2.812334	-9.184663	-1.026627	H	-2.823347	9.418354	1.534220
H	2.146949	-9.608843	-1.805812	H	-3.130648	11.165146	1.709515
H	3.415199	-10.035871	-0.631401	C	-3.834394	8.077719	-0.969239
С	-0.582432	-7.551727	-0.109053	С	-2.584957	7.673380	-1.458594
C	-0.698744	-7.024649	-1.405935	Н	-1.839877	8.436744	-1.725083
H	-0.245479	-7.547316	-2.259990	C	-2.319102	6.302680	-1.591878
C	-1.384276	-5.818641	-1.586649	H	-1.344474	5.967931	-1.976432
H	-1.441375	-5.379392	-2.594304	С	-3.278088	5.334479	-1.229211
С	-1.970784	-5.139509	-0.495146	С	-4.533315	5.779148	-0.752964
C	-1.883037	-5.725034	0.783987	Н	-5.290397	5.038782	-0.454677
H	-2.373595	-5.235244	1.637197	С	-4.824413	7.140740	-0.632312
C	-1.177783	-6.917920	0.988067	H	-5.797589	7.478712	-0.250755
Н	-1.098814	-7.370718	1.985957	С	-2.977386	3.862395	-1.328842
C	-2.621282	-3.794395	-0.674061	Н	-3.133757	3.364689	-0.350223
H	-1.844269	-2.999535	-0.683384	H	-3.656140	3.366522	-2.054020
H	-3.315166	-3.563562	0.156857	H	-1.935020	3.677996	-1.648192
Н	-3.168082	-3.722840	-1.635092	N	-1.630761	1.264106	2.828179
N	1.066574	0.323542	-0.062219	N	-0.096050	2.762667	0.921004
N	-0.311274	-1.145328	1.983551	N	-4.771345	-4.437283	7.479141
N	4.315491	5.651494	-4.967518	H	-4.064388	-4.934816	8.025571
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N	6.683319	4.815176	-6.389160	H	-5.927949	-5.069695	4.518274
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Н	2.606249	-7.142600	-3.096492	N	-4.679177	9.990846	0.770120
N	1.951629	-8.599469	-0.015029	H	-5.390190	10.736183	0.773493
H	2.367042	-8.353249	0.888887	S	-3.891480	-5.996035	4.304546
S	7.924723	4.031876	-5.513574	S	-4.202699	9.828668	-0.871694
S							
	0.333264	-9.066557	0.149370	F	-0.779564	-2.278354	6.094504
F	0.259147	4.089637	-3.025238	F	-2.145062	-3.934468	7.744228
F	1.601275	5.555701	-4.854957	F	-4.785417	-1.434938	3.683737
F	4.402505	2.789473	-1.076125	F	-6.142926	-3.050465	5.295723
F	5.733590	4.156753	-2.939632	F	-0.671101	6.019800	3.798645
F	2.984428	-3.945328	1.550353	F	-1.990326	8.303446	4.186518
F	3.854070	-6.226625	0.518608	F	-4.543592	4.054953	1.860758
F	0.339468	-3.131347	-2.317345	F	-5.886014	6.376052	2.226409
F	1.280783	-5.409127	-3.418179	0	-3.778221	-4.838420	3.379347
0	7.431646	2.654367	-5.308229	0	-2.967613	-6.167823	5.453222
0							
	8.377963	4.896080	-4.396533	0	-2.943301	10.567001	-1.124131
0	0.046139	-9.971171	-0.991631	0	-5.435864	10.129260	-1.627300
0	0.130745	-9.488640	1.553153				
С	-1.968909	-0.981314	3.830775		ZNATELT		
C	-2.215422	0.400339	3.729826	E.T.J	MEI		
C	-3.128394	1.121529	4.593469				
H	-3.702825	0.675016	5.411727		rmation 10.		
C	-3.095612	2.432420	4.195559	Multi	plicity: 4		
H	-3.635804	3.284364	4.621706	Charg			
C	-2.151106	2.511461	3.099314		-3c) = -6436.94130	6932763 Hartree	
C	-1.791280	3.714990	2.465390		/def2-TZVP) = -643		
С	-0.792228	3.816302	1.476457		- D3(BJ)/def2-TZV		
С	-0.368992	5.064362	0.874470	E(PBE	0 - D3(BJ)/def2-TZ	VP) = -6435.14514	4706639 Hartree
Н	-0.765644	6.054701	1.114671		h-3c) = -6428.3360		
C	0.599369	4.752121	-0.042359		) = -197.36108 Kca		
H	1.167837	5.437648	-0.679095		) = -368.28448  Kca		
С	0.734772	3.310341	-0.034233	E(ωB9	7X-V/def2-TZVP) =	-6440.93455640081	4 Hartree
С	-2.733703	-1.770775	4.834343		1-xTB) = $-241.6195$		
C	-2.096290	-2.435903	5.902120		2-xTB) = $-236.7981$		
<u> </u>	2.000290	2.30000	J. JUZIZU	- (GEW			

E (GFN-	FF) = -31.2393234	64338 Hartree		С	4.706332	-6.190087	0.322478
Q 11				C	0.354351	-2.623683	2.280683
Coordin Co	-0.519231	0.314856	0.002990	H H	0.777483 -0.293684	-2.947209 -1.744873	3.252514 2.453428
Si	-2.193774	2.477909	0.379173	Н	-0.283126	-3.437382	1.886483
0	-0.778459	2.365647	-0.698573	C	2.200007	-5.543584	1.479597
C	-1.578993	1.196086	1.583572	H	1.221230	-5.307025	1.919756
C C	0.261373 -0.650363	4.119194 3.016267	-1.998621 -1.914222	C H	4.617281 4.091597	-4.113767 -3.185928	-1.023735 -1.284738
C	0.446268	4.757513	-3.279981	C	4.114147	-7.047905	1.296349
C	-3.691956	2.022771	-0.666596	Н	4.643875	-7.966883	1.590632
H	-3.763584	2.718650	-1.526450	С	5.844471	-4.425693	-1.592280
H	-4.621984	2.136545	-0.075403	H	6.292456	-3.743157	-2.330236
H C	-3.651164 -1.356350	0.988579 2.588284	-1.056361 -3.030846	C H	3.289827 4.103274	-1.725784 -1.470326	1.968245 1.263150
Н	-2.034498	1.731331	-2.946773	Н	3.164447	-0.903446	2.699281
C	0.992908	4.592404	-0.874096	H	3.598296	-2.630002	2.533720
H	0.838055	4.106222	0.095673	С	2.889871	-6.724362	1.860746
C	-0.288243	4.289103	-4.409179	H	2.435109	-7.389429	2.610989
H C	-0.136984 1.881380	4.781023 5.650389	-5.382088 -1.000301	C H	5.964810 6.490185	-6.478060 -7.400880	-0.284382 0.008413
Н	2.439842	6.004084	-0.120447	C	6.520877	-5.618528	-1.221303
C	-2.430475	4.293962	0.817214	H	7.493698	-5.858398	-1.677553
H	-1.597396	4.758822	1.371989	Si	0.092959	-1.983038	-1.493856
H	-3.353175	4.394956	1.425413	0	-1.058799	-0.670660	-1.896847
H C	-2.582830 -1.172747	4.865006 3.230062	-0.122170 -4.282782	C C	-2.069954 -2.173909	-0.667429 -0.878966	-4.105280 -2.690161
Н	-1.730821	2.858592	-5.154743	C	-3.242337	-0.898659	-4.917111
C	1.368527	5.841516	-3.371377	C	-1.011519	-3.347892	-0.825156
H	1.512256	6.327315	-4.349066	H	-1.695550	-3.691912	-1.627144
C	2.073030	6.278772	-2.259423	H	-0.399131	-4.210076	-0.497229
H Si	2.782028 -0.486657	7.115483 1.880688	-2.350510 2.942491	H C	-1.633093 -3.373108	-2.999494 -1.280135	0.021523 -2.115191
0	-1.630635	2.364863	4.158711	Н	-3.413172	-1.413178	-1.027177
C	-1.578514	4.286934	5.604421	C	-0.871533	-0.217501	-4.729132
C	-1.315066	2.892334	5.375942	Н	0.000648	-0.004984	-4.100328
C	-1.264154	4.855431	6.892556	С	-4.455233	-1.319481	-4.296489
C H	0.711396 1.302712	0.626576 1.100818	3.678319 4.486964	H C	-5.340732 -0.816459	-1.494098 -0.019901	-4.926586 -6.100703
н	1.414844	0.312015	2.882263	Н	0.116383	0.334951	-6.564276
Н	0.224698	-0.279075	4.081636	C	0.919932	-2.605979	-3.061173
С	-0.782483	2.107292	6.397849	H	1.474535	-1.825104	-3.611315
H	-0.602610	1.039049	6.213264	H	1.639537	-3.390472	-2.748432
C	-2.140583	5.117463	4.594407	H	0.177422	-3.058706	-3.748442
H C	-2.386555 -0.711426	4.662429 4.022254	3.626308 7.909289	C H	-4.518153 -5.455270	-1.499484 -1.813394	-2.923518 -2.440152
Н	-0.474263	4.462739	8.889644	C	-3.145777	-0.687657	-6.324978
C	-2.376810	6.463702	4.832792	Н	-4.038092	-0.868808	-6.944337
H	-2.812371	7.094478	4.042801	С	-1.960862	-0.262025	-6.907037
C	0.580204	3.412988	2.654309	H	-1.906486	-0.105610	-7.995101
H H	0.050199 1.462458	4.283334 3.187413	2.229337 2.025277	Si O	2.418822 3.812043	0.115095 -0.887041	-0.959096 -1.192984
H	0.958798	3.717715	3.652793	C	5.520218	-0.917869	-2.881475
C	-0.482761	2.677230	7.662188	Ċ	5.056260	-0.501303	-1.585491
H	-0.063182	2.034855	8.451435	С	6.859888	-0.569097	-3.288198
C	-1.520045	6.243449	7.101017	С	2.833384	1.498691	0.252597
H C	-1.279194 -2.061200	6.679823 7.031918	8.083103 6.096192	H H	3.642592 1.923937	2.152037 2.122070	-0.129856 0.361558
Н	-2.250980	8.100911	6.277254	Н	3.119447	1.120684	1.252998
Si	-2.946120	0.181373	2.372242	C	5.899298	0.223208	-0.743576
0	-3.356910	-1.006458	1.168562	H	5.538881	0.510807	0.253820
С	-5.506647	-2.072307	0.884684	С	4.700114	-1.677968	-3.762858
C C	-4.153051 -6.319657	-2.098654 -3.256672	1.368427	H	3.689442	-1.949204	-3.431598
C	-2.549962	-0.766769	1.028728 3.956916	C H	7.686799 8.706514	0.184793 0.449054	-2.404553 -2.723359
Н	-3.442347	-1.367607	4.226784	C	5.175075	-2.085018	-5.001322
H	-2.361705	-0.049503	4.778759	H	4.532022	-2.679179	-5.668135
H	-1.691935	-1.459619	3.881722	С	2.108000	0.917181	-2.636646
C	-3.649295	-3.251058	1.969078	H	2.140808	0.174286	-3.456474
H C	-2.610497 -6.063642	-3.250134 -0.919828	2.326126 0.260738	H H	1.139820 2.910045	1.450593 1.657913	-2.682425 -2.832364
Н	-5.431457	-0.030900	0.146241	C	7.210690	0.567832	-1.159934
C	-5.768364	-4.414737	1.650687	Н	7.854992	1.140457	-0.475332
H	-6.395798	-5.312707	1.756479	C	7.312769	-1.002564	-4.569984
C	-7.370331	-0.925591	-0.206176	H	8.335664	-0.739392	-4.882327
H C	-7.784597 -4.499402	-0.027330 1.174247	-0.688713 2.787830	C H	6.492593 6.863159	-1.743606 -2.071827	-5.408388 -6.391535
Н	-4.923632	1.741383	1.937967	п	0.003139	-2.0/102/	-0.391333
Н	-4.224175	1.896153	3.583735	Conf	ormation 12.		
H	-5.294264	0.506057	3.177975	Mult	iplicity: 4		
C	-4.460175	-4.405612	2.109963		ge: 0	084.608	
H	-4.035518	-5.302021	2.586801		7-3c) = -6436.930224		*****
C H	-7.658512 -8.278365	-3.225196 -4.128904	0.536361 0.645203		6/def2-TZVP) = -6437 E - D3(BJ)/def2-TZVP		
C	-8.175121	-2.088188	-0.067108		E0 - D3(BJ)/def2-TZV		
H	-9.210543	-2.084488	-0.440307	E(PB	Eh-3c) = -6428.32161	3829956 Hartree	
Si	1.705317	-2.153374	1.042330		(6) = -190.96799  Kcal		
0	2.095774	-3.561147	0.108714		(7) = -316.01737  Kcal		0 112 22
C C	1.080578 4.021032	-0.982526 -4.981917	-0.273653 -0.066373		97X-V/def2-TZVP) = -0.0000000000000000000000000000000000		o narciee
C	2.748519	-4.681487	0.531034		N2-xTB) = -236.79130		
				•			

E (GFN-F	F) = -31.314329	122815 Hartree		C	5.633611 3.153443	4.219681	-1.087003
Coordin	a+ae•			Н	3.153443	0.474932 1.233730	1.421582 1.753380
Co	-0.808621	-0.180561	1.293930	H	2.772728	-0.044567	2.320179
Si	-3.261116	-2.851498	0.967150	Н	3.687722	-0.255953	0.786748
0	-3.898316	-2.112642	-0.459024	С	4.768693	1.534670	-1.363600
C	-2.424696	-1.494634	1.936082	Н	4.423951	0.499806	-1.484916
С	-5.920102	-2.835472	-1.587059	С	3.324262	4.910192	-0.523288
C	-4.486580	-2.723066	-1.530396	H	2.270407	4.636698	-0.374868
C	-6.523289	-3.454666	-2.744659	C	6.556926	3.193212	-1.444956
С	-2.208373	-4.310961	0.394054	H	7.611049	3.460939	-1.614875
H	-2.691499	-4.747688	-0.504660	С	3.744624	6.226517	-0.395550
H	-2.169106	-5.102484	1.166548	Н	3.019719	7.013157	-0.136062
H	-1.172333	-4.037019	0.119636	С	1.094970	2.724715	1.590267
C	-3.712150	-3.182404	-2.594761	H	0.320181	3.325024 2.333026	1.077021
H C	-2.621596	-3.064317 -2.345870	-2.548685 -0.551413	H H	0.656759 1.923329	3.405865	2.527924 1.874508
Н	-6.765473 -6.301270	-1.854231	0.311394	С	6.125798	1.882008	-1.582918
C	-5.694125	-3.924558	-3.804408	Н	6.834866	1.089470	-1.867599
Н	-6.164807	-4.392829	-4.682174	C	6.027928	5.583377	-0.944181
C	-8.144594	-2.471654	-0.633280	Н	7.084529	5.844735	-1.113463
Н	-8.780973	-2.084108	0.176865	С	5.108586	6.565062	-0.604332
С	-4.717131	-3.569045	1.943848	Н	5.433909	7.611684	-0.501222
H	-5.410121	-2.779079	2.297854	Si	1.090146	-1.360105	-0.900135
H	-4.337626	-4.102821	2.840917	0	2.568288	-1.009531	-1.719755
H	-5.305147	-4.290374	1.340222	C	4.441038	-2.344299	-2.417022
С	-4.317827	-3.781590	-3.728118	C	3.177381	-1.722219	-2.707899
H	-3.677197	-4.132456	-4.551361	С	5.138175	-3.032928	-3.477215
С	-7.944598	-3.570290	-2.792929	С	-0.078665	-2.303992	-2.033446
H	-8.401051	-4.046015	-3.675077	H	0.395769	-3.248401	-2.368061
C	-8.740365	-3.094266	-1.762100	H	-0.981047	-2.562451	-1.446474
H	-9.835178	-3.191397	-1.819837	H	-0.385472	-1.719894	-2.919526
Si O	-3.517389 -2.217635	-0.028420	2.264961	C H	2.637979	-1.799599	-3.990610 -4.198169
C	-2.217633	1.201831 3.278937	2.223638 3.485643	С	1.684541 5.026846	-1.298001 -2.295351	-1.119479
C	-2.370842	2.576299	2.240230	Н	4.482825	-1.776512	-0.318940
C	-2.315202	4.722532	3.463655	C	4.553737	-3.093177	-4.775803
C	-4.794891	0.476482	0.983740	Н	5.092076	-3.619382	-5.578803
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Н	-4.549403	0.155956	-0.042590	С	1.574915	-2.586174	0.450462
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H	-2.683766	2.704270	0.118882	H	0.678154	-2.943279	0.994482
С	-2.101413	2.617149	4.735992	H	2.064407	-3.463611	-0.020662
H	-2.094670	1.521228	4.753378	C	3.328794	-2.489494	-5.018228
С	-2.509886	5.400595	2.225116	H	2.882662	-2.527790	-6.023719
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C	-1.970807	3.336291	5.915197	Н	6.932690	-4.154801	-3.991963
H	-1.848697	2.803536	6.870365	C	6.949076	-3.562133	-1.910908
C	-4.427410	0.165696	3.908774	H	7.924311	-4.029650	-1.705717
H H	-3.820949 -5.252895	0.024308 -0.576833	4.818515 3.933167	Si O	-0.494270	1.141443 0.567819	-1.663649 -3.188300
н Н	-4.887240	1.174908	3.949749	C	0.086180 0.101500	1.373130	-5.444011
C	-2.658209	4.683745	1.048754	C	0.759890	1.218678	-4.176622
Н	-2.816927	5.206048	0.093674	C	0.814136	2.019634	-6.520201
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Н	-2.208339	6.529565	4.673075	Н	-0.989772	3.368946	-2.605868
С	-1.999829	4.755948	5.894084	H	-0.703200	3.524139	-0.838072
H	-1.891838	5.319514	6.832960	Н	0.685031	3.315404	-1.951458
Si	-1.373469	-2.066183	3.349292	C	2.063798	1.670571	-4.000274
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C	2.045125	-1.400545	4.463201	С	-1.224240	0.902701	-5.666527
C	0.944860	-0.605430	4.002391	H	-1.745672	0.401995	-4.838128
C	2.906444	-0.839959	5.480658	С	2.144657	2.483179	-6.299990
C H	-1.800628 -1.007954	-1.623265 -2.024647	5.132759 5.796698	H C	2.679958 -1.835956	2.976998 1.065452	-7.125440 -6.901667
н	-2.764077	-2.086448	5.426021	Н	-2.860651	0.696397	-7.061733
н Н	-1.862038	-0.534519	5.426021	н С	-2.297866	0.696397	-1.718330
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C	2.340586	-2.694405	3.946320	Н	-2.811351	1.071331	-2.584995
Н	1.710768	-3.102506	3.148709	C	2.750746	2.306143	-5.064699
С	2.647137	0.468062	5.985594	Н	3.780744	2.654820	-4.893525
H	3.315189	0.880688	6.756651	С	0.151043	2.170085	-7.774580
C	3.426633	-3.417487	4.417745	H	0.691493	2.664433	-8.597353
H	3.644220	-4.411197	3.998194	C	-1.142744	1.706368	-7.963718
С	-0.880956	-3.883897	3.388730	H	-1.635415	1.832365	-8.940122
H	-0.365774	-4.229349	2.474029				
H	-1.786059	-4.510951	3.527757		ormation 17.		
H	-0.213647	-4.061024	4.255258		iplicity: 4		
С	1.577561	1.207062	5.506078	Charg		999696 11	
H C	1.375275	2.219389	5.887152		7-3c) = -6436.925473 5/def2-TZVP) = -6437		rt roo
Н	4.009031 4.661599	-1.617047 -1.188229	5.944024 6.720261		5/def2-TZVP) = -643/ E - D3(BJ)/def2-TZVP		
С	4.265222	-2.878258	5.428526		E - D3(BJ)/de12-TZVP E0 - D3(BJ)/def2-TZV		
Н	5.123735	-3.460476	5.795714		Eh-3c) = -6428.30255		1.30130 Hartree
Si	1.777678	1.352545	0.485280		6) = -203.78526  Kcal		
0	2.528418	2.203605	-0.817926		7) = -376.19146 Kcal		
C	0.421678	0.271345	-0.254829		97X-V/def2-TZVP) = -		2 Hartree
C	4.248505	3.881108	-0.862011		N1-xTB) = -241.62269		
C	3.842559	2.509246	-0.996848	E (GFN	12-xTB) = $-236.78855$	3791529 Hartree	

E (GFN-I	FF) = -31.2430488	23054 Hartree		С	0.040417	5.236550	5.701437
~ 1:				C	-1.949806	1.349822	3.041267
Coordin Co	-0.135588	0.096099	-0.543206	H H	-2.435327 -2.648892	2.289401 0.811764	3.374975 2.373518
Si	-1.391496	-1.527286	-2.397848	H	-1.781264	0.724517	3.938548
0	0.353128	-1.284840	-2.139171	С	0.051281	2.406219	5.630182
C	-1.864548	0.154369	-1.731866	H	0.078356	1.307854	5.605146
C	2.035966	-1.896527	-3.770519	С	0.761122	5.308588	3.336545
C	1.361131	-2.151119	-2.533140	H	1.053781	4.773677	2.423378
C C	3.130538 -1.819927	-2.766374 -3.052294	-4.134568 -1.391830	C H	-0.297912 -0.560801	4.480897 5.015459	6.862278 7.787720
Н	-1.183370	-3.887796	-1.749954	C	0.773164	6.695471	3.378570
H	-2.879782	-3.341419	-1.522359	Н	1.069721	7.269684	2.487740
H	-1.646029	-2.906711	-0.311403	С	-0.745674	3.150026	0.908351
C	1.723001	-3.214292	-1.719406	H	0.159768	3.541056	0.406305
H	1.201641	-3.357297	-0.766211	H	-1.440532	2.775560	0.130603
C	1.671046	-0.833889	-4.647079	H	-1.242834	3.995018	1.426431
H C	0.818859 3.489388	-0.191847 -3.843589	-4.390016 -3.271563	C H	-0.281321 -0.526998	3.095062 2.514038	6.824209 7.726086
Н	4.328271	-4.495912	-3.558615	С	0.057932	6.663078	5.704389
C	2.362996	-0.624420	-5.831937	Н	-0.211282	7.188919	6.633853
Н	2.060102	0.196239	-6.500129	С	0.411971	7.378753	4.570379
C	-1.689955	-1.943590	-4.204944	H	0.422105	8.479098	4.594036
H	-1.469103	-1.095273	-4.875724	Si	0.238818	-1.272162	2.265190
H	-2.756574	-2.225781	-4.330579	0	1.213641	-2.430779	1.422911
H C	-1.075000	-2.820040 -4.064678	-4.496203 -2.092459	C C	2.578364	-4.129453	2.473265
Н	2.794225 3.070610	-4.893110	-1.423123	C	1.387273 2.783123	-3.742830 -5.526783	1.766435 2.774046
C	3.819182	-2.515318	-5.358432	C	-1.553551	-1.867283	2.178524
Н	4.655286	-3.176784	-5.634270	Н	-1.581893	-2.972398	2.264659
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Si	-1.212190	1.586814	-2.724336	С	0.462617	-4.710627	1.374099
O C	-1.161466	1.143943	-4.394872	H	-0.430700	-4.400302	0.815314
C	-2.068498 -0.959744	2.262516 1.998002	-6.314936 -5.441219	C H	3.558431 3.397188	-3.177702 -2.117381	2.874342 2.637181
C	-1.872362	3.143326	-7.440001	C	1.810411	-6.485340	2.362408
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H	-1.679069	3.900318	-3.414609	С	4.698939	-3.582554	3.554349
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H	-3.215001	3.088365	-2.994270	С	0.769389	-1.278734	4.073964
С	0.283428	2.577219	-5.688422	H	1.749576	-0.785690	4.210189
H C	1.125946 -3.349366	2.351980 1.681000	-5.019885 -6.095723	H H	0.015518 0.846024	-0.761101 -2.324316	4.701194 4.437790
Н	-3.475686	1.002072	-5.241407	C	0.677109	-6.080787	1.674951
C	-0.587172	3.721236	-7.660873	Н	-0.070460	-6.821603	1.352843
H	-0.444834	4.391202	-8.522289	С	3.966580	-5.903063	3.476082
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H	-5.393653	1.505742	-6.767961	С	4.903496	-4.954479	3.859155
C	0.604261	1.941232	-2.234313	H	5.810888	-5.264389	4.399984
H H	1.318485 0.827712	1.303702 1.838151	-2.788589 -1.139931	Si O	2.394344 3.277865	0.688912 0.084011	1.085316 2.436842
H	0.844809	3.004072	-2.445047	C	5.554444	0.363879	3.160288
C	0.464152	3.438582	-6.802446	C	4.162029	0.705260	3.267900
H	1.455611	3.883090	-6.978162	С	6.488351	0.972961	4.077978
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C	-4.223759	2.832638	-8.054811	H	2.451808	2.946153	-0.032683
H Si	-5.068989 -3.641107	3.048769 0.290071	-8.725807 -1.212023	H C	2.523016 3.731655	3.111546 1.609117	1.763295 4.235255
0	-3.919295	-1.133407	-0.273968	Н	2.663586	1.852485	4.286042
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H H	-5.182133 -4.072259	1.633678	0.180096	C H	7.387473	-0.867994	2.110821
H H	-3.503918	2.713934 1.866384	-0.716231 0.757891	н С	7.743570 3.127822	-1.583647 -0.270077	1.354319 -0.360040
C	-5.283559	-0.935085	1.687715	Н	2.982283	-1.356532	-0.211732
Н	-4.555012	-0.233218	2.116313	Н	2.693175	0.001715	-1.342171
С	-5.780165	-2.958104	-1.451981	H	4.216004	-0.060847	-0.412943
H	-4.886593	-2.667631	-2.020255	С	4.661679	2.204429	5.124766
C	-7.354389	-2.205347	1.892698	Н	4.293203	2.917096	5.878512
H	-8.248952	-2.497889	2.463179	C	7.867947	0.625282	3.971591
C H	-6.692880 -6.523456	-3.857939 -4.288351	-1.983106 -2.981735	H C	8.580543 8.310575	1.087921 -0.273605	4.672547 3.012139
C	-4.829548	0.229832	-2.682276	Н	9.379335	-0.529192	2.948031
Н	-4.565342	-0.581875	-3.389246			******	
H	-4.806213	1.185653	-3.245551		formation 18.		
Н	-5.871830	0.062421	-2.341148		ciplicity: 4		
С	-6.436957	-1.310620	2.421821		rge: 0	CARES	
H	-6.595403	-0.883756	3.423809		97-3c) = -6436.924701		******
C H	-8.065114 -8.957060	-3.692205 -3.978261	0.019152 0.598344		)6/def2-TZVP) = -6437 BE - D3(BJ)/def2-TZVP		
н С	-7.846205	-4.227896	-1.241025		BEO - D3(BJ)/def2-TZV BEO - D3(BJ)/def2-TZV		
Н	-8.565462	-4.942644	-1.668938		BEh-3c) = -6428.30358		
Si	-0.348736	1.769700	2.136065		M6) = -187.22108  Kcal		
0	0.706318	2.448838	3.327008		(47) = -379.82743  Kcal		
С	0.549224	0.335098	1.339192		397X-V/def2-TZVP) = -		9 Hartree
C C	0.387464 0.361981	4.547749 3.110695	4.480913 4.468659		FN1-xTB) = -241.62332 FN2-xTB) = -236.78416		
C	0.301301	J. 11009J	1. 100000	TO) T	, - 200./0410	nattree	

E (GFN-	FF) = -31.2385905	39073 Hartree		С	0.654855	4.545926	3.972175
				C	-0.690503	-0.227819	4.297878
Coordi				H	-1.103184	0.643191	4.846691
Co	0.050673	-0.300452	-0.397082	H	-1.213087	-1.141869	4.643517
Si	-0.393277 0.599062	-0.107640	-3.215536	H	0.385620	-0.306032	4.544906
0 C	-0.678194	-1.230448 1.090682	-2.239281 -1.824365	C H	1.808003 2.245906	2.108784 1.161898	3.124556 2.793890
C	2.657880	-2.261778	-2.989202	C	-1.488015	3.919734	2.793696
C	1.269119	-2.363361	-2.645672	Н	-2.080382	3.197458	2.342202
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C	-1.846336	-1.100352	-3.879105	H	2.597218	4.964297	4.874315
H	-1.471560	-2.077702	-4.248848	С	-2.052063	5.116654	3.334201
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H	-2.654123	-1.262207	-3.145141	С	-2.805546	0.379668	2.140208
C	0.612920	-3.587847	-2.669669	H	-2.969440	0.543883	1.058908
H C	-0.453848 3.353746	-3.625509 -1.018941	-2.408933 -3.033055	H H	-3.461483 -3.091588	-0.443169 1.303249	2.477477 2.681244
Н	2.807545	-0.087435	-2.839350	C	2.566660	3.038090	3.879342
C	2.675990	-4.722402	-3.290791	Н	3.609370	2.789940	4.130170
Н	3.231680	-5.642318	-3.527573	C	0.041925	5.766181	4.385398
С	4.701706	-0.971077	-3.360783	Н	0.644817	6.484658	4.962756
H	5.214552	0.002071	-3.405069	С	-1.279659	6.049873	4.074841
C	0.613762	0.374834	-4.728738	H	-1.732409	6.997994	4.402736
H	1.567223	0.871261	-4.481824	Si	-1.635602	-2.636752	0.971049
H	0.009209	1.086357	-5.329827	0	-2.551825	-2.700695	2.440390
H	0.804141	-0.520635	-5.355794	C	-3.714987	-4.457867	3.587855
C	1.322510	-4.772249	-2.994474	C	-3.722855	-3.359161	2.660682
H C	0.788605 4.759498	-5.734268 -3.389903	-2.996816 -3.619222	C C	-4.950397 -1.088111	-5.151619 -4.423896	3.858453 0.680432
Н	5.304328	-4.318436	-3.850119	Н	-2.011678	-5.032788	0.585370
C	5.412866	-2.167062	-3.646494	Н	-0.507509	-4.539443	-0.255086
Н	6.483068	-2.119781	-3.898342	Н	-0.497786	-4.851122	1.512608
Si	0.800027	2.132425	-1.366517	С	-4.915663	-2.965163	2.053748
0	1.807366	2.395282	-2.750833	H	-4.914240	-2.110803	1.362216
C	3.821174	3.706919	-2.898973	С	-2.522396	-4.871255	4.246449
C	2.416767	3.541775	-3.156705	H	-1.595869	-4.318529	4.040142
C	4.476553	4.906262	-3.361214	С	-6.147528	-4.728479	3.208926
С	0.521292	3.802880	-0.566737	H	-7.086245	-5.263154	3.419528
H	1.510761	4.256428	-0.353202	C	-2.536961	-5.937878	5.133883
H H	-0.023712 -0.031184	3.704574 4.498795	0.390305 -1.227479	H C	-1.608672 -2.741701	-6.246591	5.638398
п С	1.710892	4.498795	-3.847496	Н	-3.121248	-2.213927 -1.175536	-0.488636 -0.501085
Н	0.640769	4.364654	-4.046760	H	-2.141787	-2.346279	-1.411625
C	4.580410	2.724715	-2.201203	H	-3.599371	-2.913461	-0.552623
Н	4.071423	1.817918	-1.852782	C	-6.123991	-3.655577	2.330943
С	3.719161	5.893342	-4.058166	Н	-7.050384	-3.325233	1.836605
H	4.225626	6.806660	-4.405449	С	-4.925832	-6.244505	4.775207
C	5.933906	2.910030	-1.957038	H	-5.867193	-6.777408	4.982319
H	6.499246	2.144273	-1.403580	С	-3.748333	-6.631730	5.398075
С	1.993635	1.109535	-0.274382	H	-3.750918	-7.477229	6.102905
H	2.659875	0.462598	-0.871719	Si	1.258343	-2.181559	1.885816
H	1.592233 2.630617	0.513389	0.587211	0 C	2.356546	-0.895099	2.264330
H C	2.366040	1.841950 5.700317	0.263809 -4.294155	C	4.773784 3.529153	-0.895819 -0.951215	2.239353 2.958300
Н	1.786475	6.463380	-4.835758	C	6.006884	-0.865264	2.990658
C	5.870203	5.061059	-3.096233	Ċ	2.184900	-3.203472	0.600724
Н	6.372315	5.976016	-3.447924	Н	3.134768	-3.553145	1.055841
С	6.584221	4.089167	-2.410293	H	1.621046	-4.090851	0.258822
H	7.657677	4.231264	-2.212985	H	2.450105	-2.607049	-0.292878
Si	-2.318780	1.959013	-1.914982	С	3.527708	-0.974627	4.352141
0	-3.523001	0.708626	-1.887504	H	2.563905	-0.997542	4.879689
С	-5.695080	0.834638	-2.954040	C	4.831242	-0.864297	0.816997
C	-4.875197	0.846838	-1.771153	H	3.891850	-0.888404	0.252880
C C	-7.128364 -2.752226	0.941411 3.123433	-2.809813 -0.504821	C H	5.963119 6.908809	-0.896460 -0.872752	4.415394 4.977918
Н	-3.852193	3.123433	-0.475967	H C	6.908809	-0.872752	0.152125
H	-2.284503	4.118665	-0.623416	Н	6.065039	-0.800338	-0.947996
Н	-2.425384	2.703632	0.463078	C	1.084526	-3.233586	3.446694
C	-5.474906	0.941035	-0.515029	Н	0.525773	-2.718120	4.249485
H	-4.839134	0.934341	0.380242	H	0.561375	-4.182877	3.219161
С	-5.142245	0.710352	-4.259997	H	2.093787	-3.489576	3.829505
H	-4.055078	0.608472	-4.356845	С	4.745997	-0.950775	5.077178
С	-7.699400	1.044569	-1.507910	H	4.714207	-0.969269	6.177094
H	-8.792748	1.124059	-1.409797	C	7.239013	-0.802212	2.273716
С	-5.955887	0.705491	-5.383615	H	8.178413	-0.777371	2.847958
H C	-5.509617 -2.511131	0.606758 2.901000	-6.384890 -3.545328	C H	7.262683 8.224170	-0.774016 -0.728987	0.887274 0.353253
Н	-2.290823	2.266802	-4.427838	11	0.224170	-0.720907	0.333233
Н	-1.801916	3.755521	-3.564331	Confo	ormation 21.		
H	-3.537472	3.304369	-3.664200		iplicity: 4		
C	-6.883874	1.038475	-0.387336		ge: 0		
Н	-7.324073	1.111400	0.618912		7-3c) = -6436.948845	705947 Hartree	
С	-7.933710	0.935647	-3.987598		6/def2-TZVP) = -6437		
H	-9.026030	1.020356	-3.875236		E - D3(BJ)/def2-TZVP		
C	-7.364614	0.823105	-5.247058		E0 - D3(BJ)/def2-TZV		4875779 Hartree
H	-8.003837	0.819751	-6.143065		Eh-3c) = $-6428.34072$		
Si O	-0.989467	-0.001910	2.455061		6) = -179.27535  Kcal		
C	-0.230935 -0.320421	1.504651 -1.344256	2.008497 1.303981		7) = -372.20256 Kcal 97X-V/def2-TZVP) = -		7 Hartree
C	-0.132862	3.601353	3.213498		N1-xTB) = -241.63215		. 1141 01 00
C	0.483880	2.373675	2.786242		N1-XIB) = $-241.03213N2-XIB$ ) = $-236.80747$		
-				,	, , , , , , , , , , , , , , , , , , , ,		

E (GFN-	FF) = -31.3343060	81172 Hartree		C C	-0.125853 3.264111	-5.425672 -1.768533	2.296056
Coordin	nates:			Н	3.288581	-1.768533	1.323341
Co	-0.295620	-0.328207	-0.240347	Н	4.272861	-1.642723	0.225221
Si	0.267711	1.803243	2.161075	Н	3.051661	-0.875477	1.271628
0	1.301969	0.485178	2.623982	С	0.760548	-2.750243	2.548084
C C	-1.058405 2.606073	1.082967 0.217269	1.055291 4.642393	H C	1.075675 -0.327183	-1.700961 -5.153744	2.633269 -0.151231
C	2.500638	0.638989	3.273600	Н	-0.208650	-4.531698	-1.046363
C	3.888267	0.313683	5.300306	C	0.224158	-4.893071	3.571611
C	1.334087	3.102094	1.323696	Н	0.136667	-5.539601	4.458085
H	2.229405	3.323684	1.935863	С	-0.783662	-6.458729	-0.263260
H H	0.758383 1.654165	4.042209 2.777435	1.229140 0.317059	H C	-1.031244 2.506306	-6.868045 -3.600531	-1.254245 -1.580024
C	3.623030	1.119461	2.602494	Н	1.810008	-3.957084	-2.358258
Н	3.535694	1.389393	1.542989	Н	3.484180	-3.399718	-2.067153
С	1.493744	-0.302658	5.363222	H	2.664361	-4.418392	-0.847162
H	0.526994	-0.370897	4.850494	С	0.673463	-3.587122	3.689974
C	5.009227	0.827474	4.584613	H	0.954906	-3.175894	4.671398
H C	5.980849 1.629917	0.898416 -0.719261	5.096928 6.680154	C H	-0.598104 -0.693452	-6.763120 -7.391550	2.142044 3.041393
Н	0.759223	-1.119310	7.222178	C	-0.928848	-7.268866	0.894032
C	-0.330582	2.600370	3.770692	Н	-1.295936	-8.301671	0.796433
H	-0.900347	1.917855	4.428500	Si	0.133956	-0.889534	-2.968497
H	-0.972539	3.476480	3.546591	0	-1.393844	-0.796278	-2.032537
H C	0.547293 4.874093	2.961268 1.219424	4.346033 3.261562	C C	-3.477429 -2.442060	-1.377328 -1.690321	-3.160369 -2.221727
Н	5.737457	1.605356	2.698055	C	-4.551373	-2.329232	-3.331833
C	3.988044	-0.120054	6.656081	Č	0.060615	-2.578177	-3.803515
H	4.965488	-0.047383	7.158566	H	-0.776987	-2.585382	-4.530528
C	2.888542	-0.626866	7.332799	Н	1.002921	-2.763997	-4.358011
H	2.988995	-0.958157	8.377635	H	-0.105699	-3.412402	-3.097021
Si O	-2.362456 -2.910785	0.169429 -1.040437	2.055523 0.943674	C H	-2.469436 -1.679785	-2.877494 -3.066848	-1.509093 -0.775028
C	-4.970236	-2.265232	0.689222	C	-3.497341	-0.172997	-3.918811
C	-3.639782	-2.163000	1.220958	Н	-2.671063	0.536028	-3.792739
C	-5.708287	-3.488449	0.891880	C	-4.540711	-3.546116	-2.591218
C	-1.809671	-0.709163	3.627154	H	-5.371246	-4.255541	-2.722142
H H	-2.641622 -1.608688	-1.357199 0.022567	3.969588 4.432673	C H	-4.536472 -4.535574	0.104614	-4.794592 -5.365241
н	-0.916823	-1.340567	3.488413	С	0.006005	1.045987 0.399646	-4.331033
C	-3.083943	-3.233152	1.918412	Н	-0.224670	1.406122	-3.934520
H	-2.055069	-3.156045	2.289712	Н	0.951489	0.461097	-4.906874
С	-5.553918	-1.219831	-0.078189	H	-0.794471	0.105668	-5.038476
H	-4.965792	-0.310969	-0.249023	C	-3.515932	-3.812328	-1.697927
C H	-5.107524 -5.675819	-4.559679 -5.491441	1.616709 1.760245	H C	-3.515207 -5.603256	-4.735606 -2.009436	-1.099422 -4.240122
C	-6.819288	-1.363264	-0.627845	Н	-6.426132	-2.731212	-4.360225
Н	-7.247973	-0.552469	-1.235963	C	-5.602867	-0.820215	-4.953657
С	-3.863230	1.168533	2.639893	H	-6.426625	-0.591665	-5.646734
H	-4.391785	1.742753	1.857927	Si	2.720888	0.603496	-2.148963
H	-3.540243	1.881145	3.427230	0	3.753302	0.858118	-0.781575
H C	-4.594034 -3.818868	0.471145 -4.430239	3.099945 2.111861	C C	5.588824 5.096508	2.331638 1.051222	-0.290840 -0.729030
Н	-3.339805	-5.263057	2.648698	C	7.010038	2.513658	-0.115529
C	-7.011528	-3.595565	0.322485	C	2.219936	2.341374	-2.654559
H	-7.577338	-4.527772	0.478170	H	3.119242	2.990065	-2.646946
C	-7.555747	-2.560059	-0.423602	H	1.772353	2.395124	-3.664153
H	-8.559855	-2.665938	-0.862342	H	1.482493	2.749321	-1.939410
Si O	-1.887025 -0.773458	2.401730 2.847450	-0.000400 -1.265423	C H	6.000686 5.619176	0.029414 -0.941187	-1.022386 -1.367074
C	-0.366878	4.948750	-2.398851	C	4.713443	3.422456	-0.025862
C	-1.049332	3.683576	-2.310840	Н	3.637185	3.279402	-0.177358
C	-0.611056	5.798421	-3.541039	C	7.897155	1.437478	-0.410953
С	-3.472621	1.819242	-0.834462	H	8.979523	1.584854	-0.277024
H H	-3.844273 -4.269991	2.597700 1.637170	-1.528583 -0.091288	C H	5.206362 4.512470	4.641255 5.472269	0.416859 0.616204
H H	-3.312138	0.882854	-1.398312	н С	3.778194	-0.165450	-3.520714
C	-1.927314	3.310240	-3.328580	Н	4.111265	-1.192602	-3.269396
H	-2.437022	2.343294	-3.257525	Н	3.183427	-0.231621	-4.455639
C	0.550558	5.384827	-1.402855	Н	4.678446	0.444891	-3.737887
H	0.736100	4.727146	-0.547782	C	7.395982	0.227589	-0.865377
C H	-1.521277 -1.699466	5.376793 6.033351	-4.553721 -5.418797	H C	8.081668 7.480369	-0.601027 3.779258	-1.099465 0.346797
C	1.206073	6.602022	-1.515430	Н	8.564148	3.915992	0.487238
Н	1.916536	6.916114	-0.735338	C	6.601852	4.819583	0.611556
C	-2.280170	4.026485	0.886576	H	6.985904	5.787626	0.967753
H	-1.376435	4.534608	1.275134				
H	-2.973132	3.858859	1.735204		ormation 28.		
H C	-2.771847 -2.163527	4.721661 4.154406	0.174841 -4.442618		iplicity: 4 ge: 0		
Н	-2.163527	3.821382	-5.224033		ge: 0 7-3c) = -6436.938432	602682 Hartree	
C	0.078311	7.045156	-3.622660		6/def2-TZVP) = -6437		rtree
H	-0.109994	7.690294	-4.495117	E(PB	E - D3(BJ)/def2-TZVP	= -6434.683396	410443 Hartree
C	0.967537	7.441721	-2.635341		EO - D3(BJ)/def2-TZV		5577711 Hartree
H	1.491270	8.406122	-2.719217		Eh-3c) = $-6428.33189$		
Si O	1.978673 0.454818	-2.031759 -2.392588	-0.669620 0.195996		6) = -185.07246  Kcal 7) = -366.33415  Kcal		
C	1.362756	-0.560086	-1.618633		97X-V/def2-TZVP) = -		2 Hartree
C	-0.007220	-4.595288	1.119050		N1-xTB) = -241.62616		
С	0.411622	-3.234382	1.293953	E (GFI	N2-xTB) = -236.80274	4885602 Hartree	

E(GFN-FF) = -31.312004550772 Hartree				C	-1.541579 -0.597669	-4.678777 -3.940230	-5.974294
Coordi	nates:			Н	-0.317809	-4.721119	-1.061443 -1.799323
Co	0.614867	-0.324012	0.771282	Н	-0.103667	-4.190689	-0.103399
Si	1.554530	1.553354	2.747856	H	-1.693940	-3.999199	-0.920951
0	-0.106768	1.035352	2.352629	C	0.531680	-2.937864	-5.145112
С	2.440714	0.639043	1.397542	H	1.330980	-2.247118	-4.845515
C	-1.958803	2.476244	3.054221	C	-2.923919	-3.952018	-4.057591
C	-1.189669	1.273091	3.195150	H	-3.038320	-3.319937	-3.168665
C C	-3.076413 1.809333	2.681204 1.059468	3.946835 4.551391	C H	-0.325988 -0.208570	-4.598136 -5.216795	-6.714668 -7.617313
Н	1.150318	1.684221	5.187766	C	-3.950874	-4.786482	-4.474654
H	2.859573	1.252663	4.851211	Н	-4.890737	-4.828186	-3.903602
H	1.578877	0.000526	4.768228	С	1.816892	-2.376359	-2.067992
C	-1.510714	0.347120	4.179758	H	2.175015	-1.544445	-2.703075
H	-0.907534	-0.562080	4.272526	H	2.346832	-2.315056	-1.099100
C	-1.681989	3.464375	2.070531	H	2.091297	-3.331799	-2.558148
H	-0.840417	3.302386	1.391288	С	0.684194	-3.742937	-6.302852
C	-3.373782	1.708192	4.944007	H	1.618177	-3.673035	-6.881184
H C	-4.232690 -2.474380	1.878617 4.595919	5.610042 1.949191	C H	-2.617445 -2.494720	-5.527799 -6.140450	-6.371156 -7.278129
Н	-2.256226	5.333021	1.162471	C	-3.796146	-5.581906	-5.641478
C	1.569211	3.432496	2.755026	Н	-4.615896	-6.240282	-5.967303
H	1.316491	3.890732	1.783228	Si	-2.220895	-0.982911	-0.011551
H	2.571387	3.792982	3.065850	0	-2.736232	0.588948	0.485722
H	0.831759	3.784247	3.504376	С	-4.587007	2.104856	0.525252
С	-2.603435	0.563699	5.056930	C	-3.935142	0.928075	1.033495
H C	-2.834007	-0.192882 3.855511	5.822083 3.793209	C C	-5.791794 -2.009029	2.570925 -2.079599	1.165341 1.521099
Н	-3.869048 -4.731284	3.855511	4.463032	Н	-2.009029	-2.507773	1.843968
C	-3.580147	4.793997	2.814742	H	-1.324930	-2.926597	1.325206
Н	-4.215438	5.683902	2.696204	Н	-1.603221	-1.504363	2.375723
Si	3.620944	1.610672	0.332226	C	-4.517678	0.214191	2.080381
0	5.071005	1.507664	1.285598	H	-4.010232	-0.672504	2.479195
C	6.984290	2.368902	2.397200	C	-4.076386	2.811940	-0.597840
C	6.269038	2.128914	1.171408	H	-3.200581	2.398520	-1.111495
С	8.282850	2.991629	2.340694	С	-6.344294	1.824957	2.247651
C H	3.924886	0.827612	-1.369598	H C	-7.268615	2.182381	2.726630
H H	3.908401 3.141183	1.607032 0.085763	-2.157672 -1.609161	Н	-4.699662 -4.305220	3.964031 4.483597	-1.055087 -1.941420
H	4.903923	0.313211	-1.419613	C	-3.628329	-1.640536	-1.074528
C	6.829182	2.513873	-0.047131	Н	-3.646103	-1.114025	-2.047299
Н	6.284671	2.323097	-0.982723	Н	-3.549071	-2.731362	-1.246493
С	6.433233	2.012717	3.660447	H	-4.587191	-1.450533	-0.549147
H	5.434250	1.553821	3.678270	C	-5.723175	0.662960	2.677025
C	8.824286	3.367643	1.075687	H	-6.149663	0.083270	3.509977
H	9.815449	3.844343	1.038555	С	-6.394986	3.769066	0.681185
C H	7.137440 6.700844	2.248262 1.970090	4.833121 5.804523	H C	-7.307378 -5.858286	4.134740 4.456870	1.178371 -0.398038
C	3.356503	3.455959	0.033247	Н	-6.343795	5.376020	-0.760830
Н	3.474625	4.061548	0.949870	Si	-0.528845	0.765516	-1.992895
Н	2.366894	3.673187	-0.414217	0	-2.095251	0.887731	-2.714486
H	4.129848	3.789357	-0.688259	C	-2.970729	1.005627	-4.945672
C	8.105135	3.134143	-0.086247	C	-2.445479	1.662117	-3.778981
H	8.524083	3.426295	-1.061364	С	-3.408654	1.808853	-6.061176
C	8.978616	3.215000	3.565983	С	0.669526	0.742600	-3.446739
H	9.972805	3.687277	3.526811	H	0.483695	1.661486	-4.040670
C H	8.422825 8.976647	2.851124 3.033201	4.783987 5.717645	H H	1.727743 0.494138	0.757826 -0.128169	-3.124345 -4.105517
Si	3.221180	-0.993323	1.824298	C	-2.346125	3.053463	-3.749348
0	1.745879	-1.989280	1.614232	Н	-1.954241	3.546261	-2.848810
C	1.010444	-3.690898	3.171801	С	-3.058416	-0.412459	-5.027542
С	1.652856	-3.327448	1.944397	H	-2.689441	-1.004202	-4.179687
C	0.880840	-5.089241	3.500108	C	-3.298463	3.229086	-5.989533
C	4.518600	-1.695870	0.652899	H	-3.634531	3.834570	-6.845140
H	4.750525	-2.733825	0.966470	C	-3.569354	-1.026459	-6.162575
H	5.447195	-1.097678	0.745132	H	-3.624782	-2.124356	-6.210889
H C	4.216345 2.171715	-1.710225 -4.305591	-0.409051 1.103105	C H	-0.215220 -1.081629	2.333554 2.505878	-0.994754 -0.332111
Н	2.659180	-4.006953	0.166209	H	0.681913	2.201300	-0.356402
C	0.510090	-2.716917	4.076934	Н	-0.054605	3.219625	-1.640457
Н	0.624119	-1.659946	3.805583	C	-2.772489	3.831348	-4.857214
C	1.407730	-6.067138	2.606859	H	-2.686402	4.927762	-4.804181
H	1.304414	-7.132613	2.861925	C	-3.933238	1.143266	-7.208718
C	-0.104599	-3.092070	5.261658	H	-4.272149	1.753838	-8.060595
H	-0.483010	-2.324260	5.954161	С	-4.014239	-0.240980	-7.259155
C	3.870507	-1.393315	3.546935	H	-4.419784	-0.735603	-8.155228
H H	3.139125 4.746975	-1.273914 -0.747089	4.363970 3.759496	Conf-	ermation 31.		
H H	4.746975	-2.445644	3.759496		prmation 31.		
C	2.045634	-5.678617	1.439067	Charo			
Н	2.454700	-6.435151	0.753062		7-3c) = -6436.936324	584732 Hartree	
C	0.235055	-5.441282	4.722759		5/def2-TZVP) = -6437		rtree
H	0.130304	-6.508412	4.972791		- D3(BJ)/def2-TZVP		
C	-0.247071	-4.468095	5.585355		0 - D3(BJ)/def2-TZV		5979824 Hartree
H	-0.739161	-4.759810	6.525271		2h-3c) = -6428.32895		
Si	-0.044095	-2.277974	-1.764203		$S_{i}$ = -195.38077 Kcal		
0 C	-0.833450 -0.560586	-2.193992 -0.727636	-3.304776 -0.853631		7) = -367.51279 Kcal 97X-V/def2-TZVP) = -		8 Hartron
C	-1.705173	-3.873544	-4.788179		11-xTB) = $-241.62004$		0 1101 01 00
C	-0.638144	-2.995934	-4.387412		12-xTB) = $-236.79252$		
-				,	; 300.0202		

E (GFN-F	FF) = -31.2396055	09369 Hartree		C	2.974632	5.389608	-3.826295
Q 11 .				C	-0.601747	1.059090	-2.827580
Coordir Co	-0.578519	-0.780766	0.502491	H H	-0.481101 -0.925614	1.485109 0.005061	-3.844379 -2.922356
Si	-1.420593	-3.176036	-1.650673	Н	-1.384211	1.634027	-2.297270
0	-0.794595	-2.182519	-2.922356	C	3.649892	3.527861	-1.798105
C	-2.071473	-2.030546	-0.312073	H	3.899386	2.798005	-1.017149
C	-0.613515	-2.466504	-5.314127	C	0.621020	4.627727	-3.747706
C C	-0.047008 0.194765	-2.574481 -2.832411	-3.996251 -6.453641	H C	-0.140009 4.314042	3.968595 5.294428	-3.306952 -3.345732
C	-0.025708	-4.343368	-1.151181	Н	5.082174	5.955281	-3.775889
Н	0.308633	-4.896958	-2.051040	C	0.288830	5.536628	-4.742414
H	-0.358172	-5.090696	-0.407693	Н	-0.748947	5.603563	-5.103312
H	0.844721	-3.802311	-0.739816	C	2.377231	0.399719	-3.013819
С	1.268404	-3.014108	-3.846004	Н	3.378271	0.451287	-2.547444
H	1.699747	-3.071175	-2.838932	H	2.147878	-0.649332	-3.286002
C H	-1.941556 -2.537900	-2.003316 -1.709996	-5.530065 -4.659372	H C	2.400540 4.636820	0.987878 4.382565	-3.954272 -2.351429
C	1.531542	-3.284851	-6.253774	Н	5.670197	4.310008	-1.978738
Н	2.139275	-3.558174	-7.129585	C	2.594713	6.311334	-4.846955
С	-2.464592	-1.909702	-6.811604	H	3.368027	6.969461	-5.273797
H	-3.492989	-1.546173	-6.959011	С	1.284679	6.384532	-5.297438
C	-2.745297	-4.273717	-2.438593	H	1.013150	7.102546	-6.086498
H H	-3.591024 -3.154967	-3.701590 -4.985927	-2.864818 -1.692697	Si O	0.243784 -0.566462	1.869772 0.806458	0.904715 2.099816
н	-2.291470	-4.862676	-3.262265	C	-0.816791	1.610861	4.383312
C	2.052690	-3.368771	-4.972922	C	-1.382556	1.309080	3.098555
Н	3.087934	-3.707900	-4.816245	C	-1.687965	2.145908	5.404606
C	-0.376907	-2.724170	-7.756203	С	-1.169220	2.882276	0.194037
H	0.240867	-3.003743	-8.623965	H	-1.614242	3.513705	0.989324
C	-1.676822	-2.275597	-7.935038	H	-0.799917	3.541702	-0.614574
H Si	-2.098773 -3.683695	-2.197803 -1.229592	-8.948644 -0.823944	H C	-1.970481 -2.735693	2.232375 1.508089	-0.204011 2.856546
0	-3.796568	0.248337	0.080047	Н	-3.129779	1.245197	1.867996
C	-5.827958	1.345123	0.794670	C	0.553297	1.381472	4.694508
C	-4.724174	1.233793	-0.119848	Н	1.198007	0.936741	3.928881
C	-6.757931	2.437647	0.632955	С	-3.069347	2.349924	5.116313
С	-3.871762	-0.751813	-2.635010	H	-3.720792	2.760782	5.902726
H	-4.784310	-0.131586	-2.743572	C	1.058745	1.684723	5.950054
H H	-4.010036 -3.008883	-1.652742 -0.181723	-3.262760 -3.023091	H C	2.119873 1.413619	1.494620 3.034078	6.171450 1.803010
C	-4.571913	2.165687	-1.145142	Н	2.199351	2.518592	2.383223
Н	-3.718428	2.070600	-1.830491	Н	1.903170	3.667070	1.034344
C	-6.023738	0.421311	1.860308	Н	0.848914	3.693054	2.492825
H	-5.303663	-0.396108	1.982999	С	-3.581306	2.029483	3.869083
С	-6.568544	3.368625	-0.429384	Н	-4.648645	2.173660	3.644945
H	-7.282223	4.198396	-0.545049	C	-1.131342	2.448113	6.683186
C H	-7.089746 -7.222998	0.561255 -0.159088	2.737311 3.558693	H C	-1.795340 0.211462	2.861017 2.228215	7.458642 6.952219
C	-5.231226	-2.247785	-0.422439	Н	0.621641	2.468845	7.944793
Н	-5.273392	-2.621788	0.618177	Si	2.512279	-0.283214	0.462954
H	-5.283458	-3.124876	-1.099825	0	3.797251	0.744434	-0.089795
H	-6.139124	-1.632905	-0.593296	С	5.890249	1.374425	0.907967
C	-5.497064	3.229363	-1.297911	C	5.137509	0.534936	0.014577
H C	-5.349226 -7.841693	3.951527 2.549854	-2.114977 1.554272	C C	7.317874 2.799953	1.189344 -2.014740	1.004785 -0.222251
Н	-8.549259	3.384854	1.431942	Н	3.830562	-2.355058	0.001080
C	-8.007191	1.634917	2.583477	Н	2.106886	-2.709137	0.292286
H	-8.849478	1.739960	3.284090	Н	2.629999	-2.075838	-1.313440
Si	-2.158875	-2.884278	1.343554	С	5.795283	-0.417127	-0.764264
0	-0.480971	-2.512131	1.823002	H	5.213157	-1.026470	-1.469399
C C	1.008520 0.053074	-3.745294 -2.693948	3.283757	C H	5.265389	2.388479	1.687717
C	1.614446	-3.887404	3.090589 4.587054	С	4.182307 7.950313	2.533110 0.190493	1.583913 0.207901
C	-3.262269	-2.109038	2.655437	Н	9.039631	0.054831	0.287604
Н	-2.990844	-2.517518	3.649565	C	6.010373	3.185950	2.544669
H	-4.323317	-2.369101	2.472652	H	5.513136	3.968611	3.137622
H	-3.173453	-1.007421	2.693731	C	2.765607	-0.424632	2.326569
C H	-0.294139	-1.848190	4.136060	H	2.941133 1.914255	0.558553	2.802430
H C	-1.007852 1.389043	-1.034917 -4.637563	3.963150 2.242682	H H	3.669799	-0.920074 -1.041244	2.830981 2.508006
Н	0.921664	-4.526123	1.258431	С	7.199761	-0.587429	-0.660484
C	1.239925	-2.998564	5.636969	Н	7.692366	-1.348026	-1.285502
H	1.712174	-3.114126	6.624368	С	8.050403	2.025120	1.899589
C	2.331849	-5.630375	2.466941	Н	9.139972	1.883480	1.976382
H	2.615597	-6.309942	1.649129	С	7.414330	2.999508	2.654719
C	-2.423831	-4.744530	1.500166	Н	7.998510	3.635647	3.337159
H H	-1.850386 -3.502851	-5.367321 -4.956468	0.791066 1.347676	Conf	ormation 32.		
H H	-2.163090	-5.063206	2.530799		iplicity: 4		
C	0.302266	-2.003483	5.413633		ge: 0		
Н	0.021140	-1.306300	6.216431		7-3c) = -6436.926851	401521 Hartree	
С	2.579589	-4.919706	4.779563	E (M0	6/def2-TZVP) = -6437	.182742327684 Ha	
H	3.042293	-5.025617	5.773141		E - D3(BJ)/def2-TZVP		
C	2.933868	-5.772604	3.745046		E0 - D3(BJ)/def2-TZV		1344029 Hartree
H Si	3.682406 1.035565	-6.561642 1.110664	3.912747 -1.908098		Eh-3c) = -6428.31107 6) = -200.04709 Kcal		
0	1.363410	2.805327	-1.703262		6) = -200.04709 Kcal 7) = -377.90056 Kcal		
C	0.924324	0.482076	-0.138251		97X-V/def2-TZVP) = -		6 Hartree
C	1.958891	4.527566	-3.270446	E (GF	N1-xTB) = -241.61981	3306696 Hartree	
C	2.332691	3.591193	-2.246147	E (GFI	N2-xTB) = -236.78789	3830313 Hartree	

E (GFN-	FF) = -31.2493588	00879 Hartree		С	3.074672	-4.926367	-3.547140
				C	3.647643	-1.902327	0.879351
Coordi	nates: 0.091996	0.422823	0.157372	H H	4.285514 4.256198	-2.729291 -1.307567	0.506718 1.590559
Si	-2.658438	0.422023	0.380856	H	2.806535	-2.350954	1.439236
0	-1.429894	1.562082	1.154541	С	2.676067	-2.154135	-3.923406
C	-1.475070	-0.891578	0.034426	H	2.514844	-1.080435	-4.074983
C	-1.590522	2.956142	3.119562	С	2.587927	-4.689451	-1.138018
C	-1.625378	2.823424	1.694352	H	2.315171	-4.053632	-0.289223
C C	-1.753205 -3.347849	4.269594 1.478251	3.692799 -1.079165	C H	3.219626 3.485858	-4.345149 -4.992900	-4.840176 -5.689138
Н	-3.838573	2.402109	-0.712504	н С	2.776879	-6.052433	-0.959982
H	-4.101359	0.851999	-1.594586	Н	2.659700	-6.494768	0.041033
Н	-2.578475	1.762804	-1.821204	C	4.725742	-0.499277	-1.520139
С	-1.842616	3.932647	0.884940	Н	4.630905	0.171192	-2.392690
H	-1.885428	3.809327	-0.203631	Н	5.435546	-0.027982	-0.809680
С	-1.413709	1.839795	3.982183	Н	5.175920	-1.452689	-1.865423
H	-1.307843	0.845381	3.534727	C	3.024339	-2.984959	-5.017746
C H	-1.940023 -2.035637	5.391036 6.392514	2.834109 3.278714	H C	3.134462 3.263101	-2.534699 -6.323197	-6.015968 -3.326056
C	-1.389167	2.002770	5.359755	Н	3.526633	-6.957802	-4.186640
Н	-1.254917	1.126605	6.012362	C	3.117679	-6.878055	-2.063678
С	-4.053525	0.310631	1.620246	Н	3.265183	-7.958575	-1.915187
H	-3.727661	-0.096104	2.594293	Si	2.018324	1.938278	-1.568691
H	-4.817054	-0.368275	1.189099	0	3.262612	3.091310	-1.235618
H	-4.526838	1.297835	1.798591	С	5.144091	4.086891	-2.334373
C H	-1.992214 -2.131589	5.220585	1.460654	C C	3.731135	4.059099	-2.071520 -3.183735
С	-1.718309	6.088535 4.399797	0.799805 5.111782	C	5.676321 0.327982	5.124411 2.781566	-1.517519
Н	-1.831257	5.404343	5.547293	Н	0.178100	3.460463	-2.381841
C	-1.542193	3.294057	5.930091	Н	-0.484649	2.023569	-1.578204
H	-1.519343	3.415413	7.023649	H	0.202297	3.350373	-0.579157
Si	-1.369683	-2.226191	1.342081	С	2.898412	5.020964	-2.643169
0	-2.813032	-3.157694	1.136503	H	1.821375	4.998565	-2.427227
C	-4.168477	-4.332610	2.740803	C	6.026908	3.114899	-1.785218
C	-3.156451	-4.340765	1.719013	H	5.603214	2.328382	-1.147164
C C	-4.585591 0.151284	-5.586083 -3.318818	3.321855 1.092982	C H	4.792975 5.206445	6.092024 6.880562	-3.746737 -4.393579
Н	-0.093624	-4.308000	0.664952	C	7.387211	3.158512	-2.055605
Н	0.679372	-3.488083	2.052683	Н	8.057933	2.398939	-1.626009
H	0.838045	-2.816169	0.387130	С	2.279926	1.449161	-3.369296
C	-2.613032	-5.550889	1.290049	H	3.265552	0.996904	-3.581887
H	-1.871182	-5.549824	0.480019	H	1.482198	0.767007	-3.719013
C	-4.781295	-3.125431	3.180079	H	2.207776	2.382250	-3.965740
H	-4.469849	-2.184684	2.710187	C	3.434100	6.033797	-3.479949
C H	-3.993619 -4.317962	-6.800641 -7.752765	2.866579 3.313352	H C	2.753521 7.080186	6.781708 5.139455	-3.914998 -3.436379
C	-5.757776	-3.141213	4.165393	Н	7.488649	5.932283	-4.082490
Н	-6.224572	-2.199357	4.491621	C	7.918407	4.180606	-2.886620
С	-1.361644	-1.741029	3.167323	Н	8.998837	4.209319	-3.094822
H	-2.201698	-1.095838	3.482366	Si	2.548160	1.366265	1.471536
H	-0.409222	-1.255187	3.456134	0	1.663752	2.852416	1.533370
H	-1.440911	-2.686136	3.745164	C	1.549995	5.175722	2.081925
C H	-3.031728 -2.586166	-6.776188 -7.715547	1.868439 1.507339	C C	1.660124 1.420858	3.806173 6.209203	2.505581 3.079166
C	-5.590160	-5.563297	4.334909	C	4.353531	1.828116	1.736322
Н	-5.907106	-6.519190	4.780741	Н	4.472422	2.336536	2.715075
C	-6.162914	-4.370526	4.750857	Н	5.020322	0.942524	1.727515
H	-6.937872	-4.374766	5.532484	Н	4.671580	2.525885	0.937693
Si	-1.741167	-1.624370	-1.675563	C	1.717456	3.506808	3.867168
0	-3.456087	-1.526080	-1.886238	H	1.784916	2.462698	4.194691
C	-5.022214	-3.250064	-2.481781	C	1.578777	5.536093	0.707022
C C	-4.189084 -5.823306	-2.141423 -3.894627	-2.859122 -3.493099	H C	1.758103 1.470592	4.742779 5.861540	-0.027107 4.460119
C	-0.885179	-0.628399	-3.029688	Н	1.378630	6.656129	5.216107
Н	-1.066427	-1.092660	-4.020228	C	1.433297	6.858960	0.315231
Н	0.205909	-0.666924	-2.835334	Н	1.480449	7.123227	-0.752256
Н	-1.209116	0.429043	-3.078383	C	1.915119	0.253112	2.871602
C	-4.170107	-1.695237	-4.179022	H	0.879750	0.546273	3.135024
H	-3.539764	-0.833697	-4.442580	Н	1.910346	-0.813574	2.581573
C H	-5.067881	-3.723823	-1.140415	H C	2.535217	0.352423	3.786007
С	-4.448143 -5.773055	-3.219188 -3.415119	-0.387555 -4.835766	Н	1.631052 1.665042	4.537360 4.265275	4.836225 5.901719
Н	-6.386147	-3.912484	-5.602906	C	1.257213	7.556852	2.640051
C	-5.868642	-4.805556	-0.800857	Н	1.145334	8.346172	3.400147
H	-5.885392	-5.167229	0.238873	С	1.251825	7.876228	1.290024
С	-1.258691	-3.421544	-1.937212	H	1.130004	8.923172	0.972316
H	-1.791344	-4.098718	-1.244043				
H	-0.166041	-3.566433	-1.833572		rmation 5.		
H	-1.541991	-3.706306	-2.971502		plicity: 4		
C H	-4.964193 -4.932240	-2.337914 -1.968609	-5.164853 -6.201455	Charg	re: U '-3c) = -6436.931627	283002 Hartroo	
С	-6.637369	-5.000198	-3.105269		-30) = -6436.931627 5/def2-TZVP) = -6437		rtree
Н	-7.250834	-5.496602	-3.873766		: - D3(BJ)/def2-TZVP		
C	-6.658972	-5.447606	-1.791654	E (PBE	0 - D3(BJ)/def2-TZV	P) = -6435.13334	
H	-7.291175	-6.305081	-1.513977	E(PBE	h-3c) = -6428.31427	6683425 Hartree	
Si	3.112951	-0.856858	-0.606280		= -201.67427 Kcal		
0	2.132312	-1.879189	-1.606221		() = -375.26832  Kcal		7
C C	2.083421 2.726845	0.653496 -4.089387	-0.201197 -2.421618		7X-V/def2-TZVP) = - (1-xTB) = -241.62064		, uartree
C	2.726845	-2.681818	-2.642775		(1-xTB) = -241.62064 (2-xTB) = -236.79234		
~	,	001010	2.012//0	_ , 511	, 200.75254	III., Marcroe	

E (GFN-	FF) = -31.2511172	99767 Hartree		С	2.581587	-6.725551	1.057943
Coordin	12+00.			C H	-1.779129 -1.424627	-4.657950 -5.434620	0.379482 1.088009
Co	-0.457656	0.165330	-0.100154	H	-2.862251	-4.502309	0.551632
Si	0.418786	2.753575	0.258132	Н	-1.652692	-5.055590	-0.645969
0	0.090691	1.853944	-1.259339	С	1.348850	-5.330776	-1.071591
C	0.596645	1.219179	1.322497	H	0.880412	-4.786161	-1.901922
C	0.768432	2.385779	-3.515277	C	2.106452	-4.840761	2.585741
C	-0.225819	2.418731	-2.486413	H	1.699923	-3.833892	2.743149
C	0.443777	2.952310	-4.801626	C	2.511820	-7.305387	-0.242628
C	-1.077316	3.863178	0.530152	H	2.944992	-8.304013	-0.405063
H	-1.175671	4.557619	-0.327998	C	2.718381	-5.525164	3.626262
H H	-0.922438 -2.025969	4.453961 3.303578	1.452562	H C	2.784567 -0.912628	-5.063020 -2.545149	4.622962 2.451103
C	-1.469516	2.993921	0.634037 -2.719229	Н	-0.360386	-1.600539	2.431103
Н	-2.218389	3.009254	-1.918793	H	-1.962676	-2.391930	2.764742
C	2.053255	1.809472	-3.313770	Н	-0.475430	-3.326250	3.104523
Н	2.290137	1.389130	-2.329486	C	1.911206	-6.615051	-1.283581
С	-0.844705	3.521495	-5.012715	Н	1.864571	-7.060177	-2.289137
Н	-1.090408	3.929879	-6.004029	С	3.199682	-7.399724	2.152788
С	2.986272	1.780656	-4.340177	H	3.628860	-8.398804	1.978048
H	3.974901	1.328636	-4.168227	C	3.266337	-6.817343	3.409584
C	1.884602	3.873610	-0.081886	H	3.748901	-7.353566	4.240853
H	2.788981	3.335170	-0.416690	Si	-3.043901	-1.181528	-0.400090
H	2.123826	4.431683	0.845867	0	-3.882799	-1.886825	-1.732070
H	1.603958	4.604735	-0.867364	C	-5.793719	-3.310400	-1.988520
С	-1.778292	3.542314	-3.989948	C	-5.233954	-1.991838	-1.877176
H	-2.779329	3.964101	-4.161323	C	-7.216740	-3.449325	-2.179337
C H	1.428556 1.175826	2.907649 3.331528	-5.831025 -6.814937	C H	-3.152855 -4.171007	0.705071 1.076156	-0.527305 -0.289078
C	2.671614	2.334260	-5.609894	Н	-2.478332	1.194317	0.215084
Н	3.417655	2.334260	-6.418471	н	-2.866127	1.041542	-1.540224
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C	5.378830	2.492812	2.835419	C	-4.982546	-4.477573	-1.908303
C	4.343077	1.548662	3.158531	Н	-3.901184	-4.353445	-1.763376
C	6.624139	2.441600	3.562200	С	-8.032197	-2.281380	-2.249172
C	2.447301	-1.181501	2.203086	H	-9.116967	-2.395919	-2.395281
H	3.511002	-1.462617	2.340126	С	-5.547063	-5.740929	-2.012680
H	2.002527	-1.905698	1.491319	H	-4.908473	-6.634967	-1.947861
H	1.933747	-1.289761	3.175724	С	-4.035010	-1.689040	1.123495
C	4.557807	0.598635	4.156669	H	-4.009621	-2.776839	1.326130
H	3.754200	-0.104466	4.412403	H	-3.702566	-1.149044	2.031123
C	5.197981	3.488745	1.834881	H	-5.093207	-1.409871	0.938732
H	4.241734	3.518249	1.298450	C	-7.461584	-1.023430	-2.133072
C H	6.808556 7.762508	1.448443	4.568094 5.115720	H C	-8.092767 -7.760313	-0.123300	-2.188383
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C	3.400853	0.473394	-0.086675	Н	-7.386554	-6.890534	-2.288034
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H	4.413519	0.140475	0.222816	C	-2.362808	0.288882	-5.055189
С	5.792729	0.549379	4.852547	С	-1.186291	-0.248448	-4.427327
H	5.932670	-0.211702	5.635288	C	-2.293805	0.704241	-6.434251
C	7.631252	3.402767	3.249878	С	-1.306343	-3.387708	-3.222664
H	8.581208	3.366742	3.805986	H	-0.933122	-3.358294	-4.266944
C	7.425902	4.366627	2.273428	H	-1.014539	-4.360463	-2.781003
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Si	-0.161615	1.549793	3.006751	C	-0.023703	-0.427838	-5.177424
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C C	1.241811	4.551818	4.945671	C	-3.590785	0.417692	-4.350373
C	0.052040 1.131707	3.955919 5.361057	4.401736 6.134690	H C	-3.637753 -1.084641	0.025162 0.513404	-3.328115 -7.164097
C	-2.032553	1.269267	3.046148	Н	-1.041604	0.824058	-8.219160
Н	-2.423886	1.418945	4.072604	C	-4.703609	0.981530	-4.957489
Н	-2.253600	0.222914	2.754154	Н	-5.652258	1.055267	-4.404217
H	-2.587289	1.943019	2.364974	С	1.264069	-1.851345	-2.348143
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H	-2.084013	3.719298	4.574042	H	1.700080	-2.311111	-1.441060
C	2.517101	4.359997	4.342524	H	1.652982	-2.389498	-3.235937
H	2.582066	3.722829	3.450212	C	0.016921	-0.055350	-6.544398
C	-0.145994	5.543934	6.742344	H	0.953553	-0.198888	-7.103495
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C	3.650891	4.948086	4.886465	H	-3.399767	1.620273	-8.072674
H	4.630351	4.787393	4.411555	C	-4.628852	1.438692	-6.300641
C H	0.556491 1.647616	0.678946 0.841876	4.514282 4.595218	Н	-5.513592	1.890405	-6.775044
H H	0.342084	-0.407581	4.595218	Confo	rmation 6.		
H H	0.080526	1.129416	5.410143		plicity: 4		
C	-1.273662	4.955456	6.191263	Charg			
Н	-2.258687	5.103423	6.659936	_	-3c) = $-6436.929409$	9885716 Hartree	
C	2.318546	5.949326	6.663928		/def2-TZVP) = -6437		rtree
Н	2.238560	6.568140	7.571630		- D3(BJ)/def2-TZVE		
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H	4.454041	6.210870	6.479312		h-3c) = -6428.31843		
Si	-0.801898	-3.065308	0.641127		) = -198.38159  Kcal		
0	0.858843	-3.492207	0.387022		) = -371.42271  Kcal		
C	-1.242946	-1.666547	-0.517211		7X-V/def2-TZVP) = -		o Hartree
C C	2.015712 1.384182	-5.416466 -4.736710	1.286197 0.187967		(1-xTB) = -241.61986 (2-xTB) = -236.78999		
_	1.001102	1.750/10	0.10/50/	- (G:N	_ 112, 200.70993		

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Coordi	nates: 1.015841	-0.037062	-0.287927	H H	3.819653 3.458569	1.638685 0.258176	-3.450368 -4.526461
Si	-1.962202	-0.040221	1.046870	H	2.115050	1.236289	-3.844172
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C C	-3.299149 -5.547339	-2.123139 -2.901105	-0.142914 -0.860588	H C	4.158916 5.724773	-0.660442 3.695463	1.002580 0.512098
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H	-0.695700	-1.710995	2.473215	C	4.858400	-1.057710	-2.020349
C H	-3.186033	-3.264643	0.650932	H H	5.023377	-1.633241	-1.092562 -2.888809
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C H	-5.777326	-0.642658	-2.566110	H	7.371443	2.887678	2.515602
С	-5.868128 -3.580516	0.227391 0.860829	-3.234029 1.389814	C H	6.685618 7.406481	0.850373 0.626795	2.774004 3.574978
Н	-4.061623	1.248369	0.473028	Si	1.860168	-2.904536	-0.726978
Н	-3.379581	1.703403	2.079696	0	2.728182	-2.253476	0.662094
H	-4.297554	0.167870	1.874963	С	4.244606	-3.538394	2.059849
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H	-4.104390	-5.113131	1.336188	C	4.492155	-4.177378 -4.278221	3.332483
C H	-6.716346 -7.528044	-2.691899 -3.433294	-1.652055 -1.591607	C H	2.942374 3.271769	-4.278221 -4.956816	-1.428914 -0.615957
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Si	-1.087216	2.393025	-0.773172	С	1.992394	-2.970491	2.830748
0	-1.572779	3.732794	0.216316	H	1.020538	-2.500409	2.637291
C	-3.254328	5.427246	-0.081903	C	5.278359	-3.539639	1.081048
C C	-1.885939 -3.589324	4.995529 6.781008	-0.186044 -0.453516	H C	5.083405 3.471212	-3.056648 -4.193849	0.117002 4.326455
C	0.353878	2.941977	-1.860270	Н	3.673443	-4.683183	5.291215
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H	1.216549	3.261151	-1.247813	C	0.271973	-3.606864	-0.015391
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H C	0.138192 -4.281731	5.553412 4.559248	-0.677526 0.384991	H H	-0.241875 0.480054	-4.234960 -4.218592	-0.765671 0.884966
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C	-2.561175	7.659238	-0.905799	Н	1.452175	-3.615434	4.837736
H	-2.824759	8.690889	-1.184267	C	5.765183	-4.781765	3.556670
C	-5.594993	4.998507	0.473320	H	5.950250	-5.270044	4.526384
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C H	-2.565523 -3.505832	2.165726 1.971060	-1.917839 -1.371004	H Si	7.725800 0.605197	-5.238224 -1.777045	2.776053 -3.282399
H	-2.417519	1.372917	-2.673426	0	0.174744	-3.427543	-3.019939
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С	-1.250283	7.215896	-0.985069	C	-0.140646	-4.385812	-3.935846
H	-0.457248	7.899915	-1.323886	С	-1.845373	-5.762677	-5.087253
C	-4.950546	7.195753	-0.351595	C	1.484760	-1.746011	-4.957140 -5.669794
H C	-5.207066 -5.933068	8.227400 6.326366	-0.638972 0.098550	H H	0.894817 1.540940	-2.358816 -0.719175	-5.366436
Н	-6.977948	6.665805	0.168327	H	2.509246	-2.169533	-4.922092
Si	0.315291	1.816326	1.915877	С	0.858120	-5.046759	-4.648669
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C	-1.405873	3.934016	4.499475	C	-2.570487	-4.082919	-3.417328
C C	-0.864541 -1.363930	2.618584 4.509346	4.298221 5.821165	H C	-2.313904 -0.796312	-3.312906 -6.416024	-2.677226 -5.800041
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Н	2.018674	1.086121	3.582850	C	-3.895868	-4.423066	-3.647166
H	2.393372	0.378537	2.001690	H	-4.695281	-3.912289	-3.092881
H	1.094294	-0.333713	3.006313	С	-0.968862	-0.766659	-3.391159
C	-0.314339	1.914262	5.367472	H	-1.483853	-0.789799	-2.410012
H C	0.079724 -1.982424	0.902347 4.671892	5.197130 3.427653	H H	-0.719624 -1.658242	0.286231 -1.149434	-3.635738 -4.170460
Н	-2.001253	4.212332	2.430749	C	0.526397	-6.063778	-5.579938
C	-0.787174	3.761958	6.890746	Н	1.334919	-6.569333	-6.130071
H	-0.759493	4.206092	7.897454	С	-3.218832	-6.089930	-5.289788
С	-2.503502	5.939765	3.643870	H	-3.469493	-6.876715	-6.018435
H	-2.948730	6.496435	2.804975	C H	-4.220695	-5.433791	-4.590222
C H	1.233238 0.596419	3.440053 4.244109	1.690164 1.281260	Н	-5.275693	-5.696088	-4.762428
Н	2.123205	3.306445	1.044189	THE	MITD		
H	1.594706	3.757063	2.690358	F.OD	NIB		
C	-0.276946	2.492833	6.663083				
H	0.160524	1.916550	7.492760		rmation 18.		
C H	-1.908145 -1.880391	5.815401 6.260643	6.004542 7.011805	Multip Charge	olicity: 5		
н С	-2.465192	6.514863	4.942768		e: U -3c) = -4543.371079	9649190 Hartree	
Н	-2.879417	7.522117	5.106103		/def2-TZVP) = -4543		rtree
Si	3.131435	-0.324418	-2.117740	E(PBE	- D3(BJ)/def2-TZVI	= -4541.719550	568001 Hartree
0	2.959939	0.768499	-0.718535		) - D3(BJ)/def2-TZV		2467126 Hartree
C	1.639432	-1.366221	-1.778880		n-3c) = -4537.45663 = 211.25911 Kcal		
C C	4.815486 3.887171	1.397228 1.720007	0.720233 -0.323766		= 211.25911 Kcal/ = -4.53441 Kcal/r		
-				, .==//	/*		

E (GFN1- E (GFN2-	-xTB) = $-154.6714$	-4545.914083603027 73112078 Hartree 70400669 Hartree 57928 Hartree	Hartree	Н Н Н Н	1.013876 -3.873379 0.207167 -2.235303 -1.983242	-1.240867 -2.107679 -3.554804 -4.009521 -2.727617	3.254204 2.559671 2.861908 2.540775
0				C	-3.035242	-3.372018	-2.156876
Coordi		0.070305	0 000000				-1.470051
Fe	0.376637	-0.072395	0.898803	C	-1.351874	-3.429864	-3.208341
Si	1.117302	3.188491	0.988490	C	-3.436345	-4.673342	-1.811996
Si	-0.298077	1.479881	3.174612	C	-1.737403	-4.734603	-3.546907
Si	-1.343653	-1.020482	-1.637776	C	-2.782137	-5.359506	-2.847083
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N	0.573749	1.668078	1.669572	H	-0.533625	-2.948196 -5.157245	-3.768839
N C	0.115505 -0.196318	-1.131469 3.844085	-0.673439 -0.207103	H H	-4.260538 -1.218128	-5.157245	-1.264590 -4.356595
C	-0.658339	5.177688	-0.203694	н	-3.085954	-6.384755	-3.109229
C	-1.663762	5.596072	-1.091080	C	-1.016960	-0.038247	-3.231240
C	-2.216096	4.689395	-2.010937	C	-2.024863	0.088617	-4.214793
C	-1.765089	3.359242	-2.037548	C	0.204162	0.633201	-3.447379
C	-0.774702	2.948788	-1.133657	C	-1.824485	0.872086	-5.362165
C	2.711717	2.858866	0.004651	Ċ	0.413493	1.418274	-4.592178
C	3.965969	2.821081	0.655634	C	-0.603735	1.542549	-5.551002
C	5.135072	2.453159	-0.028983	Н	-2.984673	-0.439154	-4.084049
C	5.074324	2.116475	-1.390966	Н	0.997287	0.547493	-2.690346
С	3.844384	2.176235	-2.065680	Н	-2.623072	0.960340	-6.115333
С	2.680631	2.552780	-1.375133	Н	1.372615	1.941216	-4.734106
C	1.460531	4.469275	2.335968	Н	-0.446353	2.160762	-6.448276
C	-1.744061	2.688311	3.326833				
С	-2.076229	3.312759	4.550462		rmation 2.		
С	-3.135156	4.231259	4.631769	Multi	plicity: 5		
С	-3.882518	4.544591	3.484865	Charg			
С	-3.568647	3.935472	2.259241		-3c) = -4543.368423		
C	-2.510096	3.018041	2.184504		/def2-TZVP) = -4543		
С	-2.705035	-0.142701	-0.662276		- D3(BJ)/def2-TZVE		
C	2.505795	-1.876210	0.701584	•	0 - D3(BJ)/def2-TZ\	,	3654015 Hartree
C	2.991122	-0.575535	1.000022	•	h-3c) = -4537.45673		
C	3.596891	-0.297312	2.241713		) = 209.06869 Kcal/		
C	3.758851	-1.318059	3.188090		) = -3.64883  Kcal/n		0
C C	3.330463	-2.625395	2.887811	•	7X-V/def2-TZVP) = -		2 Hartree
C	2.708358 2.616330	-2.896229 -1.681294	1.660341 -2.363718		1-xTB) = $-154.668702-xTB$ ) = $-153.62570$		
Н	-0.239350	5.904063	0.510795		-FF) = -21.59418489		
H	-2.018944	6.638165	-1.065003	E (GIN	-FF) = -21.59410403	77013 Haltiee	
H	-2.998721	5.020651	-2.711026	Coord	inates:		
Н	-2.178098	2.636623	-2.758431	Fe	0.631272	-0.563765	0.017905
Н	-0.447543	1.897417	-1.142957	Si	-0.288124	2.626766	-0.557936
Н	4.034226	3.077917	1.725798	Si	2.567212	1.390641	-0.489757
H	6.098653	2.423612	0.503083	Si	-0.475642	-3.566304	-0.324298
Н	5.987396	1.817417	-1.928128	Si	-1.317444	-1.743247	2.021299
H	3.791154	1.932155	-3.138512	N	0.819029	1.267384	-0.445150
H	1.728073	2.613376	-1.922895	N	-0.409671	-2.055397	0.557942
H	2.233156	4.108297	3.044478	С	-1.604740	2.237051	-1.867608
H	0.539289	4.682247	2.915942	С	-1.290077	1.377998	-2.943028
H	1.822956	5.420965	1.896729	С	-2.218113	1.105699	-3.960655
H	-1.495476	3.084157	5.458675	С	-3.487310	1.704646	-3.925406
H	-3.376095	4.709070	5.594153	C	-3.816078	2.575946	-2.873871
H	-4.708938	5.269587	3.546204	C	-2.883459	2.836859	-1.856897
H	-4.139746	4.183563	1.351469	C	0.654015 0.701777	4.157994	-1.181600
H H	-2.261175 -3.040552	2.568505 -0.756142	1.211643 0.195998	C C	1.448725	4.457033 5.541495	-2.563292 -3.048837
Н	-3.577148	0.055994	-1.317951	C	2.161560	6.358704	-2.156265
H	-2.357138	0.830558	-0.263064	C	2.117816	6.087381	-0.779649
H	2.945941	0.030336	0.245637	C	1.369521	5.000634	-0.300249
Н	3.945828	0.723220	2.453960	Č	-1.114763	3.014807	1.091273
Н	4.232293	-1.101719	4.158205	Č	3.247208	2.544893	0.840331
H	3.474820	-3.433167	3.622063	C	2.607209	2.604132	2.099023
H	2.359332	-3.917204	1.437367	C	3.065285	3.472301	3.102185
H	2.073736	-1.744165	-3.328294	С	4.179403	4.294673	2.865264
H	3.505517	-2.342602	-2.415020	C	4.832691	4.242174	1.623048
H	2.981417	-0.641511	-2.239727	C	4.367498	3.375106	0.621726
C	0.816903	1.563760	4.697556	С	0.585058	-4.912764	0.473077
H	1.671972	0.870998	4.559915	С	-0.262869	-0.579420	3.095790
H	1.223705	2.585277	4.839334	С	-0.800871	0.552894	3.747971
H	0.278960	1.268661	5.621575	С	-0.032137	1.301609	4.653490
С	1.085238	-4.003171	-1.007358	С	1.293120	0.925932	4.929274
C	-0.005499	-4.514910	-0.268949	C	1.852959	-0.185006	4.278368
C	1.829728	-4.904288	-1.799500	С	1.081883	-0.926486	3.369676
C	-0.342198	-5.874549	-0.318794	C	-1.630888	-3.312737	3.031163
C	1.497349	-6.267823	-1.854427	H	-0.288449	0.921494	-2.972304
C H	0.409712 -0.616119	-6.755209 -3.825424	-1.113649 0.332194	H H	-1.953821 -4.219914	0.423312 1.495776	-4.783719 -4.720106
H H	2.682334	-3.825424 -4.539082	-2.393981	н Н	-4.219914 -4.808577	3.052086	-2.844570
н Н	-1.207584	-6.246740	0.251072	H H	-3.163001	3.516958	-1.036411
н	2.087748	-6.952723	-2.482937	н	0.140794	3.829041	-3.274182
Н	0.142491	-7.822277	-1.161496	Н	1.471181	5.753256	-4.129147
C	-0.962785	-0.302149	2.984174	Н	2.747072	7.211197	-2.534505
C	-2.345440	-0.591821	2.830454	Н	2.674637	6.721288	-0.072447
C	-0.048991	-1.400279	3.007316	H	1.362114	4.798857	0.782043
C	-2.796856	-1.906706	2.674718	H	-0.357717	3.260196	1.862298
С	-0.513082	-2.724281	2.842928	H	-1.694620	2.140984	1.447672
С	-1.877645	-2.976240	2.668190	H	-1.802831	3.879720	0.999359
H	-3.069647	0.238230	2.830640	H	1.731409	1.965915	2.296132

Н	2.548233	3.505569	4.073421	С	5.888413	1.486701	-0.329585
H	4.540892	4.976614	3.650891	С	4.651430	0.842693	-0.179003
H	5.706550	4.884688	1.432484	C	1.699327	-1.447589	-2.533152
H	4.879746	3.359158	-0.353131	C	1.584508	-0.827247	-3.800146
H	1.617091	-4.538652	0.617061	С	1.152994	-1.542693	-4.927568
Н	0.628246	-5.837768	-0.137845	C	0.808216	-2.899695	-4.809016
H	0.175941	-5.181295	1.467522	С	0.902754	-3.531748	-3.559531
H	-1.845039	0.845253	3.551772	С	1.349338	-2.814307	-2.437274
H	-0.471506	2.179137	5.153085	С	2.366076	-1.651340	0.459355
H	1.893170	1.501850	5.650486	С	0.933128	2.939832	-2.739238
H	2.895468	-0.475040	4.482285	Č	0.080723	2.171088	-3.563176
H	1.529797	-1.801524	2.870801	С	-0.069137	2.457671	-4.927826
H	-2.251236	-4.034330	2.462275	С	0.646931	3.520607	-5.502537
H	-2.154197	-3.070851	3.978258	C	1.507612	4.291059	-4.703939
H	-0.669281	-3.796296	3.295980	С	1.645532	4.003780	-3.335972
С	3.262294	1.803553	-2.191758	C	-4.200354	-2.112060	1.388829
Н			-2.953180				
	2.817367	1.130678		С	-1.446355	-1.595470	4.300251
H	3.016651	2.846661	-2.474382	С	-0.137192	-2.067475	4.553789
H	4.363142	1.672319	-2.219920	C	0.085041	-3.251387	5.273570
C	-2.978319	-0.894467	1.684199	С	-1.004369	-3.989872	5.764132
С	-3.193059	-0.120212	0.522748	С	-2.311696	-3.530177	5.541606
C	-4.049563	-1.022947	2.597343	C	-2.525847	-2.343828	4.821135
C	-4.431139	0.492728	0.274094	С	-3.368749	0.749959	3.678487
С	-5.289294	-0.409823	2.359186	H	4.030083	0.060357	-3.450929
C	-5.482900	0.346839	1.192987	H	6.209770	1.220164	-3.730550
H	-2.381583	-0.001766	-0.214814	H	7.418898	2.139834	-1.733538
Н	-3.920986	-1.620333	3.513983	Н	6.416870	1.878439	0.553633
H	-4.569708	1.082290	-0.643844	H	4.223757	0.745368	0.832465
H	-6.109328	-0.530363	3.084121	H	1.817120	0.242680	-3.910763
H	-6.456460	0.823207	0.999213	H	1.075850	-1.033819	-5.901576
С	3.094266	-0.395688	-0.027465	H	0.463661	-3.462670	-5.690304
C	3.707451	-0.711098	1.214766	H	0.620697	-4.590009	-3.449615
С	2.948069	-1.445351	-0.980285	H	1.398901	-3.333929	-1.467320
C	4.137831	-2.011606	1.502278	H	1.372787	-2.070982	0.716958
C	3.388321	-2.752893	-0.690645	H	2.765237	-1.132184	1.353814
C	3.976468	-3.035791	0.548390	H	3.045458	-2.497997	0.234014
Н	3.844618	0.086746	1.960472	H	-0.459280	1.313217	-3.134309
Н	2.552332	-1.233829	-1.986344	Н	-0.741472	1.840885	-5.545461
H	4.609653	-2.232499	2.472434	H	0.538495	3.747653	-6.574481
H	3.272924	-3.541921	-1.447579	H	2.077234	5.120500	-5.151212
H	4.325560	-4.056033	0.770915	H	2.326045	4.619704	-2.726810
С	0.173348	-3.202957	-2.073705	H	-4.020989	-2.574231	2.380237
C	-0.056025	-1.941279	-2.668520	Н	-4.743590	-2.848531	0.762753
C	0.920171	-4.147670	-2.811320	H	-4.849076	-1.223963	1.528411
С	0.464556	-1.622624	-3.933950	H	0.728652	-1.498098	4.178937
C	1.444157	-3.838608	-4.076924	H	1.114057	-3.599050	5.455236
С	1.224272	-2.569742	-4.638115	H	-0.833642	-4.920948	6.326404
Н	-0.656149	-1.185318	-2.130212	Н	-3.170035	-4.098922	5.932067
Н	1.113769	-5.144663	-2.383865	Н	-3.560077	-1.996802	4.663245
H	0.279177	-0.630652	-4.373481	H	-3.514766	1.651355	3.050628
H	2.030068	-4.590086	-4.628970	H	-3.396101	1.046519	4.746979
H	1.638475	-2.321116	-5.627118	H	-4.222156	0.067549	3.494701
С	-2.261307	-4.192332	-0.448544	C	2.460037	3.516769	-0.129679
Ċ	-2.631203	-5.497825	-0.054537	Н	2.568392	3.281388	0.946159
C	-3.277696	-3.330304	-0.919665	H	3.421882	3.291434	-0.630211
С	-3.966222	-5.928002	-0.124972	H	2.255138	4.602780	-0.228745
C	-4.613943	-3.750119	-0.984656	С	-0.305928	1.144858	3.520059
C	-4.960723	-5.052180	-0.588200	С	-0.437205	2.258594	4.378424
H	-1.865570	-6.195129	0.321917	С	0.950461	0.933827	2.904402
Н	-3.024236	-2.304774	-1.229930	C	0.637869	3.130334	4.610679
H	-4.232041	-6.949784	0.188734	C	2.031909	1.800660	3.133733
H	-5.389889	-3.052799	-1.337233	С	1.877466	2.902375	3.988772
H	-6.008972	-5.384977	-0.638550	H	-1.402298	2.456510	4.871063
				H	1.093007	0.067962	2.235819
Conform	ation 21.			Н	0.510399	3.994558	5.281238
	icity: 5			H	2.999948	1.610767	2.645303
Charge:				H	2.723108	3.583065	4.171886
	c) = $-4543.36709$			С	-0.584517	2.971117	-0.016266
E(M06/d	lef2-TZVP) = -454	3.371282237613 Ha:	rtree	С	-1.836927	2.529485	-0.550391
E(PBE -	D3(BJ)/def2-T7.V	$^{7}P) = -4541.7173945$	545529 Hartree	С	-0.613124	3.763676	1.164692
E (PBEO	- D3(BJ)/def2-T7	(VP) = -4542.042593	3890112 Hartree	С	-3.050932	2.861696	0.092114
		05720653 Hartree	JOJUITE HUICICE	C	-1.819382	4.094453	1.788508
	= 217.16784 Kcal			С	-3.043072	3.640654	1.253661
E(PM7)	= -3.22646 Kcal/	mol		H	-1.884732	2.017151	-1.525420
E(ωB97X	-V/def2-TZVP) =	-4545.913271856990	) Hartree	H	0.332949	4.107872	1.609815
		58260097 Hartree		H	-4.000569	2.517120	-0.342375
		63228533 Hartree		Н	-1.810430	4.703642	2.705004
E (GFN-F	F) = -21.4561727	01/02 Hartree		H	-3.991824	3.909791	1.743187
				С	-1.540385	-3.255184	0.349321
Coordin	ates:			C	-0.594171	-3.642996	1.324090
Fe	-0.549608	0.606329	0.378808	С	-1.737662	-4.112828	-0.757062
Si	2.234839	-0.462468	-1.002214	C	0.137688	-4.834043	1.197152
			-0.898110		-1.009546		-0.890033
Si	1.061394	2.516232		C		-5.305936	
Si	-2.545359	-1.663011	0.591133	С	-0.065240	-5.667529	0.085371
Si	-1.732991	-0.067501	3.204537	H	-0.431214	-3.002997	2.204190
N	1.062057	0.786006	-0.626295	H	-2.466298	-3.841473	-1.538056
N	-1.645314	-0.478986	1.510025	Н	0.869291	-5.111011	1.972389
C	3.942445	0.327563	-1.290134	H	-1.179784	-5.957165	-1.761913
C					0.507340		
	4.536362	0.470396	-2.564019	H		-6.602377	-0.019209
С	5.771816	1.119070	-2.725282	С	-2.862120	-0.918637	-1.132236
С	6.449796	1.632316	-1.608913	С	-1.930886	-1.077062	-2.185871

С							
	-4.036486	-0.175815	-1.398606	H	3.208954	3.048837	2.008112
C	-2.166179	-0.520838	-3.455184	H	4.212877	1.627799	2.462404
С	-4.268546	0.397996	-2.657642	С	0.549000	-1.275897	-4.004023
C	-3.331781	0.223765	-3.691512	C	1.577735	-0.884494	-4.892528
Н	-1.010431	-1.659181	-2.029483	Č	-0.785774	-1.104063	-4.433789
H	-4.788214	-0.041303	-0.604080	Č	1.287046	-0.329917	-6.149856
H	-1.428616	-0.681483	-4.255650	C	-1.085287	-0.543095	-5.684498
H	-5.188887	0.974893	-2.839163	C	-0.048060	-0.150218	-6.545123
H	-3.515716	0.662360	-4.684577	Н	2.632164	-1.003303	-4.596500
	0.010/10	0.002000	1.001077	Н	-1.618391	-1.391676	-3.774913
Conforma	ation 23.			Н	2.106897	-0.029536	-6.820880
Multipli				H	-2.135734	-0.404405	-5.983168
Charge:	4			H	-0.280002	0.294340	-7.525309
_	c) = -4543.36725	6545556 Hartroo		C	2.117357	-0.854246	2.129496
		3.369366511494 Hai	rtroo	C	1.113613	-1.802172	2.503030
		P) = -4541.7159284		C	3.372454	-1.360851	1.694178
		VP) = -4542.041236		C	1.365231	-3.189816	2.404426
		76490443 Hartree	JOUUTIZ HAICIEE	C	3.616062	-2.735386	1.609450
	= 224.33014 Kcal			C	2.605561	-3.655182	1.956263
	= -5.19854 Kcal/			Н	0.178586	-1.469704	2.987016
		-4545.914275737952	) Hartree	H	4.170981	-0.656249	1.414835
		88547662 Hartree	. Hartree	H	0.584167	-3.900018	2.709381
		01352972 Hartree		H	4.597572	-3.100148	1.269845
	F(x) = -21.5863692			H	2.798099	-4.736484	1.887043
E (GIN II	21.3003032	DI/II HAICIEE		C	-3.016323	-0.617987	-1.477232
Coordina	+os•			C	-4.421479	-0.716849	-1.352515
Fe	0.293224	-0.557382	0.489965	C	-2.480987	0.563092	-2.032341
re Si	-0.318058	2.729944	0.489965	C	-5.258958	0.328572	-2.032341
Si	1.780039	1.025225	2.289629	C	-3.312116	1.613521	-2.454939
Si	-1.872455	-1.998980	-0.863010	C	-4.704229	1.496334	-2.323275
Si	0.961984	-1.995329	-2.294669	Н	-4.873194	-1.621012	-0.910502
N	0.435890	1.209398	1.179754	п Н	-1.391202	0.662469	-2.133541
N N	-0.190058	-1.555752	-1.055108	H H	-6.351024	0.862469	-2.133541
C	-0.190038	3.061257	-1.117022	н Н	-2.861186	2.524295	-2.877424
C	0.653506	2.161943	-1.939623	H	-5.362057	2.317095	-2.649121
C	0.783972	2.376736	-3.320990	C	-2.161989	-2.092119	1.022767
C	0.703372	3.518696	-3.904201	C	-2.577775	-0.944148	1.740570
C	-0.479728	4.441013	-3.101816	C	-1.968617	-3.289527	1.750625
C	-0.614006	4.210426	-1.723668	C	-2.769602	-0.983897	3.132053
C	0.487958	4.153474	1.698071	C	-2.165735	-3.337057	3.132033
C	1.484314	4.963825	1.106250	C	-2.556343	-2.179572	3.835401
C	2.140991	5.963049	1.842084	Н	-2.776670	-0.008795	1.197252
Ċ	1.810454	6.173110	3.190980	Н	-1.654432	-4.203026	1.219822
С	0.815074	5.388071	3.794548	H	-3.101399	-0.079832	3.665761
С	0.159662	4.393795	3.052190	H	-2.015207	-4.281019	3.686096
С	-2.173903	2.718836	1.088950	H	-2.703954	-2.214031	4.925695
С	1.242461	1.408441	4.062429				
С	-0.085119	1.121742	4.451606	Conform	nation 24.		
C	-0.541386	1.412067	5.745658	Multipl	icity: 5		
	0.011000	1.112007			itorcy. o		
C	0.326904	2.005722	6.677151	Charge:	: 0		
C	0.326904 1.650081	2.005722 2.298124	6.677151 6.308429	Charge: E(B97-3	: 0 3c) = -4543.361856		
C C	0.326904 1.650081 2.102091	2.005722 2.298124 1.997789	6.677151 6.308429 5.013433	Charge: E(B97-3 E(M06/c	: 0 3c) = -4543.361856 def2-TZVP) = -4543	3.365468626444 Ha	
C C	0.326904 1.650081 2.102091 -2.351934	2.005722 2.298124 1.997789 -3.640660	6.677151 6.308429 5.013433 -1.660069	Charge: E(B97-3 E(M06/c E(PBE -	: 0 Bc) = -4543.361856 def2-TZVP) = -4543 - D3(BJ)/def2-TZVP	3.365468626444 Ha P) = -4541.711997	926952 Hartree
C C C	0.326904 1.650081 2.102091 -2.351934 1.006242	2.005722 2.298124 1.997789 -3.640660 -3.887921	6.677151 6.308429 5.013433 -1.660069 -2.434027	Charge: E(B97-3 E(M06/c E(PBE - E(PBE0	: 0 8c) = -4543.361856 def2-TZVP) = -4543 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI	3.365468626444 Ha P) = -4541.711997 JP) = -4542.03706	926952 Hartree
0 0 0 0	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414	Charge: E(B97-3 E(M06/c E(PBE - E(PBE0 E(PBEh-	0 = -4543.361856 def2-TZVP) = -4543 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI -3c) = -4537.44783	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree	926952 Hartree
000000	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500	Charge: E(B97-3 E(M06/c E(PBE - E(PBE0 E(PBEh- E(PM6)	0 0 8c) = -4543.361856 def2-TZVP) = -454'. - D3(BJ)/def2-TZV'. - D3(BJ)/def2-TZ'. -3c) = -4537.4478'. = 215.50676 Kcal/.	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree /mol	926952 Hartree
C C C C C C	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208	Charge: E(B97-3 E(M06/c E(PBE - E(PBE0 E(PBEh- E(PM6) E(PM7)	: 0 8c) = -4543.361856 def2-TzVP) = -454: - D3(BJ)/def2-TzVI - D3(BJ)/def2-TzVI - 3c) = -4537.4478: = 215.50676 Kcal/r = -3.31226 Kcal/r	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree /mol	926952 Hartree 9662785 Hartree
C C C C C C	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196	Charge: E(B97-3 E(M06/c E(PBE - E(PBE0 E(PBEh- E(PM6) E(PM7) E(ωB97)	: 0 - (36)	3.365468626444 Ha P) = -4541.711997 PP) = -4542.03706 33398744 Hartree /mol nol -4545.91257766085	926952 Hartree 9662785 Hartree
C C C C C C C	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683	Charge: E (B97-3 E (M06/c E (PBE - E (PBE0 E (PBEh- E (PM6) E (PM7) E (WB97X E (GFN1-	0 0 3c) = -4543.361856 def2-TZVP) = -4542 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI -3c) = -4537.44783 = 215.50676 Kcal/ = -3.31226 Kcal/r (-V/def2-TZVP) = -4XTB) = -154.66613	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree /mol mol -4545.91257766085 39085289 Hartree	926952 Hartree 9662785 Hartree
0 0 0 0 0 0 0 0 0	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232	Charge: E (B97-3 E (M06/c E (PBE - E (PBE0- E (PBE0- E (PM6) E (GFN1- E (GFN1- E (GFN2-	0 0 3c) = -4543.361856 lef2-TZVP) = -4543 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI -3c) = -4537.44783 = 215.50676 Kcal/ = -3.31226 Kcal/f (-V/def2-TZVP) = - -xTB) = -154.66613 -xTB) = -153.62568	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree  /mol nol -4545.91257766085 39085289 Hartree 52613226 Hartree	926952 Hartree 9662785 Hartree
С С С С С С С С С С С С С С С С С С С	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744	Charge: E (B97-3 E (M06/c E (PBE - E (PBE0- E (PBE0- E (PM6) E (GFN1- E (GFN1- E (GFN2-	0 0 3c) = -4543.361856 def2-TZVP) = -4542 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI -3c) = -4537.44783 = 215.50676 Kcal/ = -3.31226 Kcal/r (-V/def2-TZVP) = -4XTB) = -154.66613	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree  /mol nol -4545.91257766085 39085289 Hartree 52613226 Hartree	926952 Hartree 9662785 Hartree
С С С С С С С С С С С С С С С С С С С	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202	Charge: E (B97-3 E (M06/c E (PBE - E (PBE) - E (PM6) E (PM7) E (B972- E (GFN2- E (GFN-F	0 0 8c) = -4543.361856 def2-TZVP) = -4543. - D3(BJ)/def2-TZV1 - D3(BJ)/def2-TZV1 -3c) = -4537.44783 = 215.50676 Kcal/r -V/def2-TZVP) = - -VTB) = -154.66613 -VTB) = -153.62563 -VF) = -21.58421891	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree  /mol nol -4545.91257766085 39085289 Hartree 52613226 Hartree	926952 Hartree 9662785 Hartree
С С С С С С С С С С С С Н Н Н	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470 3.687431	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202 -4.988117	Charge: E (B97-3 E (M06/c E (PBE - E (PBE0-E) E (PM6) E (PM7) E (\omega B97\omega E) E (GFN1-E) Coordin	3c) = -4543.361856 def2-TZVP) = -4543 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - 3c) = -4537.44783 = 215.50676 Kcal/r - V/def2-TZVP) = -454.66613 - XTB) = -153.62565 FF) = -21.58421891	3.365468626444 Ha P) = -4541.711997 PP) = -4542.03706 33398744 Hartree /mol mol -4545.91257766085 39085289 Hartree 52613226 Hartree 18269 Hartree	926952 Hartree 9662785 Hartree 6 Hartree
С С С С С С С С С С С Н Н Н Н Н Н	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728 0.307233	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470 3.687431 5.341002	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202 -4.988117 -3.554884	Charge: E(B97-3 E(M06/c) E(PBE-6 E(PBE0) E(PBEh-6 E(PM7) E(GFN1-6 E(GFN2-6 Coordin	3c) = -4543.361856 def2-TZVP) = -4542 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI -3c) = -4537.44783 = 215.50676 Kcal, = -3.31226 Kcal, = -3.31226 Kcal, = V-V/def2-TZVP) = -4.000000000000000000000000000000000000	3.365468626444 Ha P) = -4541.711997 PP) = -4542.03706 333398744 Hartree /mol nol -4545.91257766085 39085289 Hartree 22613226 Hartree 18269 Hartree	926952 Hartree 9662785 Hartree 6 Hartree -0.539992
С С С С С С С С С С С С С Н Н Н Н Н Н Н	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728 0.307233 -0.924351 -1.166439	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470 3.687431 5.341002 4.940860	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202 -4.988117 -3.554884 -1.109231	Charge: E (B97-3 E (M06/c E (PBE o E (PBE o E (PBE o E (PBE o E (PM7) E (GB97X E (GFN1-E (GFN2-E (GFN-E GFN-E GFN-E GFN-E GFN-E GFN-E GFN-E GFN-E Si	0 0 3c) = -4543.361856 lef2-TZVP) = -4542 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI -3c) = -4537.44783 = 215.50676 Kcal/e = -3.31226 Kcal/f (-V/def2-TZVP) = -2.2TB) = -154.66613 -2.TB) = -153.62568 FF) = -21.58421891 mates: 0.495859 -0.565781	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree mol mol 4545.91257766085 39085289 Hartree 22613226 Hartree 18269 Hartree  0.118908 -2.863932	926952 Hartree 9662785 Hartree 6 Hartree -0.539992 0.145283
С С С С С С С С С С С С С Н Н Н Н Н Н Н	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728 0.307233 -0.924351 -1.166439 1.754040	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470 3.687431 5.341002 4.940860 4.804079	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202 -4.988117 -3.554884 -1.109231 0.049628	Charge: E (B97-3 E (M06/c E (PBE - E (PBE0-E (PBE0-E (PM7)) E (\omega B97x) E (GFN1-E (GFN2-E (GFN-F Coording Fe Si Si	0 0 8c) = -4543.361856 lef2-TZVP) = -4544 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI -3c) = -4537.44783 = 215.50676 Kcal/r (-V/def2-TZVP) = - -xTB) = -154.66613 -xTB) = -153.62568 FF) = -21.58421893 nates: 0.495859 -0.565781 -0.688596	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree Vmol mol -4545.91257766085 39085289 Hartree 52613226 Hartree 8269 Hartree 0.118908 -2.863932 -1.340070	926952 Hartree 9662785 Hartree 6 Hartree -0.539992 0.145283 -2.658982
С С С С С С С Н Н Н Н Н Н Н Н Н Н Н Н Н	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728 0.307233 -0.924351 -1.166439 1.754040 2.915557	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470 3.687431 5.341002 4.940860 4.804079 6.580993	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202 -4.988117 -3.554884 -1.109231 0.049628 1.361450	Charge: E(B97-3 E(M06/c E(PBE- E(PBE0) E(PBEh- E(PM6)) E(GFN1- E(GFN2- E(GFN-F  Coordin Fe Si Si Si	3c) = -4543.361856 def2-TZVP) = -4543 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - C4537.44783 = 215.50676 Kcal/r - V/def2-TZVP) = -45466613 - XTB) = -153.62567 FF) = -21.58421893  mates:  0.495859 -0.565781 -0.688596 -0.569655	3.365468626444 Ha P) = -4541.711997 P) = -4542.03706 33398744 Hartree fmol mol -4545.91257766085 39085289 Hartree 52613226 Hartree 18269 Hartree  0.118908 -2.863932 -1.340070 2.186997	926952 Hartree 9662785 Hartree 6 Hartree -0.539992 0.145283 -2.658982 1.501566
C C C C C C C H H H H H H H H H H H H H	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728 0.307233 -0.924351 -1.166439 1.754040 2.915557 2.327652	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470 3.687431 5.341002 4.940860 4.804079 6.580993 6.952590	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202 -4.988117 -3.554884 -1.109231 0.049628 1.361450 3.771846	Charge: E(B97-3 E(M06/c E(PBE- E(PBE0) E(PBEh- E(PM6) E(FM7) E(GFN1- E(GFN2- E(GFN-F Coording Fe Si Si Si	3c) = -4543.361856 def2-TZVP) = -4542 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI -3c) = -4537.44783 = 215.50676 Kcal, = -3.31226 Kcal, (-V/def2-TZVP) = -4754.66613	3.365468626444 Ha P) = -4541.711997 PP) = -4542.03706 33398744 Hartree  /mol mol -4545.91257766085 39085289 Hartree 52613226 Hartree 18269 Hartree  0.118908 -2.863932 -1.340070 2.186997 1.760730	926952 Hartree 9662785 Hartree 6 Hartree -0.539992 0.145283 -2.658982 1.501566 1.173960
С С С С С С С С С С С Н Н Н Н Н Н Н Н Н	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728 0.307233 -0.924351 -1.166439 1.754040 2.915557 2.327652 0.551315	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470 3.687431 5.341002 4.940860 4.804079 6.580993 6.952590 5.544237	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202 -4.988117 -3.554884 -1.109231 0.049628 1.361450 3.771846 4.851933	Charge: E(B97-3 E(M06/c) E(PBE-6 E(PBE-6 E(PM6)) E(PM7) E(GFN1-6 E(GFN2-6 Coordin Fe Si Si Si N	10 0 13c) = -4543.361856 1def2-TZVP) = -4542 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI -3c) = -4537.44783 = 215.50676 Kcal, = -3.31226 Kcal, = -7.31226 Kcal, = -7.3126 Kcal, = -7.31226 K	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree /mol mol 4545.91257766085 39085289 Hartree 22613226 Hartree 18269 Hartree 0.118908 -2.863932 -1.340070 2.186997 1.760730 -1.601696	926952 Hartree 9662785 Hartree 6 Hartree -0.539992 0.145283 -2.65892 1.501566 1.173960 -1.005788
C C C C C C C H H H H H H H H H H H H H	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728 0.307233 -0.924351 -1.166439 1.754040 2.915557 2.327652 0.551315 -0.608503	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470 3.687431 5.341002 4.940860 4.804079 6.580993 6.952590 5.544237 3.781276	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202 -4.988117 -3.554884 -1.109231 0.049628 1.361450 3.771846 4.851933 3.549522	Charge: E (B97-3 E (M06/c E (PBE o E (PM7) E (GFN1-E (GFN2-E (GFN-E o E (GFN-E o E (GFN o E (	10 0 10 0 10 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree  mol mol -4545.91257766085 39085289 Hartree 52613226 Hartree 18269 Hartree  0.118908 -2.863932 -1.340070 2.186997 1.760730 -1.601696 1.490376	926952 Hartree 9662785 Hartree 6 Hartree -0.539992 0.145283 -2.658982 1.501566 1.173960 -1.005788 0.734852
С С С С С С С Н Н Н Н Н Н Н Н Н Н Н Н Н	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728 0.307233 -0.924351 -1.166439 1.754040 2.915557 2.327652 0.551315 -0.608503 -2.375801	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470 3.687431 5.341002 4.940860 4.804079 6.580993 6.952590 5.544237 3.781276 2.438198	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202 -4.988117 -3.554884 -1.109231 0.049628 1.361450 3.771846 4.851933 3.549522 2.142542	Charge: E(B97-3 E(M06/c E(PBE- E(PBE0) E(PBEh- E(PM6)) E(GFN1- E(GFN2- E(GFN-F  Coordin Fe Si Si Si Si N N C	3c) = -4543.361856 def2-TZVP) = -4543. def2-TZVP) = -4543 D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - C4537.44783 = 215.50676 Kcal/r (-V/def2-TZVP) = -4543.66613 XTB) = -154.66613 XTB) = -153.62565 FF) = -21.58421893  mates:  0.495859 -0.565781 -0.688596 -0.569655 2.516335 -0.166181 0.837062 0.120421	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree Vmol mol mol -4545.91257766085 39085289 Hartree 62613226 Hartree 62613226 Hartree 6269 Hartree 70.118908 62.863932 61.340070 62.186997 61.760730 61.601696 61.490376 64.534007	926952 Hartree 9662785 Hartree 6 Hartree -0.539992 0.145283 -2.658982 1.501566 1.173960 -1.005788 0.734852 -0.437425
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СССССССНННННННН	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728 0.307233 -0.924351 -1.166439 1.754040 2.915557 2.327652 0.551315 -0.608503 -2.375801 -2.693674 -2.693674	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470 3.687431 5.341002 4.940860 4.804079 6.580993 6.952590 5.544237 3.781276 2.438198 2.004272 3.723303	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202 -4.988117 -3.554884 -1.109231 0.049628 1.361450 3.771846 4.851933 3.549522 2.142542 0.419911 0.910490	Charge: E(B97-3 E(M06/c) E(PBE-6 E(PBE0) E(PBEh-E(PM6)) E(GFN1-E(GFN2-E(GFN-E) Coordin Fe Si Si Si N N C C C C	10 0 13c) = -4543.361856 1def2-TZVP) = -4542 1-D3(BJ)/def2-TZVI 1-D3(BJ)/def2-TZVI 1-3c) = -4537.44783 1= 215.50676 Kcal, 1= -3.31226 Kcal, 1-3.31226 Ccal, 1-	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree /mol mol 14545.91257766085 39085289 Hartree 18269 Hartree 18269 Hartree  0.118908 -2.863932 -1.340070 2.186997 1.760730 -1.601696 1.490376 -4.534007 -4.594910 -5.821847	926952 Hartree 9662785 Hartree 6 Hartree -0.539992 0.145283 -2.658982 1.501566 1.173960 -1.005788 0.734852 -0.437425 -1.353168 -1.739111
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СССССССННННННННН	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728 0.307233 -0.924351 -1.166439 1.754040 2.915557 2.327652 0.551315 -0.608503 -2.693674 -2.693674 -2.698500 -0.777321	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470 3.687431 5.341002 4.940860 4.804079 6.580993 6.952590 5.544237 3.781276 2.438198 2.004272 3.723303 0.685352	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202 -4.988117 -3.554884 -1.109231 0.049628 1.361450 3.771846 4.851933 3.549522 2.142542 0.419911 0.910490 3.714923	Charge: E(B97-3 E(M06/c) E(PBE-6 E(PBE0-6 E(PBE0-6 E(PM7) E(M97) E(GFN1-6 E(GFN-6 Coordin Fe Si Si Si N N C C C C C	10 0 13c) = -4543.361856 1def2-TZVP) = -4542 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI -3c) = -4537.44783 = 215.50676 Kcal, = -3.31226 Kcal, = -7.31226	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree  mol mol -4545.91257766085 39085289 Hartree 52613226 Hartree 18269 Hartree  0.118908 -2.863932 -1.340070 2.186997 1.760730 -1.601696 1.490376 -4.534007 -4.594910 -5.821847 -7.020327	926952 Hartree 9662785 Hartree 6 Hartree -0.539992 0.145283 -2.658982 1.501566 1.173960 -1.005788 0.734852 -0.437425 -1.353168 -1.739111 -1.209540
ССССССНННННННННН	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728 0.307233 -0.924351 -1.166439 1.754040 2.915557 2.327652 0.551315 -0.608503 -2.693674 -2.608500 -0.777321 -1.580718	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470 3.687431 5.341002 4.940860 4.804079 6.580993 6.952590 5.544237 3.781276 2.438198 2.004272 3.723303 0.685352 1.181731	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202 -4.988117 -3.554884 -1.109231 0.049628 1.361450 3.771846 4.851933 3.549522 2.142542 0.419911 0.910490 3.714923 6.029333	Charge: E(B97-3 E(M06/c E(PBE- E(PBE0) E(PBEh- E(PM6)) E(GFN1- E(GFN2- E(GFN-F  Coordin Fe Si Si Si Si N C C C C C	10	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree Vmol mol mol -4545.91257766085 39085289 Hartree 2.613226 Hartree 1.8269 Hartree 1.8269 Hartree 1.8269 Hartree 1.863932 -1.340070 2.186997 1.760730 -1.601696 1.490376 -4.534007 -4.594910 -5.821847 -7.020327 -6.982930	926952 Hartree 9662785 Hartree 6 Hartree -0.539992 0.145283 -2.658982 1.501566 1.173960 -1.005788 0.734852 -0.437425 -1.353168 -1.739111 -1.209540 -0.296082
ССССССННННННННННН	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728 0.307233 -0.924351 -1.166439 1.754040 2.915557 2.327652 0.551315 -0.608503 -2.375801 -2.693674 -2.608500 -0.777321 -1.580718 -0.028894	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470 3.687431 5.341002 4.940860 4.804079 6.580993 6.952590 5.544237 3.781276 2.438198 2.004272 3.723303 0.685352 1.181731 2.242816	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202 -4.988117 -3.554884 -1.109231 0.049628 1.361450 3.771846 4.851933 3.549522 2.142542 0.419911 0.910490 3.714923 6.029333 7.691773	Charge: E(B97-3 E(M06/c E(PBE-6(PBE0-6(PM6)) E(PM7)) E(GFN1-6(GFN2-6(GFN-6)) Coordin Fe Si Si Si N N C C C C C C C	10 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	3.365468626444 Ha P) = -4541.711997 PP) = -4542.03706 33398744 Hartree Finol F	926952 Hartree 9662785 Hartree 6 Hartree 6 Hartree -0.539992 0.145283 -2.658982 1.501566 1.173960 -1.005788 0.734852 -0.437425 -1.353168 -1.739111 -1.209540 -0.296082 0.083995
СССССССННННННННННН	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728 0.307233 -0.924351 -1.166439 1.754040 2.915557 2.327652 0.551315 -0.608503 -2.375801 -2.693674 -2.608500 -0.777321 -1.580718 -0.028894 2.332184	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470 3.687431 5.341002 4.940860 4.804079 6.580993 6.952590 5.544237 3.781276 2.438198 2.004272 3.723303 0.685352 1.181731 2.242816 2.768480	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202 -4.988117 -3.554884 -1.109231 0.049628 1.361450 3.771846 4.851933 3.549522 2.142542 0.419911 0.910490 3.7714923 6.029333 7.691773 7.033692	Charge: E(B97-3 E(M06/c) E(PBE-6 E(PBE0) E(PBE) E(PM7) E(GFN1-6 E(GFN2-6 COORDING Si Si N N C C C C C C C C C C C C C C C C C	3c) = -4543.361856 def2-TZVP) = -4543. def2-TZVP) = -4543 D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI3.31226 Kcal/r (-V/def2-TZVP) = -2.75842189121.58421891 - D45859 - D45859 - D565781 - D688596 - D569655 - D569655 - D566181 - D837062 - D166181 - D837062 - D120421 - D193269 - D756202 - D185294 - D372345 - D446936 - D372345	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree Vmol nol -4545.91257766085 39085289 Hartree 52613226 Hartree 18269 Hartree 0.118908 -2.863932 -1.340070 2.186997 1.760730 -1.601696 1.490376 -4.534007 -4.594910 -5.821847 -7.020327 -6.982930 -5.751905 -3.013032	926952 Hartree 9662785 Hartree 6 Hartree 6 Hartree -0.539992 0.145283 -2.658982 1.501566 1.173960 -1.005788 0.734852 -0.437425 -1.353168 -1.739111 -1.209540 -0.296082 0.083995 0.345691
ССССССННННННННННННН	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728 0.307233 -0.924351 -1.166439 1.754040 2.915557 2.327652 0.551315 -0.608503 -2.375801 -2.693674 -2.608500 -0.777321 -1.580718 -0.028894 2.332184 3.139523 -2.136556 -3.436762	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470 3.687431 5.341002 4.940860 4.804079 6.580993 6.952590 5.544237 3.781276 2.438198 2.004272 3.723303 0.685352 1.181731 2.242816 2.768480 2.246439 -3.622941 -3.828393	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202 -4.988117 -3.554884 -1.109231 0.049628 1.361450 3.771846 4.851933 3.549522 2.142542 0.419911 0.910490 3.714923 6.029333 7.691773 7.033692 4.738181 -2.747399 -1.525814	Charge: E(B97-3 E(M06/c E(PBE-6(PBE0-6(PM6)) E(PM7)) E(GFN1-6(GFN2-6(GFN-6)) Coordin Fe Si Si Si N N C C C C C C C C C C C C C C C C C	3c) = -4543.361856 def2-TZVP) = -4543. D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI3.31226 Kcal/r - V/def2-TZVP) = -454.66613. ETB) = -154.66613. ETB) = -153.62565 ET) = -21.58421893  Dates:  0.495859 -0.565781 -0.688596 -0.569655 2.516335 -0.166181 0.837062 0.120421 1.193269 1.756202 1.251591 0.185294 -0.372345 -2.446936 -3.132861 -4.532945 -5.275846	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree Vmol mol mol -4545.91257766085 39085289 Hartree 82613226 Hartree 8269 Hartree 8269 Hartree 1.340070 2.186997 1.760730 -1.601696 1.490376 -4.534007 -4.594910 -5.821847 -7.020327 -6.982930 -5.751905 -3.013032 -2.213639 -2.248019 -3.091716	926952 Hartree 9662785 Hartree 9662785 Hartree 6 Hartree 6 Hartree -0.539992 0.145283 -2.658982 1.501566 1.173960 -1.005788 0.734852 -0.437425 -1.353168 -1.739111 -1.209540 -0.296082 0.083995 0.345691 1.288390 1.389214 0.548305
СССССССННННННННННННН	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728 0.307233 -0.924351 -1.166439 1.754040 2.915557 2.327652 0.551315 -0.608503 -2.375801 -2.693674 -2.608500 -0.777321 -1.580718 -0.028894 2.332184 3.139523 -2.136556 -3.436762 -1.784113	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470 3.687431 5.341002 4.940860 4.940860 4.804079 6.580993 6.952590 5.544237 3.781276 2.438198 2.004272 3.723303 0.685352 1.181731 2.242816 2.768480 2.246439 -3.828393 -4.489727	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202 -4.988117 -3.554884 -1.109231 0.049628 1.361450 3.771846 4.851933 3.549522 2.142542 0.419911 0.910490 3.7714923 6.029333 7.691773 7.033692 4.738181 -2.747399 -1.525814 -1.231222	Charge: E(B97-3 E(M06/c E(PBE-6 E(PBE0) E(PBE)-E(PM6) E(GFN1-6 E(GFN2-6 E(GFN-6 Coordin Fe Si Si N N C C C C C C C C C C C C C C C C C	3c) = -4543.361856 def2-TZVP) = -4543 -D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - 3c) = -4537.44783 = 215.50676 Kcal/r = -3.31226 Kcal/r -V/def2-TZVP) = -4543.626615 -XTB) = -154.66613 -XTB) = -153.62566 -0.565781 -0.688596 -0.565781 -0.688596 -0.569655 -0.569655 -0.166181 -0.837062 0.120421 1.193269 1.756202 1.251591 0.185294 -0.372345 -2.446936 -3.132861 -4.532945 -5.275846 -4.613425	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree Vmol nol -4545.91257766085 39085289 Hartree 18269 Hartree 18269 Hartree 0.118908 -2.863932 -1.340070 2.186997 1.760730 -1.601696 1.490376 -4.534007 -4.594910 -5.821847 -7.020327 -6.982930 -5.751905 -3.013032 -2.213639 -2.248019 -3.091716 -3.897881	926952 Hartree 9662785 Hartree 9662785 Hartree 6 Hartree 6 Hartree -0.539992 0.145283 -2.658982 1.501566 1.173960 -1.005788 0.734852 -0.437425 -1.353168 -1.739111 -1.209540 -0.296082 0.083995 0.345691 1.288390 1.389214 0.548305 -0.391217
СССССССИНННННННННННННН	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728 0.307233 -0.924351 -1.166439 1.754040 2.915557 2.327652 0.551315 -0.608503 -2.375801 -2.693674 -2.608500 -0.777321 -1.580718 -0.028894 2.332184 3.139523 -2.136556 -3.436762 -1.784113 0.958173	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470 3.687431 5.341002 4.940860 4.804079 6.580993 6.952590 5.544237 3.781276 2.438198 2.004272 3.723303 0.685352 1.181731 2.242816 2.768480 2.246439 -3.622941 -3.828393 -4.489727 -3.984907	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202 -4.988117 -3.554884 -1.109231 0.049628 1.361450 3.771846 4.851933 3.549522 2.142542 0.419911 0.910490 3.714923 6.029333 7.691773 7.033692 4.738181 -2.747399 -1.525814 -1.231222 -4.607826	Charge: E(B97-3 E(M06/c) E(PBE-6 E(PBE0) E(PBE) E(PM7) E(GFN1-6 E(GFN2-6 E(GFN-6 Coordin Fe Si Si N N C C C C C C C C C C C C C C C C C	3c) = -4543.361856 def2-TZVP) = -4543 -D3(BJ)/def2-TZVI -D3(BJ)/def2-TZVI -3c) = -4537.44783 = 215.50676 Kcal/ = -3.31226 Kcal/r -V/def2-TZVP) = -454366613 -XTB) = -153.62566 -153.62566 -1565781 -0.688596 -0.569781 -0.688596 -0.569655 -2.516335 -0.166181 -0.837062 -0.120421 -1.193269 -1.756202 -1.251591 -0.185294 -0.372345 -2.446936 -3.132861 -4.532945 -5.275846 -4.613425 -3.214867	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree Vmol nol -4545.91257766085 39085289 Hartree 18269 Hartree 18269 Hartree 0.118908 -2.863932 -1.340070 2.186997 1.760730 -1.601696 1.490376 -4.534007 -4.594910 -5.821847 -7.020327 -6.982930 -55.751905 -3.013032 -2.213639 -2.248019 -3.091716 -3.897881 -3.8956400	926952 Hartree 9662785 Hartree 9662785 Hartree 6 Hartree 6 Hartree -0.539992 0.145283 -2.658982 1.501566 1.173960 -1.005788 0.734852 -0.437425 -1.353168 -1.739111 -1.209540 -0.296082 0.083995 0.345691 1.288390 1.389214 0.548305 -0.391217 -0.488915
СССССССННННННННННННННН	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728 0.307233 -0.924351 -1.166439 1.754040 2.915557 2.327652 0.551315 -0.608503 -2.375801 -2.693674 -2.608500 -0.777321 -1.580718 -0.028894 2.332184 3.139523 -2.136556 -3.436762 -1.784113 0.958173	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470 3.687431 5.341002 4.940860 4.804079 6.580993 6.952590 5.544237 3.781276 2.438198 2.004272 3.723303 0.685352 1.181731 2.242816 2.768480 2.246439 -3.622941 -3.828393 -4.489727 -3.984907 -6.481349	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202 -4.988117 -3.554884 -1.109231 0.049628 1.361450 3.771846 4.851933 3.549522 2.142542 0.419911 0.910490 3.714923 6.029333 7.691773 7.033692 4.738181 -2.747399 -1.525814 -1.231222 -4.607826 -4.702538	Charge: E(B97-3 E(M06/c E(PBE-6)PBE-6 E(PBE0)E(PBE0-6 E(PM6))E(PM7) E(GFN1-6 E(GFN2-6 E(GFN-6 Coordin Fe Si	E 0	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree  (mol mol mol mol mol mol mol mol mol mol	926952 Hartree 9662785 Hartree 9662785 Hartree 6 Hartree 6 Hartree -0.539992 0.145283 -2.658982 1.501566 1.173960 -1.005788 0.734852 -0.437425 -1.353168 -1.739111 -1.209540 -0.296082 0.083995 0.345691 1.288390 1.389214 0.548305 -0.391217 -0.488915 1.824000
СССССССНННННННННННННННН	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728 0.307233 -0.924351 -1.166439 1.754040 2.915557 2.327652 0.551315 -0.608503 -2.375801 -2.693674 -2.608500 -0.777321 -1.580718 -0.028894 2.332184 3.139523 -2.136556 -3.436762 -1.784113 0.958173 0.994053 1.055994	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470 3.687431 5.341002 4.940860 4.804079 6.580993 6.952590 5.544237 3.781276 2.438198 2.004272 3.72303 0.685352 1.181731 2.242816 2.768480 2.246439 -3.622941 -3.828393 -4.489727 -3.984907 -6.481349 -7.820937	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202 -4.988117 -3.554884 -1.109231 0.049628 1.361450 3.771846 4.851933 3.549522 2.142542 0.419911 0.910490 3.714923 6.029333 7.691773 7.033692 4.738181 -2.747399 -1.525814 -1.231222 -4.607826 -4.702538 -2.585274	Charge: E(B97-3 E(M06/c E(PBE- E(PBE0) E(PBEh- E(PM6)) E(GFN1- E(GFN2- E(GFN-F  Coordin Fe Si Si Si N C C C C C C C C C C C C C C C C C C	3c) = -4543.361856 def2-TZVP) = -4543. def2-TZVP) = -4543 D3(BJ)/def2-TZVI - C-4537.44783 = 215.50676 Kcal/r - XTB) = -154.66613 XTB) = -154.66613 XTB) = -153.62565 - C-156421893 - C-1565781 - C-1688596 - C-166181 - C-166	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree Vmol mol mol -4545.91257766085 39085289 Hartree 322613226 Hartree 18269 Hartree 18269 Hartree 18269 Hartree 18269 Hartree 18269 Hartree 18269 Hartree 1.760730 -1.601696 1.490376 -4.534007 -4.594910 -5.821847 -7.020327 -6.982930 -5.751905 -3.013032 -2.213639 -2.248019 -3.091716 -3.897881 -3.856400 -2.452999 -1.507794	926952 Hartree 9662785 Hartree 9662785 Hartree 6 Hartree 6 Hartree -0.539992 0.145283 -2.658982 1.501566 1.173960 -1.005788 0.734852 -0.437425 -1.353168 -1.739111 -1.209540 -0.296082 0.083995 0.345691 1.288390 1.389214 0.548305 -0.391217 -0.488915 1.824000 -2.911442
СССССССННННННННННННННННН	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728 0.307233 -0.924351 -1.166439 1.754040 2.915557 2.327652 0.551315 -0.608503 -2.375801 -2.693674 -2.608500 -0.777321 -1.580718 -0.028894 2.332184 3.139523 -2.136556 -3.436762 -1.784113 0.958173 0.994053 1.0555994 1.086237	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470 3.687431 5.341002 4.940860 4.804079 6.580993 6.952590 5.544237 3.781276 2.438198 2.004272 3.723303 0.685352 1.181731 2.242816 2.768480 2.246439 -3.622941 -3.828393 -4.489727 -3.984907 -6.481349 -7.820937 -6.647723	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202 -4.988117 -3.554884 -1.109231 0.049628 1.361450 3.771846 4.851933 3.549522 2.142542 0.419911 0.910490 3.714923 6.029333 7.691773 7.033692 4.738181 -2.747399 -1.525814 -1.231222 -4.607826 -4.702538 -2.585274 -0.366831	Charge: E(B97-3 E(M06/c E(PBE-6 E(PBE0) E(PBE)-6 E(PM7) E(GFN1-6 E(GFN2-6 E(GFN-6 Coordin Fe Si Si N N C C C C C C C C C C C C C C C C C	3c) = -4543.361856 def2-TZVP) = -4543 -D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI -3-3.31226 Kcal/r -V/def2-TZVP) = -2.758 -154.66613 -2.758 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.569655 -0.5696	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree Vmol nol -4545.91257766085 39085289 Hartree 52613226 Hartree 18269 Hartree 0.118908 -2.863932 -1.340070 2.186997 1.760730 -1.601696 1.490376 -4.534007 -4.594910 -5.821847 -7.020327 -6.982930 -5.751905 -3.013032 -2.213639 -2.248019 -3.091716 -3.897881 -3.856400 -2.452999 -1.507794 -0.851054	926952 Hartree 9662785 Hartree 9662785 Hartree 6 Hartree 6 Hartree -0.539992 0.145283 -2.658982 1.501566 1.173960 -1.005788 0.734852 -0.437425 -1.353168 -1.739111 -1.209540 -0.296082 0.083995 0.345691 1.288390 1.389214 0.548305 -0.391217 -0.488915 1.824000 -2.911442 -2.043135
ССССССССннннннннннннннннннн	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728 0.307233 -0.924351 -1.166439 1.754040 2.915557 2.327652 0.551315 -0.608503 -2.375801 -2.693674 -2.608500 -0.777321 -1.580718 -0.028894 2.332184 3.139523 -2.136556 -3.436762 -1.784113 0.958173 0.994053 1.055994 1.086237 1.086237 1.086237	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470 3.687431 5.341002 4.940860 4.804079 6.580993 6.952590 5.544237 3.781276 2.438198 2.004272 3.723303 0.685352 1.181731 2.242816 2.768480 2.246439 -3.622941 -3.828393 -4.489727 -3.984907 -6.481349 -7.820937 -6.647723 -4.151448	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202 -4.988117 -3.554884 -1.109231 0.049628 1.361450 3.771846 4.851933 3.549522 2.142542 0.419911 0.910490 3.714923 6.029333 7.691773 7.033692 4.738181 -2.747399 -1.525814 -1.231222 -4.607826 -4.702538 -2.585274 -0.366831 -0.273317	Charge: E(B97-3 E(M06/c) E(PBE-6 E(PBE0) E(PBE) E(PM7) E(GFN1-6 E(GFN2-6 E(GFN-6 Coordin Fe Si Si N N C C C C C C C C C C C C C C C C C	3c) = -4543.361856 def2-TZVP) = -4543 -D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI -3c) = -4537.44783 = 215.50676 Kcal/ = -3.31226 Kcal/ -XTB) = -154.66613 -XTB) = -153.6256 FF) = -21.58421893 dates:  0.495859 -0.565781 -0.688596 -0.569655 -2.516335 -0.166181 0.83762 0.120421 1.193269 1.756202 1.251591 0.185294 -0.372345 -2.446936 -3.132861 -4.532945 -5.275846 -4.613425 -3.214867 0.184058 -2.553661 -3.455857 -4.842050	3.365468626444 Ha P) = -4541.711997 P) = -4542.03706 33398744 Hartree Pmol mol mol -4545.91257766085 39085289 Hartree 18269 Hart	926952 Hartree 9662785 Hartree 9662785 Hartree 6 Hartree 6 Hartree -0.539992 0.145283 -2.658982 1.501566 1.173960 -1.005788 0.734852 -0.437425 -1.353168 -1.739111 -1.209540 -0.296082 0.083995 0.345691 1.288390 1.389214 0.548305 -0.391217 -0.488915 1.824000 -2.911442 -2.043135 -2.208520
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СССССССННННННННННННННННННННН	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728 0.307233 -0.924351 -1.166439 1.754040 2.915557 2.327652 0.551315 -0.608503 -2.375801 -2.693674 -2.608500 -0.777321 -1.580718 -0.028894 2.332184 3.139523 -2.136556 -3.436762 -1.784113 0.958173 0.994053 1.055994 1.086237 1.033950 2.735922 3.437488	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470 3.687431 5.341002 4.940860 4.804079 6.580993 6.952590 5.544237 3.781276 2.438198 2.004272 3.723303 0.685352 1.181731 2.242816 2.768480 2.246439 -3.622941 -3.828393 -4.489727 -3.984907 -6.481349 -7.820937 -6.647723 -4.151448 -0.291283 -1.700635	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202 -4.988117 -3.554884 -1.109231 0.049628 1.361450 3.771846 4.851933 3.549522 2.142542 0.419911 0.910490 3.714923 6.029333 7.691773 7.033692 4.738181 -2.747399 -1.525814 -1.231222 -4.607826 -4.702538 -2.585274 -0.366831 -0.273317 -1.691754 -2.553452	Charge: E(B97-3 E(M06/c E(PBE- E(PBE0) E(PBEh- E(PM6)) E(GFN1- E(GFN2- E(GFN-F  Coordin Fe Si Si Si N N C C C C C C C C C C C C C C C C C	3c) = -4543.361856 def2-TZVP) = -4543. def2-TZVP) = -4543 D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI154.66613 XTB) = -154.66613 XTB) = -153.62565 - D1.66181 - D1.688596 - D1.	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree Vmol mol mol -4545.91257766085 39085289 Hartree 52613226 Hartree 18269 Hartree 0.118908 -2.863932 -1.340070 2.186997 1.760730 -1.601696 1.490376 -4.534007 -4.594910 -5.821847 -7.020327 -6.982930 -5.751905 -3.013032 -2.213639 -2.248019 -3.091716 -3.897881 -3.856400 -2.452999 -1.507794 -0.851054 -0.971492 -1.765233 -2.433975	926952 Hartree 9662785 Hartree 9662785 Hartree 6 Hartree 6 Hartree 6 Hartree 7 0.539992 0.145283 -2.658982 1.501566 1.173960 -1.005788 0.734852 -0.437425 -1.353168 -1.739111 -1.209540 -0.296082 0.083995 0.345691 1.288390 1.389214 0.548305 -0.391217 -0.488915 1.824000 -2.911442 -2.043135 -2.208520 -3.245678 -4.112991
ССССССССннннннннннннннннннннннн	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728 0.307233 -0.924351 -1.166439 1.754040 2.915557 2.327652 0.551315 -0.608503 -2.375801 -2.693674 -2.608500 -0.777321 -1.580718 -0.028894 2.332184 3.139523 -2.136556 -3.436762 -1.784113 0.958173 0.994053 1.055994 1.086237 1.033950 2.735922 3.437488 2.980393	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470 3.687431 5.341002 4.940860 4.804079 6.580993 6.952590 5.544237 3.781276 2.438198 2.004272 3.723303 0.685352 1.181731 2.242816 2.768480 2.246439 -3.622941 -3.828393 -4.489727 -3.984907 -6.481349 -7.820937 -6.647723 -4.151448 -0.291283 -1.700635 -1.855017	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202 -4.988117 -3.554884 -1.109231 0.049628 1.361450 3.771846 4.851933 3.549522 2.142542 0.419911 0.910490 3.714923 6.029333 7.691773 7.033692 4.738181 -2.747399 -1.525814 -1.231222 -4.607826 -4.702538 -2.585274 -0.366831 -0.273317 -1.691754 -2.553452 -0.835411	Charge: E(B97-3 E(M06/c E(PBE-6 E(PBE0) E(PBE0) E(PM7) E(GFN1-6 E(GFN2-6 COORDING Si Si Si N N C C C C C C C C C C C C C C C C C	30	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree Vmol nol -4545.91257766085 39085289 Hartree 52613226 Hartree 18269 Hart	926952 Hartree 9662785 Hartree 9662785 Hartree 6 Hartree 6 Hartree 6 Hartree 6 Hartree 7 0.539992 0.145283 -2.658982 1.501566 1.173960 -1.005788 0.734852 -0.437425 -1.353168 -1.739111 -1.209540 -0.296082 0.083995 0.345691 1.288390 1.389214 0.548305 -0.391217 -0.488915 1.824000 -2.911442 -2.043135 -2.208520 -3.245678 -4.112991 -3.946923
ССССССССНннннннннннннннннннннннн	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728 0.307233 -0.924351 -1.166439 1.754040 2.915557 2.327652 0.551315 -0.608503 -2.375801 -2.693674 -2.608500 -0.777321 -1.580718 -0.028894 2.332184 3.139523 -2.136556 -3.436762 -1.784113 0.958173 0.994053 1.055994 1.086237 1.033950 2.735922 3.437488 2.980393 3.352879	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470 3.687431 5.341002 4.940860 4.804079 6.580993 6.952590 5.544237 3.781276 2.438198 2.004272 3.723303 0.685352 1.181731 2.242816 2.768480 2.246439 -3.622941 -3.828393 -4.489727 -3.984907 -6.481349 -7.820937 -6.647723 -4.151448 -0.291283 -1.700635 -1.855017 1.962516	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202 -4.988117 -3.554884 -1.109231 0.049628 1.361450 3.771846 4.851933 3.549522 2.142542 0.419911 0.910490 3.714923 6.029333 7.691773 7.033692 4.738181 -2.747399 -1.525814 -1.231222 -4.607826 -4.702538 -2.585274 -0.366831 -0.273317 -1.691754 -2.553452 -0.835411 1.846526	Charge: E(B97-3 E(M06/c) E(PBE-6 E(PBE0) E(PBE) E(PM7) E(GFN1-6 E(GFN2-6 E(GFN-6 COORDINATION N CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	3c) = -4543.361856 def2-TZVP) = -4543 -D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI -3c) = -4537.44783 = 215.50676 Kcal/r = -3.31226 Kcal/r -V/def2-TZVP) = -4543.62661 -3.45859 -0.565781 -0.688596 -0.565781 -0.688596 -0.569655 -0.5668596 -0.569655 -0.166181 -0.837062 -0.120421 -1.193269 -1.756202 -1.251591 -0.185294 -0.372345 -2.446936 -3.132861 -4.532945 -5.275846 -4.613425 -3.214867 -0.184058 -2.553661 -3.455857 -4.842050 -5.358326 -4.481446 -3.092830 -2.118251	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree Vmol nol -4545.91257766085 39085289 Hartree 18269 Hartree	926952 Hartree 9662785 Hartree 9662785 Hartree 6 Hartree 6 Hartree 6 Hartree 6 Hartree 7 0.539992 0.145283 -2.658982 1.501566 1.173960 -1.005788 0.734852 -0.437425 -1.353168 -1.739111 -1.209540 -0.296082 0.083995 0.345691 1.288390 1.389214 0.548305 -0.391217 -0.488915 1.824000 -2.911442 -2.043135 -2.208520 -3.245678 -4.112991 -3.946923 0.569847
ССССССССннннннннннннннннннннннн	0.326904 1.650081 2.102091 -2.351934 1.006242 0.993390 1.011498 1.045269 1.061539 1.039337 2.685122 1.082488 1.311728 0.307233 -0.924351 -1.166439 1.754040 2.915557 2.327652 0.551315 -0.608503 -2.375801 -2.693674 -2.608500 -0.777321 -1.580718 -0.028894 2.332184 3.139523 -2.136556 -3.436762 -1.784113 0.958173 0.994053 1.055994 1.086237 1.033950 2.735922 3.437488 2.980393	2.005722 2.298124 1.997789 -3.640660 -3.887921 -4.565607 -5.969677 -6.720751 -6.062827 -4.661224 -1.394733 1.253502 1.640470 3.687431 5.341002 4.940860 4.804079 6.580993 6.952590 5.544237 3.781276 2.438198 2.004272 3.723303 0.685352 1.181731 2.242816 2.768480 2.246439 -3.622941 -3.828393 -4.489727 -3.984907 -6.481349 -7.820937 -6.647723 -4.151448 -0.291283 -1.700635 -1.855017	6.677151 6.308429 5.013433 -1.660069 -2.434027 -3.671414 -3.727500 -2.542208 -1.300196 -1.250683 -1.798232 -1.486744 -3.945202 -4.988117 -3.554884 -1.109231 0.049628 1.361450 3.771846 4.851933 3.549522 2.142542 0.419911 0.910490 3.714923 6.029333 7.691773 7.033692 4.738181 -2.747399 -1.525814 -1.231222 -4.607826 -4.702538 -2.585274 -0.366831 -0.273317 -1.691754 -2.553452 -0.835411	Charge: E(B97-3 E(M06/c E(PBE-6 E(PBE0) E(PBE0) E(PM7) E(GFN1-6 E(GFN2-6 COORDING Si Si Si N N C C C C C C C C C C C C C C C C C	30	3.365468626444 Ha P) = -4541.711997 VP) = -4542.03706 33398744 Hartree Vmol nol -4545.91257766085 39085289 Hartree 52613226 Hartree 18269 Hart	926952 Hartree 9662785 Hartree 9662785 Hartree 6 Hartree 6 Hartree 6 Hartree 6 Hartree 7 0.539992 0.145283 -2.658982 1.501566 1.173960 -1.005788 0.734852 -0.437425 -1.353168 -1.739111 -1.209540 -0.296082 0.083995 0.345691 1.288390 1.389214 0.548305 -0.391217 -0.488915 1.824000 -2.911442 -2.043135 -2.208520 -3.245678 -4.112991 -3.946923

С	3.199017	-0.775195	0.043297	E (PBE	h-3c) = -4537.45026	5528681 Hartree	
C	3.584986	-2.124501	0.040247	E (PM6)	) = 208.04060 Kcal/	mol	
C	4.046836	-2.717193	1.225829	E (PM7	= -5.85628  Kcal/m	iol	
C	4.125190	-1.952510	2.401309	E(ωB9	7X-V/def2-TZVP) = -	4545.91034197421	9 Hartree
C	3.736935	-0.601490	2.393990	E (GFN	1-xTB) = $-154.67002$	0074520 Hartree	
C	2.764909	2.659450	2.814887	E (GFN:	2-xTB) = $-153.62593$	2708899 Hartree	
H	1.586645	-3.656066	-1.771781	E (GFN	-FF) = -21.59641688	5984 Hartree	
H	2.590130	-5.844252	-2.458336				
H	1.687947	-7.985417	-1.510403	Coord	inates:		
H	-0.215801	-7.920211	0.120349	Fe	0.022662	-0.139476	0.109807
H	-1.213160	-5.739518	0.797101	Si	-0.586809	0.511578	-2.929910
H	-2.567517	-1.548648	1.962172	Si	-2.231860	1.813413	-0.642683
H	-5.045387	-1.615845	2.131235	Si	1.562970	-2.244027	1.165721
H	-6.374014	-3.119691	0.623603	Si	3.044395	0.557279	1.280897
H	-5.191091	-4.554521	-1.059689	N	-1.028284	0.684748	-1.243694
H	-2.710061	-4.488839	-1.236658	N	1.686610	-0.501638	0.997152
Н	-0.214452	-1.501980	2.228586	С	-2.091798	0.013894	-3.966663
Н	1.285954	-2.365634	1.756215	C	-2.331694	0.561023	-5.246267
Н	-0.056093	-3.257353	2.548819	C	-3.454546	0.181788	-5.999677
Н	-3.069552	-0.250389	-1.207330	C	-4.360076	-0.758174	-5.483515
Н	-5.522224	-0.458267	-1.512194	C	-4.137040	-1.316180	-4.214336
Н	-6.447071	-1.868564	-3.372909	C	-3.014901	-0.931778	-3.466404
Н	-4.880250	-3.062445	-4.924481	C	0.724349	-0.856042	-3.116930
Н	-2.420963	-2.836196	-4.637722	C	2.089415	-0.566609	-2.887936
Н	-2.146320	2.009987	-0.468119	C	3.090803	-1.515801	-3.144148
H	-3.030893	1.972990	1.094206	C	2.743225	-2.787561	-3.628708
H	-2.162040	0.514123	0.533642	C	1.392169	-3.101769	-3.848728
H	2.866184	-0.315290	-0.907409	C	0.396788	-2.142767	-3.600462
H	3.517719	-2.717585	-0.883195	C	0.164846	2.099172	-3.637031
H	4.338255	-3.778335	1.232817	C	-3.971208	1.459699	-1.307245
п Н	4.485313	-2.414866	3.333415	C	-4.553556	2.291969	-2.288895
H	3.797332	-0.019940	3.328115	C	-5.804705	1.992649	-2.850856
H	2.355313	3.686757	2.739240	C	-6.513327	0.858928	-2.425270
H	3.850323	2.745538	3.027135	C	-5.958169	0.021429	-1.444801
H	2.268254	2.156837	3.666922	C	-4.697603	0.315298	-0.905005
С	0.222065	-2.384084	-3.943040	С	2.696523	-3.250080	0.049750
H	1.318965	-2.256460	-3.844125	С	2.788202	2.218174	0.384821
H	-0.003875	-3.462169	-3.819018	С	3.241883	2.418144	-0.938480
H	-0.062929	-2.076754	-4.970131	С	3.012754	3.625275	-1.618149
С	3.415530	2.774539	-0.152676	С	2.320830	4.667833	-0.981127
С	4.571826	2.317002	-0.821475	С	1.889476	4.505973	0.345147
С	2.921445	4.058126	-0.481368	С	2.133082	3.298555	1.019711
C	5.202463	3.103354	-1.801300	С	4.663885	-0.195937	0.644722
С	3.552209	4.851626	-1.450864	H	-1.632508	1.302906	-5.664715
C	4.691541	4.372062	-2.119978	H	-3.626335	0.625166	-6.993119
H	4.986013	1.325529	-0.577605	H	-5.245003	-1.052027	-6.069100
H	2.016191	4.440438	0.016744	H	-4.852079	-2.042505	-3.797840
H	6.099158	2.725277	-2.316864	H	-2.859537	-1.355742	-2.462176
H	3.149664	5.848859	-1.689311	H	2.376004	0.428140	-2.514693
H	5.184552	4.989832	-2.886525	H	4.148391	-1.263646	-2.967403
C	-0.168677	0.492544	-2.865575	H	3.525781	-3.534182	-3.833349
C	-1.096780	1.557259	-3.026658	H	1.113794	-4.096303	-4.231113
C	1.223997	0.822354	-2.871235	H	-0.656813	-2.391525	-3.804346
C	-0.663895	2.882689	-3.150371	H	0.898058	2.523105	-2.921799
C	1.654476	2.161838	-2.990827	H	-0.615807	2.866296	-3.813111
C	0.711974	3.187683	-3.115975	H	0.684290	1.905650	-4.597746
H	-2.173327	1.327761	-3.061262	H	-4.015752	3.188476	-2.635319
H	1.979937	0.019502	-2.904171	H	-6.228533	2.647150	-3.628073
H	-1.402654	3.689050	-3.279632	H	-7.495723	0.623897	-2.863145
H	2.728545	2.396902	-2.992570	H	-6.504773	-0.874817	-1.110594
H	1.052615	4.230434	-3.198522	H	-4.255402	-0.376204	-0.173817
C	-0.486442	4.082728	1.460940	H	2.583105	-2.954763	-1.010173
C	-0.612728	4.743087	0.216147	H	2.469862	-4.331523	0.148734
C	-0.221069	4.869674	2.603206	H	3.758769	-3.105241	0.328711
С	-0.475575	6.135709	0.114025	H	3.801168	1.618764	-1.449794
C	-0.079231	6.264227	2.507069	H	3.376705	3.753617	-2.649238
C	-0.205113	6.899778	1.261783	H	2.130068	5.611831	-1.513968
H	-0.800545	4.153053	-0.695321	H	1.366580	5.326837	0.859958
H	-0.118548	4.382398	3.586361	H	1.819871	3.199045	2.071479
H	-0.576302	6.628842	-0.865710	Н	4.933133	-1.098203	1.230083
H	0.132475	6.858447	3.409623	Н	5.499634	0.527058	0.736207
H	-0.093072	7.992357	1.184995	Н	4.570786	-0.497760	-0.418450
C	-0.757065	1.593443	3.294500	C	-1.762575	3.612062	-0.995113
С	0.079863	0.587282	3.824475	Н	-0.727713	3.792748	-0.638637
С	-1.786396	2.099104	4.121666	Н	-1.787482	3.855289	-2.075913
Č	-0.099710	0.100820	5.129483	Н	-2.445089	4.307878	-0.465219
C	-1.970084	1.620679	5.428609	C	3.252028	0.973170	3.122153
Č	-1.125810	0.618541	5.935044	C	2.487478	0.352351	4.133371
Н	0.885643	0.173354	3.198395	C	4.219643	1.926630	3.516322
Н	-2.458579	2.886768	3.741279	C	2.684894	0.663083	5.489037
Н	0.563091	-0.688836	5.516368	C	4.420196	2.244427	4.868161
Н	-2.776620	2.030646	6.056402	C	3.652305	1.609941	5.859161
Н	-1.269926	0.240653	6.959037	Н	1.727488	-0.392071	3.855693
				Н	4.824953	2.440564	2.750641
Conform	nation 26.			Н	2.082066	0.155215	6.257923
	Licity: 5			Н	5.178532	2.990925	5.151702
Charge				Н	3.810107	1.855546	6.920825
	3c) = -4543.36496	0019486 Hartree		C	-2.143410	1.566412	1.243184
		3.368737449843 Ha:	rtree	C	-3.204431	1.149453	2.075805
		P) = -4541.714985		C	-0.874816	1.768911	1.845694
		VP) = -4542.04041			-2.996469	0.890949	3.440430

С	-0.661938	1.520679	3.213935	H	-3.536444	-2.658942	-0.615362
C	-1.721320	1.061459	4.009147	H	-5.019919	-1.646842	-0.796539
Н	-4.211402	1.020592	1.649753	Н	-2.023209	-3.328534	1.551695
H				Н		-5.122794	2.524797
	-0.045955	2.181560	1.247052		-3.461465		
H	-3.837261	0.556876	4.068288	H	-4.658491	-4.733039	4.695393
H	0.332435	1.683914	3.654361	H	-4.390020	-2.545069	5.889801
H	-1.558021	0.853329	5.077716	H	-2.931606	-0.767879	4.935252
С	-0.250329	-2.504931	0.631732	H	0.347617	0.002130	-4.327624
C	-1.313657	-1.887728	1.362928	H	1.428366	-1.320157	-4.891881
С	-0.602321	-3.328117	-0.474344	H	2.072362	0.341799	-4.683081
С	-2.660412	-2.119634	1.006906	H	1.105182	4.726574	-2.292295
Ċ	-1.937263	-3.533248	-0.833786	Н	-0.759125	6.239283	-1.649620
C	-2.972296	-2.933495		H	-2.225493	5.680054	0.309428
			-0.086455				
H	-1.103298	-1.299410	2.271881	H	-1.807756	3.578819	1.613706
H	0.192683	-3.806273	-1.065782	H	0.025458	2.050124	0.954525
H	-3.458787	-1.662202	1.609025	H	3.615406	1.891410	-3.207216
H	-2.180385	-4.165973	-1.701190	H	3.286149	3.605762	-2.819420
H	-4.023495	-3.107908	-0.363451	H	2.042075	2.617705	-3.668649
С	1.841508	-2.820988	2.953244	С	-1.399269	1.014220	3.381217
С	3.163133	-2.870136	3.455100	H	-0.670793	1.763639	3.014317
C	0.788297	-3.124171	3.844927	H	-2.414070	1.447704	3.280607
C	3.424456	-3.182584	4.796752	Н	-1.185720	0.847426	4.457041
C	1.042465	-3.437807	5.190104	C	3.492494	2.196804	0.082731
				C			
C	2.361315	-3.461369	5.670627		4.753321	1.611758	-0.179794
H	4.012227	-2.638954	2.791100	С	3.312730	2.838335	1.328950
H	-0.252173	-3.117094	3.485291	C	5.785043	1.642986	0.770910
H	4.461672	-3.200914	5.165209	C	4.340000	2.871272	2.286951
H	0.205060	-3.668659	5.866938	C	5.578118	2.269135	2.011716
H	2.561892	-3.702812	6.725875	H	4.935503	1.107530	-1.141339
				H	2.351223	3.325869	1.557129
Conform	mation 27.			H	6.754048	1.172235	0.542370
	licity: 5			Н	4.172554	3.370674	3.253840
Charge				Н	6.383536	2.291987	2.761989
		1520026 #				-1.169318	2.761969
,	3c) = -4543.37351			C	0.578655		
	,	3.376078082881 на		С	0.938757	-2.488678	2.882228
		P) = -4541.722502		С	1.626421	-0.265894	2.210056
E(PBE0	- D3(BJ)/def2-TZ	VP) = -4542.04831	9576493 Hartree	C	2.280430	-2.899108	2.898619
E (PBEh-	-3c) = -4537.4593	03363538 Hartree		C	2.974330	-0.667593	2.232437
E(PM6)	= 214.02917 Kcal	/mol		C	3.300449	-1.989822	2.567644
E(PM7)	= -10.75376 Kcal	/mol		H	0.150556	-3.207045	3.158229
E(ωB97)	X-V/def2-TZVP) =	-4545.91437656069	4 Hartree	H	1.409022	0.789508	1.981420
E (GFN1	-xTB) = $-154.6734$	73282311 Hartree		H	2.535115	-3.933164	3.178933
E (GFN2	-xTB) = $-153.6333$	78270335 Hartree		H	3.762185	0.061042	1.993377
	FF) = -21.4720101			H	4.353673	-2.310399	2.582115
2 (0211	21, 21,1,20101	oo,,o marara		C	0.613066	-2.178803	-1.854274
Coordi	nn+00.			C		-2.603497	
Coordi		0 452260	0 202620		-0.519194		-2.605759
Fe	0.094271	-0.453360	-0.303630	С	0.877661	-2.844306	-0.617295
Si	-3.053055	-0.241472	-0.155846	С	-1.348831	-3.630160	-2.147859
Si	-1.238829	-0.597667	2.406487	С	0.034044	-3.881843	-0.163115
Si	1.799734	-0.806180	-2.471005	С	-1.073367	-4.272791	-0.922163
Si	2.105971	2.070796	-1.214833	H	-0.753752	-2.107934	-3.559615
N	-1.528578	-0.437300	0.689692	H	1.799208	-2.629260	-0.051389
N	1.468713	0.443058	-1.287842	H	-2.218373	-3.940216	-2.747657
С	-2.654459	0.262284	-1.943618	H	0.267362	-4.388106	0.784830
C	-1.844655	1.393129	-2.202951	H	-1.724793	-5.087300	-0.569534
С	-1.567695	1.810403	-3.514316	C	3.583085	-1.429255	-2.348196
С	-2.095468	1.098110	-4.602526	С	4.337233	-1.822436	-3.476187
Č	-2.896627	-0.032944	-4.369488	Č	4.192231	-1.527385	-1.076537
C	-3.172578	-0.441162	-3.054878	C	5.651693	-2.298012	-3.339322
C	-4.082876	1.124116	0.675519	C	5.501335	-2.009671	-0.932008
		2.418538				-2.395431	
C	-4.226891		0.130008	C	6.235209		-2.065596
С	-4.935423	3.421502	0.811972	H	3.895102	-1.755115	-4.483363
С	-5.520320	3.147972	2.058211	H	3.637278	-1.195868	-0.185792
C	-5.401190	1.862813	2.613353	H	6.225222	-2.594104	-4.231475
C	-4.694130	0.864492	1.925490	H	5.954006	-2.073676	0.070131
		-1.809994	-0.188422	H	7.265153	-2.769425	-1.957730
C	-4.106389						
		-1.921674	3.177306				
C C	-4.106389			Confor	mation 3.		
C C	-4.106389 -2.353918 -2.525706	-3.160526	2.517019				
с с с	-4.106389 -2.353918 -2.525706 -3.341304	-3.160526 -4.166232	2.517019 3.057329	Multip	licity: 5		
0 0 0 0	-4.106389 -2.353918 -2.525706 -3.341304 -4.013128	-3.160526 -4.166232 -3.948182	2.517019 3.057329 4.271571	Multip Charge	licity: 5 : 0	1290310 Hartron	
0 0 0 0 0	-4.106389 -2.353918 -2.525706 -3.341304 -4.013128 -3.861904	-3.160526 -4.166232 -3.948182 -2.723065	2.517019 3.057329 4.271571 4.940120	Multip Charge E(B97-	licity: 5 : 0 3c) = -4543.374459		
000000	-4.106389 -2.353918 -2.525706 -3.341304 -4.013128 -3.861904 -3.037534	-3.160526 -4.166232 -3.948182 -2.723065 -1.723525	2.517019 3.057329 4.271571 4.940120 4.397684	Multip Charge E(B97- E(M06/	licity: 5 : 0 3c) = -4543.374459 def2-TZVP) = -4543	3.378788184949 Ha	
00000000	-4.106389 -2.353918 -2.525706 -3.341304 -4.013128 -3.861904 -3.037534 1.374118	-3.160526 -4.166232 -3.948182 -2.723065 -1.723525 -0.407995	2.517019 3.057329 4.271571 4.940120 4.397684 -4.262565	Multip Charge E(B97- E(M06/ E(PBE	licity: 5 : 0 3c) = -4543.374459 def2-TZVP) = -4543 - D3(BJ)/def2-TZVP	3.378788184949 Ha P) = -4541.721998	648313 Hartree
00000000	-4.106389 -2.353918 -2.525706 -3.341304 -4.013128 -3.861904 -3.037534 1.374118 0.731183	-3.160526 -4.166232 -3.948182 -2.723065 -1.723525 -0.407995 3.275805	2.517019 3.057329 4.271571 4.940120 4.397684 -4.262565 -0.706762	Multip Charge E(B97- E(M06/ E(PBE E(PBE0	licity: 5 : 0 3c) = -4543.374459 def2-TZVP) = -4543 - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF	3.378788184949 Ha P() = -4541.721998 P() = -4542.05042	648313 Hartree
C C C C C C C	-4.106389 -2.353918 -2.525706 -3.341304 -4.013128 -3.861904 -3.037534 1.374118 0.731183 0.477457	-3.160526 -4.166232 -3.948182 -2.723065 -1.723525 -0.407995 3.275805 4.464785	2.517019 3.057329 4.271571 4.940120 4.397684 -4.262565 -0.706762 -1.425563	Multip Charge E(B97- E(M06/ E(PBE E(PBE0 E(PBEh	licity: 5 : 0 3c) = -4543.374459 def2-TZVP) = -4543 - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - 3c) = -4537.46256	8.378788184949 Ha P) = -4541.721998 PP) = -4542.05042 55938135 Hartree	648313 Hartree
	-4.106389 -2.353918 -2.525706 -3.341304 -4.013128 -3.861904 -3.037534 1.374118 0.731183 0.477457 -0.575048	-3.160526 -4.166232 -3.948182 -2.723065 -1.723525 -0.407995 3.275805 4.464785 5.324108	2.517019 3.057329 4.271571 4.940120 4.397684 -4.262565 -0.706762 -1.425563 -1.065591	Multip Charge E(B97- E(M06/ E(PBE E(PBE0 E(PBEh E(PM6)	licity: 5 : 0 3c) = -4543.374459 def2-TZVP) = -4543 - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZV -3c) = -4537.46256 = 197.86854 Kcal/	3.378788184949 Ha P) = -4541.721998 PP) = -4542.05042 55938135 Hartree (mol	648313 Hartree
	-4.106389 -2.353918 -2.525706 -3.341304 -4.013128 -3.861904 -3.037534 1.374118 0.731183 0.477457 -0.575048 -1.393694	-3.160526 -4.166232 -3.948182 -2.723065 -1.723525 -0.407995 3.275805 4.464785 5.324108 5.014629	2.517019 3.057329 4.271571 4.940120 4.397684 -4.262565 -0.706762 -1.425563 -1.065591 0.031405	Multip Charge E (B97- E (M06/ E (PBE E (PBE0 E (PBEh E (PM6)) E (PM7)	licity: 5 : 0 3c) = -4543.374459 def2-TZVP) = -4543 - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF -3c) = -4537.46256 = 197.86854 Kcal/m = -2.31902 Kcal/m	3.378788184949 Ha P) = -4541.721998 PP) = -4542.05042 55938135 Hartree (mol	648313 Hartree 6495231 Hartree
	-4.106389 -2.353918 -2.525706 -3.341304 -4.013128 -3.861904 -3.037534 1.374118 0.731183 0.477457 -0.575048 -1.393694 -1.156778	-3.160526 -4.166232 -3.948182 -2.723065 -1.723525 -0.407995 3.275805 4.464785 5.324108 5.014629 3.842441	2.517019 3.057329 4.271571 4.940120 4.397684 -4.262565 -0.706762 -1.425563 -1.065591 0.031405 0.767322	Multip Charge E (B97- E (M06/ E (PBE E (PBE0) E (PBEh E (PM6) E (PM7) E (\omegaB97	licity: 5 : 0 3c) = -4543.374459 def2-TZVP) = -4543 - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF -3c) = -4537.46256 = 197.86854 Kcal/m Z-V/def2-TZVP) = -	8.378788184949 Ha P) = -4541.721998 PP) = -4542.05042 S5938135 Hartree mol tol 4545.91844677672	648313 Hartree 6495231 Hartree
	-4.106389 -2.353918 -2.525706 -3.341304 -4.013128 -3.861904 -3.037534 1.374118 0.731183 0.477457 -0.575048 -1.393694	-3.160526 -4.166232 -3.948182 -2.723065 -1.723525 -0.407995 3.275805 4.464785 5.324108 5.014629	2.517019 3.057329 4.271571 4.940120 4.397684 -4.262565 -0.706762 -1.425563 -1.065591 0.031405	Multip Charge E (B97- E (M06/ E (PBE E (PBE0) E (PBEh E (PM6) E (PM7) E (\omegaB97	licity: 5 : 0 3c) = -4543.374459 def2-TZVP) = -4543 - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF -3c) = -4537.46256 = 197.86854 Kcal/m = -2.31902 Kcal/m	8.378788184949 Ha P) = -4541.721998 PP) = -4542.05042 S5938135 Hartree mol tol 4545.91844677672	648313 Hartree 6495231 Hartree
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0 0 0 0 0 0 0 0 0 0 0 0 0 0	-4.106389 -2.353918 -2.525706 -3.341304 -4.013128 -3.861904 -3.037534 1.374118 0.731183 0.477457 -0.575048 -1.393694 -1.156778 -0.107843 2.824745	-3.160526 -4.166232 -3.948182 -2.723065 -1.723525 -0.407995 3.275805 4.464785 5.324108 5.014629 3.842441 2.989365 2.599465	2.517019 3.057329 4.271571 4.940120 4.397684 -4.262565 -0.706762 -1.425563 -1.065591 0.031405 0.767322 0.395112 -2.883673	Multip Charge E (B97- E (M06/ E (PBE E (PBE0 E (PBE0 E (PM6) E (PM7) E (GFN1 E (GFN1	licity: 5 : 0 3c) = -4543.374459 def2-TZVP) = -4543 - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF -3c) = -4537.46256 = 197.86854 Kcal/ = -2.31902 Kcal/ x-V/def2-TZVP) = - xTB) = -154.67443 -xTB) = -153.63378	8.378788184949 Ha P) = -4541.721998 PP) = -4542.05042 55938135 Hartree (mol 101 4545.91844677672 4526022 Hartree 12870437 Hartree	648313 Hartree 6495231 Hartree
C C C C C C C C C C C H	-4.106389 -2.353918 -2.525706 -3.341304 -4.013128 -3.861904 -3.037534 1.374118 0.731183 0.477457 -0.575048 -1.393694 -1.156778 -0.107843 2.824745 -1.422716	-3.160526 -4.166232 -3.948182 -2.723065 -1.723525 -0.407995 3.275805 4.464785 5.324108 5.014629 3.842441 2.989365 2.599465 1.968708	2.517019 3.057329 4.271571 4.940120 4.397684 -4.262565 -0.706762 -1.425563 -1.065591 0.031405 0.767322 0.395112 -2.883673 -1.367488	Multip Charge E (B97- E (M06/ E (PBE E (PBE0 E (PBE0 E (PM6) E (PM7) E (GFN1 E (GFN1	licity: 5 : 0 3c) = -4543.374459 def2-TZVP) = -4543 - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZV -3c) = -4537.46256 = 197.86854 Kcal/m X-V/def2-TZVP) = - xTB) = -154.67443	8.378788184949 Ha P) = -4541.721998 PP) = -4542.05042 55938135 Hartree (mol 101 4545.91844677672 4526022 Hartree 12870437 Hartree	648313 Hartree 6495231 Hartree
C C C C C C C C C H H	-4.106389 -2.353918 -2.525706 -3.341304 -4.013128 -3.861904 -3.037534 1.374118 0.731183 0.477457 -0.575048 -1.393694 -1.156778 -0.107843 2.824745 -1.422716 -0.934781	-3.160526 -4.166232 -3.948182 -2.723065 -1.723525 -0.407995 3.275805 4.464785 5.324108 5.014629 3.842441 2.989365 2.599465 1.968708 2.696571	2.517019 3.057329 4.271571 4.940120 4.397684 -4.262565 -0.706762 -1.425563 -1.065591 0.031405 0.767322 0.395112 -2.883673 -1.367488 -3.677230	Multip Charge E (B97- E (M06/ E (PBE E (PBE0 E (PBE0) E (PM7) E (GF7) E (GFN1 E (GFN2-	licity: 5 : 0 3c) = -4543.374459 def2-TZVP) = -4543 - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - 3c) = -4537.46256 = 197.86854 Kcal/ = -2.31902 Kcal/π X-V/def2-TZVP) =xTB) = -154.67443 -xTB) = -153.63378 FF) = -21.59103959	8.378788184949 Ha P) = -4541.721998 PP) = -4542.05042 55938135 Hartree (mol 101 4545.91844677672 4526022 Hartree 12870437 Hartree	648313 Hartree 6495231 Hartree
С С С С С С С С С С Н Н Н	-4.106389 -2.353918 -2.525706 -3.341304 -4.013128 -3.861904 -3.037534 1.374118 0.731183 0.477457 -0.575048 -1.393694 -1.156778 -0.107843 2.824745 -1.422716 -0.934781 -1.882611	-3.160526 -4.166232 -3.948182 -2.723065 -1.723525 -0.407995 3.275805 4.464785 5.324108 5.014629 3.842441 2.989365 2.599465 1.968708 2.696571 1.421260	2.517019 3.057329 4.271571 4.940120 4.397684 -4.262565 -0.706762 -1.425563 -1.065591 0.031405 0.767322 0.395112 -2.883673 -1.367488 -3.677230 -5.633324	Multip Charge E(B97- E(M06/ E(PBE E(PBE0) E(PBEh E(PM6) E(GFN7) E(GFN1 E(GFN2 E(GFN-	licity: 5 : 0 3c) = -4543.374459 def2-TZVP) = -4543 - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - 3c) = -4537.46256 = 197.86854 Kcal/r = -2.31902 Kcal/r X-V/def2-TZVP) =xTB) = -154.67443 -xTB) = -153.63378 FF) = -21.59103959 nates:	8.378788184949 Ha c) = -4541.721998 dP) = -4542.05042 f5938135 Hartree mol nol -4545.91844677672 f5226022 Hartree f2870437 Hartree f4908 Hartree	648313 Hartree 6495231 Hartree 5 Hartree
С С С С С С С С С С Н Н Н Н	-4.106389 -2.353918 -2.525706 -3.341304 -4.013128 -3.861904 -3.037534 1.374118 0.731183 0.477457 -0.575048 -1.393694 -1.156778 -0.107843 2.824745 -1.422716 -0.934781 -1.882611 -3.312208	-3.160526 -4.166232 -3.948182 -2.723065 -1.723525 -0.407995 3.275805 4.464785 5.324108 5.014629 3.842441 2.989365 2.599465 1.968708 2.696571 1.421260 -0.597137	2.517019 3.057329 4.271571 4.940120 4.397684 -4.262565 -0.706762 -1.425563 -1.065591 0.031405 0.767322 0.395112 -2.883673 -1.367488 -3.677230 -5.633324 -5.219064	Multip Charge E (B97- E (M06/ E (PBE E (PBE0 E (PBE0) E (PM6) E (QM7) E (GFN1 E (GFN2 Coordi Fe	licity: 5 : 0 3c) = -4543.374459 def2-TZVP) = -4543 - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZV -3c) = -4537.46256 = 197.86854 Kcal/n X-V/def2-TZVP) =xTB) = -154.67443 -xTB) = -153.63378 FF) = -21.59103959 nates: 0.243001	8.378788184949 Ha c) = -4541.721998 dP) = -4542.05042 f5938135 Hartree (mol nol 454545.91844677672 4525022 Hartree 12870437 Hartree 14908 Hartree 0.299894	648313 Hartree 6495231 Hartree 5 Hartree 0.414860
СССССССССН Н Н Н Н Н	-4.106389 -2.353918 -2.525706 -3.341304 -4.013128 -3.861904 -3.037534 1.374118 0.731183 0.477457 -0.575048 -1.393694 -1.156778 -0.107843 2.824745 -1.422716 -0.934781 -1.882611 -3.312208 -3.803185	-3.160526 -4.166232 -3.948182 -2.723065 -1.723525 -0.407995 3.275805 4.464785 5.324108 5.014629 3.842441 2.989365 2.599465 1.968708 2.696571 1.421260 -0.597137 -1.329474	2.517019 3.057329 4.271571 4.940120 4.397684 -4.262565 -0.706762 -1.425563 -1.065591 0.031405 0.767322 0.395112 -2.883673 -1.367488 -3.677230 -5.633324 -5.219064 -2.893241	Multip Charge E(B97- E(M06/ E(PBE) E(PBE0) E(PBE0) E(PM6) E(PM7) E(GFN1 E(GFN2) C(GFN1 Coordi Fe Si	licity: 5 : 0 3c) = -4543.374459 def2-TZVP) = -4543 - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF -3c) = -4537.46256 = 197.86854 Kcal/r X-V/def2-TZVP) =xTB) = -154.67443 -xTB) = -153.63378 FF) = -21.59103959 nates:	8.378788184949 Ha c) = -4541.721998 dP) = -4542.05042 f5938135 Hartree fmol aol .4545.91844677672 f5226022 Hartree f2870437 Hartree d4908 Hartree 0.299894 2.810784	648313 Hartree 6495231 Hartree 5 Hartree 0.414860 -1.014597
	-4.106389 -2.353918 -2.525706 -3.341304 -4.013128 -3.861904 -3.037534 1.374118 0.731183 0.477457 -0.575048 -1.393694 -1.156778 -0.107843 2.824745 -1.422716 -0.934781 -1.882611 -3.312208 -3.803185 -3.772645	-3.160526 -4.166232 -3.948182 -2.723065 -1.723525 -0.407995 3.275805 4.464785 5.324108 5.014629 3.842441 2.989365 2.599465 1.968708 2.696571 1.421260 -0.597137 -1.329474 2.653382	2.517019 3.057329 4.271571 4.940120 4.397684 -4.262565 -0.706762 -1.425563 -1.065591 0.031405 0.767322 0.395112 -2.883673 -1.367488 -3.677230 -5.633324 -5.219064 -2.893241 -0.844957	Multip Charge E(B97- E(M06/ E(PBE E(PBE) E(PBE) E(PM7) E(\omegas) E(GFN1 E(GFN2 E(GFN- Coordi Fe Si Si	licity: 5 : 0 3c) = -4543.374459 def2-TZVP) = -4543 - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - 3c) = -4537.4626 = 197.86854 Kcal/ = -2.31902 Kcal/π X-V/def2-TZVP) =xTB) = -154.67443 -xTB) = -153.63378 FF) = -21.59103959 nates:	8.378788184949 Ha 2) = -4541.721998 2P) = -4542.05042 55938135 Hartree 201 201 202 203 204 204 205 206 207 207 208 208 208 208 208 208 208 208 208 208	648313 Hartree 6495231 Hartree 5 Hartree 0.414860 -1.014597 -1.252314
СССССССССНННННН	-4.106389 -2.353918 -2.525706 -3.341304 -4.013128 -3.861904 -3.037534 1.374118 0.731183 0.477457 -0.575048 -1.393694 -1.156778 -0.107843 2.824745 -1.422716 -0.934781 -1.882611 -3.312208 -3.803185 -3.772645 -5.030276	-3.160526 -4.166232 -3.948182 -2.723065 -1.723525 -0.407995 3.275805 4.464785 5.324108 5.014629 3.842441 2.989365 2.599465 1.968708 2.696571 1.421260 -0.597137 -1.329474 2.653382 4.423909	2.517019 3.057329 4.271571 4.940120 4.397684 -4.262565 -0.706762 -1.425563 -1.065591 0.031405 0.767322 0.395112 -2.883673 -1.367488 -3.677230 -5.633324 -5.219064 -2.893241 -0.844957 0.365420	Multip Charge E (B97- E (M06/ E (PBE) E (PBE) E (PE) E (E) E (E) E (GFN1 E (GFN2 E (GFN- Coordi Fe Si Si	licity: 5 : 0 3c) = -4543.374459 def2-TZVP) = -4543 - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - 3c) = -4537.46256 = 197.86854 Kcal/r Z-V/def2-TZVP) = -xTB) = -154.67443 -xTB) = -153.63378 FF) = -21.59103959 nates:	8.378788184949 Ha 2) = -4541.721998 2P) = -4542.05042 55938135 Hartree mol nol .4545.91844677672 55226022 Hartree 12870437 Hartree 44908 Hartree  0.299894 2.810784 0.696002 -2.534421	648313 Hartree 6495231 Hartree 5 Hartree 0.414860 -1.014597 -1.252314 -0.390110
СССССССССССННННННН	-4.106389 -2.353918 -2.353918 -2.525706 -3.341304 -4.013128 -3.861904 -3.037534 1.374118 0.731183 0.477457 -0.575048 -1.393694 -1.156778 -0.107843 2.824745 -1.422716 -0.934781 -1.882611 -3.312208 -3.803185 -3.772645 -5.030276 -6.074484	-3.160526 -4.166232 -3.948182 -2.723065 -1.723525 -0.407995 3.275805 4.464785 5.324108 5.014629 3.842441 2.989365 2.599465 1.968708 2.696571 1.421260 -0.597137 -1.329474 2.655382 4.423909 3.933493	2.517019 3.057329 4.271571 4.940120 4.397684 -4.262565 -0.706762 -1.425563 -1.065591 0.031405 0.767322 0.395112 -2.883673 -1.367488 -3.677230 -5.633324 -5.219064 -2.893241 -0.844957 0.365420 2.595039	Multip Charge E (B97- E (M06/ E (PBE E (PBE0 E (PBE0) E (PM6) E (GFN1 E (GFN2 E (GFN- Coordi Fe Si Si Si	licity: 5 : 0 3c) = -4543.374459 def2-TZVP) = -4543 - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - 3c) = -4537.46256 = 197.86854 Kcal/m X-V/def2-TZVP) =xTB) = -154.67443 -xTB) = -153.63378 FF) = -21.59103959 nates:	8.378788184949 Ha p) = -4541.721998 pr) = -4542.05042 F5938135 Hartree fmol tol 4545.91844677672 4526022 Hartree 62870437 Hartree 64908 Hartree 62870437 Hartree 64908 Hartree 62870437 Hartree 64908 Hartree 62870437 Hartree 64908 Hartree 62870437 Hartree 63870437 Hartree 64908 Hartree	648313 Hartree 6495231 Hartree 5 Hartree 0.414860 -1.014597 -1.252314 -0.390110 2.540258
СССССССССННННННН	-4.106389 -2.353918 -2.353918 -2.525706 -3.341304 -4.013128 -3.861904 -3.037534 1.374118 0.731183 0.477457 -0.575048 -1.393694 -1.156778 -0.107843 2.824745 -1.422716 -0.934781 -1.882611 -3.312208 -3.803185 -3.772645 -5.030276 -6.074484 -5.863035	-3.160526 -4.166232 -3.948182 -2.723065 -1.723525 -0.407995 3.275805 4.464785 5.324108 5.014629 3.842441 2.989365 2.599465 1.968708 2.696571 1.421260 -0.597137 -1.329474 2.6553382 4.423909 3.933493 1.636694	2.517019 3.057329 4.271571 4.940120 4.397684 -4.262565 -0.706762 -1.425563 -1.065591 0.031405 0.767322 0.395112 -2.883673 -1.367488 -3.677230 -5.633324 -5.219064 -2.893241 -0.844957 0.365420 2.595039 3.587237	Multip Charge E (B97- E (M06/ E (PBE E (PBE0 E (PBE0) E (PM7) E (GFN1 E (GFN2 E (GFN- Coordi Fe Si Si Si N	licity: 5 : 0 3c) = -4543.374459 def2-TZVP) = -4543 - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP - 3c) = -4537.46256 = 197.86854 Kcal/m X-V/def2-TZVP) =xTB) = -154.67443 -xTB) = -153.63378 FF) = -21.59103959 nates:	8.378788184949 Ha c) = -4541.721998 dP) = -4542.05042 f5938135 Hartree fmol nol -4545.91844677672 f5226022 Hartree f2870437 Hartree f4908 Hartree 0.299894 2.810784 0.696002 -2.534421 -1.455849 1.254927	648313 Hartree 6495231 Hartree 5 Hartree 0.414860 -1.014597 -1.252314 -0.390110 2.540258 -0.614003
СССССССССНННННННН	-4.106389 -2.353918 -2.353706 -3.341304 -4.013128 -3.861904 -3.037534 1.374118 0.731183 0.477457 -0.575048 -1.393694 -1.156778 -0.107843 2.824745 -1.422716 -0.934781 -1.882611 -3.312208 -3.803185 -3.772645 -5.030276 -6.074484 -5.863035 -4.607723	-3.160526 -4.166232 -3.948182 -2.723065 -1.723525 -0.407995 3.275805 4.464785 5.324108 5.014629 3.842441 2.989365 2.599465 1.968708 2.696571 1.421260 -0.597137 -1.329474 2.653382 4.423909 3.933493 1.636694 -0.134983	2.517019 3.057329 4.271571 4.940120 4.397684 -4.262565 -0.706762 -1.425563 -1.065591 0.031405 0.767322 0.395112 -2.883673 -1.367488 -3.677230 -5.633324 -5.219064 -2.893241 -0.844957 0.365420 2.595039 3.587237 2.383890	Multip Charge E (B97- E (M06/ E (PBE E (PBE) E (PBE) E (PM7) E (\omega FN- E (GFN1- Coordi Fe Si Si Si N N	licity: 5 : 0 3c) = -4543.374459 def2-TZVP) = -4543 - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - S45466 - 1.564375 - 1.324981 - 1.047330 - 1.177305	8.378788184949 Ha c) = -4541.721998 dP) = -4542.05042 fS938135 Hartree fmol lol lol los226022 Hartree lole lol lol lol lol lol lol lol lol	648313 Hartree 6495231 Hartree 5 Hartree 0.414860 -1.014597 -1.252314 -0.390110 2.540258 -0.614003 0.806669
СССССССССННННННН	-4.106389 -2.353918 -2.353918 -2.525706 -3.341304 -4.013128 -3.861904 -3.037534 1.374118 0.731183 0.477457 -0.575048 -1.393694 -1.156778 -0.107843 2.824745 -1.422716 -0.934781 -1.882611 -3.312208 -3.803185 -3.772645 -5.030276 -6.074484 -5.863035	-3.160526 -4.166232 -3.948182 -2.723065 -1.723525 -0.407995 3.275805 4.464785 5.324108 5.014629 3.842441 2.989365 2.599465 1.968708 2.696571 1.421260 -0.597137 -1.329474 2.6553382 4.423909 3.933493 1.636694	2.517019 3.057329 4.271571 4.940120 4.397684 -4.262565 -0.706762 -1.425563 -1.065591 0.031405 0.767322 0.395112 -2.883673 -1.367488 -3.677230 -5.633324 -5.219064 -2.893241 -0.844957 0.365420 2.595039 3.587237	Multip Charge E (B97- E (M06/ E (PBE E (PBE0 E (PBE0) E (PM7) E (GFN1 E (GFN2 E (GFN- Coordi Fe Si Si Si N	licity: 5 : 0 3c) = -4543.374459 def2-TZVP) = -4543 - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP - 3c) = -4537.46256 = 197.86854 Kcal/m X-V/def2-TZVP) =xTB) = -154.67443 -xTB) = -153.63378 FF) = -21.59103959 nates:	8.378788184949 Ha c) = -4541.721998 dP) = -4542.05042 f5938135 Hartree fmol nol -4545.91844677672 f5226022 Hartree f2870437 Hartree f4908 Hartree 0.299894 2.810784 0.696002 -2.534421 -1.455849 1.254927	648313 Hartree 6495231 Hartree 5 Hartree 0.414860 -1.014597 -1.252314 -0.390110 2.540258 -0.614003

С	1.981221	3.672186	0.515400	Н	3.207546	0.363065	-5.176954
С	3.303778	3.578856	0.971578	С	0.014857	-3.557035	-0.776730
C	4.131457	2.533887	0.521925	C	-0.006303	-4.472830	-1.852978
C	3.636180	1.602298	-0.400384	С	-1.142150	-3.449510	0.023402
C	2.305032	1.690367	-0.850419	С	-1.139770	-5.258292	-2.113648
C	-1.221906	4.218101	-0.096140	Č	-2.281131	-4.231344	-0.229387
С	-2.065467	3.933081	1.000106	С	-2.280136	-5.139147	-1.300141
C	-2.700538	4.961711	1.713437	H	0.875366	-4.566568	-2.508957
C	-2.497620	6.301488	1.344579	Н	-1.161630	-2.719642	0.845990
C	-1.660048	6.606395	0.259291	Н	-1.137374	-5.965425	-2.958137
С	-1.031911	5.572255	-0.453373	Н	-3.173904	-4.112673	0.402731
C	-0.257788	3.196419	-2.864768	H	-3.172014	-5.750689	-1.507284
C	-2.414460	-0.262048	-2.888180				
C	-2.398402	-1.675400	-2.927063	Confo	rmation 32.		
C	-2.246910	-2.369988	-4.138328		plicity: 5		
C	-2.109243	-1.663503	-5.342785	Charg			
C	-2.133426	-0.259032	-5.329947	E(B97	(-3c) = -4543.37369	6662202 Hartree	
C	-2.287461	0.428524	-4.115992	E (M06	f/def2-TZVP) = -4543	3.376943832447 Ha	rtree
С	2.932384	-3.702078	0.199283		- D3(BJ)/def2-TZV		
C	3.139808	-1.327182	3.066865		10 - D3(BJ)/def2-TZ		
							0394390 naittee
C	4.087499	-0.818753	2.152126		h-3c) = -4537.4600		
C	5.434521	-0.660088	2.513195	E(PM6	5) = 210.61454 Kcal,	/mol	
C	5.859286	-1.012323	3.804223	E(PM7	= -10.93816  Kcal	/mol	
C	4.931469	-1.519603	4.729107		7X-V/def2-TZVP) =		5 Hartree
							5 Hartree
С	3.585359	-1.672748	4.362002		(1-xTB) = -154.6733		
C	0.531240	-2.989410	3.306781	E (GFN	(2-xTB) = -153.6326	37687937 Hartree	
H	1.342545	4.499442	0.864296	E (GFN	I-FF) = -21.61371769	93457 Hartree	
H	3.695200	4.323326	1.682044				
Н	5.166725	2.453508	0.886968	Coord	linates:		
						0 257655	0 270402
Н	4.281495	0.801347	-0.789222	Fe	0.028378	-0.357655	-0.372483
H	1.956209	0.973881	-1.610976	Si	0.246205	-2.084556	2.231529
H	-2.222065	2.883327	1.294121	Si	2.223320	0.308302	1.636357
H	-3.360841	4.716714	2.560264	Si	-2.451292	1.739544	-1.147839
Н	-2.995675	7.110186	1.901522	Si	-1.352943	-0.738386	-2.764696
H	-1.499515	7.655133	-0.035508	N	0.886975	-0.761903	1.272987
H	-0.381190	5.829594	-1.305435	N	-1.345588	0.418111	-1.451467
H	-1.253037	3.422119	-3.296828	С	-1.420053	-2.579202	1.462102
Н	0.174996	2.331371	-3.406750	C	-2.442553	-1.617629	1.281080
Н	0.398457	4.073502	-3.039616	С	-3.692625	-1.969374	0.747467
H	-2.493612	-2.250577	-1.994150	C	-3.948560	-3.299457	0.380190
H	-2.228295	-3.469954	-4.130520	С	-2.946123	-4.270842	0.544659
H	-1.985871	-2.205848	-6.293005	С	-1.699330	-3.911501	1.080299
Н	-2.034977	0.303508	-6.271741	C	-0.020873	-1.514978	4.026015
H	-2.308102	1.529413	-4.131823	С	-1.291621	-1.198372	4.554316
H	3.867146	-3.159408	0.444049	C	-1.434059	-0.703931	5.861444
H	3.153573	-4.456349	-0.583169	С	-0.303172	-0.518732	6.672038
Н	2.615062	-4.246555	1.111385	Č	0.969493	-0.841192	6.171871
Н	3.750435	-0.542974	1.141005	С	1.104563	-1.337328	4.865935
H	6.157462	-0.260893	1.783916	C	1.370260	-3.602085	2.270970
H	6.915366	-0.892572	4.091676	С	3.754216	-0.672358	2.174240
Н	5.260689	-1.797929	5.742398	С	4.135680	-1.819613	1.439998
Н				C	5.261442		
	2.871592	-2.068623	5.103165			-2.574965	1.801250
H	-0.550471	-3.042971	3.071522	C	6.027221	-2.201862	2.918135
H	0.649061	-2.997235	4.409951	C	5.661896	-1.071250	3.665841
H	1.004450	-3.909866	2.909956	C	4.538524	-0.314434	3.293320
С	-3.770487	2.140603	-1.571496	С	-4.067551	1.513973	-2.104013
	-3.984484	2.686125	-0.631944	C	-0.926153	0.080377	-4.418230
H							
H	-3.370767	2.875169	-2.299670	C	0.003735	1.144610	-4.445563
H	-4.726011	1.748857	-1.976204	С	0.378176	1.752431	-5.653066
C	0.403028	0.095818	3.143855	С	-0.181714	1.311375	-6.863155
C	-0.760869	0.027089	3.946489	C	-1.114282	0.261249	-6.857319
	0.878765					-0.348537	
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Confor	mation 5.			Н	-0.747423	-0.792566	6.156197
Multip	licity: 5			Н	1.553310	1.829313	3.577079
Charge				Н	0.268793	1.458857	5.694122
_		4641640					
	3c) = -4543.36429			C	-2.690344	0.526731	0.865652
E(M06/	def2-TZVP) = -454	3.369541128376 Ha	rtree	С	-3.624744	-0.084127	-0.016421
E (PRE	- D3(BJ)/def2-TZV	P) = -4541 714858	146132 Hartree	С	-2.370258	-0.164586	2.078023
		•					
	- D3(BJ)/def2-TZ		42/1005 Hartree	C	-4.183317	-1.333715	0.268425
E (PBEh	-3c) = -4537.4503	86252622 Hartree		C	-2.946817	-1.424523	2.360170
E (PM6)	= 210.47233 Kcal	/mol		С	-3.836828	-2.012150	1.456507
	= -2.08331 Kcal/			Н	-3.911935	0.441454	-0.939570
			_				
E(ωB97	X-V/def2-TZVP) =	-4545.91318139223	0 Hartree	H	-1.760573	0.324116	2.856807
E (GFN1	-xTB) = $-154.6674$	15494971 Hartree		H	-4.903369	-1.786417	-0.430878
F (CFN2	-xTB) = $-153.6228$	33951079 Hartree		Н	-2.701722	-1.925514	3.307559
E (GFN-	FF) = -21.4522006	43952 Hartree		H	-4.286439	-2.990978	1.684194
				C	-0.388203	-1.463256	-2.616841
Coordi	nates:			C	0.279058	-0.708395	-3.608196
Fe	-0.432185	-0.190236	0.559097	C	-1.801993	-1.482155	-2.650959
Si	1.228972	2.549288	-0.206720	С	-0.429842	-0.010137	-4.599604
Si	-1.859078	2.225320	0.540553	C	-2.517878	-0.799571	-3.645909
Si	0.566195	-2.533208	-1.362706	C	-1.831801	-0.068377	-4.629490
Si	0.678076	-2.803744	1.716878	H	1.379579	-0.677662	-3.621903
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C	3.435108	2.703477	1.667789		-2.390404		
С	3.435108						-1.524767
C C	3.435108 4.088521	3.113683	2.842087	C	-0.078704	-4.315661	-1.524767
C C	3.435108 4.088521 3.465084	3.113683 4.021751	2.842087 3.712021	C C	-0.078704 -1.360446	-4.315661 -4.650496	-1.028318
C C	3.435108 4.088521	3.113683	2.842087	C	-0.078704	-4.315661	
C C C	3.435108 4.088521 3.465084 2.186701	3.113683 4.021751 4.515196	2.842087 3.712021 3.400453	C C C	-0.078704 -1.360446 0.681864	-4.315661 -4.650496 -5.343278	-1.028318 -2.125492
0 0 0 0	3.435108 4.088521 3.465084 2.186701 1.537886	3.113683 4.021751 4.515196 4.090595	2.842087 3.712021 3.400453 2.230798	C C C	-0.078704 -1.360446 0.681864 -1.866986	-4.315661 -4.650496 -5.343278 -5.954758	-1.028318 -2.125492 -1.133762
0 0 0 0 0	3.435108 4.088521 3.465084 2.186701 1.537886 0.812884	3.113683 4.021751 4.515196 4.090595 4.025639	2.842087 3.712021 3.400453 2.230798 -1.323437	C C C	-0.078704 -1.360446 0.681864 -1.866986 0.185170	-4.315661 -4.650496 -5.343278 -5.954758 -6.653338	-1.028318 -2.125492 -1.133762 -2.229463
0 0 0 0 0 0	3.435108 4.088521 3.465084 2.186701 1.537886	3.113683 4.021751 4.515196 4.090595	2.842087 3.712021 3.400453 2.230798	0 0 0 0 0	-0.078704 -1.360446 0.681864 -1.866986	-4.315661 -4.650496 -5.343278 -5.954758	-1.028318 -2.125492 -1.133762 -2.229463 -1.735095
0 0 0 0 0 0	3.435108 4.088521 3.465084 2.186701 1.537886 0.812884 0.268529	3.113683 4.021751 4.515196 4.090595 4.025639 3.781933	2.842087 3.712021 3.400453 2.230798 -1.323437	C C C	-0.078704 -1.360446 0.681864 -1.866986 0.185170 -1.092449	-4.315661 -4.650496 -5.343278 -5.954758 -6.653338 -6.961260	-1.028318 -2.125492 -1.133762 -2.229463 -1.735095
0000000	3.435108 4.088521 3.465084 2.186701 1.537886 0.812884 0.268529 -0.098375	3.113683 4.021751 4.515196 4.090595 4.025639 3.781933 4.835925	2.842087 3.712021 3.400453 2.230798 -1.323437 -2.606414 -3.454952	C C C C H	-0.078704 -1.360446 0.681864 -1.866986 0.185170 -1.092449 -1.964258	-4.315661 -4.650496 -5.343278 -5.954758 -6.653338 -6.961260 -3.878213	-1.028318 -2.125492 -1.133762 -2.229463 -1.735095 -0.524348
C C C C C C C C	3.435108 4.088521 3.465084 2.186701 1.537886 0.812884 0.268529 -0.098375 0.074452	3.113683 4.021751 4.515196 4.090595 4.025639 3.781933 4.835925 6.165844	2.842087 3.712021 3.400453 2.230798 -1.323437 -2.606414 -3.454952 -3.038556	C C C C C H H	-0.078704 -1.360446 0.681864 -1.866986 0.185170 -1.092449 -1.964258 1.688264	-4.315661 -4.650496 -5.343278 -5.954758 -6.653338 -6.961260 -3.878213 -5.122952	-1.028318 -2.125492 -1.133762 -2.229463 -1.735095 -0.524348 -2.515100
C C C C C C C	3.435108 4.088521 3.465084 2.186701 1.537886 0.812884 0.268529 -0.098375 0.0774452 0.628496	3.113683 4.021751 4.515196 4.090595 4.025639 3.781933 4.835925 6.165844 6.431979	2.842087 3.712021 3.400453 2.230798 -1.323437 -2.606414 -3.454952 -3.038556 -1.777221	C C C C C H H H	-0.078704 -1.360446 0.681864 -1.866986 0.185170 -1.092449 -1.964258 1.688264 -2.867804	-4.315661 -4.650496 -5.343278 -5.954758 -6.653338 -6.961260 -3.878213 -5.122952 -6.191563	-1.028318 -2.125492 -1.133762 -2.229463 -1.735095 -0.524348 -2.515100 -0.738342
C C C C C C C C	3.435108 4.088521 3.465084 2.186701 1.537886 0.812884 0.268529 -0.098375 0.074452	3.113683 4.021751 4.515196 4.090595 4.025639 3.781933 4.835925 6.165844	2.842087 3.712021 3.400453 2.230798 -1.323437 -2.606414 -3.454952 -3.038556	C C C C C H H	-0.078704 -1.360446 0.681864 -1.866986 0.185170 -1.092449 -1.964258 1.688264	-4.315661 -4.650496 -5.343278 -5.954758 -6.653338 -6.961260 -3.878213 -5.122952	-1.028318 -2.125492 -1.133762 -2.229463 -1.735095 -0.524348 -2.515100
	3.435108 4.088521 3.465084 2.186701 1.537886 0.812884 0.268529 -0.098375 0.074452 0.628496 0.996876	3.113683 4.021751 4.515196 4.090595 4.025639 3.781933 4.835925 6.165844 6.431979 5.371249	2.842087 3.712021 3.400453 2.230798 -1.323437 -2.606414 -3.454952 -3.038556 -1.777221 -0.932991	С С С С С Н Н Н Н	-0.078704 -1.360446 0.681864 -1.866986 0.185170 -1.092449 -1.964258 1.688264 -2.867804 0.798626	-4.315661 -4.650496 -5.343278 -5.954758 -6.653338 -6.961260 -3.878213 -5.122952 -6.191563 -7.438977	-1.028318 -2.125492 -1.133762 -2.229463 -1.735095 -0.524348 -2.515100 -0.738342 -2.698986
	3.435108 4.088521 3.465084 2.186701 1.537886 0.812884 0.268529 -0.098375 0.074452 0.628496 0.996876 2.365494	3.113683 4.021751 4.515196 4.090595 4.025639 3.781933 4.835925 6.165844 6.431979 5.371249 1.365664	2.842087 3.712021 3.400453 2.230798 -1.323437 -2.606414 -3.454952 -3.038556 -1.777221 -0.932991 -1.139820	C C C C C H H H	-0.078704 -1.360446 0.681864 -1.866986 0.185170 -1.092449 -1.964258 1.688264 -2.867804	-4.315661 -4.650496 -5.343278 -5.954758 -6.653338 -6.961260 -3.878213 -5.122952 -6.191563	-1.028318 -2.125492 -1.133762 -2.229463 -1.735095 -0.524348 -2.515100 -0.738342
	3.435108 4.088521 3.465084 2.186701 1.537886 0.812884 0.268529 -0.098375 0.074452 0.628496 0.996876 2.365494 -2.672007	3.113683 4.021751 4.515196 4.090595 4.025639 3.781933 4.835925 6.165844 6.431979 5.371249 1.365664 3.052513	2.842087 3.712021 3.400453 2.230798 -1.323437 -2.606414 -3.454952 -3.038556 -1.777221 -0.932991 -1.139820 -0.947328	С С С С С Н Н Н Н	-0.078704 -1.360446 0.681864 -1.866986 0.185170 -1.092449 -1.964258 1.688264 -2.867804 0.798626	-4.315661 -4.650496 -5.343278 -5.954758 -6.653338 -6.961260 -3.878213 -5.122952 -6.191563 -7.438977	-1.028318 -2.125492 -1.133762 -2.229463 -1.735095 -0.524348 -2.515100 -0.738342 -2.698986
	3.435108 4.088521 3.465084 2.186701 1.537886 0.812884 0.268529 -0.098375 0.074452 0.628496 0.996876 2.365494	3.113683 4.021751 4.515196 4.090595 4.025639 3.781933 4.835925 6.165844 6.431979 5.371249 1.365664	2.842087 3.712021 3.400453 2.230798 -1.323437 -2.606414 -3.454952 -3.038556 -1.777221 -0.932991 -1.139820	С С С С С Н Н Н Н	-0.078704 -1.360446 0.681864 -1.866986 0.185170 -1.092449 -1.964258 1.688264 -2.867804 0.798626 -1.483471	-4.315661 -4.650496 -5.343278 -5.954758 -6.653338 -6.961260 -3.878213 -5.122952 -6.191563 -7.438977	-1.028318 -2.125492 -1.133762 -2.229463 -1.735095 -0.524348 -2.515100 -0.738342 -2.698986
00000000000000	3.435108 4.088521 3.465084 2.186701 1.537886 0.812884 0.268529 -0.098375 0.074452 0.628496 0.996876 2.365494 -2.672007 -2.642655	3.113683 4.021751 4.515196 4.090595 4.025639 3.781933 4.835925 6.165844 6.431979 5.371249 1.365664 3.052513 2.412269	2.842087 3.712021 3.400453 2.230798 -1.323437 -2.606414 -3.454952 -3.038556 -1.777221 -0.932991 -1.139820 -0.947328 -2.206383	С С С С С Н Н Н Н	-0.078704 -1.360446 0.681864 -1.866986 0.185170 -1.092449 -1.964258 1.688264 -2.867804 0.798626	-4.315661 -4.650496 -5.343278 -5.954758 -6.653338 -6.961260 -3.878213 -5.122952 -6.191563 -7.438977	-1.028318 -2.125492 -1.133762 -2.229463 -1.735095 -0.524348 -2.515100 -0.738342 -2.698986
0 0 0 0 0 0 0 0 0 0 0 0 0 0	3.435108 4.088521 3.465084 2.186701 1.537886 0.812884 0.268529 -0.098375 0.074452 0.628496 0.996876 2.365494 -2.672007 -2.642655 -3.243264	3.113683 4.021751 4.515196 4.090595 4.025639 3.781933 4.835925 6.165844 6.431979 5.371249 1.365664 3.052513 2.412269 2.995742	2.842087 3.712021 3.400453 2.230798 -1.323437 -2.606414 -3.454952 -3.038556 -1.777221 -0.932991 -1.139820 -0.947328 -2.206383 -3.330423	С С С С С Н Н Н Н	-0.078704 -1.360446 0.681864 -1.866986 0.185170 -1.092449 -1.964258 1.688264 -2.867804 0.798626 -1.483471	-4.315661 -4.650496 -5.343278 -5.954758 -6.653338 -6.961260 -3.878213 -5.122952 -6.191563 -7.438977	-1.028318 -2.125492 -1.133762 -2.229463 -1.735095 -0.524348 -2.515100 -0.738342 -2.698986
0000000000000000	3.435108 4.088521 3.465084 2.186701 1.537886 0.812884 0.268529 -0.098375 0.074452 0.628496 0.996876 2.365494 -2.672007 -2.642655 -3.243264 -3.867471	3.113683 4.021751 4.515196 4.090595 4.025639 3.781933 4.835925 6.165844 6.431979 5.371249 1.365664 3.052513 2.412269 2.995742 4.248941	2.842087 3.712021 3.400453 2.230798 -1.323437 -2.606414 -3.454952 -3.038556 -1.777221 -0.932991 -1.139820 -0.947328 -2.206383 -3.330423 -3.221795	С С С С С Н Н Н Н	-0.078704 -1.360446 0.681864 -1.866986 0.185170 -1.092449 -1.964258 1.688264 -2.867804 0.798626 -1.483471	-4.315661 -4.650496 -5.343278 -5.954758 -6.653338 -6.961260 -3.878213 -5.122952 -6.191563 -7.438977	-1.028318 -2.125492 -1.133762 -2.229463 -1.735095 -0.524348 -2.515100 -0.738342 -2.698986
0 0 0 0 0 0 0 0 0 0 0 0 0	3.435108 4.088521 3.465084 2.186701 1.537886 0.812884 0.268529 -0.098375 0.074452 0.628496 0.996876 2.365494 -2.672007 -2.642655 -3.243264	3.113683 4.021751 4.515196 4.090595 4.025639 3.781933 4.835925 6.165844 6.431979 5.371249 1.365664 3.052513 2.412269 2.995742	2.842087 3.712021 3.400453 2.230798 -1.323437 -2.606414 -3.454952 -3.038556 -1.777221 -0.932991 -1.139820 -0.947328 -2.206383 -3.330423	С С С С С С Н Н Н Н Н Н	-0.078704 -1.360446 0.681864 -1.866986 0.185170 -1.092449 -1.964258 1.688264 -2.867804 0.798626 -1.483471	-4.315661 -4.650496 -5.343278 -5.954758 -6.653338 -6.961260 -3.878213 -5.122952 -6.191563 -7.438977	-1.028318 -2.125492 -1.133762 -2.229463 -1.735095 -0.524348 -2.515100 -0.738342 -2.698986

	olicity: 2			С	5.477088	-7.532335	-0.460906
Charge	e: 0			C	2.768783	-6.723711	0.340754
E(B97-	-3c) = -5613.021580	0151656 Hartree		C	1.780479	-2.827713	1.268852
	def2-TZVP) = -5612		tree	С	3.074118	-1.992937	1.444129
	- D3(BJ)/def2-TZVI			C	4.257967	-2.914392	1.809026
	) - D3(BJ)/def2-TZV		824234 Hartree	С	3.377244	-1.279979	0.118789
E (PBEh	1-3c) = -5604.82270	09670281 Hartree		C	2.832445	-0.941639	2.550275
E(PM6)	= 180.72323 Kcal,	/mol		C	-2.532092	4.419254	5.701993
E(PM7)	= 67.30399 Kcal/r	nol		С	-3.837729	4.592212	4.902915
	7X-V/def2-TZVP) = -		R Hartree	C	-4.010718	3.221287	2.772593
	-xTB) = $-265.5392$		, marcice	C	-4.047371	3.599710	1.402668
	2-xTB) = $-259.27138$			С	-4.338369	2.629655	0.429704
E (GFN-	-FF) = -33.82149242	21922 Hartree		C	-4.554693	1.298139	0.821416
				C	-4.433694	0.920227	2.200438
Coordi	nates:			С	-4.173586	1.891840	3.184916
Cu	-1.360647	0.573347	0.442464	C	-3.632483	5.412734	2.505860
N	-0.811586	2.417758	1.091880	C	-3.305952	6.819899	2.872818
N	-1.778689	1.329365	-1.393860	C	-4.954596	0.268771	-0.204973
N	-1.833886	-1.291849	-0.228677	C	-4.598555	-0.524342	2.598318
N	-0.868227	-0.199834	2.252303	H	0.568031	4.647708	3.202908
С	-0.277515	2.740294	2.322166	H	-0.098582	5.687669	0.759315
С	-0.798179	3.580142	0.349960	Н	-2.218381	3.769580	-3.666928
C	-1.730559	2.659488	-1.760648	Н	-2.746186	1.257981	-4.616084
С	-2.190202	0.635978	-2.513822	H	-2.622628	-3.609347	-2.541006
C	-2.191013	-1.638867	-1.518277	H	-1.989952	-4.650588	-0.101225
C	-1.707832	-2.476606	0.462854	H	-0.643437	-2.606542	4.589821
С	-0.947989	-1.523915	2.629408	Н	-0.047496	-0.102802	5.513444
С	-0.456357	0.496160	3.370872	Н	0.932589	6.545675	-3.990754
C	0.100713	4.142451	2.350568	Н	-0.650087	8.447436	-3.529979
С	-0.227729	4.664288	1.125968	H	-2.499342	8.174482	-1.854228
C	-2.153813	2.812592	-3.138533	H	-2.769890	5.963543	-0.644522
C	-2.418267	1.552655	-3.613918	H	-0.678340	-3.003557	-6.350720
C	-2.333760	-3.078107	-1.627848	H	-2.891072	-2.915375	-7.541312
C	-2.023812	-3.598486	-0.399521	Н	-4.875989	-1.841181	-6.438074
C				Н			
	-0.624862	-1.662221	4.035126		-4.628690	-0.851999	-4.140395
С	-0.330132	-0.405376	4.499923	H	1.558457	-6.031616	3.326628
C	-1.247460	3.725341	-0.974719	H	-0.360719	-7.545135	3.840961
С	-2.347511	-0.760863	-2.607336	H	-2.712218	-6.796455	3.335376
С	-1.266685	-2.608255	1.791624	Н	-3.098826	-4.513368	2.378657
Č	-0.123276	1.864270	3.415633	Н	-0.376253	4.399824	7.363985
0	2.073226	4.693643	-4.614880	Н	1.931787	3.711921	8.071370
0	1.269341	-3.169770	-5.223627	H	3.293291	2.180604	6.612546
0	1.091408	-2.797257	0.250964	H	2.315571	1.345635	4.454653
0	-2.424256	4.929674	6.812225	Н	0.653724	3.349381	-2.122772
N	0.831618	4.125412	-2.763265	Н	-0.276559	-1.567926	-2.953086
N	-0.210090	-1.994077	-3.882787	Н	2.183677	-3.683363	3.078576
N	3.223957	-3.104645	-3.174743	H			
					-1.840607	3.292658	4.140668
N	5.288475	-3.763083	-3.828662	H	4.241427	1.518654	-4.343298
N	1.453020	-3.598845	2.369927	H	3.853174	3.070446	-5.176584
N	-1.592656	3.640054	5.074352	H	4.450994	3.085542	-3.490966
N	-3.769051	4.407212	3.469484	Н	1.946881	0.581718	-4.802004
N	-3.795280	4.959796	1.275988	Н	0.467757	1.499978	-4.350661
C							-5.700903
	-1.089015	5.053710	-1.643110	H	1.506891	2.068259	
С	-0.027732	5.220044	-2.579991	H	2.877248	0.829841	-2.336782
C	0.120166	6.445945	-3.260939	H	2.823200	2.429368	-1.549960
C	-0.772357	7.493919	-2.993471	H	1.301667	1.559350	-1.962458
C	-1.806807	7.343458	-2.055842	Н	2.304914	-1.226633	-3.123100
C	-1.963806	6.122025	-1.381392	Н	1.578846	-2.457151	-2.071716
C	-2.538388	-1.362387	-3.964089	Н	6.481440	-5.987696	-2.496401
		-1.976755					
С	-1.417663		-4.598300	H	1.828943	-4.600412	-1.083480
С	-1.554225	-2.533977	-5.886561	H	5.282382	-1.830037	-5.577208
C	-2.794831	-2.477783	-6.536082	H	3.483044	-1.872800	-5.724837
C	-3.905042	-1.876938	-5.922544	H	4.264257	-0.784309	-4.531511
C	-3.768882	-1.323365	-4.640270	Н	5.581127	-7.359356	0.632164
Č	-1.008394	-3.980133	2.312351	Н	4.897888	-8.474322	-0.571356
C	0.318422	-4.419764	2.578000	Н	6.489697	-7.711705	-0.870130
C	0.526973	-5.700629	3.131438	H	2.666033	-7.806539	0.114222
C							
	-0.549133	-6.550502	3.410265	H	3.322303	-6.663572	1.304014
С	-1.858973	-6.135053	3.124995	H	1.753384	-6.317295	0.510795
C	-2.075061	-4.861924	2.582019	H	5.195541	-2.323543	1.844319
С	0.447701	2.400867	4.689584	H	4.145595	-3.385593	2.809002
С	-0.309430	3.276440	5.517780	Н	4.386897	-3.719274	1.056706
C	0.233033	3.739280	6.736220	Н	4.260965	-0.622620	0.240227
С	1.520294	3.342088	7.119962	H	3.597368	-2.009301	-0.683728
С	2.280929	2.485719	6.309346	H	2.518012	-0.659015	-0.200065
C	1.737692	2.020067	5.104014	H	3.736435	-0.310375	2.673726
C	1.765714	3.881388	-3.746263	H	1.981500	-0.282367	2.286594
C	2.361749	2.442753	-3.713147	Н	2.601005	-1.403942	3.530713
C	3.813864	2.533135	-4.210953	Н	-4.582899	3.882442	5.322161
C	1.517265	1.599973	-4.697050	H	-4.206456	5.607982	5.139018
С	2.330361	1.794869	-2.314382	H	-4.406186	2.918683	-0.629005
C	1.003185	-2.569064	-4.190068	H	-4.094859	1.595569	4.242495
C	2.034660	-2.303839	-3.073514	H	-2.349194	6.879945	3.432681
С	3.533622	-4.219287	-2.401734	H	-3.211871	7.413478	1.946486
Č	4.839236	-4.601958	-2.819305	Н	-4.091088	7.283117	3.507172
C	5.469529	-5.687980	-2.184267	Н	-5.981253	-0.110371	-0.011362
C	4.804245	-6.372795	-1.154336	H	-4.937073	0.695137	-1.225696
С	3.482456	-5.980244	-0.761325	H	-4.284407	-0.612861	-0.195824
С	2.839813	-4.900409	-1.393434	H	-3.862414	-1.170012	2.075232
C	4.314538	-2.890724	-4.020838	H	-4.452894	-0.663416	3.686456
C	4.332256	-1.781876	-5.017159	H	-5.604779	-0.912673	2.333273

				~	0.600550	0.00000	0.000540
Confor	mation 15.			C C	-2.603572 -2.035535	-0.092096 -0.371546	2.238542 0.892436
	licity: 2			C	-3.485138	0.789426	8.075749
Charge				C	-5.852018	2.011368	6.836616
	3c) = -5613.03488	7372199 Hartree		C	0.707292	-3.047780	4.587540
E(M06/	def2-TZVP) = -5612	2.897545713929 Ha	rtree	С	0.124539	-3.874111	3.410201
E(PBE ·	- D3(BJ)/def2-TZV	P) = -5610.951484	627647 Hartree	С	0.542745	-3.220636	2.076294
	- D3(BJ)/def2-TZ		2259526 Hartree	С	0.702089	-5.293449	3.489032
	-3c) = -5604.83839			С	-1.413550	-3.922108	3.518153
	= 188.52835 Kcal,			C	3.142024	-4.473369	-1.716116
	= 51.88305 Kcal/r		4 77	C C	1.659446	-4.338802 -3.042525	-2.131230
	X-V/def2-TZVP) = - -xTB) = -265.5525		4 hartree	C	1.803013 1.241696	-1.817164	-4.281931 -4.724946
	-xTB) = $-259.28354$			C	1.487520	-1.378691	-6.037857
	FF) = -33.83695599			C	2.293116	-2.160869	-6.880401
	,			C	2.852876	-3.397500	-6.414664
Coordi	nates:			С	2.605357	-3.843835	-5.104346
Cu	1.352590	1.461207	0.287010	С	0.642907	-2.047157	-2.649228
N	2.484604	0.789626	-1.264748	С	0.088320	-1.783194	-1.294225
N	0.314708	2.640160	-0.997144	C	2.578274	-1.689380	-8.284680
N	0.262403	2.179056	1.846835	C H	3.719922	-4.221226	-7.332389
N C	2.344701 3.524448	0.233238 -0.117356	1.560983 -1.191216	н Н	4.907214 3.429798	-1.029620 0.454462	-2.733510 -4.476468
C	2.354917	1.119915	-2.599933	H	-0.532553	3.966961	-3.974418
C	0.473872	2.724287	-2.368121	Н	-1.929557	4.989517	-1.877598
Ċ	-0.663037	3.559289	-0.665550	Н	-2.034191	4.132926	3.345656
С	-0.705603	3.163800	1.790220	H	-0.791184	2.393996	5.034863
С	0.332980	1.783765	3.168716	H	3.121803	-1.172462	4.521746
C	2.134529	0.093151	2.920622	H	4.678343	-2.019784	2.459906
С	3.404267	-0.596856	1.247298	H	-0.725413	1.950549	-7.318585
С	4.072518	-0.355755	-2.512564	H	1.201057	3.095667	-8.443596
C	3.336019	0.399607	-3.387882	H	3.266307	3.659271	-7.124209
C C	-0.439070	3.710129	-2.914190 -1.859256	H H	3.350865	3.136723	-4.675684
C	-1.147260 -1.254585	4.223904 3.400070	3.111383	н Н	-5.615389 -5.036948	5.138760 7.577283	1.215009 1.032174
C	-0.620545	2.533371	3.963315	H	-2.650263	8.282595	0.680780
C	3.075906	-0.862255	3.472675	Н	-0.857703	6.532160	0.504824
C	3.858665	-1.294527	2.434075	Н	0.541491	-2.137386	7.296190
C	1.406528	2.005754	-3.145155	H	1.264994	-0.415961	8.969746
C	-1.144500	3.832239	0.629493	H	1.869509	1.900905	8.200480
C	1.185682	0.794552	3.693670	H	1.810704	2.447394	5.756341
C	3.981765	-0.766098	-0.026268	H	5.805562	-4.935356	-1.182270
0	-2.534567	2.394312	-5.597952	H	8.089813	-4.281951	-0.359724
0	-6.116710	2.967987	1.388366	H	8.474405	-1.990457	0.598321
0	1.523770	-3.514625	5.380324	H	6.559880	-0.370813	0.735413
O N	3.762986 -0.799670	-5.517348 1.157068	-1.885151 -4.756326	H H	-0.484241 -2.976096	0.378974 2.535142	-4.137907 1.080205
N	-3.825021	3.109958	1.080282	H	-0.422882	-1.363666	3.970761
N	-3.819860	0.553233	2.433066	Н	2.989843	-2.524977	-1.117553
N	-1.999927	-0.374382	3.385485	Н	-3.665580	-1.492535	-3.837679
N	0.263337	-1.743283	4.658353	H	-3.146609	-1.027721	-5.488983
N	3.630655	-3.324436	-1.147900	H	-1.923808	-1.253785	-4.196087
N	1.390194	-3.178728	-2.957737	H	-5.250025	0.489927	-3.690381
N	0.526649	-1.228761	-3.686447	H	-4.654691	2.152355	-4.052004
C	1.386843	2.227724	-4.621998	Н	-4.795261	0.960172	-5.367266
C	0.241882	1.870346	-5.384904	H	-3.457323	0.197924	-1.909903
C C	0.180707 1.260709	2.203650 2.844556	-6.753861 -7.373659	H H	-1.731649 -2.873557	0.496251 1.870113	-2.292799 -2.228084
C	2.415298	3.159308	-6.638279	Н	-5.803478	0.509671	1.722590
C	2.469052	2.856472	-5.271332	Н	-4.524138	0.498790	0.464782
Ċ	-2.213171	4.873081	0.768607	Н	-1.783829	-0.315593	6.252432
С	-3.566911	4.487430	0.976150	H	-5.850797	1.804253	4.108449
C	-4.579251	5.465130	1.066581	H	-1.068290	-0.880872	1.033569
C	-4.241075	6.820617	0.960136	H	-2.690151	-1.016390	0.270906
C	-2.909432	7.216775	0.762527	H	-1.837016	0.560028	0.321110
С	-1.906521	6.241088	0.665670	H	-3.474513	1.831265	8.460802
C	1.121351	0.485838	5.153836	H	-4.317548	0.273041	8.599693
C C	0.737575	-0.807081	5.601152	H H	-2.537548	0.307366	8.383220 7.574558
C	0.809663 1.216445	-1.123405 -0.156476	6.973481 7.901258	Н	-6.285758 -5.421994	1.303525 2.848577	7.426711
C	1.553332	1.138306	7.473291	Н	-6.682209	2.418873	6.229011
C	1.510317	1.448863	6.107851	Н	0.129391	-3.804421	1.226266
C	5.128040	-1.723967	-0.146682	Н	0.167405	-2.181994	1.990883
C	4.926228	-3.020997	-0.696193	H	1.645899	-3.184379	1.971544
C	5.994855	-3.938596	-0.766558	H	0.315257	-5.909595	2.651790
C	7.260987	-3.560326	-0.301008	H	1.807544	-5.275440	3.438855
C	7.477729	-2.281884	0.235640	Н	0.427180	-5.781469	4.443757
С	6.410542	-1.374915	0.311113	H	-1.830750	-4.550229	2.703211
C	-2.136027	1.477154	-4.881722	H	-1.727666	-4.369407	4.482838
C	-3.099002	0.611523	-4.025377	H	-1.871496	-2.915821	3.441816
C C	-2.942434	-0.874360	-4.410070 -4.298254	H H	1.400650	-5.266563 -4.288059	-2.677618 -1.221634
C	-4.534119 -2.767260	1.080097 0.808712	-4.298254 -2.530357	H H	1.027171 1.067395	-4.288059 -0.428110	-1.221634 -6.395363
C	-5.006943	2.451985	1.306947	H H	3.050590	-4.781573	-4.738608
C	-4.814753	0.925183	1.446112	Н	0.877763	-1.751415	-0.514089
C	-3.975961	0.716320	3.808495	Н	-0.392626	-0.791185	-1.311565
C	-2.827730	0.118747	4.389083	Н	-0.661806	-2.539569	-0.983403
C	-2.672160	0.133470	5.786169	H	2.209835	-2.410718	-9.045012
С	-3.654694	0.749558	6.577289	H	2.100466	-0.710992	-8.482966
С	-4.810449	1.347641	5.972311	H	3.668134	-1.576384	-8.466726
С	-4.974618	1.329671	4.575723	Н	4.612329	-3.653595	-7.672002

Н	4.074796	-5.143722	-6.834930	С	3.689443	-2.056987	0.686488
Н	3.174435	-4.519304	-8.252934	C C	3.334123 3.539358	-3.342310 -3.631658	0.155262 -1.205482
				С	4.889061	-1.295654	-3.629555
	mation 27. licity: 2			C C	5.295858	-0.861972 -1.800354	-4.996555
Charge				C	3.560382 2.748204	-1.800354	2.167101 1.062253
	3c) = -5613.04255	5915213 Hartree		С	-4.437230	-3.598228	0.013168
	def2-TZVP) = -5612			C	-4.940022	-2.503692	-0.964769
	- D3(BJ)/def2-TZV - D3(BJ)/def2-TZV			C C	-5.855384 -5.738677	-3.176425 -1.455334	-1.996935 -0.159689
E (PBEh	(-3c) = -5604.83952	22715391 Hartree		С	-3.751128	-1.837212	-1.685791
	= 174.80311 Kcal,			C	-1.665776	3.926443	3.029058
	= 47.79992 Kcal/r X-V/def2-TZVP) = -		5 Hartree	C C	-2.622947 -3.387509	3.373691 1.273794	1.947387 3.089218
E (GFN1	-xTB) = $-265.5597$	76830230 Hartree		С	-3.435204	-0.089792	2.706008
	-xTB) = $-259.28728$			C C	-3.958154	-1.041034	3.599443
E (GrN-	FF) = $-33.8506147$	70990 naitiee		C	-4.407797 -4.344878	-0.621202 0.762531	4.860993 5.234754
	nates:			С	-3.832735	1.719328	4.340383
Cu N	1.047128 2.034567	-0.274766 1.410012	-0.178021 0.366673	C C	-2.527609 -1.867646	0.973364 1.304174	1.040317 -0.255036
N	1.394981	0.156118	-2.130589	C	-4.957680	-1.636915	5.831252
N	0.029503	-1.934061	-0.723305	С	-4.830566	1.195558	6.594514
N C	0.532691 2.183092	-0.599190 1.911720	1.758905 1.642266	H H	3.361845 4.163704	3.635652 3.975152	2.511781 -0.082111
C	2.797590	2.214496	-0.457116	Н	2.539110	1.981417	-4.712160
С	2.119358	1.218265	-2.627270	H	1.003480	-0.162542	-5.457465
C C	0.898422 -0.113023	-0.519652 -2.429072	-3.225816 -2.002726	H H	-0.885579 -1.345255	-4.383683 -4.960581	-2.839474 -0.209629
C	-0.495590	-2.888894	0.121926	H	-1.120663	-2.084758	4.282348
С	-0.231414	-1.636203	2.250098	H	0.111528	0.246129	4.990156
C C	0.756885 3.078774	0.253548 3.051908	2.821899 1.629767	H H	3.498966 5.701802	6.508425 5.886618	-3.491546 -4.525511
C	3.481633	3.222907	0.328438	H	6.588104	3.545379	-4.304603
С	2.054795	1.233180	-4.076102	H	5.219133	1.817894	-3.036277
C C	1.286987 -0.683813	0.158179 -3.761791	-4.448808 -1.960771	H H	1.148669 -1.213762	-4.345128 -4.175413	-6.974899 -7.814309
C	-0.912214	-4.051289	-0.639894	H	-2.920598	-2.860800	-6.519523
С	-0.512533	-1.423675	3.658081	H	-2.244986	-1.729951	-4.381151
C C	0.098218 2.835307	-0.247896 2.159954	4.012529 -1.863853	H H	-4.604341 -3.512000	-5.237268 -6.638332	2.230115 3.987852
C	0.198777	-1.742322	-3.191047	Н	-1.114306	-6.216882	4.627614
С	-0.694848	-2.741997	1.510211	H	0.162796	-4.394511	3.470537
C 0	1.532894 1.630978	1.427224 7.068090	2.795409 -2.462834	H H	-0.348453 1.579368	4.876451 4.930396	5.298999 6.913185
0	3.188315	-4.616261	-6.145886	Н	3.471636	3.298952	6.672172
0	-4.870137	-4.748301	-0.014543	H H	3.449923	1.644477	4.778415
N	-1.867772 1.906269	5.011926 4.812774	3.563373 -2.097165	н Н	1.489555 2.221926	4.011742 -2.609250	-1.616709 -3.868209
N	2.074721	-3.174103	-4.712684	H	-3.132534	-2.202539	0.868823
N N	4.431288 4.882959	-2.592671 -0.534660	-3.371808 -2.549535	H H	-0.586650 -1.631439	2.225387 7.290401	2.719702 -0.477399
N	-3.477060	-3.181178	0.922517	Н	-0.015925	8.064927	-0.644798
N	-0.604676	3.094003	3.265316	Н	-0.949295	7.654886	-2.104919
N N	-2.811604 -2.895327	1.939257 -0.239304	2.007846 1.431934	H H	-0.553691 0.676728	5.607715 4.451579	1.008624 0.397623
С	3.632772	3.196073	-2.589414	H	1.125976	6.144437	0.746874
C C	3.139942 3.895378	4.527745 5.489698	-2.704328 -3.409716	H H	-1.972657 -1.289461	4.879098 5.171012	-1.135419 -2.763784
C	5.122883	5.125460	-3.980109	Н	-0.619893	3.869841	-1.731590
С	5.618180	3.817049	-3.861512	H	4.570706	-4.646944	-3.733566
C C	4.868786 -0.189765	2.855497 -2.383888	-3.167181 -4.486549	H H	5.273849 4.468447	-3.625030 -0.068356	-5.001726 0.241516
С	0.770240	-3.122622	-5.231181	H	3.263927	-4.619415	-1.605993
C	0.393560	-3.768281	-6.427924	Н	5.566366	0.208122	-4.965852
C C	-0.928905 -1.884205	-3.667898 -2.935496	-6.880207 -6.158827	H H	6.167319 4.467484	-1.435692 -0.992889	-5.376784 -5.723935
С	-1.508767	-2.301530	-4.965279	Н	2.555642	-2.064385	2.551172
C	-1.489333	-3.788642	2.214347	Н	4.291686	-2.410038	2.741009
C C	-2.855098 -3.563503	-4.013895 -5.052347	1.873082 2.519020	H H	3.742527 3.441686	-0.735891 -4.658312	2.408389 1.888560
С	-2.939923	-5.835951	3.497532	H	1.810388	-4.036629	1.536714
С	-1.603455	-5.601582	3.858112	H	2.508276	-5.320560	0.507421
C C	-0.891450 1.548369	-4.581229 2.311633	3.215574 4.002766	H H	-6.257762 -5.304918	-2.417269 -3.939474	-2.698039 -2.581387
C	0.461632	3.216602	4.172648	H	-6.701403	-3.691328	-1.503586
C C	0.482791 1.567836	4.166036 4.188038	5.213372 6.100841	H H	-6.157005 -6.584897	-0.690386 -1.929411	-0.846719 0.377599
C	2.628471	4.188038 3.278513	5.966105	H H	-5.101320	-0.935721	0.377599
С	2.615318	2.348736	4.914148	H	-4.120690	-1.066783	-2.394555
C C	1.240760 -0.051735	6.016006 5.924513	-1.964623 -1.102949	H H	-3.059004 -3.167406	-1.337361 -2.583597	-0.981094 -2.258794
С	-0.701914	7.314375	-1.102949	H H	-3.585798	3.907036	2.078836
C	0.322308	5.501354	0.335917	H	-2.220893	3.644231	0.950321
C C	-1.028950 3.159757	4.901753 -3.878743	-1.720535 -5.166508	H H	-4.006010 -3.779412	-2.102455 2.779950	3.319330 4.629665
С	4.422345	-3.703046	-4.298491	H	-0.905752	1.837403	-0.101362
C	4.087883	-2.630837	-2.018684	H	-1.650588	0.364786	-0.793807
C C	4.397300 4.200045	-1.334871 -1.056533	-1.523212 -0.158546	H H	-2.505781 -6.011169	1.942347 -1.416270	-0.901684 6.106085

Н	-4.924755	-2.657259	5.403945	С	0.805770	0.445480	-4.629887
Н	-4.385096	-1.649311	6.783086	C	0.158424	-0.771984	-4.350270
Н	-4.275290	0.685356	7.410057	C	-1.221123	-0.895339	-4.591454
H	-4.715336	2.286747	6.737985	C	-1.974343	0.223676	-5.080049
H	-5.901933	0.944138	6.745692	C	-1.330749	1.436337	-5.385259
11	-3.901933	0.944136	0.743032	C	2.211886	2.061506	-4.927363
C	mation 3.			C	3.441178	2.904705	-4.932833
	licity: 2			C	-1.910403	-2.219169	-4.376250
_				C	-3.464661	0.099741	-5.267950
Charge:	: 0 3c) = -5613.02829	2440165 Hartree		C	-4.996432	-0.141808	2.680740
	,			C			
		2.884558904302 Ha			-3.596456	0.091272	3.322648
		P) = -5610.944305		C	-3.606124	1.534245	3.871107
		VP) = -5611.17783	2988/53 Hartree	C	-3.465850	-0.908126	4.487282
	-3c) = -5604.8259			С	-2.415489	-0.084851	2.348751
,	= 180.56968 Kcal	, -		C	-0.046969	-4.302792	3.080133
	= 63.92277 Kcal/			С	-0.150686	-2.903834	3.722150
		-5614.58283420961	6 Hartree	С	2.194313	-2.400376	4.462776
	-xTB) = $-265.5384$			С	2.788814	-2.245178	5.745706
	-xTB) = $-259.2676$			С	4.149966	-1.901053	5.829527
E (GFN-I	FF) = -33.8274631	37018 Hartree		С	4.899146	-1.736038	4.652707
				С	4.292000	-1.944826	3.370337
Coordin				С	2.925768	-2.271548	3.273500
Cu	-0.760790	-0.044570	-1.390913	С	0.720854	-2.740369	6.111633
N	0.825794	-1.294839	-1.188298	С	-0.573054	-3.098818	6.761627
N	0.489014	1.551391	-1.425073	С	6.344016	-1.311018	4.728059
N	-2.350265	1.214471	-1.548919	C	5.129200	-1.840149	2.122320
N	-2.021806	-1.618510	-1.170337	H	2.385812	-4.265933	-0.931033
C	0.790672	-2.667775	-1.060933	H	4.083912	-2.129231	-1.150368
C	2.159424	-0.945113	-1.224912	H	3.464658	3.116132	-1.313975
С	1.864713	1.517848	-1.350157	H	1.324558	4.810525	-1.486918
С	0.138791	2.882405	-1.515496	H	-3.912248	4.147095	-2.083286
С	-2.316667	2.582146	-1.731432	H	-5.608239	2.017335	-1.802153
С	-3.683943	0.861858	-1.542677	H	-5.007356	-3.128506	-0.804861
C	-3.400105	-1.572888	-1.130785	H	-2.866467	-4.828713	-0.614908
C	-1.676761	-2.939171	-0.969208	H	6.595813	1.437699	1.023691
C	2.138454	-3.203093	-1.025759	H	8.022160	1.020191	-1.002599
C	2.989380	-2.131801	-1.131742	H	6.968677	0.299804	-3.166348
С	2.399641	2.866269	-1.366107	H	4.449831	0.021639	-3.283286
С	1.326456	3.715508	-1.456900	H	-0.754919	7.311173	-4.231118
С	-3.663002	3.097042	-1.899307	H	-1.791350	8.715329	-2.425035
С	-4.514054	2.030614	-1.758861	H	-2.533145	7.652598	-0.270723
С	-3.939766	-2.896383	-0.882078	H	-2.229584	5.180583	0.052998
С	-2.868027	-3.747124	-0.787240	H	-7.644211	-0.465233	1.828912
С	2.668945	0.364110	-1.286203	H	-9.413255	-0.828007	0.074626
С	-1.164473	3.389857	-1.694480	H	-8.774515	-1.009900	-2.345830
С	-4.199649	-0.426516	-1.299270	H	-6.353658	-0.829914	-3.005735
С	-0.369012	-3.457977	-0.931750	H	0.150892	-6.914924	2.168300
0	5.311709	1.661100	2.833676	H	0.190856	-8.678083	0.374464
0	0.164607	6.091374	-5.817234	H	-0.018955	-8.026190	-2.041364
0	-6.012909	-0.205363	3.367896	H	-0.275552	-5.600497	-2.652221
0	0.060237	-5.316618	3.758556	H	2.899637	1.076032	0.867293
N	3.891340	1.184609	1.089578	H	-0.237407	3.660170	-3.803397
N	-0.330461	4.645553	-4.073913	H	-4.065061	-0.169680	0.868461
N	0.976999	2.546880	-5.378660	H	-0.183160	-3.319729	1.291435
N	2.135330	0.819205	-4.483879	H	2.389322	1.990262	5.343201
N	-4.985413	-0.238113	1.307498	H	3.332652	0.534869	4.868501
N	-0.107141	-4.253189	1.706020	H	4.155307	2.116075	5.007208
N	0.859617	-2.688371	4.722387	H	0.808136	1.425704	3.474410
N	1.848556	-2.469284	6.742625	H	1.291779	1.443116	1.768560
С	4.150299	0.549178	-1.219668	H	1.792024	0.071346	2.837768
С	4.750130	0.957650	0.005710	H	1.851474	3.797659	3.635397
С	6.150595	1.125698	0.071418	H	3.609457	4.007363	3.329206
С	6.931435	0.887201	-1.067956	H	2.489138	3.686266	1.959996
С	6.345238	0.484119	-2.278823	H	0.040291	3.584222	-6.939593
С	4.953394	0.318210	-2.349728	H	1.681051	4.137360	-6.554524
С	-1.326498	4.864055	-1.882644	H	0.737789	-1.623507	-3.965969
C	-0.905806	5.476453	-3.097523	H	-1.912730	2.289780	-5.766028
С	-1.079388	6.864476	-3.283846	H	4.256331	2.344252	-4.441866
С	-1.662270	7.633708	-2.268226	H	3.766236	3.170639	-5.961111
С	-2.079073	7.042902	-1.065580	H	3.281147	3.850606	-4.375125
С	-1.910147	5.663023	-0.883041	H	-2.795512	-2.127420	-3.715952
С	-5.658077	-0.546070	-0.980432	H	-2.274168	-2.640863	-5.338008
С	-6.029026	-0.441281	0.393647	H	-1.226786	-2.958743	-3.918782
С	-7.384769	-0.545474	0.766085	H	-3.726575	-0.701987	-5.990502
С	-8.356840	-0.748170	-0.223816	H	-3.965674	-0.160613	-4.311219
C	-8.002947	-0.850056	-1.578442	H	-3.907700	1.045800	-5.632877
С	-6.652173	-0.749107	-1.949258	H	-2.670740	1.742031	4.430387
C	-0.202341	-4.910348	-0.607158	H	-3.686445	2.273606	3.047859
C	-0.080983	-5.290361	0.759740	H	-4.466148	1.680542	4.552901
C	0.059476	-6.649220	1.108029	H	-2.537881	-0.710176	5.062043
C	0.079757	-7.619126	0.096289	H	-4.334519	-0.820274	5.166791
C	-0.037311	-7.257459	-1.254954	H	-3.433403	-1.953737	4.116358
С	-0.179010	-5.903974	-1.598698	H	-1.458431	0.064550	2.889319
С	4.169036	1.555296	2.389802	H	-2.388419	-1.100520	1.901095
C	2.912227	1.925597	3.224624	H	-2.422952	0.658717	1.523264
C	3.214219	1.622889	4.700229	H	-0.092623	-2.096649	2.959649
C	1.641281	1.168496	2.788572	H	-1.148962	-2.825402	4.196028
C	2.705758	3.445153	3.021455	Н	4.615968	-1.755830	6.815663
C	0.166492	4.975377	-5.308930	H	2.470676	-2.442684	2.284745
C	0.738673	3.780438	-6.097999	H	-0.921612	-4.096518	6.423239
C	0.052226	1.521032	-5.174270	H	-0.417085	-3.122340	7.854300

Н	-1.376861	-2.364721	6.539185	С	2.283065	2.976507	4.617700
H	6.485859	-0.323164	4.238969	C	1.304362	1.870627	6.648360
H	6.682155	-1.224539	5.778315	C	1.803696	1.651458	7.962256
H	7.018213	-2.026193	4.211204	C	1.024749	0.916823	8.874447
H	5.908666	-2.632064	2.092984	С	-0.235087	0.435389	8.482067
H	4.510066	-1.941886	1.211579	С	-0.743147	0.716721	7.171054
Н	5.665752	-0.872230	2.066399	C	0.036884	1.430740	6.241538
11	3.003732	-0.072230	2.000399				
				С	3.330344	2.775606	6.932592
	mation 31.			C	4.554337	3.562599	6.604720
Multipl	licity: 2			С	-1.053407	-0.407232	9.427683
Charge:	: 0			C	-2.129948	0.264793	6.795996
E(B97-3	3c) = -5613.00167	5257173 Hartree		С	-0.187571	1.479090	-4.375557
		2.861948446687 Ha	rtree	Č	-1.685087	1.868297	-4.332315
		(P) = -5610.919969		C	-2.067153	2.759289	-5.532147
						0.584321	
		VP) = -5611.15211	3263//5 Hartree	С	-2.526253		-4.369967
	-3c) = -5604.8047			С	-1.928502	2.612549	-2.998358
E(PM6)	= 197.04998 Kcal	/mol		C	-0.400439	-3.965715	-4.553482
E(PM7)	= 82.38588 Kcal/	mol		С	-1.222361	-2.693601	-4.849936
E (0B97)	X-V/def2-TZVP) =	-5614.55762201572	1 Hartree	С	-1.041286	-1.762012	-7.188387
		24803432 Hartree		Č	-1.808089	-1.982716	-8.366864
				C	-1.483469	-1.273112	-9.537520
	-xTB) = $-259.2531$						
E (GFN-F	FF) = -33.8015688	1/2292 Hartree		С	-0.412190	-0.365483	-9.525745
				С	0.352743	-0.165627	-8.329826
Coordin	nates:			C	0.038447	-0.869771	-7.153200
Cu	0.130463	0.077038	0.057900	С	-2.675281	-3.251083	-6.855095
N	-0.358028	-1.803844	0.637650	С	-3.521110	-4.244548	-6.133545
N	-1.206353	0.835531	1.383997	C	-0.055562	0.397450	-10.778255
			-0.539991	C			-8.328242
N	0.594545	1.958151			1.513278	0.798514	
N	1.508623	-0.670043	-1.227446	H	-0.321843	-5.165979	0.500909
C	0.155862	-2.985892	0.142065	H	-2.174008	-4.142864	2.236662
С	-1.347596	-2.160529	1.533439	H	-3.569034	0.720452	3.776789
С	-2.047568	0.122788	2.215896	H	-2.776127	3.255745	3.120214
Ċ	-1.420011	2.169402	1.673269	Н	0.568181	5.320321	-0.423061
C	0.145663	3.142656	0.009162	Н	2.146207	4.286690	-2.404786
С	1.437312	2.306665	-1.574275	H	3.715889	-0.578489	-3.765187
C	2.237152	0.031410	-2.162469	H	3.235718	-3.086568	-2.811875
C	1.813916	-2.002524	-1.425823	H	-2.947365	-3.341488	6.421899
С	-0.531036	-4.116920	0.734504	H	-5.424064	-3.446059	6.011111
C	-1.459636	-3.604225	1.604831	Н	-6.390348	-2.529227	3.879435
C	-2.816535	1.031058	3.044890	Н	-4.853820	-1.532352	2.158689
С	-2.421039	2.302615	2.713590	H	0.035464	6.628265	4.205247
C	0.742309	4.269929	-0.679477	H	-1.605027	8.200426	3.126285
C	1.527117	3.749912	-1.677891	H	-2.880740	7.486582	1.084274
С	3.053141	-0.875023	-2.946708	H	-2.503790	5.190858	0.128437
С	2.808339	-2.136518	-2.474081	H	2.138522	3.533317	-6.571885
C	-2.139560	-1.279745	2.297911	Н	4.633792	3.661804	-6.659016
C	-0.780737	3.266300	1.061912	Н	6.000316	2.671281	-4.790763
С	2.167460	1.418496	-2.385349	H	4.840034	1.628351	-2.831673
C	1.178949	-3.103845	-0.819445	H	0.845291	-6.387725	-4.132544
0	-0.801050	-3.021974	6.860105	H	2.218028	-8.027073	-2.810443
0	1.541378	5.227627	5.118347	H	3.125047	-7.385523	-0.556617
0	0.217441	0.339519	-4.147884	H	2.647950	-5.095089	0.360300
0	-0.359729	-4.928083	-5.309963	Н	-0.634479	-1.918701	3.895860
N	-1.135072	-2.296574	4.702912	Н	0.587879	3.220751	2.837575
N	0.575919	4.121524	3.324996	H	0.228207	3.384568	-4.990787
N	2.314868	2.567250	5.995803	Н	0.120887	-2.992053	-2.833357
N	3.056833	2.232583	8.104391	H	2.986193	-2.266253	6.703048
N	0.667933	2.530934	-4.643208	H	1.626434	-1.196026	7.190378
N	0.209938	-3.889435	-3.319753	H	1.583240	-2.930449	7.618553
N	-1.628119	-2.575465	-6.223865	H	2.648647	-1.410192	4.364518
N	-2.808380	-2.912795	-8.125434	H	1.173919	-1.725670	3.432617
C	-3.062554	-1.874202	3.315428	Н	1.168897	-0.473951	4.739199
C	-2.521730	-2.386718	4.530988	Н	2.690237	-3.969709	4.833407
C	-3.384672	-2.954974	5.493722	H	1.338567	-4.713887	5.754280
C	-4.763613	-3.001332	5.251219	H	1.087032	-4.191070	4.052679
С	-5.306432	-2.490513	4.061928	H	1.929274	2.128151	3.991129
C	-4.450349	-1.931330	3.101687	H	3.314225	3.216223	4.289438
C	-1.041393	4.633012	1.615421	H	1.411869	0.715955	9.884593
C	-0.323336	5.048191	2.773398	H	-0.366498	1.652508	5.240388
C	-0.530473	6.334384	3.312794	Н	5.174407	3.634414	7.515381
C	-1.447132	7.198672	2.698871	Н	5.162145	3.086038	5.805859
C	-2.161327	6.802105	1.557355	Н	4.285165	4.584471	6.266020
C	-1.953395	5.521296	1.022430	H	-2.060289	0.024137	9.610333
C	2.847114	1.983199	-3.585055	H	-1.209446	-1.423105	9.004917
С	2.083770	2.522748	-4.656282	H	-0.548636	-0.516930	10.406442
C	2.742542	3.126186	-5.746859	Н	-2.270448	-0.819854	6.972224
C	4.139834	3.187945	-5.797817	Н	-2.902623	0.784725	7.402810
С	4.901594	2.632100	-4.758379	H	-2.342906	0.467547	5.730276
C	4.253415	2.038946	-3.667065	Н	-3.161303	2.937238	-5.532252
C	1.493776	-4.466206	-1.352884	Н	-1.593376	3.764139	-5.496258
C	0.979657	-4.840360	-2.630326	H	-1.800771	2.275906	-6.494084
С	1.248457	-6.125458	-3.146952	H	-3.601178	0.837587	-4.280022
C	2.015137	-7.027443	-2.397130	Н	-2.376532	0.033234	-5.319096
C	2.522181	-6.672236	-1.137555	H	-2.253076	-0.085752	-3.533348
С	2.257007	-5.393902	-0.624113	Н	-2.996372	2.900658	-2.913820
Ċ	-0.346681	-2.623407	5.788515	Н	-1.673368	1.966454	-2.134992
C	1.178152	-2.535181	5.510493	Н	-1.312111	3.530179	-2.915923
C	1.886907	-2.211921	6.834536	Н	-2.122049	-2.722425	-4.196452
C	1.545277	-1.476100	4.451146	H	-0.658530	-1.781950	-4.557724
C	1.594822	-3.937449	5.006591	H	-2.072106	-1.436319	-10.452985
С	1.425974	4.242067	4.400364	H	0.627285	-0.711325	-6.238271

Н	-4.037504	-3.796516	-5.257598	С	-2.713231	-2.021961	3.200999
Н	-4.285710	-4.624637	-6.833528	C	-1.042204	-2.916968	-4.040539
H	-2.904287	-5.091287	-5.769179	C	-0.511247	-4.361398	-4.212135
H	0.981806	0.181794	-11.113718	С	1.877878	-5.202799	-4.248343
H	-0.736970	0.141113	-11.611963	С	2.891820	-5.232074	-3.252240
H	-0.108797	1.497170	-10.625692	C	4.190666	-5.639168	-3.603913
H	1.196288	1.830474	-8.596017	C	4.464197	-6.018067	-4.927457
H	2.000948	0.841943	-7.335671	С	3.422390	-6.008344	-5.913015
H	2.288336	0.515079	-9.072534	С	2.121376	-5.603078	-5.567895
	2.200000	0.010079	3.072001	C	1.113307	-4.501519	-2.267444
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	mation 32.			С	0.144526	-4.003189	-1.250501
Multip.	licity: 2			С	5.857084	-6.448250	-5.316946
Charge	: 0			C	3.723732	-6.432754	-7.328657
E (B97-	3c) = -5613.01241	1494140 Hartree		С	-3.258162	0.847791	-2.550493
	•	.2.873146275971 Ha	x+x00	C	-3.746772	-0.145905	-1.463973
		$^{\prime}P) = -5610.925860$		С	-4.516926	0.532220	-0.315392
E(PBE0	- D3(BJ)/def2-T2	(VP) = -5611.15960	3419211 Hartree	С	-4.639128	-1.181750	-2.182203
E (PREh	-3c) = -5604.8085	12107461 Hartree		С	-2.505036	-0.846010	-0.882617
				C			
	= 209.68398 Kcal				0.081595	5.311450	5.502785
E(PM7)	= 71.95218 Kcal/	mol		C	1.569323	5.202220	5.110336
E (ωB97)	X-V/def2-TZVP) =	-5614.57021062863	O Hartree	С	2.017091	4.106296	2.867263
	-xTB) = $-265.5361$			С	2.677073	2.898020	2.513480
				C			
	-xTB) = $-259.2651$				2.925907	2.622609	1.157627
E (GFN-	FF) = -33.8110771	.11268 Hartree		C	2.514833	3.541392	0.176892
				С	1.796205	4.725567	0.550421
Coordi	nates:			C	1.552677	5.013706	1.905728
		1 21222	0 400650				
Cu	-0.004864	1.349080	0.403652	С	2.566692	2.898641	4.672375
N	-0.203351	1.130173	2.404906	C	2.658917	2.510205	6.108373
N	1.297212	-0.209530	0.339172	С	2.881937	3.311326	-1.267343
	0.160037	1.548063	-1.601024	C	1.294738	5.665870	-0.516074
N							
N	-1.427627	2.805019	0.436943	H	-1.490214	1.698663	5.462174
С	-1.066606	1.809337	3.240751	Н	0.484805	-0.194804	5.417442
C	0.504660	0.260614	3.204649	Н	3.136054	-2.709022	1.638046
С	1.786564	-0.907150	1.424193	H	3.088991	-2.689303	-1.080678
С	1.806012	-0.834732	-0.782135	H	1.387479	0.891251	-4.663308
C	0.909891	0.768049	-2.450868	H	-0.357226	2.984331	-4.598690
C	-0.464521	2.482938	-2.395815	Н	-3.482193	5.103166	-0.907758
C	-1.919447	3.490546	-0.652919	Н	-3.709026	4.861625	1.808391
C	-2.119289	3.275977	1.534427	H	1.229715	-4.407214	5.579974
С	-0.908262	1.340433	4.605940	Н	3.490154	-3.933969	6.574197
С	0.078548	0.388299	4.584408	H	4.814741	-1.940429	5.816081
C	2.631799	-1.997229	0.975757	Н	3.841565	-0.405108	4.048004
C	2.625863	-1.969358	-0.395943	H	1.038956	-2.781257	-6.112167
С	0.845012	1.295409	-3.802601	Н	3.493244	-2.885825	-6.532010
С	-0.020180	2.355611	-3.769025	H	5.093908	-1.926657	-4.843325
C	-2.945377	4.423798	-0.236210	Н	4.189508	-0.796575	-2.794274
C	-3.056808	4.305088	1.127600	H	-5.337173	3.108292	-4.603756
С	1.460591	-0.677885	2.772912	Н	-4.774581	5.202485	-5.875515
C	1.597129	-0.413909	-2.109087	Н	-2.659445	6.447968	-5.349129
С	-1.500469	3.336653	-1.986164	H	-1.130709	5.605908	-3.548101
С	-1.968164	2.822791	2.860117	Н	-2.415745	5.711696	6.525071
0	-0.924530	-4.551480	4.919844	Н	-4.892894	5.318912	6.670190
0				Н	-6.015813		
	-2.260147	-2.772449	-3.970041			3.747147	5.060748
0	-2.354474	0.568037	-3.337433	Н	-4.639435	2.589122	3.305830
0	-0.249586	6.063360	6.413971	H	-0.161235	-2.215069	2.915854
N	0.046371	-2.895102	3.651675	H	-0.670114	-0.969816	-3.702253
N	-0.175762	-1.849751	-3.935101	H	-4.687466	2.184747	-1.924138
N	0.751952	-4.705444	-3.600440	H	-0.307979	3.959856	4.025354
N	2.381618	-4.803342	-2.036500	H	-4.318691	-4.279557	3.153604
N	-3.937759	2.048710	-2.604366	Н	-3.090179	-5.451604	3.756816
	-0.759098				-3.610907		4.799353
N		4.541704	4.740648	H		-4.104811	
N	1.967433	4.098292	4.263012	H	-2.908546	-3.845086	1.094559
N	2.995340	2.174181	3.654756	H	-1.219803	-3.281712	1.235547
С	2.052638	-1.576540	3.811672	Н	-1.632515	-4.974953	1.655482
C	1.301288	-2.704442	4.248988	Н	-3.673414	-1.897746	2.658178
С	1.827884	-3.550459	5.247585	H	-2.861265	-1.667051	4.240523
С	3.086998	-3.267642	5.796114	H	-1.983705	-1.340502	2.715001
C	3.830801	-2.154352	5.372548	Н	-1.337115	-4.988835	-3.819076
C	3.307811	-1.308628	4.381042	Н	-0.443696	-4.582779	-5.295865
C	2.122679	-1.206309	-3.258660	H	4.982861	-5.653101	-2.840239
С	1.224635	-1.815826	-4.184544	H	1.330073	-5.594437	-6.334253
C	1.739441	-2.372542	-5.370438	Н	0.585773	-4.141846	-0.248789
C	3.118698	-2.418391	-5.610140	Н	-0.068647	-2.922281	-1.384188
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C	4.008809	-1.884638	-4.669819	H	-0.824625	-4.540363	-1.300798
С	3.504968	-1.266552	-3.516131	H	5.874593	-7.487318	-5.710027
C	-2.369744	3.900024	-3.061707	Н	6.279675	-5.806535	-6.119757
C	-3.565944	3.195520	-3.368913	Н	6.547126	-6.404297	-4.452874
C	-4.419975	3.671913	-4.377313	H	4.513243	-5.801144	-7.789863
С	-4.099205	4.838763	-5.086686	H	4.099736	-7.477120	-7.375348
C	-2.915655	5.532980	-4.794268	Н	2.824553	-6.370407	-7.971482
C							
	-2.056965	5.062060	-3.788623	H	-4.768059	-0.224230	0.456055
С	-2.777821	3.486209	3.927312	H	-3.913094	1.322091	0.175880
С	-2.149750	4.368731	4.852626	Н	-5.486328	0.966121	-0.643631
C	-2.921565	5.027491	5.833613	Н	-4.996543	-1.941092	-1.455819
С	-4.302562	4.800613	5.899359	H	-5.528745	-0.698344	-2.636699
С	-4.932130	3.926060	5.000557	H	-4.063400	-1.697083	-2.975003
C	-4.165574	3.278233	4.021239	Н	-2.811926	-1.620981	-0.152944
C	-0.997613	-3.721110	4.018362	Н		-1.329016	-1.683904
					-1.918968		
С	-2.280887	-3.505223	3.164777	H	-1.846413	-0.121104	-0.360527
C	-3.391204	-4.386824	3.751407	H	1.848625	6.158061	4.617700
С	-1.987532	-3.926133	1.708450	Н	2.132246	5.169419	6.062494

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H	3.458909	1.703553	0.874832	C	-6.381267	4.682524	0.403932
H	1.002429	5.925247	2.185958	С	-4.297247	3.314208	0.049768
Н	1.658328	2.502767	6.588308	Č	-4.420870	4.956129	1.968626
H	3.086691	1.493699	6.169620	С	3.983376	-1.831078	3.085798
H	3.305272	3.200503	6.691281	С	3.702619	-2.659739	1.824259
H	3.644128	4.048168	-1.602766	С	2.722103	-4.836566	1.122605
	3.301374			C			
H		2.298999	-1.418718		1.636002	-5.638695	1.568416
H	2.016510	3.419744	-1.949202	С	1.310136	-6.809903	0.860368
H	0.586956	5.148750	-1.198907	С	2.035731	-7.146635	-0.294935
H	0.765040	6.532152	-0.075671	С	3.104263	-6.304159	-0.749108
H	2.121076	6.054070	-1.148257	С	3.453410	-5.145926	-0.030885
				С	1.723837	-3.942224	2.911196
Confor	rmation 33.			С	1.372793	-2.979301	3.996034
	olicity: 2			Č	1.666609	-8.379448	-1.083539
Charge				C	3.849013	-6.647203	-2.014986
E(B97-	-3c) = -5613.03001	3708073 Hartree		С	1.053717	6.328107	-1.189082
E (M06)	def2-TZVP) = -561	2 885498672970 на	rtree	С	0.106644	6.274603	0.043863
	- D3(BJ)/def2-TZV			C		6.256765	1.282939
		•			1.031504		
E (PBE)	) - D3(BJ)/def2-TZ	VP) = -5611.17901	1379139 Hartree	С	-0.743021	7.556393	0.037219
E (PBEł	n-3c) = -5604.8275	98142869 Hartree		С	-0.812898	5.038903	0.071583
E (PM6)	= 171.04173 Kcal	/mol		С	-1.278298	-4.595512	-2.533913
	= 51.00600 Kcal/			С	-0.310953	-4.712005	-1.337164
E (ωB97	7X-V/def2-TZVP) =	-5614.58431704325	4 Hartree	С	1.422620	-2.913711	-1.615756
E (GFN1	1-xTB) = $-265.5511$	05162363 Hartree		С	1.703030	-1.710939	-0.919302
	2-xTB) = $-259.2721$			Č	2.795500	-0.922793	-1.324216
	,						
E (GFN-	-FF) = -33.8235262	85600 Hartree		С	3.581934	-1.340182	-2.410237
				С	3.273408	-2.553869	-3.109134
Coordi	inates:			С	2.180808	-3.342581	-2.710949
		0 660407	0 054600				
Cu	-0.465208	0.669407	0.054689	С	0.015453	-2.627208	0.104905
N	-2.298700	-0.147250	-0.166549	C	-1.073527	-2.937464	1.070149
N	-0.730723	0.698676	2.062061	С	4.764751	-0.507248	-2.837254
N	1.234752	1.733250	0.260948	C	4.129934	-2.995689	-4.268445
N	-0.305913	0.837166	-1.963209	H	-4.748598	-1.739371	-1.828745
С	-2.817030	-0.669557	-1.329869	H	-5.283262	-1.333772	0.826139
С	-3.231748	-0.378756	0.820388	H	-2.325866	0.180757	4.975135
С	-1.857398	0.338020	2.765583	H	0.300239	0.889378	5.255879
С	0.246611	0.967542	2.992176	H	3.968455	2.791586	1.905232
С	1.960434	1.863643	1.424354	H	3.948462	3.430060	-0.757962
Č	1.964333	2.341222	-0.732710	Н	0.942965	1.937032	-4.885023
C	0.598030	1.598818	-2.671350	H	-1.055761	0.095228	-5.155762
С	-1.076675	0.176280	-2.892588	H	-7.132745	1.336057	3.974464
С	-4.120239	-1.256334	-1.072440	H	-7.369860	-0.713402	5.417253
C				Н			
	-4.392008	-1.046089	0.257730		-5.607570	-2.502751	5.368337
C	-1.592709	0.402012	4.192318	H	-3.607323	-2.226559	3.868686
C	-0.272396	0.753327	4.332278	H	5.000119	-0.415682	5.222013
C	3.203869	2.561831	1.154780	Н	5.022977	1.503035	6.840736
C	3.191393	2.887620	-0.181166	H	3.449041	3.436413	6.530543
С	0.380183	1.425316	-4.097579	H	1.837425	3.419682	4.598880
С	-0.622794	0.498816	-4.234298	H	2.792023	6.724541	-3.325750
C	-3.068051	-0.113734	2.197303	Н	4.420971	5.935812	-5.074849
C	1.539025	1.456065	2.707099	H	4.749055	3.477319	-5.474950
C	1.631878	2.375566	-2.108429	H	3.456452	1.818994	-4.099684
С	-2.218951	-0.601677	-2.608456	H	-2.929992	-4.684645	-4.758602
0							
	-6.911795	3.115907	2.656179	H	-4.482151	-3.662696	-6.454950
0	4.679660	-2.253173	4.003224	H	-4.976912	-1.201667	-6.389668
0	1.594200	7.370835	-1.548809	H	-3.925690	0.226375	-4.608195
0	-1.646132	-5.598714	-3.135228	H	-4.188493	1.767225	1.752322
N	-5.050459	1.810352	2.300747	H	2.766718	-0.410695	2.249307
N	3.400304	-0.583852	3.038230	H	0.774702	4.317562	-1.361772
N	2.777665	-3.766656	2.009579	H	-1.254142	-2.585835	-2.195135
N	1.039132	-5.053766	2.673943	H	-5.994956	5.524081	-0.205374
			-1.780635	Н		3.994999	
N	1.278567	5.101884			-6.936568		-0.265513
N	-1.671009	-3.305790	-2.794241	H	-7.096727	5.073056	1.151199
N	0.341286	-3.481313	-0.946103	H	-3.967862	4.086045	-0.674774
N	0.805137	-1.553683	0.135275	H	-3.365683	2.886189	0.479647
C	-4.247431	-0.314175	3.095098	H	-4.811458	2.514764	-0.521671
С	-5.251681	0.696906	3.127525	H	-3.997477	5.761023	1.332620
C	-6.374733	0.543744	3.968283	H	-5.074663	5.423512	2.731147
С	-6.490270	-0.603654	4.764707	H	-3.581563	4.455446	2.494369
C	-5.506231	-1.604761	4.741342	Н	3.352148	-2.015637	0.990582
С	-4.389308	-1.452687	3.905522	H	4.680772	-3.088229	1.526699
C	2.523481	1.523094	3.830018	H	0.479286	-7.443995	1.205491
С	3.436363	0.443380	3.998180	H	4.257857	-4.493063	-0.401567
C	4.327301	0.440036	5.092652	Н	0.511728	-3.397532	4.546212
С	4.322320	1.514681	5.992163	H	2.210786	-2.826382	4.704724
C	3.442767	2.594889	5.822279	H	1.086448	-1.985965	3.593764
С	2.545522	2.589731	4.743505	H	1.303551	-8.124464	-2.103340
C	2.402996	3.324126	-2.966103	Н	2.533204	-9.059643	-1.221504
C	2.213164	4.724439	-2.754711	H	0.863967	-8.951540	-0.580588
С	2.948170	5.656069	-3.517577	H	4.366875	-7.627180	-1.938331
C	3.852464	5.199828	-4.486091	Н	3.165259	-6.728697	-2.887438
С	4.036615	3.826824	-4.713186	Н	4.609389	-5.879438	-2.255067
C	3.310805	2.898847	-3.951467	H	0.425216	6.273463	2.212208
С	-2.842880	-1.408843	-3.704063	H	1.663852	5.344590	1.300356
Č	-2.559597	-2.804398	-3.757777	Н	1.698297	7.141328	1.283131
С	-3.156615	-3.611493	-4.747807	H	-1.324806	7.638772	0.977570
C	-4.019727	-3.027043	-5.684636	H	-0.093292	8.445721	-0.065568
С	-4.297611	-1.651559	-5.650737	H	-1.456476	7.557040	-0.812002
Č	-3.708962	-0.851358	-4.659242	Н	-1.510410	5.111428	0.929799
C	-5.839946	2.921383	2.088523	H	-1.429714	4.958611	-0.847042
С	-5.221823	3.955466	1.104327	H	-0.260114	4.084660	0.210846

				_			
Н	-0.868558	-5.123512	-0.473610	C	0.023493	-4.333080	2.902556
H	0.451437	-5.473381	-1.592132	C	-1.446187	-4.484187	3.373902
H	3.039944	0.009106	-0.795799	С	-2.102319	-5.579711	2.519686
H	1.948757	-4.277360	-3.242286	С	-2.129725	-3.122431	3.106977
Н	-0.842580	-3.865585	1.636313	Ċ	-1.566584	-4.843930	4.866406
Н	-1.155496	-2.104335	1.787676	C	-0.165965	3.773626	0.917024
H	-2.053802	-3.062218	0.565752	С	0.860351	3.728583	2.065175
H	4.707709	-0.226891	-3.910448	C	0.832121	6.215740	2.475010
H	4.830838	0.426347	-2.246780	C	0.726198	7.003080	3.655255
H	5.722794	-1.057026	-2.715447	С	0.707686	8.405219	3.544794
H	5.192214	-3.123592	-3.969702	С	0.792403	9.001344	2.276402
Н	3.779064	-3.959066	-4.685088	C	0.897877	8.189287	1.098952
H	4.126785	-2.249670	-5.091621	C	0.919444	6.786576	1.197089
п	4.120/03	-2.249070	-3.091621				
				С	0.718684	4.948146	4.312811
	mation 34.			C	0.657753	3.722679	5.159781
Multip	licity: 2			С	0.775514	10.504753	2.147825
Charge	: 0			С	0.989258	8.842078	-0.257695
E(B97-	3c) = -5612.992167	069223 Hartree		С	-5.440792	-2.307545	-1.862157
	def2-TZVP) = -5612		rtree	C	-5.117805	-3.040198	-0.535417
	- D3(BJ)/def2-TZVI			C	-5.402772	-2.208770	0.725764
	- D3(BJ)/def2-TZ\	,	1448125 Hartree	С	-5.959805	-4.332549	-0.526581
	-3c) = -5604.79323			С	-3.619019	-3.399810	-0.592741
E(PM6)	= 205.14573 Kcal/	'mol		С	3.280123	-0.091701	-4.914678
E(PM7)	= 88.65215 Kcal/m	nol		C	3.525868	0.992580	-3.837517
E(ωB97	X-V/def2-TZVP) = -	-5614.54936503053	1 Hartree	С	5.141489	-0.352233	-2.478054
E (GEN1	-xTB) = $-265.51283$	84951264 Hartree		C	5.183300	-0.761091	-1.119506
	-xTB) = $-259.24626$			C		-1.572697	
					6.245275		-0.681019
F(GEN-	FF) = -33.78277121	./143 martree		C	7.239236	-1.962444	-1.592959
				С	7.176380	-1.539322	-2.961736
Coordi				C	6.118950	-0.727582	-3.409504
Cu	-0.958062	-0.782300	-0.525896	C	3.374956	0.416796	-1.331300
N	0.645183	-1.993010	-0.755282	С	2.080615	1.104501	-1.055810
N	-0.435994	-0.463933	1.410389	Ċ	8.378726	-2.838546	-1.134205
	-2.558504	0.440629	-0.293050	C	8.245243	-1.974009	-3.932636
N							
N	-1.483387	-1.076192	-2.462910	Н	2.781327	-3.961227	-2.457247
C	1.063471	-2.586454	-1.929849	H	3.325276	-3.774802	0.213930
C	1.531141	-2.401950	0.218130	H	1.472221	-0.782431	4.157965
С	0.611734	-1.054597	2.086142	H	-0.500642	1.081153	4.396780
С	-0.991389	0.458143	2.275378	Н	-4.494992	2.689761	1.289212
C	-2.835535	1.230152	0.803170	Н	-5.371493	2.032905	-1.216364
				H			
С	-3.550637	0.692556	-1.216868		-3.530108	-1.028905	-5.132432
С	-2.646880	-0.664852	-3.085480	Н	-1.188126	-2.374049	-5.552409
C	-0.788941	-1.812495	-3.398097	H	2.950022	-4.423408	5.336075
C	2.251644	-3.385838	-1.690425	H	5.314794	-3.651689	5.054097
С	2.524361	-3.291501	-0.352530	H	5.919939	-2.167563	3.112166
C	0.715225	-0.498663	3.419546	Н	4.114995	-1.432007	1.500328
C	-0.271913	0.448767	3.534045	Н	-2.042224	5.828143	3.103299
						5.429433	
С	-4.042670	1.995745	0.571403	H	-3.070225		5.360711
С	-4.492844	1.653858	-0.682700	H	-3.684779	3.092447	6.053250
C	-2.692357	-1.170422	-4.443033	H	-3.249466	1.172785	4.499601
C	-1.522011	-1.852370	-4.649755	Н	-8.211714	-0.422820	-3.222158
С	1.515668	-2.000553	1.564844	H	-8.239128	1.149555	-5.192345
C	-2.083212	1.298404	1.991248	Н	-6.102545	2.226711	-5.948348
C	-3.639301	0.146377	-2.513655	Н	-3.965235	1.761695	-4.722844
		-2.486663		H			
С	0.429650		-3.182201		3.409619	-2.156093	-6.762459
0	0.382206	-4.621910	1.766389	Н	2.759848	-4.409856	-7.669852
0	0.182956	3.667974	-0.256899	H	1.059429	-5.811571	-6.464689
0	-5.154050	-2.798181	-2.949874	H	-0.011540	-4.928790	-4.368301
0	3.814005	-0.047892	-6.018348	H	0.562855	-3.732412	4.798861
N	0.883362	-3.771757	3.830793	H	-2.111427	3.911047	0.460081
N	-1.481882	3.975092	1.269186	Н	-6.162797	-0.669627	-0.828787
N	0.818510	4.896935	2.919841	Н	2.071600	-0.962417	-3.517978
N	0.660710	6.184954	4.774835	H	-3.192058	-5.623774	2.719275
N	-6.073718	-1.081084	-1.760227	H	-1.936649	-5.375972	1.445687
N	2.442724	-1.082189	-4.466375	H	-1.667221	-6.575426	2.739252
N	3.982228	0.410710	-2.591704	H	-3.209719	-3.184103	3.355449
N	4.079721	-0.264078	-0.439818	Н	-1.678655	-2.314014	3.717269
C	2.555480	-2.533096	2.492917	H	-2.034452	-2.829385	2.044076
С	2.219332	-3.369199	3.590316	Н	-2.630819	-5.018526	5.124952
C	3.222398	-3.763308	4.498055	Н	-1.005566	-5.767593	5.116378
C	4.546205	-3.336498	4.332225	Н	-1.221131	-4.026053	5.535007
С	4.884086	-2.515810	3.244556	H	0.678787	2.824943	2.680195
С	3.893556	-2.118183	2.335949	H	1.851141	3.618871	1.579074
C	-2.395398	2.408627	2.940394	H	0.630764	9.022780	4.452491
C	-2.064729	3.737561	2.555892	Н	1.002062	6.166785	0.291876
С	-2.321109	4.813237	3.422316	Н	0.712570	4.036139	6.216943
С	-2.894465	4.583255	4.680741	Н	-0.298274	3.179052	5.009594
C	-3.228716	3.275847	5.068692	Н	1.488216	3.018445	4.948704
C	-2.983103	2.198483	4.203286	H	1.689912	10.886369	1.645370
C				н Н			
	-4.884521	0.424696	-3.289083		-0.083171	10.859047	1.537741
С	-6.096261	-0.184554	-2.872693	H	0.707275	10.992085	3.139200
C	-7.291702	0.077186	-3.557941	H	0.111138	9.490872	-0.463389
С	-7.298340	0.947102	-4.658785	H	1.882898	9.497479	-0.340392
С	-6.102849	1.547047	-5.082917	Н	1.048526	8.087698	-1.065382
C	-4.903958	1.285651	-4.401986	Н	-5.118267	-2.786727	1.628399
C	1.103677	-3.080196	-4.380905	Н	-4.809141	-1.270528	0.746581
				н Н			
C	2.090813	-2.307342	-5.055150		-6.480057	-1.959942	0.830200
C	2.674891	-2.785523	-6.246122	H	-5.697749	-4.958615	0.351040
С	2.297598	-4.040824	-6.741670	H	-7.044878	-4.105714	-0.478848
				H	-5.768930	4 015070	
С	1.346239	-4.825357	-6.070907			-4.915278	-1.448310
C C	1.346239 0.751073	-4.825357 -4.337652	-6.070907 -4.897159	Н	-3.353246	-4.915278	-1.448310 0.244743

	2 221 4 6 4	2 222722	1 540005	~	1 760640	4 060055	- 060400
Н	-3.381464	-3.902702	-1.548907	С	-1.768643	4.068257	5.960409
H	-2.982907	-2.493528	-0.520460	С	-2.033055	2.940762	5.169309
H	4.284410	1.684814	-4.254165	С	-6.564624	-1.008450	1.992948
Н	2.598290	1.569030	-3.648401	C	-6.345424	-1.313682	3.496064
Н	6.293272	-1.907278	0.366085	С	-6.133683	-2.827559	3.644772
H	6.061267	-0.418486	-4.463944	C	-7.545339	-0.867144	4.354649
H	1.259865	0.736030	-1.707711	С	-5.069668	-0.560583	3.940373
H	1.790113	0.886016	-0.013213	C	-1.274724	-0.960745	-5.153300
H	2.123589	2.206405	-1.175003	С	-1.290972	0.495743	-4.644311
H	9.364298	-2.349955	-1.290095	C	1.043393	0.772646	-3.768133
H	8.290105	-3.083641	-0.058470	C	1.577674	1.437674	-2.634904
H	8.415295	-3.795911	-1.696776	C	2.966883	1.624863	-2.539690
H	8.302964	-3.080736	-4.012445	С	3.803967	1.130188	-3.552438
H	8.056511	-1.572829	-4.946624	C	3.247747	0.428281	-4.672510
H	9.254228	-1.633681	-3.615462	C	1.855260	0.257013	-4.787360
				С	-0.578799	1.478848	-2.391417
0	rmation 6.			C		1.752201	-1.880818
					-1.951894		
Multi	plicity: 2			С	5.293400	1.353248	-3.458508
Charg	e: 0			С	4.158438	-0.116858	-5.742534
E (B97	-3c) = -5613.008103	273340 Hartree		С	4.296646	-2.932384	0.549618
	/def2-TZVP) = -5612		rtroo	C	4.158675	-1.934461	-0.629986
	- D3(BJ)/def2-TZVI			С	4.679632	-0.579772	-0.100943
E (PBE	0 - D3(BJ)/def2-TZV	7P) = -5611.15810	0151668 Hartree	C	5.051577	-2.428108	-1.778863
E (PBE	h-3c) = -5604.81023	34962992 Hartree		С	2.708324	-1.783597	-1.134035
E (PM6	= 174.12711  Kcal	/mol		С	1.645222	3.865382	1.990064
	,						
	) = 73.59270  Kcal/r		4 ***	C	2.235723	3.081530	0.804923
	7X-V/def2-TZVP) = -		4 Hartree	С	4.538087	3.670835	-0.061476
E (GFN	1-xTB) = $-265.52236$	57452833 Hartree		C	4.970233	4.599756	-1.050904
E (GFN	2-xTB) = $-259.25550$	06262497 Hartree		С	6.327452	4.624177	-1.420397
	-FF) = $-33.80808840$			C	7.228848	3.728971	-0.821412
T (GEW.	11,33.00000840	,110, Hatcies					
				С	6.774518	2.801519	0.173277
Coord	inates:			C	5.422072	2.778852	0.558421
Cu	-1.951721	-1.104665	0.916956	С	2.838696	4.871036	-0.877376
N	-2.995400	0.556304	1.380629	C	1.433414	5.332285	-1.058445
	-3.153684	-1.396874	-0.676268	C	8.682790	3.737522	-1.225744
N							
N	-0.896758	-2.755224	0.438086	C	7.746113	1.836579	0.805336
N	-0.751932	-0.798893	2.509193	H	-3.486468	3.557417	2.812602
С	-2.621682	1.538658	2.274921	Н	-5.425776	2.847276	1.022416
Č	-4.174106	0.976125	0.804057	Н	-6.002912	-1.164212	-2.442029
С	-4.376896	-0.802299	-0.912103	H	-4.233511	-2.993028	-3.429542
C	-2.976006	-2.335528	-1.668971	H	0.156667	-5.262363	-1.541209
С	-0.968399	-3.465851	-0.741982	H	1.359448	-5.204962	0.903387
C	0.069229	-3.370489	1.208475	Н	1.679296	-1.529013	4.714082
C	0.211326	-1.656248	2.999302	Н	0.553241	0.940835	5.074868
C	-0.708065	0.331198	3.300231	H	-9.323148	1.386718	0.902248
C	-3.566164	2.637154	2.224480	H	-9.728977	2.474700	-1.313152
С	-4.544321	2.274870	1.330730	H	-7.917611	2.460388	-3.061139
С	-5.003288	-1.408082	-2.069541	Н	-5.700882	1.422955	-2.531867
C	-4.115192	-2.330131	-2.565515	Н	-1.073289	-3.417665	-6.380733
C	-0.008529	-4.554251	-0.723111	H	-1.465876	-5.891861	-6.475596
С	0.596997	-4.525831	0.507313	H	-2.067748	-7.154452	-4.386373
С	0.876613	-1.054341	4.139890	Н	-2.269163	-5.916684	-2.212393
С	0.315765	0.186001	4.317230	Н	4.984704	-4.481862	2.732354
C		0.296525		Н	4.487218		4.833129
	-4.894505		-0.200406			-5.770206	
С	-1.895691	-3.239033	-1.779263	H	2.180872	-5.711729	5.832620
С	0.581022	-2.894604	2.434735	H	0.382104	-4.369958	4.701829
C	-1.539139	1.463458	3.174381	H	0.907511	5.322337	4.193570
Ō	-6.247736	-1.787492	1.101798	Н	-0.493853	5.810444	6.219235
0	-1.377172	-1.201355	-6.351272	H	-2.386195	4.278700	6.845969
0	5.311486	-3.598544	0.736934	H	-2.857567	2.257553	5.424617
0	2.087874	4.941061	2.370487	H	-7.507372	0.752212	2.507261
N	-7.095868	0.245437	1.722475	H	-1.140850	-1.535628	-3.196869
N	-1.207331	-1.900420	-4.152462	Н	2.404518	-2.389383	1.092953
N	-0.341835	0.804288	-3.594392	H	0.288421	2.329729	2.089377
N	0.544296	1.845353	-1.793546	H	-5.898443	-3.077578	4.698656
N	3.206566	-2.943551	1.401117	H	-7.038314	-3.392244	3.343680
N	0.577319	3.195803	2.555040	Н	-5.302147	-3.168609	3.000199
N	3.164023	3.856030	0.025515	H	-7.391799	-1.181671	5.406803
N	3.893496	5.332893	-1.526164	Н	-7.670909	0.236930	4.380446
С	-6.249810	0.816159	-0.532869	H	-8.494378	-1.319818	4.002317
C	-7.287533	0.808321	0.440595	H	-4.860197	-0.768662	5.009966
C	-8.526827	1.409246	0.142378	H	-4.190671	-0.879334	3.346890
Č	-8.755101	2.008281	-1.102223	Н	-5.174242	0.536111	3.813717
~							
С	-7.747060	1.996434	-2.078551	H	-1.109863	1.128716	-5.537085
C	-6.510890	1.404700	-1.787296	H	-2.313224	0.712721	-4.273620
C	-1.762797	-3.995374	-3.059236	H	3.400233	2.168507	-1.691778
C	-1.421754	-3.289168	-4.249927	Н	1.430197	-0.259551	-5.661360
C	-1.319285	-3.982234	-5.474260	Н	-1.874169	2.237133	-0.891851
~							
С	-1.548551	-5.363650	-5.513696	H	-2.516846	2.430695	-2.554697
C	-1.881255	-6.071130	-4.348551	H	-2.541681	0.822686	-1.755878
C	-1.986430	-5.382775	-3.131896	H	5.853423	0.394185	-3.425545
C	1.662650	-3.681949	3.105229	H	5.677992	1.909332	-4.339330
C	2.978078	-3.703409	2.555599	H	5.559594	1.935789	-2.555831
~							
С	3.986141	-4.466268	3.184748	H	4.758382	0.687523	-6.218608
C	3.691069	-5.181023	4.352919	H	4.889586	-0.841966	-5.325625
C	2.404857	-5.150002	4.913852	Н	3.587257	-0.631272	-6.538581
C	1.400246	-4.400262	4.285083	Н	4.658970	0.184616	-0.900422
C							
	-1.252256	2.651180	4.036760	H	4.051700	-0.211160	0.736419
С			3.691894	H	5.720844	-0.670752	0.266929
	-0.178072	3.521124					
С	-0.178072 0.084103	4.659513	4.484844	H	5.062213	-1.679379	-2.595638
				H H	5.062213 6.085001		

				_			
H	4.675302	-3.385474	-2.192407	C	-5.941835	0.391669	4.324840
H	2.693988	-1.151516	-2.043410	С	-5.769828	0.277250	5.710901
H	2.256896	-2.763685	-1.388889	C	-4.516096	-0.037798	6.257554
H	2.040150	-1.272928	-0.406369	С	-3.419180	-0.230621	5.404435
H	2.766561	2.192669	1.206266	C	-0.884941	-3.691224	-4.023837
H	1.426758	2.687244	0.143210	С	-0.902900	-2.266545	-4.635661
H	6.668325	5.336984	-2.186420	С	-0.088213	-2.292271	-5.935404
H	5.085142	2.067780	1.327894	C	-0.275059	-1.255973	-3.654368
H	1.040479	5.789205	-0.126195	С	-2.366298	-1.873118	-4.931981
H	1.415362	6.088515	-1.862730	Ċ	3.536947	0.872174	-4.495350
H	0.770197	4.486052	-1.337287	C	2.325825	1.831816	-4.513534
H	9.004488	2.755819	-1.635371	C	3.384484	3.718323	-3.242405
H	8.879524	4.505077	-1.998441	С	3.022829	4.440613	-2.074454
H	9.351311	3.947439	-0.363461	C	3.873118	5.457020	-1.603130
H	8.586215	2.361327	1.308276	C	5.060252	5.738557	-2.297982
H	7.248008	1.198107	1.560049	С	5.404668	5.000949	-3.479292
H	8.208119	1.164913	0.050009	С	4.560978	3.982014	-3.956649
**	0.200113	1.101313	0.00000	C			
					1.464759	2.968277	-2.371015
Conformati	on 8.			C	0.270832	2.100530	-2.161723
Multiplici	tv: 2			C	5.984897	6.819685	-1.795655
Charge: 0	-			С	6.685166	5.311415	-4.212448
_	FC12 00	E 400000000 TT					
		5490200966 Hartree		С	2.468825	2.956970	5.903330
		5612.885267637605 Hart		C	2.338416	1.493405	6.413202
E(PBE - D3	(BJ)/def2-	TZVP) = -5610.94151163	5044 Hartree	C	3.479095	0.650122	5.800861
		-TZVP) = -5611.1742331		С	2.467421	1.513445	7.942158
	- ( - , ,	,	23037 Hartree				
		27478043128 Hartree		С	0.971335	0.897469	6.010243
E(PM6) = 1	.89.76412 K	cal/mol		C	-5.953936	0.740822	1.284890
E(PM7) = 6	0.34417 Kc	al/mol		С	-5.592595	0.732350	-0.218419
		= -5614.580917187273	Hartree	C	-5.500382	-1.706567	-0.793166
			110T CT CC				
		43211639934 Hartree		С	-4.485754	-2.561784	-1.292841
E (GFN2-xTE	= -259.2	74736636298 Hartree		C	-4.784362	-3.914673	-1.533974
E (GFN-FF)	= -33.8312	25456046 Hartree		C	-6.076547	-4.390861	-1.262339
2 (011, 11)	00.0012	20100010 110120100		C	-7.088440	-3.510305	-0.753041
Coordinate				С	-6.798198	-2.155048	-0.517418
Cu	0.399218	-0.512176	1.051048	C	-3.562894	-0.610092	-1.032381
N	-1.182084	-1.714729	1.482698	С	-2.574427	0.503630	-0.959244
N	1.141866	-1.938041	-0.170454	C	-6.397863	-5.845148	-1.502655
N	2.006020	0.671874	0.658846	C	-8.468887	-4.040882	-0.462060
N	-0.378528	0.941199	2.222755	Н	-4.055682	-2.582942	3.008349
С	-2.203331	-1.445495	2.373586	Н	-3.196003	-4.388557	1.154839
	-1.476432	-2.938530	0.916111	H	1.154306	-4.841794	-1.873714
C	0.536537	-3.127417	-0.525895	H	3.409742	-3.356587	-2.212240
C	2.365348	-1.919796	-0.811723	Н	5.087027	1.370261	-0.508686
С	3.135609	0.318231	-0.054272	Н	3.967219	3.389307	0.957317
C	2.238247	1.947402	1.135593	H	-0.626678	4.041766	3.504424
C	0.116021	2.221547	2.393058	H	-2.665958	2.370402	4.235150
C	-1.538697	0.873502	2.969902	Н	-2.047871	-6.270040	-3.657788
	-3.154984	-2.540242	2.386217	Н	-2.204337	-8.325539	-2.229758
						-8.176370	
	-2.717777	-3.453309	1.460999	H	-1.744588		0.237370
C	1.395106	-3.870803	-1.428845	Н	-1.063370	-5.981257	1.238356
С	2.530640	-3.123452	-1.602729	Н	5.975943	-0.406046	-4.582674
C	4.106909	1.395393	-0.019879	Н	7.814554	-1.825402	-3.624465
C	3.548929	2.406282	0.719731	Н	7.593572	-2.781356	-1.310907
C	-0.780104	2.992171	3.232066	Н	5.510581	-2.327386	0.019350
C	-1.801435	2.152803	3.599215	H	2.936784	5.613069	5.233850
С	-0.705104	-3.604010	-0.055404	Н	2.876687	7.589477	3.680868
					2.123989		
C	3.327828	-0.893841	-0.744582	Н		7.302148	1.299605
C	1.354105	2.707603	1.924107	H	1.448839	5.004858	0.480780
C	-2.374755	-0.252429	3.103139	H	-6.910984	0.651709	3.882608
	-0.375152	-4.651960	-4.596548	Н	-6.634360	0.439460	6.372271
Ō	4.253661	0.714603	-5.477715	Н	-4.388943	-0.126513	7.346485
0	2.754436	3.897746	6.638976	H	-2.424446	-0.460627	5.815499
0	-7.036348	1.160275	1.678188	H	-1.881684	-2.949577	-2.322870
	-1.483916	-3.793745	-2.783065	Н	3.012957	0.508130	-2.553377
N	3.699815	0.264544	-3.274611	Н	1.982093	2.227143	4.056699
N	2.366756	2.783956	-3.422672	H	-4.099935	-0.067115	1.578206
N	1.825437	3.954362	-1.567926	H	-0.102700	-1.291397	-6.413438
N	2.248965	3.084602	4.545838	H	0.964195	-2.575923	-5.739643
N	-4.930046	0.277873	2.071233	Н	-0.498827	-3.032728	-6.647647
	-4.895187	-0.460047	-0.653032	Н	-0.299180	-0.242602	-4.107152
	-3.297607	-1.848264	-1.430414	H	-0.826420	-1.202795	-2.696150
C	-1.201113	-4.890854	-0.625987	H	0.779058	-1.512491	-3.424671
	-1.506256	-4.973569	-2.012182	Н	-2.398317	-0.879553	-5.426474
	-1.849572	-6.218061	-2.580035	Н	-2.842125	-2.605554	-5.614872
	-1.932108	-7.361120	-1.774658	H	-2.974032	-1.815008	-4.007273
	-1.676990	-7.279323	-0.395823	H	2.349057	2.348704	-5.493448
C	-1.307862	-6.050543	0.167713	H	1.386158	1.247729	-4.449889
C	4.599972	-1.103161	-1.507811	Н	3.614018	6.015890	-0.691621
C	4.745421	-0.549649	-2.809806	Н	4.835593	3.405847	-4.853219
C	5.901499	-0.821462	-3.570744	Н	-0.303422	2.513605	-1.313812
С	6.914979	-1.619886	-3.024703	H	-0.388461	2.050073	-3.052468
C	6.793230	-2.156339	-1.733487	Н	0.559667	1.061049	-1.895966
C	5.634050	-1.899367	-0.986728	Н	6.996375	6.422556	-1.564603
C	1.787177	4.063326	2.388288	Н	6.131917	7.621447	-2.550518
C	2.223615	4.228859	3.735768	H	5.589380	7.290365	-0.875468
C	2.612912	5.506702	4.191818	Н	6.714765	6.366055	-4.560294
C	2.572030	6.597641	3.312785	Н	7.574944	5.175408	-3.561304
C	2.153207	6.439137	1.982152	Н	6.811265	4.658998	-5.097273
C	1.763521	5.170985	1.523911	H	3.435962	-0.387778	6.190769
С	-3.560042	-0.122119	4.010294	H	3.413831	0.593092	4.694630
	-4.839839	0.184590	3.470048	Н	4.470520	1.072439	6.060712
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H	2.414646	0.481352	8.343413	Н	2.552173	6.421994	0.420277
H	3.426564	1.969767	8.251776	H	4.399899	4.757821	0.784821
Н	1.657908	2.113379	8.401497	Н	3.881421	2.319979	0.965103
H	0.859072	-0.115275	6.449764	H	1.086846	-3.389701	-2.774796
H	0.132742	1.523861	6.375232	H	3.382394	-4.223346	-3.296928
H	0.850774	0.783226	4.912569	Н	5.387844	-2.776170	-2.851503
H	-6.544585	0.842970	-0.773322	H	5.059594	-0.477088	-1.889830
H	-4.968882	1.620861	-0.442683	H	2.757971	0.362852	-1.393927
H	-4.015352	-4.597949	-1.918480	Н	-2.021238	-1.598120	-0.981853
H	-7.568191	-1.481067	-0.112015	H	-3.986061	-1.794918	-2.512930
H	-2.598294	1.026954	0.018697	H	-3.679500	-1.586798	-5.001811
H	-1.562947	0.080087	-1.080295	Н	-1.375852	-1.186950	-5.925647
H	-2.733990	1.262576	-1.753856	H	0.576923	-0.959618	-4.391974
H	-7.207335	-5.970280	-2.253177	H	-3.716380	-1.409069	1.531490
H	-5.508864	-6.396057	-1.864704	H	-5.482451	0.171097	2.343517
			-0.576943				
H	-6.752757	-6.345972		H	-4.857429	2.479532	3.108032
H	-8.443195	-4.861203	0.286437	H	-2.440533	3.174605	3.100813
H	-9.134582	-3.247867	-0.071500	H	-0.677366	1.568954	2.323935
H	-8.944413	-4.466476	-1.371204	H	-0.103251	-2.885060	-0.117118
				H	0.374545	-5.168998	0.754815
	DT 1737			H	-0.177658	-5.759591	3.139398
	BLEN			Н	-1.211177	-4.017005	4.626708
				H	-1.660649	-1.724196	3.760844
Confo	ormation 1.			Н	0.461986	2.527794	-1.839765
	iplicity: 3			Н	-0.229372	1.258005	-2.936932
Char	ge: 0			H	-1.515262	3.933266	-2.076928
E(B97	7-3c) = -2729.96686	6050881 Hartree		Н	-1.447641	3.228034	-3.727549
	6/def2-TZVP) = -272		rtroo	Н	-3.738642	2.830254	-2.284757
	· ·						
E (PBI	E - D3(BJ)/def2-TZV	P) = -2728.978699	280144 Hartree	H	-2.995528	1.398224	-3.079608
E (PBE	E0 - D3(BJ)/def2-TZ	VP) = -2729.12628	0344690 Hartree	Н	-2.988750	0.611033	-0.788833
	Eh-3c) = -2726.1156			Н	-2.716347	2.260852	-0.123186
				п	-2./1034/	2.200032	-0.123100
E(PM6	6) = 93.42146 Kcal/	mol					
E (PM	7) = 107.36848  Kcal	/mol		Confor	mation 16.		
	97X-V/def2-TZVP) =		C II		olicity: 3		
	· · · · · · · · · · · · · · · · · · ·		о нагитее	_	4		
E (GF1	N1-xTB) = -120.6214	11026550 Hartree		Charge	e: 0		
E (GFN	N2-xTB) = -119.8122	02924278 Hartree		E(B97-	-3c) = -2729.96456	1799386 Hartree	
	N-FF) = -16.9730411				def2-TZVP) = -272		rtroo
E (GFI	N-FF) = -10.9/30411	0/0/9 hartree					
				E(PBE	- D3(BJ)/def2-TZV	P) = -2728.975017	7083584 Hartree
Coord	dinates:			E (PBEC	) - D3(BJ)/def2-TZ	VP) = -2729.12242	24078092 Hartree
V	0.148242	-0.026838	0.006472		n-3c) = -2726.11402		
0	-1.054991	1.361986	-1.016424	E(PM6)	= 96.23616 Kcal/r	mol	
N	-1.096676	-0.835887	1.270135	E(PM7)	= 108.94007 Kcal	/mol	
N	0.478053	-1.000775	-1.686449		7X-V/def2-TZVP) = -		16 Hartron
							o narciee
N	1.462319	1.201804	0.773012	E (GFN1	1-xTB) = $-120.6180$	J4568258 Hartree	
С		0 401540	1.784226	E (CENT		00000000	
	2.017137	0.401549	1./84220	E (GFN2	2-xTB) = -119.8114	839283/1 Hartree	
	2.017137	0.401549			2-xTB) = -119.8114		
С	2.183254	-0.983524	1.516250		2-xTB) = -119.81148 -FF) = -16.9799628		
					,		
C C	2.183254 2.476117	-0.983524 -1.888298	1.516250 2.550522	E (GFN-	-FF) = -16.9799628		
C C	2.183254 2.476117 2.684776	-0.983524 -1.888298 -1.422505	1.516250 2.550522 3.853281	E (GFN-	FF) = -16.9799628	62299 Hartree	0 152539
0 0 0	2.183254 2.476117 2.684776 2.584644	-0.983524 -1.888298 -1.422505 -0.040640	1.516250 2.550522 3.853281 4.117271	E (GFN- Coordi V	FF) = -16.9799628 nates: -0.137933	62299 Hartree -0.071176	0.152538
C C	2.183254 2.476117 2.684776	-0.983524 -1.888298 -1.422505	1.516250 2.550522 3.853281	E (GFN-	FF) = -16.9799628	62299 Hartree	0.152538 -0.734736
0 0 0	2.183254 2.476117 2.684776 2.584644 2.244795	-0.983524 -1.888298 -1.422505 -0.040640 0.864002	1.516250 2.550522 3.853281 4.117271 3.108646	E (GFN- Coordi V	-FF) = -16.9799628 nates: -0.137933 1.417017	-0.071176 -1.148629	-0.734736
00000	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828	E (GFN- Coordi V O N	-FF) = -16.97996280 	-0.071176 -1.148629 -1.204491	-0.734736 1.597885
0 0 0 0 0 0	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306	E (GFN- Coordi V O N	-FF) = -16.97996280 nates: -0.137933 1.417017 -0.781529 1.079446	-0.071176 -1.148629 -1.204491 1.382368	-0.734736 1.597885 0.707862
00000	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828	E (GFN- Coordi V O N	-FF) = -16.97996280 	-0.071176 -1.148629 -1.204491	-0.734736 1.597885
0000000	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822	E (GFN- Coordi V O N	-FF) = -16.9799628 nates: -0.137933 1.417017 -0.781529 1.079446 -1.355697	-0.071176 -1.148629 -1.204491 1.382368	-0.734736 1.597885 0.707862 -1.369455
000000000	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334	E (GFN-Coordi V O N N N	-FF) = -16.9799628 	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462	-0.734736 1.597885 0.707862 -1.369455 -1.208206
0000000000	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110	E (GFN-Coordi V O N N N C	-FF) = -16.97996280 	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222
000000000	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104	E (GFN-Coordi V O N N N	-FF) = -16.9799628 	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953
00000000000	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104	E (GFN-Coordi VONNNNCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	Inates: -0.137933 1.417017 -0.781529 1.079446 -1.355697 -2.588101 -3.289802 -4.493929	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953
00000000000	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.99984 2.324448 3.355829 3.071705 1.764273	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302	E (GFN-Coordi VONNNNCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	-FF) = -16.97996280 	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229
	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385	E (GFN-Coordi VONNNNCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	-FF) = -16.9799628 	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123308 1.464273	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492
	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319	E (GFN- Coordi V O N N C C C C C	-FF) = -16.9799628 	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979
	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385	E (GFN- Coordi V O N N C C C C C	-FF) = -16.9799628 	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123308 1.464273	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492
	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466	Coordi V O N N C C C C	-FF) = -16.9799628 	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979 -2.639516
	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176	E (GFN- Coordi V O N N C C C C C C	-FF) = -16.97996280  Inates: -0.137933 1.417017 -0.781529 1.079446 -1.355697 -2.588101 -3.289802 -4.493929 -5.041892 -4.375826 -3.180271 -0.727732 -0.436828	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979 -2.639516 -3.245536
000000000000000000	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 4.376285 4.191175 2.902675	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182	E (GFN- Coordi V O N N C C C C C C C C C	Inates: -0.137933 1.417017 -0.781529 1.079446 -1.355697 -2.588101 -3.289802 -4.493929 -5.041892 -4.375826 -3.180271 -0.727732 -0.436828 0.281506	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341
000000000000000000	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176	E (GFN- Coordi V O N N C C C C C C	-FF) = -16.97996280  Inates: -0.137933 1.417017 -0.781529 1.079446 -1.355697 -2.588101 -3.289802 -4.493929 -5.041892 -4.375826 -3.180271 -0.727732 -0.436828	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979 -2.639516 -3.245536
000000000000000000	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059	E (GFN- Coordi V O N N C C C C C C C C C C	-FF) = -16.9799628 	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011
000000000000000000000000000000000000000	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486411	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.9799628 	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983
000000000000000000000000000000000000000	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486411 -1.598902	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.9799628 	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.993088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486411 -1.598902 -1.488147	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.97996280  Inates:	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486411 -1.598902	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.9799628 	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292 1.251933 1.220980	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477 1.315629
000000000000000000000000000000000000000	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391 -2.818577 -1.527573	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.883088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486411 -1.598902 -1.488147 -1.269310	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881 -4.324117 -4.837945	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.97996280  Inates: -0.137933 1.417017 -0.781529 1.079446 -1.355697 -2.588101 -3.289802 -4.493929 -5.041892 -4.375826 -3.180271 -0.727732 -0.436828 0.281506 0.711056 0.410783 -0.300339 2.323152 3.308057	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292 1.251933 1.220980 2.240174	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477 1.315629 1.417478
000000000000000000000000000000000000000	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391 -2.818577 -1.527573 -0.427442	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486411 -1.598902 -1.488147 -1.269310 -1.142006	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881 -4.324117 -4.837945 -3.981436	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.9799628 	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292 1.251933 1.220980 2.240174 1.984591	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018853 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477 1.315629 1.417478 2.033060
000000000000000000000000000000000000000	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391 -2.818577 -1.527573 -0.427442 -2.084969	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486441 -1.598902 -1.488147 -1.269310 -1.142006 -0.005905	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881 -4.324117 -4.837945 -3.981436 1.835610	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.9799628 	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292 1.251933 1.220980 2.240174 1.984591 0.722422	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018853 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477 1.315629 1.417478 2.033060 2.572138
000000000000000000000000000000000000000	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391 -2.818577 -1.527573 -0.427442	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486411 -1.598902 -1.488147 -1.269310 -1.142006	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881 -4.324117 -4.837945 -3.981436	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.9799628 	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292 1.251933 1.220980 2.240174 1.984591	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018853 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477 1.315629 1.417478 2.033060
000000000000000000000000000000000000000	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391 -2.818577 -1.527573 -0.427442 -2.084969 -3.446007	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486411 -1.598902 -1.488147 -1.269310 -1.142006 -0.005905 -0.399826	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881 -4.324117 -4.837945 -3.981436 1.835610 1.877220	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.97996280  Inates:	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292 1.251933 1.220980 2.240174 1.984591 0.722422 -0.281150	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477 1.315629 1.417478 2.033060 2.572138 2.519825
000000000000000000000000000000000000000	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391 -2.818577 -1.527573 -0.427442 -2.084969 -3.446007 -4.428118	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486441 -1.598902 -1.488147 -1.269310 -1.142006 -0.005905 -0.399826 0.488637	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881 -4.324117 -4.837945 -3.981436 1.835610 1.877220 2.330332	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.97996280  Inates:	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292 1.251933 1.220980 2.240174 1.984591 0.722422 -0.281150 -0.036312	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477 1.315629 1.417478 2.033060 2.572138 2.519825 1.919038
000000000000000000000000000000000000000	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391 -2.818577 -1.527573 -0.427442 -2.084969 -3.446007 -4.428118 -4.080111	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486411 -1.598902 -1.488147 -1.269310 -1.142006 -0.005905 -0.399826 0.488637 1.784581	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881 -4.324117 -4.837945 -3.981436 1.835610 1.877220 2.330332 2.756674	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.97996280  Inates:	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292 1.251933 1.220980 2.240174 1.984591 0.722422 -0.281150 -0.036312 2.558819	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477 1.315629 1.417478 2.033060 2.572138 2.519825 1.919038 0.044647
000000000000000000000000000000000000000	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391 -2.818577 -1.527573 -0.427442 -2.084969 -3.446007 -4.428118	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486441 -1.598902 -1.488147 -1.269310 -1.142006 -0.005905 -0.399826 0.488637	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881 -4.324117 -4.837945 -3.981436 1.835610 1.877220 2.330332	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.97996280  Inates:	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292 1.251933 1.220980 2.240174 1.984591 0.722422 -0.281150 -0.036312	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477 1.315629 1.417478 2.033060 2.572138 2.519825 1.919038
000000000000000000000000000000000000000	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391 -2.818577 -1.527573 -0.427442 -2.084969 -3.446007 -4.428118 -4.080111 -2.731544	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486411 -1.598902 -1.488147 -1.269310 -1.142006 -0.005905 -0.399826 0.488637 1.784581 2.173352	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881 -4.324117 -4.837945 -3.981436 1.835610 1.877220 2.330332 2.756674 2.747028	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.97996280  Inates:	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292 1.251933 1.220980 2.240174 1.984591 0.722422 -0.281150 -0.036312 2.558819 3.029563	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018853 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477 1.315629 1.417478 2.033060 2.572138 2.519825 1.919038 0.044647 0.280211
	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391 -2.818577 -1.527573 -0.427442 -2.084969 -3.446007 -4.428118 -4.080111 -2.731544 -1.739594	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486441 -1.598902 -1.488147 -1.269310 -1.142006 -0.005905 -0.399826 0.488637 1.784581 2.173352 1.283773	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881 -4.324117 -4.837945 -3.981436 1.835610 1.877220 2.330332 2.756674 2.747028 2.305100	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.97996280  Inates:	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292 1.251933 1.220980 2.240174 1.984591 0.722422 -0.281150 -0.036312 2.558819 3.029563 4.077961	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018853 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477 1.315629 1.417478 2.033060 2.572138 2.519825 1.919038 0.044647 0.280211 -0.477539
	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391 -2.818577 -1.527573 -0.427442 -2.084969 -3.446007 -4.428118 -4.080111 -2.731544 -1.739594 -0.915662	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486411 -1.598902 -1.488147 -1.269310 -1.142006 -0.005905 -0.399826 0.488637 1.784581 2.173352 1.283773 -2.141379	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881 -4.324117 -4.837945 -3.981436 1.835610 1.877220 2.330332 2.756674 2.747028 2.305100 1.759139	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.97996280  Inates:	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292 1.251933 1.220980 2.240174 1.984591 0.722422 -0.281150 -0.036312 2.558819 3.029563 4.077961 4.7721317	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477 1.315629 1.417478 2.033060 2.572138 2.519825 1.919038 0.044647 0.280211 -0.477539 -1.449126
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	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391 -2.818577 -1.527573 -0.427442 -2.084969 -3.446007 -4.428118 -4.080111 -2.731544 -1.739594 -0.915662 -0.342883	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486411 -1.598902 -1.488147 -1.269310 -1.142006 -0.005905 -0.399826 0.488637 1.784581 2.173352 1.283773 -2.141379 -3.136911	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881 -4.324117 -4.837945 -3.981436 1.835610 1.877220 2.330332 2.756674 2.747028 2.305100 1.759139 0.926773	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.97996280  Inates:	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292 1.251933 1.220980 2.240174 1.984591 0.722422 -0.281150 -0.036312 2.558819 3.029563 4.077961 4.721317 4.291048	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477 1.315629 1.417478 2.033060 2.572138 2.519825 1.919038 0.044647 0.280211 -0.477539 -1.449126 -1.665962
	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391 -2.818577 -1.527573 -0.427442 -2.084969 -3.446007 -4.428118 -4.080111 -2.731544 -1.739594 -0.915662 -0.342883 -0.074376	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486411 -1.598902 -1.488147 -1.269310 -1.142006 -0.005905 -0.399826 0.488637 1.784581 2.173352 1.283773 -2.141379 -3.136911 -4.418009	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881 -4.324117 -4.837945 -3.981436 1.835610 1.877220 2.330332 2.756674 2.747028 2.305100 1.759139 0.926773 1.423388	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.97996280  Inates:	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292 1.251933 1.220980 2.240174 1.984591 0.722422 -0.281150 -0.036312 2.558819 3.029563 4.077961 4.721317 4.291048 3.214067	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018853 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477 1.315629 1.417478 2.033060 2.572138 2.519825 1.919038 0.044647 0.280211 -0.477539 -1.449126 -1.665962 -0.944608
	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391 -2.818577 -1.527573 -0.427442 -2.084969 -3.446007 -4.428118 -4.080111 -2.731544 -1.739594 -0.915662 -0.342883 -0.074376 -0.383931	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486411 -1.598902 -1.488147 -1.269310 -1.142006 -0.005905 -0.399826 0.488637 1.784581 2.173352 1.283773 -2.141379 -3.136911 -4.418009 -4.750481	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881 -4.324117 -4.837945 -3.981436 1.835610 1.877220 2.330332 2.756674 2.747028 2.305100 1.759139 0.926773 1.423388 2.752788	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.97996280  Inates:	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292 1.251933 1.220980 2.240174 1.984591 0.722422 -0.281150 -0.036312 2.558819 3.029563 4.077961 4.721317 4.291048 3.214067 -2.593058	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477 1.315629 1.417478 2.033060 2.572138 2.519825 1.919038 0.044647 0.280211 -0.477539 -1.449126 -1.665962 -0.944608 1.356168
	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391 -2.818577 -1.527573 -0.427442 -2.084969 -3.446007 -4.428118 -4.080111 -2.731544 -1.739594 -0.915662 -0.342883 -0.074376	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486411 -1.598902 -1.488147 -1.269310 -1.142006 -0.005905 -0.399826 0.488637 1.784581 2.173352 1.283773 -2.141379 -3.136911 -4.418009	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881 -4.324117 -4.837945 -3.981436 1.835610 1.877220 2.330332 2.756674 2.747028 2.305100 1.759139 0.926773 1.423388	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.97996280  Inates:	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292 1.251933 1.220980 2.240174 1.984591 0.722422 -0.281150 -0.036312 2.558819 3.029563 4.077961 4.721317 4.291048 3.214067	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018853 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477 1.315629 1.417478 2.033060 2.572138 2.519825 1.919038 0.044647 0.280211 -0.477539 -1.449126 -1.665962 -0.944608
	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391 -2.818577 -1.527573 -0.427442 -2.084969 -3.446007 -4.428118 -4.080111 -2.731544 -1.739594 -0.915662 -0.342883 -0.074376 -0.383931 -0.966682	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486441 -1.598902 -1.488147 -1.269310 -1.142006 -0.005905 -0.399826 0.488637 1.784581 2.173352 1.283773 -2.141379 -3.136911 -4.418009 -4.750481 -3.775376	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881 -4.324117 -4.837945 -3.981436 1.835610 1.877220 2.330332 2.756674 2.747028 2.305100 1.759139 0.926773 1.423388 2.752788 3.580462	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.97996280  Inates:	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292 1.251933 1.220980 2.240174 1.984591 0.722422 -0.281150 -0.036312 2.558819 3.029563 4.077961 4.721317 4.291048 3.214067 -2.593058 -3.533849	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477 1.315629 1.417478 2.033060 2.572138 2.519825 1.919038 0.044647 0.280211 -0.477539 -1.449126 -1.665962 -0.944608 1.356168 2.274993
	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391 -2.818577 -1.527573 -0.427442 -2.084969 -3.446007 -4.428118 -4.080111 -2.731544 -1.739594 -0.915662 -0.342883 -0.074376 -0.383931 -0.966682 -1.229065	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486411 -1.598902 -1.488147 -1.269310 -1.142006 -0.005905 -0.399826 0.488637 1.784581 2.173352 1.283773 -2.141379 -3.136911 -4.418009 -4.750481 -3.775376 -2.487810	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881 -4.837945 -3.981436 1.835610 1.877220 2.330332 2.756674 2.747028 2.305100 1.759139 0.926773 1.423388 2.752788 3.580462 3.097761	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.97996280  Inates:  -0.137933 1.417017 -0.781529 1.079446 -1.355697 -2.588101 -3.289802 -4.493929 -5.041892 -4.375826 -3.180271 -0.727732 -0.436828 0.281506 0.711056 0.410783 -0.300339 2.323152 3.308057 4.540911 4.837703 3.853927 2.615591 0.670770 -0.645437 -1.184493 -0.401224 0.920898 1.451017 -0.876971 -0.348385 -0.347193	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292 1.251933 1.220980 2.240174 1.984591 0.722422 -0.281150 -0.036312 2.558819 3.029563 4.077961 4.721317 4.291048 3.214067 -2.593058 -3.533849 -4.899800	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477 1.315629 1.417478 2.033060 2.572138 2.519825 1.919038 0.044647 0.280211 -0.477539 -1.449126 -1.665962 -0.944608 1.356168 2.274993 1.967990
	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391 -2.818577 -1.527573 -0.427442 -2.084969 -3.446007 -4.428118 -4.080111 -2.731544 -1.739594 -0.915662 -0.342883 -0.074376 -0.383931 -0.966682 -1.229065 -0.467672	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486411 -1.598902 -1.488147 -1.269310 -1.142006 -0.005905 -0.399826 0.488637 1.784581 2.173352 1.283773 -2.141379 -3.136911 -4.418009 -4.750481 -3.775376 -2.487810 2.029558	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881 -4.324117 -4.837945 -3.981436 1.835610 1.877220 2.330332 2.756674 2.747028 2.305100 1.759139 0.926773 1.423388 2.752788 3.580462 3.097761 -2.176591	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.97996280  Inates:	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292 1.251933 1.220980 2.240174 1.984591 0.722422 -0.281150 -0.036312 2.558819 3.029563 4.077961 4.721317 4.291048 3.214067 -2.593058 -3.533849 -4.899800 -5.359598	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477 1.315629 1.417478 2.033060 2.572138 2.519825 1.919038 0.044647 0.280211 -0.477539 -1.449126 -1.665962 -0.944608 1.356168 2.274993 1.967990 0.746690
	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391 -2.818577 -1.527573 -0.427442 -2.084969 -3.446007 -4.428118 -4.080111 -2.731544 -1.739594 -0.915662 -0.342883 -0.074376 -0.383931 -0.966682 -1.229065 -0.467672	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486411 -1.598902 -1.488147 -1.269310 -1.142006 -0.005905 -0.399826 0.488637 1.784581 2.173352 1.283773 -2.141379 -3.136911 -4.418009 -4.750481 -3.775376 -2.487810 2.029558	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881 -4.324117 -4.837945 -3.981436 1.835610 1.877220 2.330332 2.756674 2.747028 2.305100 1.759139 0.926773 1.423388 2.752788 3.580462 3.097761 -2.176591	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.97996280  Inates:	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292 1.251933 1.220980 2.240174 1.984591 0.722422 -0.281150 -0.036312 2.558819 3.029563 4.077961 4.721317 4.291048 3.214067 -2.593058 -3.533849 -4.899800 -5.359598	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477 1.315629 1.417478 2.033060 2.572138 2.519825 1.919038 0.044647 0.280211 -0.477539 -1.449126 -1.665962 -0.944608 1.356168 2.274993 1.967990 0.746690
	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391 -2.818577 -1.527573 -0.427442 -2.084969 -3.446007 -4.428118 -4.080111 -2.731544 -1.739594 -0.915662 -0.342883 -0.074376 -0.383931 -0.966682 -1.229065 -0.467672 -1.553037	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486411 -1.598902 -1.488147 -1.269310 -1.142006 -0.005905 -0.399826 0.488637 1.784581 2.173352 1.283773 -2.141379 -3.136911 -4.418009 -4.750481 -3.775376 -2.487810 2.029558 2.984773	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881 -4.324117 -4.837945 -3.981436 1.835610 1.877220 2.330332 2.756674 2.747028 2.305100 1.759139 0.926773 1.423388 2.752788 3.580462 3.097761 -2.176591 -2.176591 -2.176591 -2.176591 -2.176591 -2.176591 -2.176591	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.97996280  Inates:	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292 1.251933 1.220980 2.240174 1.984591 0.722422 -0.281150 -0.036312 2.558819 3.029563 4.077961 4.721317 4.291048 3.214067 -2.593058 -3.533849 -4.89800 -5.359598	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018853 -0.72229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477 1.315629 1.417478 2.033060 2.572138 2.519825 1.919038 0.044647 0.280211 -0.477539 -1.449126 -1.665962 -0.944608 1.356168 2.274993 1.967990 0.746690 -0.156175
	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391 -2.818577 -1.527573 -0.427442 -2.084969 -3.446007 -4.428118 -4.080111 -2.731544 -1.739594 -0.915662 -0.342883 -0.074376 -0.383931 -0.966682 -1.229065 -0.467672 -1.553037 -2.830777	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486411 -1.598902 -1.488147 -1.269310 -1.142006 -0.005905 -0.399826 0.488637 1.784581 2.173352 1.283773 -2.141379 -3.136911 -4.418009 -4.750481 -3.775376 -2.487810 2.029558 2.984773 2.198082	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881 -4.324117 -4.837945 -3.981436 1.835610 1.877220 2.330332 2.756674 2.747028 2.305100 1.759139 0.926773 1.423388 2.752788 3.580462 3.097761 -2.176591 -2.652870 -2.652870 -2.328049	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.97996280	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292 1.251933 1.220980 2.240174 1.984591 0.722422 -0.281150 -0.036312 2.558819 3.029563 4.077961 4.721317 4.291048 3.214067 -2.593058 -3.533849 -4.899800 -5.359598 -4.436712 -3.066256	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477 1.315629 1.417478 2.033060 2.572138 2.519825 1.919038 0.044647 0.280211 -0.477539 -1.449126 -1.665962 -0.944608 1.356168 2.274993 1.967990 0.746690 -0.156175 0.147244
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ососососососососососососососососососон н н н	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391 -2.818577 -1.527573 -0.427442 -2.084969 -3.446007 -4.428118 -4.080111 -2.731544 -1.739594 -0.915662 -0.342883 -0.074376 -0.383931 -0.966682 -1.229065 -0.467672 -1.553037 -2.830777 -2.498583 2.135135 2.551897 2.92929 2.752382	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486411 -1.598902 -1.488147 -1.269310 -1.142006 -0.005905 -0.399826 0.488637 1.784581 2.173352 1.283773 -2.141379 -3.136911 -4.418009 -4.750481 -3.775376 -2.487810 2.029558 2.984773 2.198082 1.583113 -1.351848 -2.961056 -2.125693 0.332964 1.934637	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881 -4.324117 -4.837945 -3.981436 1.835610 1.877220 2.330332 2.756674 2.747028 2.305100 1.759139 0.926773 1.423388 2.752788 3.580462 3.097761 -2.176591 -2.652870 -2.328049 -0.974936 0.475670 2.320101 4.662523 5.139643	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.97996280  Inates:  -0.137933 1.417017 -0.781529 1.079446 -1.355697 -2.588101 -3.289802 -4.493929 -5.041892 -4.375826 -3.180271 -0.727732 -0.436828 0.281506 0.711056 0.410783 -0.300339 2.323152 3.308057 4.540911 4.887703 3.853927 2.615591 0.670770 -0.645437 -1.184493 -0.401224 0.920898 1.451017 -0.876971 -0.348385 -0.347193 -0.875135 -1.425607 -1.438262 -1.336956 -2.423092 -3.009812 -2.543592 -1.468686	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292 1.251933 1.220980 2.240174 1.984591 0.72222 -0.281150 -0.036312 2.558819 3.029563 4.077961 4.721317 4.291048 3.214067 -2.593058 -3.533849 -4.899800 -5.359598 -4.436712 -3.066256 -0.679454 -1.316976 -0.742121 0.481441 1.119194	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477 1.315629 1.417478 2.033060 2.572138 2.519825 1.919038 0.044647 0.280211 -0.477539 -1.449126 -1.665962 -0.944608 1.356168 2.274993 1.967990 0.746690 -0.156175 0.147244 2.784192 3.437797 4.571921 5.081167 4.440792
ососососососососососососососососососос	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391 -2.818577 -1.527573 -0.427442 -2.084969 -3.446007 -4.428118 -4.080111 -2.731544 -1.739594 -0.915662 -0.342883 -0.074376 -0.383931 -0.966682 -1.229065 -0.467672 -1.553037 -2.830777 -2.498583 2.135135 2.551897 2.929292 2.752382 2.126688 -0.334726	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486411 -1.598902 -1.488147 -1.269310 -1.142006 -0.005905 -0.399826 0.488637 1.784581 2.173352 1.283773 -2.141379 -3.136911 -4.418009 -4.750481 -3.775376 -2.487810 2.029558 2.984773 2.198082 1.583113 -1.351848 -2.961056 -2.125693 0.332964 1.934637 3.174011	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881 -4.324117 -4.837945 -3.981436 1.835610 1.877220 2.330332 2.756674 2.747028 2.305100 1.759139 0.926773 1.423388 2.752788 3.580462 3.097761 -2.176591 -2.652870 -2.328049 -0.974936 0.475670 2.320101 4.662523 5.139643 3.331250 0.482183	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.97996280  Inates:	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292 1.251933 1.220980 2.240174 1.984591 0.722422 -0.281150 -0.036312 2.558819 3.029563 4.077961 4.721317 4.291048 3.214067 -2.593058 -3.533849 -4.89800 -5.359598 -4.436712 -3.066256 -0.679454 -1.316976 -0.742121 0.481441 1.119194 0.548080 -0.457214	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477 1.315629 1.417478 2.033060 2.572138 2.519825 1.919038 0.044647 0.280211 -0.477539 -1.449126 -1.665962 -0.944608 1.356168 2.274993 1.967990 0.746690 -0.156175 0.147244 2.784192 3.437797 4.571921 5.081167 4.440792 3.313793 -1.538164
ососососососососососососососососососос	2.183254 2.476117 2.684776 2.584644 2.244795 1.738074 0.704722 0.999984 2.324448 3.355829 3.071705 1.764273 1.963244 3.252044 4.376285 4.191175 2.902675 -0.588162 -1.889980 -2.987391 -2.818577 -1.527573 -0.427442 -2.084969 -3.446007 -4.428118 -4.080111 -2.731544 -1.739594 -0.915662 -0.342883 -0.074376 -0.383931 -0.966682 -1.229065 -0.467672 -1.553037 -2.830777 -2.498583 2.135135 2.551897 2.929929 2.752382 2.126688	-0.983524 -1.888298 -1.422505 -0.040640 0.864002 2.576796 3.526644 4.893088 5.348976 4.415967 3.049311 -1.456480 -2.750839 -3.212787 -2.406289 -1.124028 -0.646767 -1.232793 -1.486411 -1.598902 -1.488147 -1.269310 -1.142006 -0.005905 -0.399826 0.488637 1.784581 2.173352 1.283773 -2.141379 -3.136911 -4.418009 -4.750481 -3.775376 -2.487810 2.029558 2.984773 2.198082 1.583113 -1.351848 -2.961056 -2.125693 0.332964 1.934637	1.516250 2.550522 3.853281 4.117271 3.108646 0.712828 0.523306 0.412822 0.503334 0.710110 0.812104 -2.043302 -2.589385 -2.879319 -2.627466 -2.088176 -1.809182 -2.572059 -2.069431 -2.933881 -4.324117 -4.837945 -3.981436 1.835610 1.877220 2.330332 2.756674 2.747028 2.305100 1.759139 0.926773 1.423388 2.752788 3.580462 3.097761 -2.176591 -2.652870 -2.328049 -0.974936 0.475670 2.320101 4.662523 5.139643 3.331250	E (GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-FF) = -16.97996280  Inates:  -0.137933 1.417017 -0.781529 1.079446 -1.355697 -2.588101 -3.289802 -4.493929 -5.041892 -4.375826 -3.180271 -0.727732 -0.436828 0.281506 0.711056 0.410783 -0.300339 2.323152 3.308057 4.540911 4.837703 3.853927 2.615591 0.670770 -0.645437 -1.184493 -0.401224 0.920898 1.451017 -0.876971 -0.348385 -0.347193 -0.875135 -1.425607 -1.438262 -1.336956 -2.423092 -3.009812 -2.543592 -1.468686 -0.864062	-0.071176 -1.148629 -1.204491 1.382368 0.103107 0.752462 1.387666 2.060990 2.123008 1.464273 0.778291 0.066213 -1.177502 -1.236031 -0.055085 1.187292 1.251933 1.220980 2.240174 1.984591 0.722422 -0.281150 -0.036312 2.558819 3.029563 4.077961 4.721317 4.291048 3.214067 -2.593058 -3.533849 -4.899800 -5.359598 -4.436712 -3.066256 -0.679454 -1.316976 -0.742121 0.481441 1.119194 0.548080	-0.734736 1.597885 0.707862 -1.369455 -1.208206 -2.265222 -2.018953 -0.727229 0.320492 0.083979 -2.639516 -3.245536 -4.448341 -5.078011 -4.492983 -3.286477 1.315629 1.417478 2.033060 2.572138 2.519825 1.919038 0.044647 0.280211 -0.477539 -1.449126 -1.665962 -0.944608 1.356168 2.274993 1.967990 0.746690 -0.156175 0.147244 2.784192 3.437797 4.571921 5.081167 4.440192 3.313793

C	3.254167	-2.609116	-0.968118	C	-0.035817	3.313721	-3.224269
С	1.798276	-2.541085	-0.527180	С	1.061395	0.681862	-2.508120
H	-2.884466	1.353766	-3.285555	С	2.274356	1.180914	-3.059003
H	-5.013866	2.547253	-2.859413	С	3.147880	0.318714	-3.723773
H	-5.984815	2.658881	-0.543722	С	2.876240	-1.062050	-3.825913
H	-4.795631	1.467235	1.338376	C	1.684166	-1.565978	-3.296457
H	-2.703037	0.228469	0.908826	С	0.762901	-0.697174	-2.683579
H	-0.772476	-2.097265	-2.744544	C	0.728899	2.067567	1.978883
H	0.502085	-2.214332	-4.903425	C	0.350819	2.266049	3.439162
H	1.274467	-0.102998	-6.021963	С	-1.165033	2.486769	3.343250
H	0.745368	2.119744	-4.973468	Č	-1.583349	1.494680	2.261332
H	-0.514027	2.222385	-2.816271	H	-3.744199	-2.357112	-1.471497
H	3.096274	3.242489	1.021574	H	-3.744728	-4.722917	-2.239050
H	5.283513	2.795616	2.094513	H	-1.668866	-6.126991	-2.050349
H	5.810093	0.530835	3.048955	H	0.411340	-5.114539	-1.053671
H	4.044252	-1.265639	2.975688	H	0.396826	-2.754590	-0.245173
H	1.828834	-0.807259	1.934520	H	-2.416401	1.224042	-1.547997
H	-1.246835	2.553298	1.069586	H	-4.399907	2.604373	-0.893187
H	-2.223934	4.391618	-0.298752	H	-5.976349	1.774957	0.886542
H	-0.816828	5.553942	-2.035866	H	-5.540710	-0.436875	1.991138
H	1.540092	4.784472	-2.431314	H	-3.532321	-1.788984	1.356974
H	2.464033	2.848749	-1.164777	H	2.571047	-3.226088	0.900922
H	0.072812	-3.169600	3.224224	Н	4.806213	-3.770838	-0.082952
H	0.078595	-5.616925	2.686970	H	6.161513	-1.976978	-1.204599
H	-0.868172	-6.434012	0.509762	H	5.254385	0.361469	-1.328008
H	-1.865519	-4.786013	-1.103365	Н	3.030039	0.901160	-0.324732
H	-1.883800	-2.331788	-0.541450	H	-0.951795	-1.631932	1.893730
H	-2.809801	-2.264800	3.036323	H	-1.450753	-2.008359	4.317251
Н	-3.853737	-1.255468	5.058734	Н	0.375361	-1.777259	6.034260
H	-3.011263	0.930565	5.969815	H	2.699909	-1.186644	5.281041
H	-1.080659	2.072996	4.830448	H	3.182231	-0.787230	2.868274
Н		1.044618	2.829862	Н	-0.972531	3.052113	0.052615
	-0.010695						
H	1.902348	0.140870	-2.305238	H	-1.754521	5.375511	-0.393746
H	2.998971	0.210350	-0.860146	H	-1.447156	6.401079	-2.672943
H				Н		5.034266	
	2.849484	-1.982570	-3.027912		-0.367973		-4.488180
H	4.321057	-1.220891	-2.332526	H	0.409558	2.725694	-4.038859
H	3.542932	-3.628649	-1.288729	H	2.528328	2.242980	-2.931303
H				Н			
	3.920039	-2.299700	-0.136075		4.082772	0.720934	-4.144684
H	1.631203	-2.792904	0.536612	H	3.593196	-1.731468	-4.322863
H	1.130907	-3.175327	-1.146792	H	1.435669	-2.634650	-3.381143
**	1.100307	0.170027	1.110,32				
				Н	-0.236081	-1.066847	-2.398898
Conform	mation 18.			H	1.626703	1.441310	1.822938
Multipl	licity: 3			H	0.846250	3.029092	1.431509
Charge:				H	0.580942	1.348305	4.018662
E(B9/-3	3c) = -2729.96243	1448459 Hartree		H	0.889726	3.117052	3.898811
			rtree				
E (M06/d	def2-TZVP) = -272	9.933890158355 Hai		H	-1.693869	2.296924	4.297112
E (M06/d E (PBE -	def2-TZVP) = -272 - D3(BJ)/def2-TZV	9.933890158355 Hai P) = -2728.9749760	017402 Hartree	H H	-1.693869 -1.388491	2.296924 3.527505	4.297112 3.028854
E (M06/d E (PBE -	def2-TZVP) = -272 - D3(BJ)/def2-TZV	9.933890158355 Hai	017402 Hartree	H	-1.693869	2.296924	4.297112
E(M06/c E(PBE - E(PBE0	def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZ	9.933890158355 Hai P) = -2728.9749760 VP) = -2729.121676	017402 Hartree	H H H	-1.693869 -1.388491 -2.430815	2.296924 3.527505 1.833289	4.297112 3.028854 1.636528
E (M06/d E (PBE - E (PBE0 E (PBEh-	def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' -3c) = -2726.1097	9.933890158355 Hai P) = -2728.9749760 VP) = -2729.121676 35138993 Hartree	017402 Hartree	H H	-1.693869 -1.388491	2.296924 3.527505	4.297112 3.028854
E (M06/d E (PBE - E (PBE0 E (PBEh-	def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZ	9.933890158355 Hai P) = -2728.9749760 VP) = -2729.121676 35138993 Hartree	017402 Hartree	H H H	-1.693869 -1.388491 -2.430815	2.296924 3.527505 1.833289	4.297112 3.028854 1.636528
E (M06/c E (PBE - E (PBE0 E (PBEh- E (PM6)	def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' -3c) = -2726.1097 = 95.03061 Kcal/s	9.933890158355 Haj P) = -2728.974976( VP) = -2729.121676 35138993 Hartree mol	017402 Hartree	H H H	-1.693869 -1.388491 -2.430815 -1.813203	2.296924 3.527505 1.833289	4.297112 3.028854 1.636528
E (M06/c E (PBE - E (PBE0 E (PBEh- E (PM6) E (PM7)	def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' -3c) = -2726.1097 = 95.03061 Kcal/s = 106.83274 Kcal	9.933890158355 Happ = -2728.974976( VP) = -2729.121676 35138993 Hartree mol /mol	017402 Hartree 6073942 Hartree	H H H H	-1.693869 -1.388491 -2.430815 -1.813203 mation 23.	2.296924 3.527505 1.833289	4.297112 3.028854 1.636528
E (M06/d E (PBE - E (PBE0 E (PBEh- E (PM6) E (PM7) E (ωB97X	def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' - D3(BJ)/def2-TZ' -3c) = -2726.1097 = 95.03061 Kcal/i = 106.83274 Kcal K-V/def2-TZVP) =	9.933890158355 Haj P) = -2728.974976( VP) = -2729.12167( 35138993 Hartree mol /mol -2730.722727107324	017402 Hartree 6073942 Hartree	H H H H Confor	-1.693869 -1.388491 -2.430815 -1.813203 mation 23. licity: 3	2.296924 3.527505 1.833289	4.297112 3.028854 1.636528
E (M06/d E (PBE - E (PBE0 E (PBEh- E (PM6) E (PM7) E (ωB97X	def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' -3c) = -2726.1097 = 95.03061 Kcal/s = 106.83274 Kcal	9.933890158355 Haj P) = -2728.974976( VP) = -2729.12167( 35138993 Hartree mol /mol -2730.722727107324	017402 Hartree 6073942 Hartree	H H H H	-1.693869 -1.388491 -2.430815 -1.813203 mation 23. licity: 3	2.296924 3.527505 1.833289	4.297112 3.028854 1.636528
E (M06/d E (PBE - E (PBE0 E (PBEh- E (PM6) E (PM7) E (ωB97X E (GFN1-	def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' -3c) = -2726.1097 = 95.03061 Kcal/; = 106.83274 Kcal X-V/def2-TZVP) = -xTB) = -120.6180	9.933890158355 Hai P) = -2728.9749760 VP) = -2729.121670 35138993 Hartree mol /mol -2730.722727107324 89184468 Hartree	017402 Hartree 6073942 Hartree	H H H Confor Multip Charge	-1.693869 -1.388491 -2.430815 -1.813203 mation 23. licity: 3	2.296924 3.527505 1.833289 0.494422	4.297112 3.028854 1.636528
E (M06/σ E (PBE - E (PBE0 E (PBEh- E (PM6) E (PM7) E (ωB97X E (GFN1- E (GFN2-	def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV -3c) = -2726.1097 = 95.03061 Kcal/ = 106.83274 Kcal K-V/def2-TZVP) = -xTB) = -120.6180 -xTB) = -119.8078	9.933890158355 Hap P) = -2728.974976( VP) = -2729.121676 35138993 Hartree mol /mol -2730.722727107326 89184468 Hartree 17577605 Hartree	017402 Hartree 6073942 Hartree	H H H Confor Multip Charge E(B97-	-1.693869 -1.388491 -2.430815 -1.813203 mation 23. licity: 3: 0 3c) = -2729.963443	2.296924 3.527505 1.833289 0.494422	4.297112 3.028854 1.636528 2.675862
E (M06/σ E (PBE - E (PBE0 E (PBEh- E (PM6) E (PM7) E (ωB97X E (GFN1- E (GFN2-	def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' -3c) = -2726.1097 = 95.03061 Kcal/; = 106.83274 Kcal X-V/def2-TZVP) = -xTB) = -120.6180	9.933890158355 Hap P) = -2728.974976( VP) = -2729.121676 35138993 Hartree mol /mol -2730.722727107326 89184468 Hartree 17577605 Hartree	017402 Hartree 6073942 Hartree	H H H Confor Multip Charge E(B97- E(M06/	-1.693869 -1.388491 -2.430815 -1.813203 mation 23. licity: 3: 0 3c) = -2729.963443 def2-TZVP) = -2729	2.296924 3.527505 1.833289 0.494422	4.297112 3.028854 1.636528 2.675862
E (M06/σ E (PBE - E (PBE0 E (PBEh- E (PM6) E (PM7) E (ωB97X E (GFN1- E (GFN2-	def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV -3c) = -2726.1097 = 95.03061 Kcal/ = 106.83274 Kcal K-V/def2-TZVP) = -xTB) = -120.6180 -xTB) = -119.8078	9.933890158355 Hap P) = -2728.974976( VP) = -2729.121676 35138993 Hartree mol /mol -2730.722727107326 89184468 Hartree 17577605 Hartree	017402 Hartree 6073942 Hartree	H H H Confor Multip Charge E(B97- E(M06/	-1.693869 -1.388491 -2.430815 -1.813203 mation 23. licity: 3: 0 3c) = -2729.963443 def2-TZVP) = -2729	2.296924 3.527505 1.833289 0.494422	4.297112 3.028854 1.636528 2.675862
E (M06/d E (PBE - E (PBE0 E (PBEh- E (PM6) E (PM7) E (GFN1- E (GFN2- E (GFN-F	def2-TZVP) = -272 - D3 (BJ)/def2-TZV - D3 (BJ)/def2-TZV - D3 (BJ)/def2-TZ' - 3c) = -2726.1097 = 95.03061 Kcal/i = 106.83274 Kcal K-V/def2-TZVP) = -xTB) = -120.6180 -xTB) = -119.8078 FF) = -16.9714983	9.933890158355 Hap P) = -2728.974976( VP) = -2729.121676 35138993 Hartree mol /mol -2730.722727107326 89184468 Hartree 17577605 Hartree	017402 Hartree 6073942 Hartree	H H H Confor Multip Charge E(B97- E(M06/ E(PBE	-1.693869 -1.388491 -2.430815 -1.813203 mation 23. licity: 3 : 0 3c) = -2729.963443 def2-TZVP) = -2729 - D3(BJ)/def2-TZVF	2.296924 3.527505 1.833289 0.494422 8487621 Hartree 9.934780274221 Ha	4.297112 3.028854 1.636528 2.675862
E (M06/6 E (PBE - E (PBE0 - E (PBE) - E (PM6) E (PM7) E (GFN1 - E (GFN2 - E (GFN - F	def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' - D3(BJ)/def2-TZ' -3c) = -2726.1097 = 95.03061 Kcal/i = 106.83274 Kcal K-V/def2-TZVP) = -xTB) = -120.6180 -xTB) = -119.8078 FF) = -16.9714983	9.933890158355 Happer	017402 Hartree 6073942 Hartree 4 Hartree	H H H Confor Multip Charge E(B97- E(M06/ E(PBE E(PBE0	-1.693869 -1.388491 -2.430815 -1.813203 mation 23. licity: 3 : 0 3c) = -2729.963443 def2-TZVP) = -2729 - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP	2.296924 3.527505 1.833289 0.494422 8487621 Hartree 9.934780274221 Ha 2) = -2728.975572 PP) = -2729.12214	4.297112 3.028854 1.636528 2.675862
E (M06/6 E (PBE - E (PBE) - E (PBE) - E (PM6) E (PM7) E (GFN1 - E (GFN2 - E (GFN - F	def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV -3c) = -2726.1097 = 95.03061 Kcal/s = 106.83274 Kcal/s K-V/def2-TZVP) = -xTB) = -120.6180 -xTB) = -119.8078 FF) = -16.9714983 hates: -0.012522	9.933890158355 Hap 9. = -2728.974976( VP) = -2729.121676 35138993 Hartree mol /mol -2730.722727107324 89184468 Hartree 17577605 Hartree 64356 Hartree	017402 Hartree 5073942 Hartree 4 Hartree -0.244565	H H H Confor Multip Charge E(B97- E(M06/ E(PBE E(PBE0)	-1.693869 -1.388491 -2.430815 -1.813203 mation 23. licity: 3 : 0 3c) = -2729.963443 def2-TZVP) = -2729 - D3 (BJ)/def2-TZV - D3 (BJ)/def2-TZV - 2726.11275	2.296924 3.527505 1.833289 0.494422 8487621 Hartree 8.934780274221 Ha 9) = -2728.975572 17P) = -2729.12214 64512889 Hartree	4.297112 3.028854 1.636528 2.675862
E (M06/6 E (PBE - E (PBE0 - E (PBE) - E (PM6) E (PM7) E (GFN1 - E (GFN2 - E (GFN - F	def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' - D3(BJ)/def2-TZ' - D3(BJ)/def2-TZ' - 3c) = -2726.1097 = 95.03061 Kcal/: = 106.83274 Kcal K-V/def2-TZVP) = -xTB) = -120.6180 -xTB) = -119.8078 FF) = -16.9714983	9.933890158355 Happer	017402 Hartree 6073942 Hartree 4 Hartree	H H H Confor Multip Charge E(B97- E(M06/ E(PBE E(PBE0)	-1.693869 -1.388491 -2.430815 -1.813203 mation 23. licity: 3 : 0 3c) = -2729.963443 def2-TZVP) = -2729 - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP	2.296924 3.527505 1.833289 0.494422 8487621 Hartree 8.934780274221 Ha 9) = -2728.975572 17P) = -2729.12214 64512889 Hartree	4.297112 3.028854 1.636528 2.675862
E (M06/6 E (PBE - E (PBE0 - E (PBE0 - E (PM7)) E (GB97X) E (GFN1- E (GFN2- E (GFN-F	def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV -3c) = -2726.1097 = 95.03061 Kcal/s = 106.83274 Kcal K-V/def2-TZVP) = -xTB) = -120.6180 -xTB) = -119.8078 FF) = -16.9714983 mates: -0.012522 -0.407392	9.933890158355 Hap P) = -2728.974976( VP) = -2729.121676 35138993 Hartree mol /mol -2730.722727107324 89184468 Hartree 64356 Hartree 64356 Hartree  0.061355 1.356650	017402 Hartree 6073942 Hartree 4 Hartree -0.244565 1.400977	H H H Confor Multip Charge E(B97- E(M06/ E(PBE0 E(PBE0 E(PBEh) E(PM6)	-1.693869 -1.388491 -2.430815 -1.813203 mation 23. licity: 3: 0 3c) = -2729.963443 def2-TZVP) = -2729 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - 20: 0 -2726.11275 = 100.67900 Kcal/	2.296924 3.527505 1.833289 0.494422 8487621 Hartree 9.934780274221 Ha P) = -2728.975572 PP) = -2729.12214 4512889 Hartree (mol	4.297112 3.028854 1.636528 2.675862
E (M06/c) E (PBE - E (PBE0 - E (PBE0 - E (PM7) E (GB97X E (GFN1- E (GFN1- E (GFN2- E (GFN-F	def2-TZVP) = -272 - D3 (BJ)/def2-TZV - D3 (BJ)/def2-TZV - D3 (BJ)/def2-TZV - D3 (BJ)/def2-TZ' - 20 (BJ)/def2-TZ' = 95.03061 Kcal/i = 106.83274 Kcal K-V/def2-TZVP) = -xTB) = -120.6180 -xTB) = -120.6180 -xTB) = -16.9714983  mates: -0.012522 -0.407392 0.213265	9.933890158355 Hap P) = -2728.974976( VP) = -2729.121676 35138993 Hartree mol /mol -2730.722727107326 89184468 Hartree 17577605 Hartree 64356 Hartree  0.061355 1.356650 1.416040	017402 Hartree 6073942 Hartree 4 Hartree -0.244565 1.400977 -1.662973	H H H Confor Multip Charge E(B97- E(M06/ E(PBE E(PBE0 E(PBE0) E(PBEN6) E(PM6) E(PM7)	-1.693869 -1.388491 -2.430815 -1.813203 mation 23. licity: 3: 0 3c) = -2729.963443 def2-TZVP) = -2729 - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF	2.296924 3.527505 1.833289 0.494422 8487621 Hartree 9.934780274221 Ha 9) = -2728.975572 PP) = -2729.12214 64512889 Hartree mol	4.297112 3.028854 1.636528 2.675862 artree 2919945 Hartree 13913105 Hartree
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E (M06/c) E (PBE - E (PBE0 - E (PBE0 - E (PM7)) E (GB97X) E (GFN1- E (GFN2- E (GFN-F V O N N N C C	def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' - D3(BJ)/def2-TZ' = 95.03061 Kcal/i = 106.83274 Kcal K-V/def2-TZVP) = -120.6180 -xTB) = -120.6180 -xTB) = -119.8078 FF) = -16.9714983  nates: -0.012522 -0.407392 0.213265 1.364834 -1.623500 -1.669136 -2.835022	9.933890158355 Hap P) = -2728.974976( VP) = -2729.121676 35138993 Hartree mol /mol -2730.722727107324 89184468 Hartree 17577605 Hartree 64356 Hartree  0.061355 1.356650 1.416040 -0.828554 -1.037301 -2.384907 -2.966303	017402 Hartree 6073942 Hartree 4 Hartree -0.244565 1.400977 -1.662973 0.863039 -0.406396 -0.802962 -1.366297	H H H H Confor Multip Charge E (B97- E (M06/ E (PBE E (PBE0 E (PBE0) E (PM6) E (PM7) E (WB97 E (GFN1) E (GFN2)	-1.693869 -1.388491 -2.430815 -1.813203 mation 23. licity: 3: 0 3c) = -2729.963443 def2-TZVP) = -2729 - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - 100.67900 Kcal/ = 104.96765 Kcal/ X-V/def2-TZVP) = - -xTB) = -120.61823 -xTB) = -119.80856 FF) = -16.86255000	2.296924 3.527505 1.833289 0.494422 8487621 Hartree 9.934780274221 Ha P) = -2728.975572 P) = -2729.12214 4512889 Hartree (mol (mol (mol 22730.72379972323 93351420 Hartree 64111014 Hartree	4.297112 3.028854 1.636528 2.675862 artree 2919945 Hartree 13913105 Hartree
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E (M06/6 E (PBE - E (PBE0 - E (PBE0 - E (PM7)) E (GB97X) E (GFN1- E (GFN1- E (GFN-F V O N N N C C C C C C C C C C	def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV = 95.03061 Kcal/i = 106.83274 Kcal K-V/def2-TZVP) = -120.6180 -xTB) = -120.6180 -xTB) = -119.8078 FF) = -16.9714983  nates: -0.012522 -0.407392 0.213265 1.364834 -1.623500 -1.669136 -2.835022 -2.827977 -1.667787 -0.507995 -0.505583 -2.824074 -3.098383 -4.217799 -5.096638 -4.851721	9.933890158355 Hai P) = -2728.974976( VP) = -2729.121676 35138993 Hartree mol /mol -2730.722727107324 89184468 Hartree 64356 Hartree 64356 Hartree 0.061355 1.356650 1.416040 -0.828554 -1.037301 -2.384907 -2.966303 -4.297216 -5.083538 -4.515704 -3.190877 -0.352444 0.877821 1.641904 1.179085 -0.062913	017402 Hartree 6073942 Hartree 6073942 Hartree 4 Hartree -0.244565 1.400977 -1.662973 0.863039 -0.406396 -0.802962 -1.366297 -1.801845 -1.701976 -1.148633 -0.697226 -0.116279 -0.758260 -0.390921 0.600522 1.217813	H H H H H Confor Multip Charge E (B87- E (M06/ E (PBE E (PBE0 E (PBE0) E (PBE0) E (PBC) E (PFN- E (GFN1) C (GFN1 V O N N N C C	-1.693869 -1.388491 -2.430815 -1.813203  mation 23. licity: 3: 0 3c) = -2729.963443 def2-TZVP) = -2729 - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP - 100.67900 Kcal/ = 104.96765 Kcal/ X-V/def2-TZVP) =xTB) = -120.61823 -xTB) = -119.80856 FF) = -16.86255000  nates:  0.084955 -0.494056 -0.212990 -1.209830 1.957445 2.973182 4.088901	2.296924 3.527505 1.833289 0.494422  8487621 Hartree 9.934780274221 Ha 9) = -2728.975572  PP) = -2729.12214 24512889 Hartree mol (mol -2730.72379972323 93351420 Hartree 44130 Hartree 44130 Hartree 44130 Hartree 04130 Hartree 04130 Hartree 04130 Hartree 04130 Hartree	4.297112 3.028854 1.636528 2.675862 artree 2919945 Hartree 3913105 Hartree 31 Hartree 0.119729 -1.845312 0.712793 0.404704 -0.176730 0.782314 0.845570
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E (M06/6 E (PBE - E (PBE0 - E (PBE0 - E (PBE0 - E (PM6)) E (PM7)) E (GFN1- E (GFN1- E (GFN2- E (GFN-F - E (	def2-TZVP) = -272 - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV = 95.03061 Kcal/i = 106.83274 Kcal K-V/def2-TZVP) = -120.6180 - TSB) = -119.8078 FF) = -16.9714983  hates: -0.012522 -0.407392 0.213265 1.364834 -1.623500 -1.669136 -2.835022 -2.827977 -1.667787 -0.507995 -0.505583 -2.824074 -3.098383 -4.217799 -5.096638 -4.851721 -3.730403 2.642836 3.166157 4.418680 5.177893 4.670534 3.420393 1.134881 -0.163580 -0.432389 0.586489 1.886662 2.163361 -0.171142 -0.812658 -1.261351 -1.095860	9.933890158355 Haip P) = -2728.974976( WP) = -2729.121676 35138993 Hartree mol /mol -2730.722727107324 89184468 Hartree 64356 Hartree 64356 Hartree 64356 Hartree 64356 Hartree 17577605 Hartree 64356 Hartree 64356 Hartree 64356 Hartree 64356 Hartree 1.037301 -2.384907 -2.966303 -4.297216 -5.083538 -4.515704 -3.190877 -0.352444 0.877821 1.641904 1.179085 -0.062913 -0.823517 -1.128260 -2.444045 -2.741872 -1.739351 -0.434197 -0.126892 -1.142984 -1.508837 -1.723584 -1.601848 -1.275226 -1.050411 2.731517 3.506092 4.804858 5.379164	017402 Hartree 6073942 Hartree 6073942 Hartree 4 Hartree 4 Hartree 6 1.400977 -1.662973 0.863039 -0.406396 -0.802962 -1.366297 -1.801845 -1.701976 -1.148633 -0.697226 -0.116279 -0.758260 -0.390921 0.600522 1.217813 0.867065 0.335604 0.405325 -0.142373 -0.772550 -0.840897 -0.284213 2.213257 2.651179 4.008815 4.968947 4.543616 3.189091 -1.934673 -0.931893 -1.196542 -2.467766	H H H H H H H Confor Multip Charge E(B87- E(M06/E(PBE E(PM6)) E(PM7)) E(GFN- E(GFN- Coordi V O N N C C C C C C C C C C C C C C C C C	-1.693869 -1.388491 -2.430815 -1.813203  mation 23. licity: 3: 0 3c) = -2729.963443 def2-TZVP) = -2729 - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP - S100.67900 Kcal/ = 104.96765 Kcal/ X-V/def2-TZVP) = -7278 -100.67900 Kcal/ = 104.96765 Kcal/ X-V/def2-TZVP) = -7278 -104.96765 Kcal/ X-V/def2-TZVP) = -7278 -109.61823 -XTB) = -119.80856 -0.212990 -1.209830 -1.209830 -1.957445 -2.973182 -4.088901 -5.042992 -4.914764 -3.813927 -2.860340 -2.230693 -3.296076 -3.469285 -2.591579 -1.549361 -1.377339 -2.176233 -2.238668 -3.177079 -4.077365 -4.002187 -3.069121 -1.102284	2.296924 3.527505 1.833289 0.494422  8487621 Hartree 9.934780274221 Ha 9) = -2728.975572 PP) = -2729.12214 4512889 Hartree (mol (mol -2730.72379972323 93351420 Hartree 94111014 Hartree 14130 Hartree 14130 Hartree 14130 Hartree 14130 Hartree 159351420 Hartree 1615769 1.490840 1.357149 0.3615769 1.490840 1.357149 0.361176 0.510216 0.393752 1.427439 1.027555 1.625654 2.634420 3.054497 -2.469245 -2.416664 2.354566 3.106823 -3.955605 -4.052584 -3.304150 -1.594729	4.297112 3.028854 1.636528 2.675862  Artree 2919945 Hartree 13913105 Hartree 1391312 0.712793 0.4404704 0.176730 0.782314 0.845570 1.862147 2.845189 2.790310 1.772476 1.390253 -2.236432 -3.489903 -3.931393 -3.090669 -1.826262 -0.269194 -1.688628 -2.403526 -1.737820 -0.388661 0.389699 1.806553
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C C							
	-1.941761	-1.022031	4.028631	С	0.173035	3.016855	3.118845
C							
	-0.634098	-1.074814	4.558687	C	1.556377	-1.385810	-2.020705
C	0.434310	-1.406426	3.722310	С	1.348240	-2.718926	-1.596645
C	0.203188	-1.699037	2.363626	C	2.360658	-3.678780	-1.737752
C	0.212629	2.717870	-0.028845	C	3.589896	-3.335779	-2.322893
С	1.368096	2.610669	-0.850218	C	3.797799	-2.018469	-2.769323
C	1.771986	3.669969	-1.669927	C	2.795178	-1.051679	-2.621987
С	1.060604	4.883361	-1.679620	C	0.141117	0.355507	-2.905473
				C			
C	-0.056091	5.018778	-0.838156		-0.215737	1.719218	-2.754114
C	-0.478299	3.960524	-0.022182	С	-0.756111	2.446940	-3.823166
С	-1.072308	1.854622	1.821399	С	-0.934440	1.846844	-5.080355
C	-2.475899	1.765263	1.686486	C	-0.548268	0.504998	-5.254092
C	-3.319379	2.038867	2.772829	C	-0.016941	-0.232838	-4.190025
C	-2.775106	2.396418	4.015983	С	-0.965838	-2.633046	1.377718
С	-1.380720	2.476205	4.164357	С	-0.522121	-3.957198	1.628114
C	-0.536267	2.213647	3.076835	С	-1.441197	-5.005844	1.752099
С	-1.795195	0.976095	-1.977732	С	-2.821464	-4.769343	1.631310
C	-1.966054	1.196470	-3.474684	C	-3.271978	-3.460033	1.396314
С	-0.521212	1.466613	-3.915787	С	-2.360094	-2.402708	1.277673
C	0.264919	0.458108	-3.088448	C	1.116280	-1.551720	2.023536
H	4.191293	-2.288074	0.095230	С	1.015346	-1.593386	3.436524
H	5.896363	-2.052622	1.892023	С	2.152336	-1.415890	4.230381
H	5.666908	-0.263575	3.642029	C	3.410194	-1.186700	3.640904
H	3.700099	1.303359	3.545937	С	3.522270	-1.160867	2.244039
H	2.004872	1.084439	1.721490	C	2.389786	-1.359532	1.437351
H	3.973032	-0.227978	-1.899131	С	-2.674904	1.569488	-0.253054
H	4.294785	-1.293881	-4.138846	C	-4.046258	1.413050	-0.897104
H	2.730595	-3.096279	-4.920308	С	-3.733934	0.538995	-2.121016
H	0.864110	-3.854705	-3.410289	С	-2.711950	-0.446529	-1.568330
H	0.578805	-2.813816	-1.152256	H	2.717130	1.012249	0.080937
H	-1.511149	-1.724736	-2.216301	H	4.005515	2.462231	-1.496734
H	-3.196564	-3.035179	-3.502596	H	3.198917	4.785326	-2.019466
H	-4.815358	-4.544700	-2.301742	H	1.084069	5.625028	-0.957638
H	-4.680161	-4.731599	0.201938	H	-0.239480	4.147004	0.556666
H	-3.014773	-3.416951	1.481333	H	-1.546080	0.150260	2.362620
Н	-3.192356		2.263158	Н	-2.622283	0.687672	4.533122
		-1.155048					
H	-2.784226	-0.753391	4.683511	H	-1.903480	2.715366	5.845286
H	-0.462410	-0.857988	5.623317	Н	-0.072975	4.174848	4.925001
H	1.460665	-1.468852	4.113801	H	0.984640	3.656851	2.745356
H	1.020503	-2.077626	1.732922	H	0.384809	-2.986332	-1.138591
H	1.952422	1.678613	-0.812456	H	2.180656	-4.707851	-1.390615
H	2.672447	3.553329	-2.293627	H	4.382812	-4.090503	-2.433314
Н	1.386360	5.718809	-2.316726	Н	4.758712	-1.738821	-3.228731
H	-0.614830	5.967701	-0.815953	H	2.957246	-0.015177	-2.954320
H	-1.356823	4.084489	0.627132	H	-0.021283	2.220925	-1.796104
H	-2.898028	1.482182	0.711417	H	-1.013098	3.507379	-3.673005
H	-4.410841	1.968819	2.646723	Н	-1.349452	2.421305	-5.921753
H	-3.436014						
	-3.436014	2.609723	4.869694	H	-0.669818	0.021831	-6.236315
Н	-0.944867	2.746635	5.138412	H	0.271022	-1.285116	-4.332227
H	-0.944867				0.271022		
H H	-0.944867 0.555961	2.282227	3.185502	H	0.271022 0.558045	-4.145399	1.717320
H	-0.944867				0.271022		
Н Н Н	-0.944867 0.555961 -2.550425	2.282227 0.301154	3.185502 -1.527515	H H	0.271022 0.558045 -1.073044	-4.145399 -6.026319	1.717320 1.940928
Н Н Н Н	-0.944867 0.555961 -2.550425 -1.763247	2.282227 0.301154 1.935843	3.185502 -1.527515 -1.421167	Н Н Н	0.271022 0.558045 -1.073044 -3.539468	-4.145399 -6.026319 -5.596940	1.717320 1.940928 1.729177
Н Н Н Н	-0.944867 0.555961 -2.550425 -1.763247 -2.364076	2.282227 0.301154 1.935843 0.281117	3.185502 -1.527515 -1.421167 -3.960574	Н Н Н Н	0.271022 0.558045 -1.073044 -3.539468 -4.351323	-4.145399 -6.026319 -5.596940 -3.253861	1.717320 1.940928 1.729177 1.322636
Н Н Н Н	-0.944867 0.555961 -2.550425 -1.763247 -2.364076	2.282227 0.301154 1.935843 0.281117	3.185502 -1.527515 -1.421167 -3.960574	Н Н Н	0.271022 0.558045 -1.073044 -3.539468 -4.351323	-4.145399 -6.026319 -5.596940	1.717320 1.940928 1.729177 1.322636
н н н н н	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965	2.282227 0.301154 1.935843 0.281117 2.033219	3.185502 -1.527515 -1.421167 -3.960574 -3.693384	Н Н Н Н	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775	1.717320 1.940928 1.729177 1.322636 1.128717
н н н н н н	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126	Н Н Н Н Н	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792
н н н н н	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965	2.282227 0.301154 1.935843 0.281117 2.033219	3.185502 -1.527515 -1.421167 -3.960574 -3.693384	Н Н Н Н	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775	1.717320 1.940928 1.729177 1.322636 1.128717
н н н н н н	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454	Н Н Н Н Н Н	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765
н н н н н н н	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424	H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.0554898 4.298295	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615
н н н н н н	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454	Н Н Н Н Н Н	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765
н н н н н н н	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424	H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909
H H H H H H H	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424	H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924
H H H H H H H H H H Conform	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424	H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909
H H H H H H H H H H Conform	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424	H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924
H H H H H H H H H M H H H H H H H H H H	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424	H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.0036154 -1.04282 -1.403078 1.714032 2.384433	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129
H H H H H H H H Conform Multipl Charge:	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424	H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842
H H H H H H H H Conform Multipl Charge:	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424	H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.0036154 -1.04282 -1.403078 1.714032 2.384433	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129
H H H H H H H H Conform Multipl Charge: E(B97-3	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387	H H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341
H H H H H H H H Conform Multipl Charge E (B97-3	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 0 -2729.95964 Mef2-TZVP) = -272	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387	H H H H H H H H H H H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610
H H H H H H H H H Conform Multipl Charge: E (B97-3 E (M06/d E (PBE -	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387	H H H H H H H H H H H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308
H H H H H H H H H Conform Multipl Charge: E (B97-3 E (M06/d E (PBE -	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387	H H H H H H H H H H H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610
H H H H H H H H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE - E(PBE0	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 Mef2-TZVP) = -272 -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387	H H H H H H H H H H H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327
H H H H H H H H H Conform Multipl Charge: E(B97-3) E(M06/d) E(PBE - E(PBEB-	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 D3(BJ)/def2-TZ D3(BJ)/def2-TZ 3c) = -2726.1079	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387	H H H H H H H H H H H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308
H H H H H H H H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE - E(PBE0 - E(PBE0 - E(PM6) -	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 D3 (BJ) /def2-TZV -D3 (BJ) /def2-TZV 3c) = -2726.1079 = 98.70431 Kcal/	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387	H H H H H H H H H H H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327
H H H H H H H H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE - E(PBE0 - E(PBE0 - E(PM6) -	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 D3(BJ)/def2-TZ D3(BJ)/def2-TZ 3c) = -2726.1079	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387	H H H H H H H H H H H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327
H H H H H H H H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE - E(PBE0 E(PBE0- E(PM6)) E(PM6)	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree	H H H H H H H H H H H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327
H H H H H H H H H H H H H H H H H H H	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV = 98.70431 Kcal/ -108.63642 Kcal	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol -2730.71829264371	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree	H H H H H H H H H H H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327
H H H H H H H H H H H H H H H H H H H	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV = 98.70431 Kcal/ -108.63642 Kcal	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree	H H H H H H H H H H H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327
H H H H H H H H H H H H H H H H H H H	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -2722 D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV = 98.70431 Kcal/ = 108.63642 Kcal :V/def2-TZVP) = xTB) = -120.6185	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol -2730.71829264371 26462890 Hartree	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree	H H H H H H H H H H H Confor	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327
H H H H H H H H H H H H H H H H H H H	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 D3(BJ)/def2-TZ D3(BJ)/def2-TZ 3c) = -2726.1079 = 98.70431 Kcal/ = 108.63642 Kcal -V/def2-TZVP) = -100.6185 xTB) = -119.8071	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol -2730.71829264371 26462890 Hartree 59859993 Hartree	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree	H H H H H H H H H H H H H H Confor	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3 : 0 3c) = -2729.95598	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577
H H H H H H H H H H H H H H H H H H H	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -2722 D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV = 98.70431 Kcal/ = 108.63642 Kcal :V/def2-TZVP) = xTB) = -120.6185	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol -2730.71829264371 26462890 Hartree 59859993 Hartree	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree	H H H H H H H H H H H H H H Confor Multip Charge E (B97- E (M06/	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3: 0 3c) = -2729.95598 def2-TZVP) = -272	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577
H H H H H H H H H H H H H H H H H H H	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 D3(BJ)/def2-TZ D3(BJ)/def2-TZ 3c) = -2726.1079 = 98.70431 Kcal/ = 108.63642 Kcal -V/def2-TZVP) = -100.6185 xTB) = -119.8071	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol -2730.71829264371 26462890 Hartree 59859993 Hartree	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree	H H H H H H H H H H H H H H Confor Multip Charge E (B97- E (M06/	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3 : 0 3c) = -2729.95598	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577
H H H H H H H H H H H H H H H H H H H	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(B	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol -2730.71829264371 26462890 Hartree 59859993 Hartree	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree	H H H H H H H H H H H H H Confor Multip Charge E(B97- E(M06/ E(PBE	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3 : 0 3c) = -2729.95598 def2-TZVP) = -272 - D3(BJ)/def2-TZV	-4.145399 -6.026319 -5.596340 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049  3537547 Hartree 9.925799006199 Ha	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577
H H H H H H H H H H Conform Multipl Charge: E(B97-3 E(M06/d- E(PBE0- E(PBE0- E(PM7)): E(GFN1- E(GFN2- E(GFN-F Coordin	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - 108.63642 Kcal -V/def2-TZVP) = xTB) = -120.6185 xTB) = -119.8071 F) = -16.9720826	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol -2730.71829264371 26462890 Hartree 59859993 Hartree 59859993 Hartree	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree	H H H H H H H H H H H H Confor Multip Charge E(B97- E(M06/ E(B98- E(PBE)	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3 : 0 3c) = -2729.95598 def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049  35537547 Hartree 9.925799006199 Ha P) = -2728.967883 VP) = -2729.11372	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577
H H H H H H H H H H H H H H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE - E(PBE) - E(PBE) - E(PBE) - E(PBE) - E(PBE) - E(PBF) - E(GFN1 - E(GFN2 - E(GFN1 - E(GFN2 - E(GFN	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 D3(BJ)/def2-TZVD D3(BJ)/def2-TZVD 98.70431 Kcal/ = 108.63642 Kcal :V/def2-TZVP) = = xTB) = -120.6185 xTB) = -119.8071 F) = -16.9720826 ates: -0.035653	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol /mol 22730.71829264371 26462890 Hartree 59859993 Hartree 59859993 Hartree	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree	H H H H H H H H H H H H H H Confor Multip Charge E(B97- E(M06/ E(PBE E(PBE0) E(PBEh)	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3 : 0 3c) = -2729.95598 def2-TZVP) = -272 - D3 (BJ)/def2-TZ' - D3 (BJ)/def2-TZ' - C3 (BJ)/def2-TZ'	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049  3537547 Hartree 9.925799006199 Hap	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577
H H H H H H H H H H Conform Multipl Charge: E(B97-3 E(M06/d- E(PBE0- E(PBE0- E(PM7)): E(GFN1- E(GFN2- E(GFN-F Coordin	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - 108.63642 Kcal -V/def2-TZVP) = xTB) = -120.6185 xTB) = -119.8071 F) = -16.9720826	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol -2730.71829264371 26462890 Hartree 59859993 Hartree 59859993 Hartree	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree	H H H H H H H H H H H H H H Confor Multip Charge E(B97- E(M06/ E(PBE E(PBE0) E(PBEh)	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3 : 0 3c) = -2729.95598 def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049  3537547 Hartree 9.925799006199 Hap	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577
H H H H H H H H H H H H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE - E(PBE0 E(PM7)) E(MB97X E(GFN1-E(GFN1-E(GFN2-E(GFN2-COording))	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 D3(BJ)/def2-TZV - D3(BJ)/def2-TZV 3c) = -2726.1079 = 98.70431 Kcal/ = 108.63642 Kcal -V/def2-TZVP) = xTB) = -120.6185 xTB) = -119.8071 F) = -16.9720826	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol -2730.71829264371 26462890 Hartree 59859993 Hartree 54530 Hartree -0.059492 0.303335	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree	H H H H H H H H H H H H H H H E (B97- E(M96/ E(PBE E(PBE) E(PBE) E(PBE) E(PBE)	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.6866488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3 : 0 3c) = -2729.95598 def2-TZVP) = -272 - D3 (BJ) / def2-TZV - D3 (BJ) / def2-TZV - D3 (BJ) / def2-TZV - 3c) = -2726.1030 = 101.67079 Kcal	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049  3537547 Hartree 9.925799006199 Ha P) = -2728.967883 VP) = -2729.11372 06289170 Hartree /mol	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577
H H H H H H H H H H H H H Conform Multipl Charge: E(B97-3 E(M06/dc E(PBE0 E(PBE0-E(PM6)): E(PM6): E(PM6): E(GFN1-E(GFN2-E(GFN2-E)) Coordin V O N	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZVP) = 98.70431 Kcal/ 108.63642 Kcal -V/def2-TZVP) = xTB) = -120.6185 xTB) = -120.6185 xTB) = -16.9720826 ates: -0.035653 -1.997416 -0.046809	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol -2730.71829264371 26462890 Hartree 54530 Hartree -0.059492 0.303335 -1.585194	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree	H H H H H H H H H H H H H H Confor Multip Charge E(B97- E(M06/ E(PBE E(PBE0) E(PBE) E(PM7)	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3 : 0 3c) = -2729.95598 def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049  3537547 Hartree 9.925799006199 Ha P) = -2728.967883 VP) = -2729.11372 06289170 Hartree /mol /mol	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577
H H H H H H H H H H H H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE - E(PBE0 E(PM7)) E(MB97X E(GFN1-E(GFN1-E(GFN2-E(GFN2-COording))	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 D3(BJ)/def2-TZV - D3(BJ)/def2-TZV 3c) = -2726.1079 = 98.70431 Kcal/ = 108.63642 Kcal -V/def2-TZVP) = xTB) = -120.6185 xTB) = -119.8071 F) = -16.9720826	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol -2730.71829264371 26462890 Hartree 59859993 Hartree 54530 Hartree -0.059492 0.303335	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree	H H H H H H H H H H H H H H H H Confor Multip Charge E(B97- E(M06/ E(PBE0 E(PBE0) E(PBE0) E(PBE0) E(PBE0) E(PBE0) E(PBE0) E(PBE0)	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3 : 0 3c) = -2729.95598 def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049  3537547 Hartree 9.925799006199 Ha P) = -2728.967883 VP) = -2729.11372 06289170 Hartree /mo1 /mo1 -2730.71475671811	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577
H H H H H H H H H H H H Conform Multipl Charge: E(B97-3 E(M06/d6 E(PBE0-E(PM6)): E(PM7) E(GFN1-E(GFN1-E(GFN2-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN1-E(GFN	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZVP) = 98.70431 Kcal/ =108.63642 Kcal -V/def2-TZVP) = 1.20.6185 xTB) = -120.6185 xTB) = -16.9720826 Mates: -0.035653 -1.997416 -0.046809 0.570884	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol -2730.71829264371 26462890 Hartree 59859993 Hartree 59859993 Hartree 54530 Hartree -0.059492 0.303335 -1.585194 -0.393892	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree 1 Hartree 0.043668 -0.529781 1.215163 -1.801395	H H H H H H H H H H H H H H H H Confor Multip Charge E(B97- E(M06/ E(PBE0 E(PBE0) E(PBE0) E(PBE0) E(PBE0) E(PBE0) E(PBE0) E(PBE0)	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3 : 0 3c) = -2729.95598 def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049  3537547 Hartree 9.925799006199 Ha P) = -2728.967883 VP) = -2729.11372 06289170 Hartree /mo1 /mo1 -2730.71475671811	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577
H H H H H H H H H H H H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE - E(PBE) - E(GFN1 - E(GFN2 - E(GFN-F Coordin V O N N N	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 IC) = -2729.95964 Mef2-TZVP) = -272 D3(BJ)/def2-TZVD D3(BJ)/def2-TZVD = 98.70431 Kcal/ = 108.63642 Kcal -V/def2-TZVP) = 108.63642 Kcal -V/def2-TZVP) = 108.63642 Kcal -109.63653 -1.997416 -0.046809 0.570884 0.343647	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol -2730.71829264371 26462890 Hartree 59859993 Hartree 59859993 Hartree 54530 Hartree -0.059492 0.303335 -1.585194 -0.393892 1.550030	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree 1 Hartree 0.043668 -0.529781 1.215163 -1.801395 1.131214	H H H H H H H H H H H H H H H H H E H H H H H H H H H H H H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.6866488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3 : 0 3c) = -2729.95598 def2-TZVP) = -272 - D3 (BJ) / def2-TZV - D3 (BJ) / def2-TZV - D3 (BJ) / def2-TZV - 3c) = -2726.1030 = 101.67079 Kcal = 106.53882 Kcal X-V/ def2-TZVP) = -xTB) = -120.6174	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049  3537547 Hartree 9.925799006199 Ha P) = -2728.967883 VP) = -2729.11372 06289170 Hartree /mo1 /mo1 /mo1 /mo1 -2730.71475671811	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577
H H H H H H H H H H H H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE - E(PBE) - E(PBE) - E(PM7) E(GFN1- E(GFN2- E(GFN2- E(GFN-F Coordin V O N N N C	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 D3(BJ)/def2-TZV D3(BJ)/def2-TZV3 = 98.70431 Kcal/ = 108.63642 Kcal -V/def2-TZVP) = -104.6185 xTB) = -119.8071 F) = -16.9720826 ates: -0.035653 -1.997416 -0.046809 0.570884 0.343647 1.135881	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol -2730.71829264371 26462890 Hartree 5985993 Hartree 5985993 Hartree 54530 Hartree -0.059492 0.303335 -1.585194 -0.393892 1.550030 2.463102	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree 1 Hartree 0.043668 -0.529781 1.215163 -1.801395 1.131214 0.405458	H H H H H H H H H H H H H H H H E H H H H H H H H H H H H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.6866488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3 : 0 3c) = -2729.95598 def2-TZVP) = -272 - D3 (BJ)/def2-TZV - D3 (BJ)/def2-TZV-3c) = -2726.1030 = 101.67079 Kcal = 106.53882 Kcal X-V/def2-TZVP) = -xTB) = -120.6174 -xTB) = -119.8076	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049  3537547 Hartree 9.925799006199 Ha P) = -2729.11372 06289170 Hartree /mol /mol /mol /mol /mol -2730.71475671811 52474203 Hartree 81266316 Hartree	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577
H H H H H H H H H H H H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE - E(PBE) - E(GFN1 - E(GFN2 - E(GFN-F Coordin V O N N N	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 IC) = -2729.95964 Mef2-TZVP) = -272 D3(BJ)/def2-TZVD D3(BJ)/def2-TZVD = 98.70431 Kcal/ = 108.63642 Kcal -V/def2-TZVP) = 108.63642 Kcal -V/def2-TZVP) = 108.63642 Kcal -109.63653 -1.997416 -0.046809 0.570884 0.343647	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol -2730.71829264371 26462890 Hartree 59859993 Hartree 59859993 Hartree 54530 Hartree -0.059492 0.303335 -1.585194 -0.393892 1.550030	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree 1 Hartree 0.043668 -0.529781 1.215163 -1.801395 1.131214	H H H H H H H H H H H H H H H H E H H H H H H H H H H H H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.6866488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3 : 0 3c) = -2729.95598 def2-TZVP) = -272 - D3 (BJ) / def2-TZV - D3 (BJ) / def2-TZV - D3 (BJ) / def2-TZV - 3c) = -2726.1030 = 101.67079 Kcal = 106.53882 Kcal X-V/ def2-TZVP) = -xTB) = -120.6174	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049  3537547 Hartree 9.925799006199 Ha P) = -2729.11372 06289170 Hartree /mol /mol /mol /mol /mol -2730.71475671811 52474203 Hartree 81266316 Hartree	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577
H H H H H H H H H H H H H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE0 E(PBE0-E(PM6)) E(PM6) E(PM6) E(GFN1-E(GFN2-E(GFN2-E) E(GFN2-F Coordin V O N N N C C C	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP) = 98.70431 Kcal/ **2 (C) = -2726.1079 = 98.70431 Kcal/ - 108.63642 Kcal - V/def2-TZVP) = xTB) = -120.6185 xTB) = -120.6185 xTB) = -19.8071 F) = -16.9720826 Ates: -0.035653 -1.997416 -0.046809 0.570884 0.343647 1.135881 2.350306	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol -2730.71829264371 26462890 Hartree 59859993 Hartree 54530 Hartree -0.059492 0.303335 -1.585194 -0.393892 1.550030 2.463102 2.017315	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree 1 Hartree 0.043668 -0.529781 1.215163 -1.801395 1.131214 0.405458 -0.173117	H H H H H H H H H H H H H H H H E H H H H H H H H H H H H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.6866488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3 : 0 3c) = -2729.95598 def2-TZVP) = -272 - D3 (BJ)/def2-TZV - D3 (BJ)/def2-TZV-3c) = -2726.1030 = 101.67079 Kcal = 106.53882 Kcal X-V/def2-TZVP) = -xTB) = -120.6174 -xTB) = -119.8076	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049  3537547 Hartree 9.925799006199 Ha P) = -2729.11372 06289170 Hartree /mol /mol /mol /mol /mol -2730.71475671811 52474203 Hartree 81266316 Hartree	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577
H H H H H H H H H H H H H Conform Multipl Charge: E(B97-3 E(M06/d6 E(PBE0-E(PBE0-E(PBE0-E(PM6))-E(GFN1-E(GFN1-E(GFN2-E(GFN1-E(GFN2-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F)-E(GFN-F	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 Mef2-TZVP) = -272 - D3(BJ)/def2-TZV- - D3(BJ)/def2-TZV	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol -2730.71829264371 26462890 Hartree 59859993 Hartree 59859993 Hartree 54530 Hartree -0.059492 0.303335 -1.585194 -0.393892 1.550030 2.463102 2.017315 2.839584	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree 1 Hartree 0.043668 -0.529781 1.215163 -1.801395 1.131214 0.405458 -0.173117 -1.048388	H H H H H H H H H H H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3 : 0 3c) = -2729.95598 def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/de	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049  3537547 Hartree 9.925799006199 Ha P) = -2729.11372 06289170 Hartree /mol /mol /mol /mol /mol -2730.71475671811 52474203 Hartree 81266316 Hartree	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577
H H H H H H H H H H H H H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE)- E(PBE)- E(PBE)- E(PBE)- E(PBE)- E(PM7) E(GFN1- E(GFN2- E(GFN-F Coordin V O N N N C C C C	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP) = 98.70431 Kcal/ **2 (C) = -2726.1079 = 98.70431 Kcal/ - 108.63642 Kcal - V/def2-TZVP) = xTB) = -120.6185 xTB) = -120.6185 xTB) = -19.8071 F) = -16.9720826 Ates: -0.035653 -1.997416 -0.046809 0.570884 0.343647 1.135881 2.350306	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol -2730.71829264371 26462890 Hartree 59859993 Hartree 54530 Hartree -0.059492 0.303335 -1.585194 -0.393892 1.550030 2.463102 2.017315	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree 1 Hartree 0.043668 -0.529781 1.215163 -1.801395 1.131214 0.405458 -0.173117	H H H H H H H H H H H H H H H H E H H H H H H H H H H H H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3 : 0 3c) = -2729.95598 def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/de	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049  3537547 Hartree 9.925799006199 Ha P) = -2729.11372 06289170 Hartree /mol /mol /mol /mol /mol -2730.71475671811 52474203 Hartree 81266316 Hartree	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577
H H H H H H H H H H H H H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE)- E(PBE)- E(PBE)- E(PBE)- E(PBE)- E(PM7) E(GFN1- E(GFN2- E(GFN-F Coordin V O N N N C C C C	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - 108.63642 Kcal -V/def2-TZVP) = xTB) = -120.6185 xTB) = -119.8071 F) = -16.9720826 Mates: -0.035653 -1.997416 -0.046809 0.570884 0.343647 1.135881 2.350306 3.073518 2.627620	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol -2730.71829264371 26462890 Hartree 59859993 Hartree 59859993 Hartree 54530 Hartree -0.059492 0.303335 -1.585194 -0.393892 1.550030 2.463102 2.017315 2.839584 4.138700	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree 9345907 Hartree 1 Hartree 1 Hartree 0.043668 -0.529781 1.215163 -1.801395 1.131214 0.405458 -0.173117 -1.048388 -1.337260	H H H H H H H H H H H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3 : 0 3c) = -2729.95598 def2-TZVP) = -272 - D3(BJ)/def2-TZ' - D3(BJ)/def2-TZ' - D3(BJ)/def2-TZ' - D3(BJ)/def2-TZ' - 3c) = -2726.1030 = 101.67079 Kcal = 106.53882 Kcal X-V/def2-TZVP) = -xTB) = -120.6174 -xTB) = -120.6174 -xTB) = -119.8076 FF) = -16.8643144	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049  3537547 Hartree 9.925799006199 Ha P) = -2728.967883 VP) = -2729.11372 06289170 Hartree /mo1 /mo1 /mo1 /mo1 /mo1 /mo1 /mo1 /mo1	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577
H H H H H H H H H H H H H H Conform Multipl Conform Charge: E(B97-3 E(M06/d E(PBE - E(PM6)) E(PBE) E(PM7) E(GFN1- E(GFN2- E(GFN1- E(GFN2- E(GFN1- Coordin V O N N N C C C C C C	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 D3(BJ)/def2-TZV D3(BJ)/def2-TZV D3(BJ)/def2-TZV = 98.70431 Kcal/ = 108.63642 Kcal :CV/def2-TZVP) = = xTB) = -120.6185 xTB) = -119.8071 F) = -16.9720826 ates: -0.035653 -1.997416 -0.046809 0.570884 0.343647 1.135881 2.350306 3.073518 2.627620 1.443821	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol 2730.71829264371 26462890 Hartree 59859993 Hartree 59859993 Hartree 54530 Hartree 54530 Hartree -0.059492 0.303335 -1.585194 -0.393892 1.550030 2.463102 2.017315 2.839584 4.138700 4.607312	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree 1 Hartree 1 Hartree 0.043668 -0.529781 1.215163 -1.801395 1.131214 0.405458 -0.173117 -1.048388 -1.337260 -0.739733	H H H H H H H H H H H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3 : 0 3c) = -2729.95598 def2-TZVP) = -272 - D3 (BJ)/def2-TZV - D3 (BJ)/def2-TZV - D3 (BJ)/def2-TZV - D3 (BJ)/def2-TZV - T30 = -2726.1030 = 101.67079 Kcal = 106.5382 Kcal X-V/def2-TZVP) = -xTB) = -120.6174 -xTB) = -119.8076 FF) = -16.8643144 nates: 0.074114	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049  3537547 Hartree 9.925799006199 Ha P) = -2728.967883 WP) = -2729.11372 06289170 Hartree /mo1 /mo1 /mo1 /mo1 /mo1 /mo1 /mo1 /mo1	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577
H H H H H H H H H H H H H H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE0 E(PBE0 E(PBE0) E(PM6)): E(MB97X E(GFN1-: E(GFN2-: E(GFN2-: Coordin V O N N N C C C C C C C	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 -D3(BJ)/def2-TZV -D3(BJ)/def2-TZVP) = 38.70431 Kcal/ = 108.63642 Kcal -V/def2-TZVP) = xTB) = -120.6185 xTB) = -120.6185 xTB) = -19.8071 F) = -16.9720826 Mates: -0.035653 -1.997416 -0.046809 0.570884 0.343647 1.135881 2.350306 3.073518 2.627620 1.443821 0.700475	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol -2730.71829264371 26462890 Hartree 59859993 Hartree 54530 Hartree -0.059492 0.303335 -1.585194 -0.393892 1.550030 2.463102 2.017315 2.839584 4.138700 4.607312 3.783924	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree 1 Hartree 1 Hartree 1 .215163 -1.801395 1.131214 0.405458 -0.173117 -1.048388 -1.337260 -0.739733 0.114948	H H H H H H H H H H H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3: 0.054129 -D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZVP) = -272 -D3(BJ)/def2-TZVP) = -2726.1030 =101.67079 Kcal =106.53882 Kcal X-V/def2-TZVP) = -120.6174 -XTB) = -120.6174 -XTB) = -120.6174 -XTB) = -120.6174 -XTB) = -120.6174 -XTB) = -120.6174 -XTB) = -120.6174	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049  3537547 Hartree 9.925799006199 Ha P) = -2728.967883 VP) = -2729.11372 06289170 Hartree /mol /mol /mol -2730.71475671811 52474203 Hartree 81266316 Hartree 00124 Hartree 00124 Hartree	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577
H H H H H H H H H H H H H H Conform Multipl Conform Charge: E(B97-3 E(M06/d E(PBE - E(PM6)) E(PBE) E(PM7) E(GFN1- E(GFN2- E(GFN1- E(GFN2- E(GFN1- Coordin V O N N N C C C C C C	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 D3(BJ)/def2-TZV D3(BJ)/def2-TZV D3(BJ)/def2-TZV = 98.70431 Kcal/ = 108.63642 Kcal :CV/def2-TZVP) = = xTB) = -120.6185 xTB) = -119.8071 F) = -16.9720826 ates: -0.035653 -1.997416 -0.046809 0.570884 0.343647 1.135881 2.350306 3.073518 2.627620 1.443821	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol 2730.71829264371 26462890 Hartree 59859993 Hartree 59859993 Hartree 54530 Hartree 54530 Hartree -0.059492 0.303335 -1.585194 -0.393892 1.550030 2.463102 2.017315 2.839584 4.138700 4.607312	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree 1 Hartree 1 Hartree 0.043668 -0.529781 1.215163 -1.801395 1.131214 0.405458 -0.173117 -1.048388 -1.337260 -0.739733	H H H H H H H H H H H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3 : 0 3c) = -2729.95598 def2-TZVP) = -272 - D3 (BJ)/def2-TZV - D3 (BJ)/def2-TZV - D3 (BJ)/def2-TZV - D3 (BJ)/def2-TZV - T30 = -2726.1030 = 101.67079 Kcal = 106.5382 Kcal X-V/def2-TZVP) = -xTB) = -120.6174 -xTB) = -119.8076 FF) = -16.8643144 nates: 0.074114	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049  3537547 Hartree 9.925799006199 Ha P) = -2728.967883 WP) = -2729.11372 06289170 Hartree /mo1 /mo1 /mo1 /mo1 /mo1 /mo1 /mo1 /mo1	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577
H H H H H H H H H H H H H H H Conform Multipl Charge: E(B97-3 E(M06/d6 E(PBE0 E(PBE0 E(PBE0) E(PBEN-E(PM6)) E(GFN1-E(GFN2-E(GFN2-E(GFN-F Coordin V O N N N C C C C C C C C C C	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588  Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 - D3(BJ)/def2-TZV D3(BJ)/def2-TZ D3(BJ)/def2-TZ-TZ D3(BJ)/def2-TZ-TZ D3(BJ)/def2-TZ-TZ D3(BJ)/def2-TZ-TZ D3(BJ	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol -2730.71829264371 26462890 Hartree 59859993 Hartree 59859993 Hartree 54530 Hartree -0.059492 0.303335 -1.585194 -0.393892 1.550030 2.463102 2.017315 2.839584 4.138700 4.607312 3.783924 1.894934	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree 1 Hartree 0.043668 -0.529781 1.215163 -1.801395 1.131214 0.405458 -0.173117 -1.048388 -1.337260 -0.739733 0.114948 2.349974	H H H H H H H H H H H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3:0 3c) = -2729.95598 def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049  3537547 Hartree 9.925799006199 Ha P) = -2728.967883 VP) = -2729.11372 06289170 Hartree /mol /mol /mol -2730.71475671811 52474203 Hartree 81266316 Hartree 00124 Hartree 00124 Hartree	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577
H H H H H H H H H H H H H H Conform Multipl Charge: E(B97-3 E(M06/de(PBE0-E(PBE0-E(PM6))): E(PBE0-E(PM7)): E(GFN1-E(GFN1-E(GFN1-E(GFN1-COORD))) COORD N N N C C C C C C C C C C C C C C C C	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 Mef2-TZVP) = -272 D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP) = 98.70431 Kcal/ = 108.63642 Kcal -V/def2-TZVP) = 7272 xTB) = -120.6185 xTB) = -119.8071 F) = -16.9720826 Mates: -0.035653 -1.997416 -0.046809 0.570884 0.343647 1.135881 2.350306 3.073518 2.627620 1.443821 0.700475 -0.241133 -1.254726	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol -2730.71829264371 26462890 Hartree 59859993 Hartree 59859993 Hartree 54530 Hartree -0.059492 0.303335 -1.585194 -0.393892 1.550030 2.463102 2.017315 2.839584 4.138700 4.607312 3.783924 1.894934 1.063193	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree 9345907 Hartree 1 Hartree 1 Hartree 0.043668 -0.529781 1.215163 -1.801395 1.131214 0.405458 -0.173117 -1.048388 -1.337260 -0.739733 0.114948 2.349974 2.902805	H H H H H H H H H H H H H H H H H H Confor Multip Charge E(B97- E(M06/ E(PBE) E(PBE) E(PBE) E(PBE) E(PBE) E(PBE) E(PBE) E(GFN1- E(GFN2- Coordi V O N N	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3 : 0 3c) = -2729.95598 def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - TS) = -2726.1030 = 101.67079 Kcal X-V/def2-TZVP) = -xTB) = -120.6174 -xTB) = -119.8076 FF) = -16.8643144 nates: 0.074114 -1.546208 -0.134847 1.309470	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049  35537547 Hartree 9.925799006199 Harbinos P) = -2728.967883 VP) = -2729.11372 06289170 Hartree /mo1 /mo1 /mo1 /mo1 /mo1 /mo1 /mo1 /mo1	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577
H H H H H H H H H H H H H H H H H H H	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 D3(BJ)/def2-TZVD - D3(BJ)/def2-TZV2 - D3(BJ)/def2-TZVD = 98.70431 Kcal/ = 108.63642 Kcal :V/def2-TZVP) = 0.210.6185 xTB) = -120.6185 xTB) = -119.8071 F) = -16.9720826 Mates: -0.035653 -1.997416 -0.046809 0.570884 0.343647 1.135881 2.350306 3.073518 2.627620 1.443821 0.700475 -0.241133 -1.254726 -1.843346	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 WP) = -2729.11703 83531869 Hartree mol /mol /mol 2-2730.71829264371 26462890 Hartree 59859993 Hartree 59859993 Hartree 54530 Hartree -0.059492 0.303335 -1.585194 -0.393892 1.550030 2.463102 2.017315 2.839584 4.138700 4.607312 3.783924 1.894934 1.063193 1.358509	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree 9345907 Hartree 1.215163 -1.801395 1.31214 0.405458 -0.173117 -1.048388 -1.337260 -0.739733 0.114948 2.349974 2.902805 4.137738	H H H H H H H H H H H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.6866488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3 : 0 3c) = -2729.95598 def2-TZVP) = -272 -D 3(BJ)/def2-TZV -D 3(BJ)/def2-TZV -D 3(BJ)/def2-TZV -D 3(BJ)/def2-TZV -S 106.53882 Kcal 106.53882 Kcal 2.047272VP) = -272 -272 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -27	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049  3537547 Hartree 9.925799006199 Ha P) = -2728.967883 VP) = -2729.11372 06289170 Hartree/mol/mol /mol /mol /mol /mol /mol /mol /	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577
H H H H H H H H H H H H H H Conform Multipl Charge: E(B97-3 E(M06/de(PBE0-E(PBE0-E(PM6))): E(PBE0-E(PM7)): E(GFN1-E(GFN1-E(GFN1-E(GFN1-COORD))) COORD N N N C C C C C C C C C C C C C C C C	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 Mef2-TZVP) = -272 D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP) = 98.70431 Kcal/ = 108.63642 Kcal -V/def2-TZVP) = 7272 xTB) = -120.6185 xTB) = -119.8071 F) = -16.9720826 Mates: -0.035653 -1.997416 -0.046809 0.570884 0.343647 1.135881 2.350306 3.073518 2.627620 1.443821 0.700475 -0.241133 -1.254726	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol -2730.71829264371 26462890 Hartree 59859993 Hartree 59859993 Hartree 54530 Hartree -0.059492 0.303335 -1.585194 -0.393892 1.550030 2.463102 2.017315 2.839584 4.138700 4.607312 3.783924 1.894934 1.063193	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree 9345907 Hartree 1 Hartree 1 Hartree 0.043668 -0.529781 1.215163 -1.801395 1.131214 0.405458 -0.173117 -1.048388 -1.337260 -0.739733 0.114948 2.349974 2.902805	H H H H H H H H H H H H H H H H H H Confor Multip Charge E(B97- E(M06/ E(PBE) E(PBE) E(PBE) E(PBE) E(PBE) E(PBE) E(PBE) E(GFN1- E(GFN2- Coordi V O N N	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3 : 0 3c) = -2729.95598 def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - TS) = -2726.1030 = 101.67079 Kcal X-V/def2-TZVP) = -xTB) = -120.6174 -xTB) = -119.8076 FF) = -16.8643144 nates: 0.074114 -1.546208 -0.134847 1.309470	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049  35537547 Hartree 9.925799006199 Harbinos P) = -2728.967883 VP) = -2729.11372 06289170 Hartree /mo1 /mo1 /mo1 /mo1 /mo1 /mo1 /mo1 /mo1	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577
H H H H H H H H H H H H H H H H H H H	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588  Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 -D3(BJ)/def2-TZVP -D3(BJ)/def2-TZVP -D3(BJ)/def2-TZVP) = 88.70431 Kcal/ =108.63642 Kcal -V/def2-TZVP) = xTB) = -120.6185 xTB) = -119.8071 F) = -16.9720826  Mates: -0.035653 -1.997416 -0.046809 0.570884 0.343647 1.135881 2.350306 3.073518 2.627620 1.443821 0.700475 -0.241133 -1.254726 -1.843346 -1.441661	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 VP) = -2729.11703 83531869 Hartree mol /mol -2730.71829264371 26462890 Hartree 5985993 Hartree 5985993 Hartree 54530 Hartree 5985993 Hartree 54530 Hartree 1.585194 -0.393892 1.550030 2.463102 2.017315 2.839584 4.138700 4.607312 3.783924 1.894934 1.063193 1.358509 2.484971	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree 9345907 Hartree 1.215163 -1.801395 1.131214 0.405458 -0.173117 -1.048388 -1.337260 -0.739733 0.114948 2.349974 2.902805 4.137738 4.874009	H H H H H H H H H H H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.686488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3: 0.30; = -2729.95598 def2-TZVP) = -272 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV-D3(BJ)/def2-TZV-D3(BJ)/def2-TZVP) = -272 - T3(BJ)/def2-TZVP) = -2726.1030 = 101.67079 Kcal = 106.53882 Kcal X-V/def2-TZVP) = -19.8076 FF) = -16.8643144 nates: 0.074114 -1.546208 -0.134847 1.309470 -0.387592 0.636731	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049  3537547 Hartree 9.925799006199 Ha P) = -2728.1372 06289170 Hartree /mol /mol /mol /mol -2730.71475671811 52474203 Hartree 81266316 Hartree 00124 Hartree 00124 Hartree 00124 Hartree 00124 Hartree	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577 Artree 2495028 Hartree 26898050 Hartree 26898050 Hartree
H H H H H H H H H H H H H H H H H H H	-0.944867 0.555961 -2.550425 -1.763247 -2.364076 -2.656965 -0.358470 -0.219436 1.287232 0.319588 Mation 24. icity: 3 0 c) = -2729.95964 lef2-TZVP) = -272 D3(BJ)/def2-TZVD - D3(BJ)/def2-TZV2 - D3(BJ)/def2-TZVD = 98.70431 Kcal/ = 108.63642 Kcal :V/def2-TZVP) = 0.210.6185 xTB) = -120.6185 xTB) = -119.8071 F) = -16.9720826 Mates: -0.035653 -1.997416 -0.046809 0.570884 0.343647 1.135881 2.350306 3.073518 2.627620 1.443821 0.700475 -0.241133 -1.254726 -1.843346	2.282227 0.301154 1.935843 0.281117 2.033219 1.328738 2.499160 0.787312 -0.544615 6467439 Hartree 9.925289336170 Ha P) = -2728.970647 WP) = -2729.11703 83531869 Hartree mol /mol /mol 2-2730.71829264371 26462890 Hartree 59859993 Hartree 59859993 Hartree 54530 Hartree -0.059492 0.303335 -1.585194 -0.393892 1.550030 2.463102 2.017315 2.839584 4.138700 4.607312 3.783924 1.894934 1.063193 1.358509	3.185502 -1.527515 -1.421167 -3.960574 -3.693384 -5.002126 -3.642454 -2.834424 -3.561387 rtree 530242 Hartree 9345907 Hartree 9345907 Hartree 1.215163 -1.801395 1.31214 0.405458 -0.173117 -1.048388 -1.337260 -0.739733 0.114948 2.349974 2.902805 4.137738	H H H H H H H H H H H H H H H H H H H	0.271022 0.558045 -1.073044 -3.539468 -4.351323 -2.713377 0.026809 2.054898 4.298295 4.502320 2.492247 -2.6866488 -2.084723 -4.742844 -4.493753 -4.625188 -3.274737 -1.967878 -3.177826 mation 25. licity: 3 : 0 3c) = -2729.95598 def2-TZVP) = -272 -D 3(BJ)/def2-TZV -D 3(BJ)/def2-TZV -D 3(BJ)/def2-TZV -D 3(BJ)/def2-TZV -S 106.53882 Kcal 106.53882 Kcal 2.047272VP) = -272 -272 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -2729.95598 -27	-4.145399 -6.026319 -5.596940 -3.253861 -1.372775 -1.741204 -1.436177 -1.036154 -1.004282 -1.403078 1.714032 2.384433 0.891443 2.391064 0.027345 1.145934 -0.789150 -1.327049  3537547 Hartree 9.925799006199 Ha P) = -2728.967883 VP) = -2729.11372 06289170 Hartree/mol/mol /mol /mol /mol /mol /mol /mol /	1.717320 1.940928 1.729177 1.322636 1.128717 3.894792 5.326765 4.272615 1.767909 0.342924 0.844686 -0.722129 -0.207842 -1.159341 -2.532610 -2.927308 -2.309327 -1.077577

С	2.996269	0.632685	2.429223				
C C	2.704231 1.378520	0.158286 0.223109	3.709622 4.190506	Coordi	nates: -0.197347	-0.051908	0.003607
C	0.353790	0.729943	3.394052	0	1.358489	-0.031908	1.191465
C	-1.462299	2.339095	1.472340	N	-1.823320	-0.608040	0.916008
C	-1.333536	3.373931	2.433787	N	0.193916	1.857244	0.138218
C	-2.409175	4.226967	2.708197	N	0.313021	-1.139769	-1.559348
С	-3.635127	4.079297	2.037725	С	0.586148	-0.228895	-2.601915
C	-3.770956	3.056933	1.084024	C	1.876465	-0.038888	-3.164024
C	-2.704442	2.194467	0.803477	C	2.103513	0.997875	-4.077522
С	1.970475	-0.516647	-2.102505	С	1.069545	1.884115	-4.432872
С	1.223818	-1.678443	-2.430122	С	-0.209757	1.706033	-3.884853
С	1.864112	-2.877774	-2.775160	C	-0.456332	0.644183	-3.003563
C	3.263329	-2.943508	-2.839968	C	0.704382	-2.477194	-1.564076
C C	4.017501	-1.790115	-2.549783	С	0.392133	-3.271596 -4.613469	-0.423820
C	3.388091 1.591098	-0.596677 1.887996	-2.181853 -2.106104	C C	0.777365 1.461434	-5.225055	-0.348835 -1.414398
C	2.246238	2.091910	-3.355352	C	1.726335	-4.468372	-2.567363
C	2.469643	3.380987	-3.851750	C	1.354883	-3.119758	-2.651619
C	2.045634	4.518215	-3.142380	C	1.542820	2.182279	0.432268
Ċ	1.380427	4.333412	-1.919406	Č	1.975041	2.234980	1.777166
С	1.155377	3.050334	-1.406567	С	3.325571	2.452217	2.085803
C	-1.438324	-2.126789	0.989781	C	4.267411	2.640089	1.058770
C	-2.453333	-1.303300	1.529258	С	3.843704	2.608926	-0.280802
C	-3.772003	-1.773275	1.643183	C	2.495988	2.380342	-0.595341
C	-4.097294	-3.078210	1.243418	C	-0.643162	2.804299	-0.467530
С	-3.085290	-3.918532	0.739946	С	-0.202972	4.082459	-0.898263
С	-1.770874	-3.453764	0.618346	С	-1.083459	4.959879	-1.544842
C	0.925442	-2.265358	1.452270	C	-2.422163	4.605029	-1.779561
C	0.722858	-2.917357	2.697552	C	-2.879199 -2.012679	3.356527	-1.323812
C C	1.793530 3.094549	-3.506418 -3.460124	3.379012 2.849153	C C	-3.020821	2.476917 -0.906582	-0.666538 0.233300
C	3.303799	-2.823648	1.615647	C	-4.286863	-0.564005	0.775541
C	2.237859	-2.240219	0.920373	C	-5.461791	-0.808386	0.053526
C	-1.625365	1.146409	-2.409932	C	-5.413041	-1.389206	-1.224586
C	-2.977331	0.952565	-3.078387	C	-4.164415	-1.734270	-1.767731
C	-3.082378	-0.578350	-3.122537	C	-2.983054	-1.507526	-1.050794
С	-2.516490	-0.986255	-1.765996	С	-1.865113	-0.479650	2.324689
H	2.223609	1.615295	0.640363	C	-2.226264	-1.576992	3.143192
H	4.026851	0.597759	2.046037	C	-2.161553	-1.472984	4.538010
H	3.498059	-0.270663	4.337638	C	-1.744889	-0.274310	5.146796
H	1.144921	-0.155321	5.197406	С	-1.414339	0.828152	4.343201
H	-0.685706	0.746394	3.752982	C	-1.483082	0.733122	2.943865
H	-0.373830	3.503314	2.955159	С	1.285401	-1.289921	2.559418
H	-2.284256	5.025468	3.455993	C	2.733062	-1.559307	2.951510
H	-4.475987	4.753332	2.257712	С	3.365432	-1.956701	1.611479
H H	-4.727000 -2.818200	2.920406 1.378012	0.554640 0.078321	C H	2.707087 2.707167	-0.977532 -0.686620	0.651169 -2.849503
H	0.126639	-1.625825	-2.399532	H	3.111628	1.133992	-4.499331
Н	1.258388	-3.768092	-3.004348	Н	1.263508	2.708761	-5.134613
Н	3.765971	-3.883090	-3.112433	Н	-1.028853	2.393819	-4.143050
Н	5.117262	-1.829603	-2.592402	Н	-1.470194	0.478086	-2.607224
Н	3.983544	0.291830	-1.924963	H	-0.191989	-2.816574	0.391806
H	2.570960	1.220078	-3.940985	H	0.518184	-5.197381	0.548404
H	2.979407	3.496971	-4.821526	H	1.760164	-6.281912	-1.356227
H	2.224740	5.528058	-3.539557	H	2.230361	-4.936935	-3.427188
H	1.028242	5.204228	-1.344304	H	1.556882	-2.556633	-3.572660
H	0.625538	2.929153	-0.450077	H	1.232031	2.084007	2.574052
H	-2.191717	-0.288940	1.860120	H	3.645491	2.482755	3.139155
H	-4.546563	-1.109825	2.058174	H	5.326534	2.812740	1.302184
H H	-5.129815 -3.328643	-3.447447 -4.947386	1.334418 0.431980	H H	4.572721 2.165909	2.751330 2.329867	-1.093541 -1.643272
H	-0.976950	-4.101566	0.216832	H	0.839413	4.384720	-0.728835
Н	-0.287766	-2.942589	3.129786	Н	-0.711000	5.943254	-1.872516
Н	1.609605	-4.000721	4.345877	H	-3.104358	5.299355	-2.291861
Н	3.933119	-3.925792	3.388340	Н	-3.930826	3.062349	-1.464701
H	4.310936	-2.788913	1.171958	H	-2.403040	1.524526	-0.277092
H	2.419406	-1.773865	-0.055573	H	-4.335726	-0.091752	1.767279
H	-1.508656	2.100324	-1.859169	H	-6.431396	-0.529737	0.495038
H	-0.779064	1.045248	-3.119661	H	-6.338805	-1.575202	-1.788897
H	-3.788021	1.385757	-2.455584	H	-4.105008	-2.202685	-2.762317
H	-3.019017	1.427735	-4.077129	H	-2.009990	-1.799675	-1.470835
H	-4.115864	-0.948206	-3.266150	H	-2.543723	-2.514207	2.661406
H	-2.456102	-0.981764	-3.945021	H	-2.432303	-2.339899	5.160560
H	-1.993049 -3.284136	-1.961080 -1.003563	-1.761435 -0.966717	H	-1.691725	-0.199298	6.243222
Н	J.ZU4130	1.000000	0.900/1/	H H	-1.110844 -1.234904	1.779311 1.591310	4.807700 2.301509
Confor	mation 26.			H	0.776200	-0.530091	3.180340
	olicity: 3			H	0.671440	-2.215000	2.553643
Charge				H	3.204336	-0.633111	3.340167
	-3c) = -2729.964216	6386315 Hartree		H	2.811942	-2.343396	3.728976
	def2-TZVP) = -2729			H	4.468780	-1.867556	1.602883
	- D3(BJ)/def2-TZVI			H	3.092754	-2.997484	1.339774
	) - D3(BJ)/def2-TZV		5287553 Hartree		2.605757	-1.360703	-0.380118
	1-3c) = -2726.11418			H	3.209948	0.010679	0.640691
	= 97.21117 Kcal/r			0			
	= 108.99983 Kcal, 7X-V/def2-TZVP) = -		1 Hartron		rmation 3. Dlicity: 3		
	/X-V/def2-TZVP) = - xTB) = -120.61764		. nartiee	Charge			
	2-xTB) = $-119.8101$				-3c) = -2729.96639	1890795 Hartree	
	-FF) = $-16.97785983$				def2-TZVP) = -272		rtree

,	E - D3(BJ)/def2-TZV E0 - D3(BJ)/def2-TZV	,		H H	-2.584306 -0.229657	0.421441 0.093132	-3.483250 -2.940167
	Eh-3c) = -2726.11500		7107333 Hartree	Н	-0.371451	-1.706822	-3.072063
	6) = 93.45212  Kcal/r			a			
	7) = 107.94963 Kcal, 97X-V/def2-TZVP) = -		2 Hartree		rmation 31. olicity: 3		
	N1-xTB) = -120.62069		Z Harcree	Charge	-		
	N2-xTB) = -119.8115				-3c) = -2729.95825		
E (GF	N-FF) = -16.97426500	06480 Hartree			<pre>/def2-TZVP) = -272 - D3(BJ)/def2-TZV</pre>		
Coor	dinates:				) - D3(BJ)/def2-TZ		
V	0.127535	0.008650	-0.008529		n-3c) = -2726.1027		
O N	-1.232230 1.551582	-0.840392 -1.322939	-1.376001 -0.143080		= 96.24529 Kcal/ = 111.94988 Kcal		
N	0.205770	1.694905	-1.045249	. ,	7X-V/def2-TZVP) =		8 Hartree
N	-0.880349	0.056511	1.660524	E (GFN)	1-xTB) = $-120.6239$	32761891 Hartree	
C C	-0.620298 -0.731751	0.995508 0.663771	2.673029 4.047177		2-xTB) = -119.8098		
C	-0.731731	1.595634	5.035375	E (GEN-	-FF) = -16.9654745	10100 Marchee	
С	0.072222	2.876213	4.689770		inates:		
C C	0.180301	3.216224	3.330701	V	0.072688	0.203866	-0.350068
C	-0.169422 -1.729648	2.297536 -1.038556	2.334178 1.922004	O N	2.167481 -1.671638	0.633990 0.330633	-0.916409 -1.204207
С	-3.084289	-0.852391	2.292552	N	0.492721	-1.708377	-0.226716
C	-3.942977	-1.951141	2.415195	N	-0.034411	1.166958	1.338637
C C	-3.473214 -2.124254	-3.257398 -3.454754	2.179112 1.845014	C C	-0.826777 -1.040424	0.730297 -0.651879	2.419543 2.649153
C	-1.254119	-2.358309	1.732957	C	-1.881062	-1.086460	3.681717
С	1.424329	2.366613	-1.279657	С	-2.519891	-0.161594	4.523275
C C	2.590672 3.823168	1.636677 2.286635	-1.616068 -1.770496	C C	-2.301754 -1.469810	1.210942 1.655924	4.315438 3.280873
C	3.920498	3.678015	-1.615934	C	0.687333	2.372185	1.485452
С	2.765660	4.414725	-1.298034	C	1.565779	2.567741	2.582263
C C	1.533581	3.772875	-1.127741	C C	2.361298	3.716169 4.700142	2.662347
C	-0.978876 -1.023550	2.251921 2.867528	-1.558546 -2.837940	C	2.301858 1.416094	4.527959	1.657012 0.581831
C	-2.236535	3.317214	-3.373413	C	0.605949	3.384779	0.501686
C	-3.438814	3.170407	-2.657280	C	1.685790	-2.147824	0.378966
C C	-3.403743 -2.192389	2.582733 2.139912	-1.382235 -0.833202	C C	2.270813 3.512636	-1.415667 -1.786986	1.443018 1.975445
C	2.296609	-1.088855	1.022234	C	4.200746	-2.906074	1.478036
С	2.386130	0.250192	1.487961	С	3.616517	-3.658640	0.443011
C C	2.875805 3.362300	0.537757 -0.494100	2.771533 3.583935	C C	2.378789 -0.403361	-3.292029 -2.703843	-0.099312 -0.691689
C	3.339375	-1.819647	3.104849	C	-0.829278	-3.750041	0.162433
С	2.804876	-2.125515	1.849852	С	-1.782576	-4.679066	-0.270814
C C	1.787689 3.099384	-2.464281 -2.777754	-0.928617 -1.364880	C C	-2.328906 -1.894679	-4.589521 -3.571011	-1.562530 -2.424404
C	3.334616	-3.892741	-2.178036	C	-0.932896	-2.645581	-1.999124
С	2.272707	-4.722184	-2.579084	C	-1.581314	1.595628	-1.806917
C C	0.971409	-4.426805	-2.142944	C C	-2.497551	2.647426 3.935217	-1.527573 -2.010226
C	0.728210 -2.640825	-3.317067 -1.187932	-1.320587 -1.195276	C	-2.259438 -1.108825	4.221532	-2.777536
С	-3.153479	-1.500850	-2.599033	С	-0.212775	3.190967	-3.085355
C C	-2.252431 -0.905099	-0.636825 -0.770848	-3.492379 -2.799283	C C	-0.457715 -2.896037	1.883180 -0.354038	-2.627551 -1.187126
Н	-1.068243	-0.344065	4.329898	C	-3.227991	-1.188925	-0.096445
H	-0.479327	1.310201	6.095425	C	-4.398993	-1.953045	-0.117572
H	0.342312	3.601948	5.471192	C	-5.278715	-1.886554	-1.211365
H H	0.532554 -0.091618	4.217236 2.575560	3.036672 1.272599	C C	-4.968662 -3.790585	-1.040649 -0.282801	-2.289111 -2.283642
Н	-3.452280	0.171038	2.460990	С	2.718607	-0.126568	-2.023629
H	-4.997188	-1.788248	2.688450	C	4.185603	-0.321357	-1.669605
H H	-4.155224 -1.736196	-4.115958 -4.472098	2.270609 1.681969	C C	4.518810 3.243452	1.016499 1.336158	-0.995132 -0.214191
Н	-0.188455	-2.505402	1.503140	Н	-0.533065	-1.380404	2.001916
H	2.513369	0.545654	-1.744046	H	-2.029596	-2.167127	3.832887
H H	4.715962 4.887595	1.694779 4.186877	-2.024758 -1.742546	H H	-3.177818 -2.796893	-0.505453 1.950953	5.335196 4.963576
Н	2.828205	5.506506	-1.168577	Н	-1.317984	2.732868	3.117417
H	0.634871	4.351949	-0.867558	H	1.618956	1.794401	3.363619
H H	-0.090666 -2.245307	2.976851 3.782157	-3.410967 -4.371718	H H	3.044626 2.932168	3.843689 5.599618	3.516500 1.722760
H H	-4.388598	3.525640	-3.083759	н Н	1.335892	5.297481	-0.201667
H	-4.329891	2.482380	-0.794731	H	-0.108893	3.274481	-0.323682
H	-2.162512	1.699898	0.175964	H	1.725802	-0.550465	1.849019
H H	2.111785 2.885318	1.085591 1.580589	0.817683 3.121536	H H	3.938860 5.172277	-1.199682 -3.199884	2.804051 1.902330
Н	3.764873	-0.272116	4.583016	Н	4.136787	-4.544728	0.046668
Н	3.726030	-2.634705	3.736673	Н	1.932176	-3.882001	-0.913188
H H	2.749275 3.929739	-3.167345 -2.124928	1.501804 -1.055813	H H	-0.409719 -2.114436	-3.812830 -5.475022	1.178053 0.413884
н Н	4.360961	-4.113313	-2.510336	н Н	-3.090745	-5.310291	-1.894645
H	2.460583	-5.595430	-3.221307	H	-2.314988	-3.488119	-3.437964
H	0.132105	-5.077780	-2.434198	H	-0.602158	-1.837105	-2.667649
H H	-0.285031 -2.699975	-3.098428 -2.037767	-0.956609 -0.489549	H H	-3.374919 -2.968006	2.430142 4.742678	-0.901137 -1.769044
H	-3.148714	-0.310007	-0.750050	H	-0.928003	5.243593	-3.142087
Н	-3.019835	-2.577305	-2.833671	H	0.672924	3.392663	-3.707168
H H	-4.228860 -2.216629	-1.259590 -0.984992	-2.703589 -4.542785	H H	0.193442 -2.551026	1.051411 -1.224135	-2.940495 0.766787
						.==.=00	,

H							5.169656
	-4.629123	-2.604715	0.739213	H	-2.058797	-3.006820	
H	-6.201093	-2.486412	-1.222767	H	-2.129995	-3.844066	2.801673
H	-5.647923	-0.977654	-3.153780	H	-0.581951	-2.857073	1.076650
Н	-3.538671	0.358158	-3.142012	Н	-0.133352	4.217476	-1.387079
H	2.137652	-1.066001	-2.101875	H	-0.722248	6.090464	0.157361
H	2.594009	0.464263	-2.960436	H	-0.551768	5.785484	2.645543
H	4.294539	-1.164202	-0.957079	H	0.258027	3.589409	3.565887
H	4.809918	-0.532349	-2.559526	H	0.874197	1.724032	2.006798
H	5.401944	0.957250	-0.329966	H	0.189646	0.423448	-2.912911
H	4.719257	1.798062	-1.757295	H	1.605201	0.534881	-4.969730
H	2.992101	2.412981	-0.182705	H	3.547493	2.130492	-5.081274
Н	3.274827	0.944224	0.820408	H	4.061327	3.582715	-3.095972
	0.27.1027	0.911221	0.020100				
				H	2.682397	3.423728	-1.025434
Confo	ormation 33.			H	-1.937186	2.046220	-0.780108
MUITI	iplicity: 3			H	-3.310380	0.873294	-0.641922
Charq	ae: 0			H	-2.636943	3.230806	1.248724
_	_	10502576 #					
E(B9/	7-3c) = -2729.96637	95235/6 Hartree		H	-4.241796	2.828467	0.540941
E (M06	6/def2-TZVP) = -272	29.934747889639 Har	rtree	H	-3.735628	1.908244	3.065902
	E - D3(BJ)/def2-TZV			H	-4.370900	0.734767	1.864554
E (PBF	E0 - D3(BJ)/def2-TZ	(VP) = -2729.125272	2920965 Hartree	H	-2.303874	-0.407305	2.469702
	Eh-3c) = -2726.1167			Н	-1.439030	1.153812	2.731717
				п	-1.439030	1.133012	2./31/1/
E (PM6	6) = 93.19738 Kcal/	mol					
	· ·						
	7) = 113.51464 Kcal			T.TT	CIZ		
E (ωB9	97X-V/def2-TZVP) =	-2730.727523297464	l Hartree	ПОБ	CIZ		
	N1-xTB) = -120.6204						
	,						
E (GFN	N2-xTB) = -119.8105	60363668 Hartree		Confor	mation 2.		
E (GFN	N-FF) = -16.9737605	,65180 Hartree		Multip	licity: 5		
				Charge	0		
~	Att and a second					7006700 #	
	dinates:				-3c) = -3593.87107		
V	0.046472	-0.065751	-0.042627	E (GFN1	-xTB) = $-169.7150$	92985715 Hartree	
_					,		
0	-1.758118	0.631859	0.737896		-xTB) = $-169.2301$		
N	0.605700	1.727397	-0.635731	E(GFN-	FF) = $-24.13656720$	05388 Hartree	
							A Committee of the Comm
N	1.067179	-0.809936	1.438999		def2-TZVP) = -3593		
N	-0.722648	-1.369695	-1.270465	E(PBE	<ul> <li>D3 (BJ) /def2-TZV!</li> </ul>	= -3592.337878	491573 Hartree
	0.170037	-2.244425	-1.903495		- D3(BJ)/def2-TZ		
С						,	02000/0 naitiee
C	1.562349	-1.982400	-1.809542	E (PBEh	(-3c) = -3588.83099	96805323 Hartree	
C		-2.862651	-2.350832		= 151.18855 Kcal,		
	2.503651						
C	2.084908	-4.019442	-3.030652	E(PM7)	= 51.26554 Kcal/r	nol	
C	0.709566	-4.280358	-3.148685		X-V/def2-TZVP) = -		7
				E (WD9/	X-V/GEIZ-IZVP)	-3390.30/03003094	/ naitree
C	-0.241061	-3.413494	-2.592570				
С	-2.100801	-1.415687	-1.592421	Coordi	nates:		
C	-2.558937	-1.025659	-2.873006	Fe	-0.103815	0.531318	-0.098951
С	-3.929662	-0.989781	-3.161766	С	-1.418516	0.004414	1.354142
C	-4.872122	-1.345502	-2.181000	C	-2.163119	-1.012507	2.007383
C	-4.426432	-1.755593	-0.913554	С	-2.533755	-0.830699	3.360032
C	-3.054671	-1.801122	-0.623410	H	-3.064790	-1.645891	3.876794
С	2.470625	-0.878102	1.470602	С	-2.306579	0.382960	4.024428
C	3.244046	0.052066	0.727566	H	-2.635499	0.508670	5.067231
С	4.639518	-0.048211	0.685154	С	-1.727343	1.458869	3.339293
C	5.308702	-1.056479	1.398839	H	-1.657034	2.439831	3.827556
С	4.553332	-1.967505	2.155894	С	-1.271989	1.271345	2.017006
C	3.155438	-1.889573	2.191791	С	-2.792504	-2.192784	1.314992
C	0.316809	-1.449804	2.451325	С	-2.120872	-3.426661	1.131880
C	0.378589	-1.014654	3.797375	C	-2.829095	-4.523539	0.600154
~	-0.469389		4.762232	H	-2.309820	-5.484709	
( '		-1 572362		11			0 461991
C		-1.572362					0.461991
C	-1.389348	-1.572362 -2.577655	4.409168	С	-4.184453	-4.417221	0.461991 0.270796
C	-1.389348	-2.577655	4.409168		-4.184453	-4.417221	0.270796
C C	-1.389348 -1.433058	-2.577655 -3.039676	4.409168 3.084077	Н	-4.184453 -4.727996	-4.417221 -5.286787	0.270796 -0.129404
C	-1.389348	-2.577655	4.409168		-4.184453	-4.417221	0.270796
C C C	-1.389348 -1.433058 -0.577982	-2.577655 -3.039676 -2.491646	4.409168 3.084077 2.114331	H C	-4.184453 -4.727996 -4.842688	-4.417221 -5.286787 -3.193356	0.270796 -0.129404 0.443351
C C C	-1.389348 -1.433058 -0.577982 0.380052	-2.577655 -3.039676 -2.491646 2.830023	4.409168 3.084077 2.114331 0.208848	H C H	-4.184453 -4.727996 -4.842688 -5.905836	-4.417221 -5.286787 -3.193356 -3.107913	0.270796 -0.129404 0.443351 0.170323
C C C C	-1.389348 -1.433058 -0.577982 0.380052 -0.051160	-2.577655 -3.039676 -2.491646 2.830023 4.083452	4.409168 3.084077 2.114331 0.208848 -0.297885	H C H C	-4.184453 -4.727996 -4.842688 -5.905836 -4.166191	-4.417221 -5.286787 -3.193356 -3.107913 -2.067656	0.270796 -0.129404 0.443351 0.170323 0.948806
C C C C	-1.389348 -1.433058 -0.577982 0.380052	-2.577655 -3.039676 -2.491646 2.830023	4.409168 3.084077 2.114331 0.208848	H C H	-4.184453 -4.727996 -4.842688 -5.905836	-4.417221 -5.286787 -3.193356 -3.107913	0.270796 -0.129404 0.443351 0.170323
C C C C C	-1.389348 -1.433058 -0.577982 0.380052 -0.051160 -0.380523	-2.577655 -3.039676 -2.491646 2.830023 4.083452 5.129469	4.409168 3.084077 2.114331 0.208848 -0.297885 0.572618	H C H C	-4.184453 -4.727996 -4.842688 -5.905836 -4.166191 -0.678797	-4.417221 -5.286787 -3.193356 -3.107913 -2.067656 -3.614317	0.270796 -0.129404 0.443351 0.170323 0.948806 1.575436
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ССССССССССССССНННННННН	-1.389348 -1.433058 -0.577982 0.380052 -0.051160 -0.380523 -0.289914 0.156214 0.497925 1.342860 1.054098 1.846557 2.929509 3.213359 2.439970 -2.601073 -3.302662 -3.525560 -2.212412 1.938433 3.574316 2.823835 0.365995 -1.313958 -1.818801 -4.266825 -5.948411 -5.154888 -2.701718 2.735866	-2.577655 -3.039676 -2.491646 2.830023 4.083452 5.129469 4.960195 3.730764 2.681705 1.901123 1.102380 1.177397 2.067684 2.880864 2.798964 1.512391 2.398689 1.415423 0.640349 -1.067968 -2.629116 -4.707879 -5.182778 -3.638928 -0.738431 -0.670999 -1.309489 -2.051032 -2.120009 0.866206	4.409168 3.084077 2.114331 0.208848 -0.297885 0.572618 1.966845 2.478413 1.613045 -1.822789 -2.956118 -4.109079 -4.173349 -3.061682 -1.897899 -0.076316 0.939763 2.097153 2.125669 -1.316473 -2.248831 -3.466416 -3.678416 -2.676001 -3.635256 -4.160191 -2.406971 -0.142227 0.367259 0.190601	Н С Н С С Н С Н Н Н С Н С Н Н Н С С С С	-4.184453 -4.727996 -4.842688 -5.905836 -4.166191 -0.678797 -0.326264 0.240780 0.251701 -0.080029 1.284161 -0.619167 -1.242020 0.419294 -0.991994 -4.930787 -4.192144 -5.637424 -4.930735 -6.093414 -6.452323 -5.926554 -5.413273 -6.693078 -6.454311 -0.633259 -1.165047 -0.439249 -0.803990 0.692613	-4.417221 -5.286787 -3.193356 -3.107913 -2.067656 -3.614317 -2.626505 -4.052148 -3.301180 -5.021909 -4.173141 -4.588188 -4.225698 -4.709499 -5.594213 -0.753704 0.034976 -0.324358 -0.278703 0.679603 -1.023668 -0.825534 -1.064134 -1.609178 0.142150 2.331007 2.489688 3.316067 3.417054 4.019540	0.270796 -0.129404 0.443351 0.170323 0.948806 1.575436 1.931718 0.425323 -0.389428 -0.008604 0.777330 2.765750 3.608522 3.134501 2.482459 1.108812 1.355988 -0.187837 -1.039554 -0.064827 -0.467178 2.278843 3.230831 2.104006 2.407623 1.160008 -0.193189 -1.095965 -2.127318 -0.691625
ССССССССССССССНННННННН	-1.389348 -1.433058 -0.577982 0.380052 -0.051160 -0.380523 -0.289914 0.156214 0.497925 1.342860 1.054098 1.846557 2.929509 3.213359 2.439970 -2.601073 -3.302662 -3.525560 -2.212412 1.938433 3.574316 2.823835 0.365995 -1.313958 -1.818801 -4.266825 -5.948411 -5.154888 -2.701718 2.735866	-2.577655 -3.039676 -2.491646 2.830023 4.083452 5.129469 4.960195 3.730764 2.681705 1.901123 1.102380 1.177397 2.067684 2.880864 2.798964 1.512391 2.398689 1.415423 0.640349 -1.067968 -2.629116 -4.707879 -5.182778 -3.638928 -0.738431 -0.670999 -1.309489 -2.051032 -2.120009 0.866206	4.409168 3.084077 2.114331 0.208848 -0.297885 0.572618 1.966845 2.478413 1.613045 -1.822789 -2.956118 -4.109079 -4.173349 -3.061682 -1.897899 -0.076316 0.939763 2.097153 2.125669 -1.316473 -2.248831 -3.466416 -3.678416 -2.676001 -3.635256 -4.160191 -2.406971 -0.142227 0.367259 0.190601	Н С Н С С Н С Н Н Н С Н С Н Н Н С Н Н Н С С С Н	-4.184453 -4.727996 -4.842688 -5.905836 -4.166191 -0.678797 -0.326264 0.240780 0.251701 -0.080029 1.284161 -0.619167 -1.242020 0.419294 -0.991994 -4.930787 -4.192144 -5.637424 -4.930735 -6.093414 -6.452323 -5.926554 -5.413273 -6.693078 -6.454311 -0.633259 -1.165047 -0.439249 -0.803990 0.692613	-4.417221 -5.286787 -3.193356 -3.107913 -2.067656 -3.614317 -2.626505 -4.052148 -3.301180 -5.021909 -4.173141 -4.588188 -4.225698 -4.709499 -5.594213 -0.753704 0.034976 -0.324358 -0.278703 0.679603 -1.023668 -0.825534 -1.064134 -1.609178 0.142150 2.331007 2.489688 3.316067 3.417054 4.019540	0.270796 -0.129404 0.443351 0.170323 0.948806 1.575436 1.931718 0.425323 -0.389428 -0.008604 0.777330 2.765750 3.608522 3.134501 2.482459 1.108812 1.355988 -0.187837 -1.039554 -0.064827 -0.467178 2.278843 3.230831 2.104006 2.407623 1.160008 -0.193189 -1.095965 -2.127318 -0.691625
СССССССССССССННННННННН	-1.389348 -1.433058 -0.577982 0.380052 -0.051160 -0.380523 -0.289914 0.156214 0.497925 1.342860 1.054098 1.846557 2.929509 3.213359 2.439970 -2.601073 -3.302662 -3.525560 -2.212412 1.938433 3.574316 2.823835 0.365995 -1.313958 -1.818801 -4.266825 -5.948411 -5.154888 -2.701718 2.735866 5.208519	-2.577655 -3.039676 -2.491646 2.830023 4.083452 5.129469 4.960195 3.730764 2.681705 1.901123 1.102380 1.177397 2.067684 2.880864 2.798964 1.512391 2.398689 1.415423 0.640349 -1.067968 -2.629116 -4.707879 -5.182778 -3.638928 -0.738431 -0.670999 -1.309489 -2.051032 -2.120009 0.866206 0.685044	4.409168 3.084077 2.114331 0.208848 -0.297885 0.572618 1.966845 2.478413 1.613045 -1.822789 -2.956118 -4.109079 -4.173349 -3.061682 -1.897899 -0.076316 0.939763 2.097153 2.125669 -1.316473 -2.248831 -3.466416 -3.678416 -2.676001 -3.635256 -4.160191 -2.406971 -0.142227 0.367259 0.190601 0.092754	Н С Н С С Н С Н Н Н С Н Н Н С Н Н Н С С С Н С Н	-4.184453 -4.727996 -4.842688 -5.905836 -4.166191 -0.678797 -0.326264 0.240780 0.251701 -0.080029 1.284161 -0.619167 -1.242020 0.419294 -0.991994 -4.930787 -4.192144 -5.637424 -4.930735 -6.093414 -6.452323 -5.926554 -5.413273 -6.693078 -6.454311 -0.633259 -1.165047 -0.439249 -0.803990 0.692613 1.243262	-4.417221 -5.286787 -3.193356 -3.107913 -2.067656 -3.614317 -2.626505 -4.052148 -3.301180 -5.021909 -4.173141 -4.588188 -4.225698 -4.709499 -5.594213 -0.753704 0.034976 -0.324358 -0.278703 0.679603 -1.023668 -0.825534 -1.064134 -1.609178 0.142150 2.331007 2.489688 3.316067 3.417054 4.019540 4.638941	0.270796 -0.129404 0.443351 0.170323 0.948806 1.575436 1.931718 0.425323 -0.389428 -0.008604 0.777330 2.765750 3.608522 3.134501 2.482459 1.108812 1.355988 -0.187837 -1.039554 -0.064827 -0.467178 2.278843 3.230831 2.104006 2.407623 1.160008 -0.193189 -1.095965 -2.127318 -0.691625 -1.414534
СССССССССССССССННННННННН	-1.389348 -1.433058 -0.577982 0.380052 -0.051160 -0.380523 -0.289914 0.156214 0.497925 1.342860 1.054098 1.846557 2.929509 3.213359 2.439970 -2.601073 -3.302662 -3.525560 -2.212412 1.938433 3.574316 2.823835 0.365995 -1.313958 -1.818801 -4.266825 -5.948411 -5.154888 -2.701718 2.735866 5.208519 6.405919	-2.577655 -3.039676 -2.491646 2.830023 4.083452 5.129469 4.960195 3.730764 2.681705 1.901123 1.102380 1.177397 2.067684 2.880864 2.798964 1.512391 2.398689 1.415423 0.640349 -1.067968 -2.629116 -4.707879 -5.182778 -3.638928 -0.738431 -0.670999 -1.309489 -2.051032 -2.120009 0.866206 0.685044 -1.129334	4.409168 3.084077 2.114331 0.208848 -0.297885 0.572618 1.966845 2.478413 1.613045 -1.822789 -2.956118 -4.109079 -4.173349 -3.061682 -1.897899 -0.076316 0.939763 2.097153 2.125669 -1.316473 -2.248831 -3.466416 -3.678416 -2.676001 -3.635256 -4.160191 -2.406971 -0.142227 0.367259 0.190601 0.092754 1.369014	Н С Н С С Н С Н Н Н С Н Н Н С Н Н Н С С С Н С Н С	-4.184453 -4.727996 -4.842688 -5.905836 -4.166191 -0.678797 -0.326264 0.240780 0.251701 -0.080029 1.284161 -0.619167 -1.242020 0.419294 -0.991994 -4.930787 -4.192144 -5.637424 -4.930735 -6.093414 -6.452323 -5.926554 -5.413273 -6.693078 -6.693078 -6.693078 -6.693078 -6.454311 -0.633259 -1.165047 -0.439249 -0.803990 0.692613 1.243262 1.107483	-4.417221 -5.286787 -3.193356 -3.107913 -2.067656 -3.614317 -2.626505 -4.052148 -3.301180 -5.021909 -4.173141 -4.588188 -4.225698 -4.709499 -5.594213 -0.753704 0.034976 -0.324358 -0.278703 0.679603 -1.023668 -0.825534 -1.064134 -1.609178 0.142150 2.331007 2.489688 3.316067 3.417054 4.019540 4.638941 3.970507	0.270796 -0.129404 0.443351 0.170323 0.948806 1.575436 1.931718 0.425323 -0.389428 -0.008604 0.777330 2.765750 3.608522 3.134501 2.482459 1.108812 1.355988 -0.187837 -1.039554 -0.064827 -0.467178 2.278843 3.230831 2.104006 2.407623 1.160008 -0.193189 -1.095965 -2.127318 -0.650513
СССССССССССССННННННННН	-1.389348 -1.433058 -0.577982 0.380052 -0.051160 -0.380523 -0.289914 0.156214 0.497925 1.342860 1.054098 1.846557 2.929509 3.213359 2.439970 -2.601073 -3.302662 -3.525560 -2.212412 1.938433 3.574316 2.823835 0.365995 -1.313958 -1.818801 -4.266825 -5.948411 -5.154888 -2.701718 2.735866 5.208519	-2.577655 -3.039676 -2.491646 2.830023 4.083452 5.129469 4.960195 3.730764 2.681705 1.901123 1.102380 1.177397 2.067684 2.880864 2.798964 1.512391 2.398689 1.415423 0.640349 -1.067968 -2.629116 -4.707879 -5.182778 -3.638928 -0.738431 -0.670999 -1.309489 -2.051032 -2.120009 0.866206 0.685044	4.409168 3.084077 2.114331 0.208848 -0.297885 0.572618 1.966845 2.478413 1.613045 -1.822789 -2.956118 -4.109079 -4.173349 -3.061682 -1.897899 -0.076316 0.939763 2.097153 2.125669 -1.316473 -2.248831 -3.466416 -3.678416 -2.676001 -3.635256 -4.160191 -2.406971 -0.142227 0.367259 0.190601 0.092754	Н С Н С С Н С Н Н Н С Н Н Н С Н Н Н С С С Н С Н	-4.184453 -4.727996 -4.842688 -5.905836 -4.166191 -0.678797 -0.326264 0.240780 0.251701 -0.080029 1.284161 -0.619167 -1.242020 0.419294 -0.991994 -4.930787 -4.192144 -5.637424 -4.930735 -6.093414 -6.452323 -5.926554 -5.413273 -6.693078 -6.454311 -0.633259 -1.165047 -0.439249 -0.803990 0.692613 1.243262	-4.417221 -5.286787 -3.193356 -3.107913 -2.067656 -3.614317 -2.626505 -4.052148 -3.301180 -5.021909 -4.173141 -4.588188 -4.225698 -4.709499 -5.594213 -0.753704 0.034976 -0.324358 -0.278703 0.679603 -1.023668 -0.825534 -1.064134 -1.609178 0.142150 2.331007 2.489688 3.316067 3.417054 4.019540 4.638941	0.270796 -0.129404 0.443351 0.170323 0.948806 1.575436 1.931718 0.425323 -0.389428 -0.008604 0.777330 2.765750 3.608522 3.134501 2.482459 1.108812 1.355988 -0.187837 -1.039554 -0.064827 -0.467178 2.278843 3.230831 2.104006 2.407623 1.160008 -0.193189 -1.095965 -2.127318 -0.691625 -1.414534
СССССССССССССССННННННННННН	-1.389348 -1.433058 -0.577982 0.380052 -0.051160 -0.380523 -0.289914 0.156214 0.497925 1.342860 1.054098 1.846557 2.929509 3.213359 2.439970 -2.601073 -3.302662 -3.525560 -2.212412 1.938433 3.574316 2.823835 0.365995 -1.313958 -1.818801 -4.266825 -5.948411 -5.154888 -2.701718 2.735866 5.208519 6.405919 5.060204	-2.577655 -3.039676 -2.491646 2.830023 4.083452 5.129469 4.960195 3.730764 2.681705 1.901123 1.102380 1.177397 2.067684 2.880864 2.798964 1.512391 2.398689 1.415423 0.640349 -1.067968 -2.629116 -4.707879 -5.182778 -3.638928 -0.738431 -0.679999 -1.309489 -2.051032 -2.120009 0.866206 0.685044 -1.129334 -2.765006	4.409168 3.084077 2.114331 0.208848 -0.297885 0.572618 1.966845 2.478413 1.613045 -1.822789 -2.956118 -4.109079 -4.173349 -3.061682 -1.897899 -0.076316 0.939763 2.097153 2.125669 -1.316473 -2.248831 -3.466416 -3.678416 -2.676001 -3.635256 -4.160191 -2.406971 -0.142227 0.367259 0.190601 0.092754 1.369014 2.721594	Н С Н С С Н С Н Н Н С Н Н Н С Н Н Н С С С Н С Н С Н	-4.184453 -4.727996 -4.842688 -5.905836 -4.166191 -0.678797 -0.326264 0.240780 0.251701 -0.080029 1.284161 -0.619167 -1.242020 0.419294 -0.991994 -4.930787 -4.192144 -5.637424 -4.930735 -6.093414 -6.452323 -5.926554 -5.413273 -6.693078 -6.454311 -0.633259 -1.165047 -0.439249 -0.803990 0.692613 1.243262 1.107483 1.966264	-4.417221 -5.286787 -3.193356 -3.107913 -2.067656 -3.614317 -2.626505 -4.052148 -3.301180 -5.021909 -4.173141 -4.588188 -4.225698 -4.709499 -5.594213 -0.753704 0.034976 -0.324358 -0.278703 0.679603 -1.023668 -0.825534 -1.064134 -1.669178 0.142150 2.331007 2.489688 3.316067 3.417054 4.019540 4.638941 3.970507 4.578996	0.270796 -0.129404 0.443351 0.170323 0.948806 1.575436 1.931718 0.425323 -0.389428 -0.008604 0.777330 2.765750 3.608522 3.134501 2.482459 1.108812 1.355988 -0.187837 -1.039554 -0.064827 -0.467178 2.278843 3.230831 2.104006 2.407623 1.160008 -0.193189 -1.095965 -2.127318 -0.691625 -1.414534 0.650513 0.967491
ССССССССССССННННННННННН	-1.389348 -1.433058 -0.577982 0.380052 -0.051160 -0.380523 -0.289914 0.156214 0.497925 1.342860 1.054098 1.846557 2.929509 3.213359 2.439970 -2.601073 -3.302662 -3.525560 -2.212412 1.938433 3.574316 2.823835 0.365995 -1.313958 -1.818801 -4.266825 -5.948411 -5.154888 -2.701718 2.735866 5.208519 6.405919 5.060204 2.575842	-2.577655 -3.039676 -2.491646 2.830023 4.083452 5.129469 4.960195 3.730764 2.681705 1.901123 1.102380 1.177397 2.067684 2.880864 2.798964 1.512391 2.398689 1.415423 0.640349 -1.067968 -2.629116 -4.707879 -5.182778 -3.638928 -0.738431 -0.670999 -1.309489 -2.051032 -2.120009 0.866206 0.685044 -1.129334 -2.765006 -2.624159	4.409168 3.084077 2.114331 0.208848 -0.297885 0.572618 1.966845 2.478413 1.613045 -1.822789 -2.956118 -4.109079 -4.173349 -3.061682 -1.897899 -0.076316 0.939763 2.097153 2.125669 -1.316473 -2.248831 -3.466416 -3.678416 -2.676001 -3.635256 -4.160191 -2.406971 -0.142227 0.367259 0.190601 0.092754 1.369014 2.721594 2.769073	Н С Н С С Н С Н Н Н С Н Н Н С Н Н Н С С С Н С Н С Н С	-4.184453 -4.727996 -4.842688 -5.905836 -4.166191 -0.678797 -0.326264 0.240780 0.251701 -0.080029 1.284161 -0.619167 -1.242020 0.419294 -0.991994 -4.930787 -4.192144 -5.637424 -4.930735 -6.093414 -6.452323 -5.926554 -5.413273 -6.693078 -6.454311 -0.633259 -1.165047 -0.439249 -0.803990 0.692613 1.243262 1.107483 1.966264 0.466784	-4.417221 -5.286787 -3.193356 -3.107913 -2.067656 -3.614317 -2.626505 -4.052148 -3.301180 -5.021909 -4.173141 -4.588188 -4.225698 -4.709499 -5.594213 -0.753704 0.034976 -0.324358 -0.278703 0.679603 -1.023668 -0.825534 -1.064134 -1.609178 0.142150 2.331007 2.489688 3.316067 3.417054 4.019540 4.638941 3.970507 4.578996 3.152543	0.270796 -0.129404 0.443351 0.170323 0.948806 1.575436 1.931718 0.425323 -0.389428 -0.008604 0.777330 2.765750 3.608522 3.134501 2.482459 1.108812 1.355988 -0.187837 -1.039554 -0.064827 -0.467178 2.278843 3.230831 2.104006 2.407623 1.160008 -0.193189 -1.095965 -2.127318 -0.691625 -1.414534 0.650513 0.967491 1.591413
ССССССССССССССННННННННННН	-1.389348 -1.433058 -0.577982 0.380052 -0.051160 -0.380523 -0.289914 0.156214 0.497925 1.342860 1.054098 1.846557 2.929509 3.213359 2.439970 -2.601073 -3.302662 -3.525560 -2.212412 1.938433 3.574316 2.823835 0.365995 -1.313958 -1.818801 -4.266825 -5.948411 -5.154888 -2.701718 2.735866 5.208519 6.405919 5.060204	-2.577655 -3.039676 -2.491646 2.830023 4.083452 5.129469 4.960195 3.730764 2.681705 1.901123 1.102380 1.177397 2.067684 2.880864 2.798964 1.512391 2.398689 1.415423 0.640349 -1.067968 -2.629116 -4.707879 -5.182778 -3.638928 -0.738431 -0.679999 -1.309489 -2.051032 -2.120009 0.866206 0.685044 -1.129334 -2.765006	4.409168 3.084077 2.114331 0.208848 -0.297885 0.572618 1.966845 2.478413 1.613045 -1.822789 -2.956118 -4.109079 -4.173349 -3.061682 -1.897899 -0.076316 0.939763 2.097153 2.125669 -1.316473 -2.248831 -3.466416 -3.678416 -2.676001 -3.635256 -4.160191 -2.406971 -0.142227 0.367259 0.190601 0.092754 1.369014 2.721594	Н С Н С С Н С Н Н Н С Н Н Н С Н Н Н С С С Н С Н С Н	-4.184453 -4.727996 -4.842688 -5.905836 -4.166191 -0.678797 -0.326264 0.240780 0.251701 -0.080029 1.284161 -0.619167 -1.242020 0.419294 -0.991994 -4.930787 -4.192144 -5.637424 -4.930735 -6.093414 -6.452323 -5.926554 -5.413273 -6.693078 -6.454311 -0.633259 -1.165047 -0.439249 -0.803990 0.692613 1.243262 1.107483 1.966264	-4.417221 -5.286787 -3.193356 -3.107913 -2.067656 -3.614317 -2.626505 -4.052148 -3.301180 -5.021909 -4.173141 -4.588188 -4.225698 -4.709499 -5.594213 -0.753704 0.034976 -0.324358 -0.278703 0.679603 -1.023668 -0.825534 -1.064134 -1.669178 0.142150 2.331007 2.489688 3.316067 3.417054 4.019540 4.638941 3.970507 4.578996	0.270796 -0.129404 0.443351 0.170323 0.948806 1.575436 1.931718 0.425323 -0.389428 -0.008604 0.777330 2.765750 3.608522 3.134501 2.482459 1.108812 1.355988 -0.187837 -1.039554 -0.064827 -0.467178 2.278843 3.230831 2.104006 2.407623 1.160008 -0.193189 -1.095965 -2.127318 -0.691625 -1.414534 0.650513 0.967491
СССССССССССССССННННННННННННН	-1.389348 -1.433058 -0.577982 0.380052 -0.051160 -0.380523 -0.289914 0.156214 0.497925 1.342860 1.054098 1.846557 2.929509 3.213359 2.439970 -2.601073 -3.302662 -3.525560 -2.212412 1.938433 3.574316 2.823835 0.365995 -1.313958 -1.818801 -4.266825 -5.948411 -5.154888 -2.701718 2.735866 5.208519 6.405919 5.060204 2.575842 1.092136	-2.577655 -3.039676 -2.491646 2.830023 4.083452 5.129469 4.960195 3.730764 2.681705 1.901123 1.102380 1.177397 2.067684 2.880864 2.798964 1.512391 2.398689 1.415423 0.640349 -1.067968 -2.629116 -4.707879 -5.182778 -3.638928 -0.738431 -0.670999 -1.309489 -2.051032 -2.120009 0.866206 0.685044 -1.129334 -2.765006 -2.624159 -0.220528	4.409168 3.084077 2.114331 0.208848 -0.297885 0.572618 1.966845 2.478413 1.613045 -1.822789 -2.956118 -4.109079 -4.173349 -3.061682 -1.897899 -0.076316 0.939763 2.097153 2.125669 -1.316473 -2.248831 -3.466416 -3.678416 -2.676001 -3.635256 -4.160191 -2.406971 -0.142227 0.367259 0.190601 0.092754 1.369014 2.721594 2.769073 4.065120	Н С Н С С Н С Н Н Н С Н С Н С Н Н Н С С С Н С Н С Н С С	-4.184453 -4.727996 -4.842688 -5.905836 -4.166191 -0.678797 -0.326264 0.240780 0.251701 -0.080029 1.284161 -0.619167 -1.242020 0.419294 -0.991994 -4.930787 -4.192144 -5.637424 -4.930735 -6.093414 -6.452323 -5.926554 -5.413273 -6.693078 -6.454311 -0.633259 -1.165047 -0.439249 -0.803990 0.692613 1.243262 1.107483 1.966264 0.466784 -2.629202	-4.417221 -5.286787 -3.193356 -3.107913 -2.067656 -3.614317 -2.626505 -4.052148 -3.301180 -5.021909 -4.173141 -4.588188 -4.225698 -4.709499 -5.594213 -0.753704 0.034976 -0.324358 -0.278703 0.679603 -1.023668 -0.825534 -1.064134 -1.609178 0.142150 2.331007 2.489688 3.316067 3.417054 4.019540 4.638941 3.970507 4.578996 3.152543 2.145000	0.270796 -0.129404 0.443351 0.170323 0.948806 1.575436 1.931718 0.425323 -0.389428 -0.008604 0.777330 2.765750 3.608522 3.134501 2.482459 1.108812 1.355988 -0.187837 -1.039554 -0.064827 -0.467178 2.278843 3.230831 2.104006 2.407623 1.160008 -0.193189 -1.095965 -2.127318 -0.691625 -1.414534 0.650513 0.967491 1.591413 -0.523700
ССССССССССССННННННННННН	-1.389348 -1.433058 -0.577982 0.380052 -0.051160 -0.380523 -0.289914 0.156214 0.497925 1.342860 1.054098 1.846557 2.929509 3.213359 2.439970 -2.601073 -3.302662 -3.525560 -2.212412 1.938433 3.574316 2.823835 0.365995 -1.313958 -1.818801 -4.266825 -5.948411 -5.154888 -2.701718 2.735866 5.208519 6.405919 5.060204 2.575842	-2.577655 -3.039676 -2.491646 2.830023 4.083452 5.129469 4.960195 3.730764 2.681705 1.901123 1.102380 1.177397 2.067684 2.880864 2.798964 1.512391 2.398689 1.415423 0.640349 -1.067968 -2.629116 -4.707879 -5.182778 -3.638928 -0.738431 -0.670999 -1.309489 -2.051032 -2.120009 0.866206 0.685044 -1.129334 -2.765006 -2.624159	4.409168 3.084077 2.114331 0.208848 -0.297885 0.572618 1.966845 2.478413 1.613045 -1.822789 -2.956118 -4.109079 -4.173349 -3.061682 -1.897899 -0.076316 0.939763 2.097153 2.125669 -1.316473 -2.248831 -3.466416 -3.678416 -2.676001 -3.635256 -4.160191 -2.406971 -0.142227 0.367259 0.190601 0.092754 1.369014 2.721594 2.769073	Н С Н С С Н С Н Н Н С Н Н Н С Н Н Н С С С Н С Н С Н С	-4.184453 -4.727996 -4.842688 -5.905836 -4.166191 -0.678797 -0.326264 0.240780 0.251701 -0.080029 1.284161 -0.619167 -1.242020 0.419294 -0.991994 -4.930787 -4.192144 -5.637424 -4.930735 -6.093414 -6.452323 -5.926554 -5.413273 -6.693078 -6.454311 -0.633259 -1.165047 -0.439249 -0.803990 0.692613 1.243262 1.107483 1.966264 0.466784	-4.417221 -5.286787 -3.193356 -3.107913 -2.067656 -3.614317 -2.626505 -4.052148 -3.301180 -5.021909 -4.173141 -4.588188 -4.225698 -4.709499 -5.594213 -0.753704 0.034976 -0.324358 -0.278703 0.679603 -1.023668 -0.825534 -1.064134 -1.609178 0.142150 2.331007 2.489688 3.316067 3.417054 4.019540 4.638941 3.970507 4.578996 3.152543	0.270796 -0.129404 0.443351 0.170323 0.948806 1.575436 1.931718 0.425323 -0.389428 -0.008604 0.777330 2.765750 3.608522 3.134501 2.482459 1.108812 1.355988 -0.187837 -1.039554 -0.064827 -0.467178 2.278843 3.230831 2.104006 2.407623 1.160008 -0.193189 -1.095965 -2.127318 -0.691625 -1.414534 0.650513 0.967491 1.591413

C H	-3.536411 -3.393194	3.215443 3.264140	0.109487 1.207602	E(GFN2-xTB) = -169.236 E(GFN-FF) = -24.05123		
н	-4.603200	2.982818	-0.088042	E(GFN-FF) = -24.03123 E(M06/def2-TZVP) = -35		ırtree
Н	-3.317524	4.219445	-0.310276	E(PBE - D3(BJ)/def2-T2		
C	-2.905341	1.981434	-2.019513	E(PBE0 - D3(BJ)/def2-		36238828 Hartree
Н	-2.228882	1.239239	-2.485569	E(PBEh-3c) = -3588.834		
H H	-2.799105 -3.945103	2.935046 1.632153	-2.575887 -2.175499	E(PM6) = 175.76578  Kca E(PM7) = 62.98373  Kca	, -	
C	0.920157	3.195365	3.043694	$E(\omega B97X-V/def2-TZVP) =$	, -	7 Hartree
Н	0.628078	2.232609	3.511006	•		
С	2.437041	3.342521	3.205013	Coordinates:		
H	2.982555	2.613624	2.581071	Fe 0.147149	0.056866	0.408117
H H	2.729253 2.787320	3.171738 4.360218	4.260543 2.934175	C 1.956544 C 2.526716	-0.213910 -0.614680	-0.499227 -1.742415
C	0.196714	4.337760	3.786368	C 3.879898	-0.320304	-2.025904
Н	-0.904970	4.287276	3.679327	н 4.300777	-0.647014	-2.989352
H	0.515758	5.319601	3.379204	C 4.708865	0.305040	-1.085454
H	0.442000	4.321405	4.868260	Н 5.765305	0.500988	-1.322871
C	1.458076	-0.350770	-0.970198	C 4.198469	0.612069	0.179435
C C	2.638682 3.371987	-0.791302 -1.886145	-0.296365 -0.805768	H 4.858324 C 2.839570	1.016641 0.361336	0.962923 0.465883
Н	4.268283	-2.224577	-0.262012	C 1.861155	-1.535451	-2.728181
C	2.997645	-2.516401	-2.000813	C 1.251789	-1.058626	-3.919840
H	3.570097	-3.377966	-2.376882	C 0.791050	-1.995507	-4.865132
C	1.938039	-1.990462	-2.749171	н 0.323154	-1.642595	-5.795599
H C	1.701839 1.183694	-2.402485 -0.901384	-3.742613 -2.257806	C 0.899099 H 0.519137	-3.372338 -4.087331	-4.636242 -5.382415
C	3.294358	-0.062850	0.852351	C 1.494898	-3.835174	-3.457853
Č	3.123367	-0.465837	2.202418	н 1.590432	-4.918887	-3.287614
C	3.957104	0.082001	3.197780	C 2.000972	-2.934911	-2.500344
H	3.835325	-0.243665	4.242157	C 1.117502	0.437902	-4.195596
С	4.948177	1.014779	2.877013	Н 1.108632	0.946597	-3.207210
H	5.601142	1.423112	3.663558	C -0.182744 H -1.080149	0.800925 0.475165	-4.929147
C H	5.087519 5.855030	1.443463 2.191684	1.551819 1.300856	H -1.080149 H -0.225044	0.475165	-4.368992 -5.940119
C	4.270723	0.925071	0.528798	н -0.251737	1.896346	-5.075183
C	2.129105	-1.552792	2.578127	C 2.333634	0.966065	-4.979396
H	1.474825	-1.703725	1.694952	Н 3.280465	0.782091	-4.437902
С	1.235187	-1.160676	3.762860	Н 2.246784	2.058957	-5.150117
H	0.684487	-0.220971	3.560475	H 2.406426	0.469889	-5.969460
H	1.821576	-1.024316	4.694851	C 2.782666	-3.476875	-1.305066
H C	0.480715 2.877086	-1.947655 -2.871017	3.963259 2.844624	H 2.939062 C 2.034916	-2.635835 -4.572434	-0.603018 -0.536534
Н	3.461015	-3.187214	1.957424	н 1.062857	-4.203679	-0.156790
Н	2.172437	-3.686928	3.100674	н 2.635170	-4.913775	0.331795
H	3.586165	-2.758764	3.691019	н 1.838541	-5.465259	-1.165894
С	4.510669	1.370512	-0.909890	C 4.176093	-3.952567	-1.752850
Н	3.668979	0.982337	-1.514084	Н 4.742093	-3.133489	-2.238972
C H	4.513700	2.898658	-1.062545	H 4.099913	-4.788351	-2.479112
н Н	3.570450 4.618815	3.338503 3.179566	-0.683082 -2.130842	H 4.767442 C 2.328235	-4.307660 0.616339	-0.883617 1.857664
H	5.355998	3.371463	-0.516270	C 2.000741	-0.508904	2.686855
C	5.800534	0.745829	-1.468933	C 1.619184	-0.268652	4.024807
H	5.758722	-0.360283	-1.423096	н 1.381913	-1.119584	4.676932
Н	6.689358	1.076928	-0.892168	C 1.581658	1.025740	4.545562
H	5.953243	1.037226	-2.528776	Н 1.280861	1.189999	5.591319
C C	0.175844 0.495427	-0.285551 0.938167	-3.194145 -3.866466	C 1.942065 H 1.925706	2.117694 3.127192	3.743265 4.174987
C	-0.380762	1.412115	-4.860161	C 2.328237	1.942373	2.404812
Н	-0.145359	2.346073	-5.389315	C 2.244972	-1.948361	2.223625
С	-1.539052	0.705347	-5.210220	н 1.919530	-2.016818	1.164462
H	-2.201341	1.089841	-6.001099	C 3.752404	-2.265734	2.258298
C	-1.853844	-0.479608	-4.542416	н 4.334074	-1.578178	1.615526
H C	-2.774271 -1.017575	-1.023391 -0.983018	-4.803450 -3.525380	H 3.933674 Н 4.143894	-3.300111 -2.186086	1.900768 3.294000
C	1.796806	1.686049	-3.583661	C 1.459626	-3.001354	3.009161
Н	1.951913	1.643147	-2.484436	н 0.380112	-2.767184	3.042220
C	2.994121	0.987407	-4.257835	Н 1.828390	-3.109988	4.050324
Н	3.121037	-0.053707	-3.907194	Н 1.564195	-3.988994	2.519393
H	3.935053	1.534510	-4.043110	C 2.739717	3.138114	1.548893
H C	2.856944	0.964728 3.163483	-5.358921 -3.997657	H 3.705388	2.877245	1.067729
Н	1.775569 0.877311	3.693879	-3.627004	C 1.714754 H 1.597930	3.371699 2.480647	0.432867 -0.215176
Н	1.803582	3.281560	-5.100856	н 2.014269	4.217866	-0.216681
H	2.668627	3.680613	-3.593484	н 0.730364	3.613152	0.870719
С	-1.431340	-2.247741	-2.787652	C 2.960028	4.433076	2.338966
H	-0.757932	-2.350540	-1.912365	н 3.690146	4.305102	3.163453
С	-2.862449	-2.130579	-2.252827	H 2.010806	4.814569	2.769599
H H	-2.976749 -3.117537	-1.227326 -3.007017	-1.623336 -1.630313	H 3.347872 C -1.849413	5.223202 0.408012	1.665281 0.210194
H H	-3.11/53/	-2.073087	-3.071619	C -1.849413 C -2.472750	1.670077	-0.023315
C	-1.267297	-3.509868	-3.649656	C -3.828686	1.743406	-0.418573
Н	-0.219395	-3.648592	-3.980954	н -4.273471	2.734646	-0.597627
H	-1.904526	-3.460334	-4.557476	C -4.616322	0.591850	-0.532315
Н	-1.566522	-4.410162	-3.074379	н -5.673543	0.667098	-0.829307
Conf-	mation 25			C -4.050696	-0.649063 -1.565077	-0.220817
	mation 25. licity: 5			H -4.661160 C -2.688175	-1.565077 -0.743997	-0.253777 0.129273
Charge				C -1.841386	2.999805	0.280288
	3c) = -3593.86473	0263530 Hartree		C -1.366693	3.847987	-0.756497
	-xTB) = $-169.7151$			C -1.013820	5.174381	-0.439586

Н	-0.662312	5.846308	-1.236464	С	-1.656742	-0.849838	3.745631
C				Н	-1.041310		4.658404
	-1.080177	5.648371	0.875087			-1.005646	
H	-0.792680	6.686341	1.103362	С	-3.099650	-0.626982	4.240191
C	-1.497854	4.792541	1.901582	H	-3.483914	-1.520298	4.772278
H	-1.538984	5.165836	2.935919	H	-3.784321	-0.406102	3.398169
С	-1.897087	3.470389	1.625412	H	-3.136489	0.232356	4.941435
С	-1.240549	3.354710	-2.196184	C	-1.111907	0.418104	3.071409
Н	-1.262252	2.244218	-2.160456	Н	-0.118360	0.246987	2.594927
C	0.091073	3.777730	-2.837897	Н	-0.967524	1.216916	3.824934
H	0.958089	3.387953	-2.271346	H	-1.794450	0.813114	2.294953
H	0.192026	4.880352	-2.896758	С	-2.269365	-3.839234	-0.452450
H	0.163105	3.396139	-3.873997	H	-2.432548	-2.848018	-0.921534
C	-2.432662	3.813207	-3.054357	C	-1.289944	-4.608844	-1.346892
H	-3.392374	3.455966	-2.633912	H	-0.317039	-4.089974	-1.410440
H	-2.346973	3.420326	-4.088596	Н	-1.702433	-4.703643	-2.372174
H	-2.477675	4.920910	-3.111760	H	-1.097764	-5.635988	-0.973111
C	-2.469736	2.603070	2.743983	C	-3.633763	-4.550633	-0.401641
Н	-2.389869	1.550149	2.407455	Н	-4.371806	-3.967814	0.182079
C	-1.697419	2.716694	4.062484	H	-3.543950	-5.552937	0.067331
H	-0.622010	2.504234	3.914971	H	-4.039813	-4.687653	-1.425098
H	-2.088908	1.986676	4.799622	С	-2.501720	1.540213	-1.794443
H	-1.793123	3.722595	4.521335	C	-2.224998	1.183638	-3.143406
C	-3.964113	2.909382	2.950200	C	-2.090827	2.209321	-4.097789
H	-4.540343	2.755556	2.017081	H	-1.892947	1.952109	-5.148798
H	-4.109154	3.962415	3.271149	C	-2.184255	3.557462	-3.729073
H	-4.396062	2,250576	3.732267	Н	-2.053512	4.344251	-4.488040
C	-2.186211	-2.102814	0.521647	C	-2.434340	3.900280	-2.396440
C	-2.235190	-2.438576	1.909726	Н	-2.506945	4.961674	-2.113332
C	-1.880678	-3.738029	2.314760	C	-2.626304	2.905382	-1.417866
H	-1.932494	-4.008072	3.380813	С	-2.164514	-0.281897	-3.570400
C	-1.480543	-4.698396	1.378489	H	-1.873153	-0.866843	-2.672268
H	-1.195578	-5.709246	1.707570	C	-3.551739	-0.778900	-4.017995
С	-1.457308	-4.368947	0.020787	H	-4.303209	-0.668365	-3.212715
H	-1.169499	-5.129485	-0.722204	H	-3.514060	-1.849894	-4.307359
С	-1.819368	-3.084617	-0.439830	H	-3.904793	-0.199766	-4.896612
C	-2.799018	-1.460420	2.938330	С	-1.120990	-0.552350	-4.663509
Н	-2.895000	-0.477859	2.437211	Н	-0.127582	-0.143517	-4.393093
C	-4.216019	-1.893019	3.354626	Н	-1.416825	-0.103943	-5.634766
				Н			-4.832708
H	-4.882324	-1.974467	2.472820		-1.013768	-1.643624	
H	-4.662148	-1.156602	4.054878	С	-3.052206	3.304049	-0.006021
H	-4.205261	-2.881259	3.860271	H	-3.019364	2.387449	0.618143
С	-1.888785	-1.254739	4.154663	С	-2.103560	4.322036	0.633159
H	-0.910433	-0.830742	3.856791	H	-1.064365	3.948083	0.636416
H	-1.699526	-2.200488	4.704160	H	-2.404983	4.534328	1.680297
H	-2.356518	-0.547247	4.869475	H	-2.101424	5.289863	0.089589
С	-1.893713	-2.921540	-1.958165	C	-4.502739	3.819681	0.002966
H	-1.050065	-3.527323	-2.354763	H	-5.208987	3.063283	-0.391509
С	-3.194933	-3.556354	-2.489701	Н	-4.601914	4.730698	-0.623326
H	-3.315237	-4.603203	-2.146569	Н	-4.822389	4.081256	1.033113
H	-3.201382	-3.551492	-3.599304	С	2.018914	0.223592	0.108859
Н	-4.078580	-2.982077	-2.143428	C	2.652397	1.483677	-0.106315
C	-1.724032	-1.517157	-2.541821	C	4.059915	1.586426	-0.213720
Н	-0.852644	-0.994682	-2.102435	Н	4.501314	2.585388	-0.349829
H	-2.616129	-0.882040	-2.394114	C	4.881830	0.457769	-0.175852
H	-1.540572	-1.608945	-3.628152	H	5.972760	0.553183	-0.289937
				С	4.289062	-0.791352	0.027556
	nation 27.			H	4.906652	-1.700441	0.089381
Multipl	licity: 5			C	2.892656	-0.905256	0.196779
Charge:	: 0			C	1.956871	2.805653	-0.249659
E(B97-3	3c) = -3593.85589	1483977 Hartree		C	1.633229	3.567113	0.907209
		64105228 Hartree		С	1.216051	4.901051	0.741210
E (GFN2-	-xTB) = $-169.2326$	63529372 Hartree		Н	0.978033	5.510689	1.625208
	FF) = $-24.0443671$			C	1.079789	5.462916	-0.534914
		3.603482345096 Ha	x+x00	Н	0.731849	6.501843	-0.643079
		$^{\prime}P) = -3592.318520$		C	1.377608	4.699952	-1.668439
		SVP) = -3592.62396	/292348 Hartree	H	1.268910	5.147002	-2.668520
		10403138 Hartree		С	1.846925	3.377334	-1.546450
	= 194.26395 Kcal			С	1.816581	2.980734	2.305787
	= 69.19441 Kcal/			H	1.704034	1.879945	2.208422
E (ωB97Σ	(-V/def2-TZVP) =	-3596.39176874106	O Hartree	C	0.766046	3.471851	3.311420
				H	-0.263792	3.345600	2.923388
Coordin	nates:			H	0.903980	4.544599	3.559584
Fe	0.034229	-0.339716	0.155920	H	0.850298	2.908607	4.263429
C	-2.019316	-0.332926	-0.047390	C	3.237171	3.255072	2.834146
C	-2.638612	-1.270936	0.836359	Н	4.009379	2.834995	2.161233
C	-4.039653	-1.353540	0.836339	H H			
					3.379704	2.806957	3.839856
H	-4.456400	-2.084667	1.694125	H	3.415774	4.347491	2.919264
C	-4.884806	-0.546421	0.218213	C	2.315223	2.622699	-2.789440
H	-5.978807	-0.620519	0.317857	H	2.517114	1.575906	-2.482175
С	-4.310846	0.345938	-0.690516	С	1.252158	2.574697	-3.890579
H	-4.953497	0.977186	-1.323088	H	0.310023	2.137496	-3.515475
C	-2.907459	0.482557	-0.810433	H	1.606439	1.965718	-4.748364
С	-1.872165	-2.320438	1.591122	H	1.011572	3.584818	-4.282866
C	-1.501301	-2.150888	2.954987	C	3.633958	3.209972	-3.324788
C	-1.019228	-3.271763	3.661692	Н	4.436055	3.183508	-2.561678
Н	-0.745440	-3.150496	4.721655	H	3.499942	4.267376	-3.634911
п С	-0.889762	-4.522637	3.051603	Н	3.986502	2.640629	-4.209835
Н	-0.505814	-5.379496	3.626336	н С	2.428326	-2.280840	0.584783
С	-1.238254	-4.676654	1.706246	C	2.428326	-2.280840	1.972533
H	-1.135547	-5.661346	1.226710	C	2.296131	-3.948404	2.364718
С	-1.743318	-3.596545	0.962135	H	2.348275	-4.212115	3.431356

С	2.052280	-4.947849	1 417400	Н	1 026201	2.354233	-0.337926
			1.417482		1.936291		
H	1.902361	-5.990116	1.738492	C	2.544557	4.186520	0.609668
C	1.986788	-4.616120	0.061650	H	1.513194	4.493823	0.862316
H	1.794164	-5.403171	-0.684476	H	2.833149	4.703590	-0.328410
С	2.168746	-3.290787	-0.384365	H	3.218912	4.541806	1.416543
C		-1.579390		C	4.071241	2.326964	
	2.919823		3.015828				-0.098547
H	2.810632	-0.577099	2.553995	H	4.240455	1.237768	-0.166365
С	2.053843	-1.596809	4.281454	H	4.868793	2.763656	0.538136
H	0.985643	-1.459786	4.037335	H	4.194909	2.748343	-1.115966
H	2.363158	-0.781840	4.967322	C	-0.778969	1.316695	4.027212
H	2.150739	-2.550606	4.840413	H	-1.130927	2.368543	3.962979
C	4.405934	-1.758845	3.377270	C	-1.732047	0.469568	3.170215
H	5.054406	-1.667828	2.485153	H	-1.783086	0.828687	2.124575
Н	4.586064	-2.756586	3.829537	Н	-2.759208	0.501649	3.585318
	4.723878			H			3.157990
H		-0.988764	4.110046		-1.406861	-0.585204	
C	2.150590	-3.066077	-1.898203	C	-0.890455	0.897209	5.497735
H	1.641973	-3.966448	-2.306670	H	-0.249367	1.510359	6.162572
С	1.347668	-1.854905	-2.395405	H	-0.621202	-0.170187	5.636556
Н	0.374939	-1.747667	-1.859513	Н	-1.938228	1.013977	5.839006
H	1.109648	-1.972006	-3.470569	C	-0.004666	-1.942814	-0.141227
H	1.900949	-0.904567	-2.275369	C	-0.734295	-2.935092	0.582295
C	3.566530	-3.065482	-2.507615	C	-1.005732	-4.189959	-0.014561
Н	4.139072	-3.962027	-2.195894	Н	-1.564487	-4.938231	0.568284
H	4.137161	-2.167519	-2.199117	С	-0.533976	-4.517903	-1.289503
H	3.508034	-3.064130	-3.615849	H	-0.752699	-5.504083	-1.726548
				C	0.272337	-3.600613	-1.970963
Conform	ation 28.			Н	0.726320	-3.870634	-2.935842
	icity: 5			C		-2.334950	-1.408713
					0.535317		
Charge:				С	-1.149459	-2.834886	2.025368
E(B97-3	c) = $-3593.85955$	5228174 Hartree		С	-2.527718	-2.831403	2.379562
•	,	73146138 Hartree		C	-2.891799	-2.887292	3.739803
•		96181251 Hartree		Н	-3.957630	-2.876407	4.015129
•							
	F) = -24.0446628			С	-1.923345	-2.946500	4.743064
E(M06/d	lef2-TZVP) = -359	3.609560879721 На	rtree	H	-2.221219	-2.983149	5.802198
E(PBE -	D3(BJ)/def2-TZV	(P) = -3592.323967	382504 Hartree	C	-0.566890	-2.961751	4.393721
E (PREO	- D3(BJ)/def2-T7	VP) = -3592.62840	7848730 Hartree	H	0.187826	-3.021879	5.189510
		09006462 Hartree	7010700 11010100	C	-0.153950	-2.919084	3.048822
	= 182.74979 Kcal			C	-3.637758	-2.763255	1.335986
E(PM7)	= 67.32603 Kcal/	mol		H	-3.154045	-2.616231	0.349578
E (ωB97X	-V/def2-TZVP) =	-3596.38662364348	1 Hartree	C	-4.574235	-1.568879	1.580927
,	•			H	-4.012864	-0.615513	1.610047
Coordin				Н	-5.120954	-1.669558	2.541006
Fe	0.273286	0.079639	0.045997	H	-5.335293	-1.496609	0.776698
C	-0.500405	1.983685	0.119988	C	-4.435679	-4.077244	1.269816
С	-1.398008	2.776463	-0.653267	H	-3.780165	-4.943091	1.050637
C	-1.957892	3.959192	-0.112348	Н	-5.210323	-4.026484	0.476988
H	-2.662100	4.534831	-0.732843	H	-4.950733	-4.283727	2.231072
C	-1.614336	4.422236	1.161430	C	1.333041	-3.032151	2.710899
H	-2.056512	5.350016	1.555391	H	1.528255	-2.298656	1.900227
С	-0.659524	3.716905	1.899403	С	2.265145	-2.693638	3.879658
Н	-0.303227	4.105076	2.866508	Н	2.018716	-1.716267	4.331898
C	-0.119259	2.518362	1.388849	H	3.314052	-2.644258	3.525847
С	-1.723275	2.616603	-2.114425	H	2.225544	-3.469043	4.672754
С	-2.908357	1.980166	-2.576690	С	1.684421	-4.432814	2.171808
Č	-3.292360	2.159316	-3.920188	Н	1.130115	-4.684644	1.248836
H	-4.215031	1.671561	-4.273452	H	1.452152	-5.206906	2.932498
C	-2.528305	2.928557	-4.805907	H	2.768338	-4.497492	1.943613
H	-2.854618	3.060383	-5.848836	C	1.513170	-1.431901	-2.105520
C	-1.336765	3.507526	-4.359404	Č	2.815063	-1.282656	-1.529270
H	-0.721220	4.095181	-5.058282	C	3.756223	-0.460245	-2.179247
C	-0.919890	3.367408	-3.020983	H	4.767669	-0.360465	-1.758324
C	-3.751899	1.040225	-1.721128	С	3.445545	0.184679	-3.380247
Н	-4.613855	0.758080	-2.364823	Н	4.189813	0.831276	-3.869884
C	-4.348056	1.645402	-0.438799	C	2.199782	-0.032297	-3.982234
H	-4.808591	2.634509	-0.633414	H	1.980600	0.433740	-4.954519
H	-3.587052	1.778396	0.353531	C	1.228781	-0.852188	-3.377852
H	-5.135778	0.976045	-0.038611	С	3.276248	-2.195517	-0.395804
C	-2.972936	-0.252130	-1.433852	Н	2.369501	-2.591733	0.096005
H	-2.573515	-0.700966	-2.364012	C	4.019728	-3.400705	-1.001716
H	-3.612737	-1.005259	-0.936496	H	3.384616	-3.929266	-1.740419
H	-2.107808	-0.058430	-0.761603	H	4.298443	-4.125567	-0.208929
C	0.360784	4.063845	-2.565945	Н	4.948237	-3.080261	-1.518757
Н				C			
	0.531134	3.783747	-1.508809		4.106980	-1.501075	0.684672
C	1.585245	3.582722	-3.358514	H	3.524070	-0.704147	1.185048
H	1.713517	2.486695	-3.265393	H	5.037044	-1.047177	0.283439
H	2.508799	4.070046	-2.981788	H	4.413446	-2.231422	1.460098
Н	1.501548	3.823290	-4.439164	C	-0.049571	-1.175993	-4.140470
C	0.215978	5.593523	-2.611002	Н	-0.752647	-1.646511	-3.422650
H	-0.634814	5.932373	-1.986724	C	-0.726343	0.069646	-4.716528
H	0.040965	5.954957	-3.645888	H	-0.881315	0.836671	-3.938235
H	1.135368	6.086537	-2.232347	H	-1.715032	-0.184527	-5.147397
C	0.954964	1.848819	2.193034	Н	-0.126408	0.528610	-5.528937
C	2.307857	1.924036	1.729543	C	0.236990	-2.196882	-5.258623
C	3.329393	1.415542	2.558654	H	0.704905	-3.123949	-4.873236
H	4.375542	1.473283	2.229598	H	0.928015	-1.766388	-6.013083
C	3.036868	0.863219	3.807452	H	-0.701486	-2.476633	-5.780163
Н	3.848946	0.471391	4.438842				
C	1.713144	0.816451	4.264725	Confor	mation 29.		
Н		0.399733	5.259254				
	1 506004			rıu±t±p.	licity: 5		
	1.506804			O1	_		
С	0.653054	1.309276	3.484731	Charge			
					: 0 3c) = -3593.858900	0479013 Hartree	

E (CEN1.	-xTB) = -169.7061	3/79/175 Hartroo		С	0.323705	-5.644565	-0.700130
	-xTB) = $-169.7001-xTB$ ) = $-169.2216$			Н	-0.200441	-6.352101	-0.038161
	FF) = -24.1314742			С	1.540292	-6.010901	-1.283076
		3.604869074244 Ha		H	1.979204	-7.000082	-1.082487
		P) = -3592.326692		C	2.189899	-5.101913	-2.121151
	-3c) = -3588.8164	VP) = -3592.61886	U3/9635 Hartree	H C	3.148157 1.640470	-5.380011 -3.832932	-2.585187 -2.386120
	= 155.92226 Kcal			C	-1.624997	-4.145082	-0.279831
E(PM7)	= 58.16683 Kcal/	mol		H	-1.853343	-5.082896	0.271749
E(ωB972	X-V/def2-TZVP) =	-3596.37132793249	1 Hartree	С	-2.759780	-3.965111	-1.299655
Coordi				H H	-2.764311 -2.661487	-4.794893 -3.017094	-2.034804 -1.859394
Fe	0.301122	0.343081	-0.113376	н Н	-3.743580	-3.957987	-0.788095
C	-0.506948	0.423135	1.702542	C	-1.564908	-3.026519	0.767892
С	-1.893170	0.569453	2.020188	H	-0.862379	-3.285354	1.583203
C	-2.409493	-0.056559	3.176670	Н	-2.558367	-2.851221	1.225983
H C	-3.484027 -1.574773	0.042679 -0.760149	3.398849 4.057430	H C	-1.217389 2.403629	-2.072423 -2.912343	0.326294 -3.340746
Н	-1.998043	-1.251649	4.946744	Н	1.943772	-1.906624	-3.283373
C	-0.191959	-0.764224	3.839494	С	3.884708	-2.762111	-2.955635
H	0.485092	-1.215699	4.581496	H	4.003447	-2.453184	-1.898633
C C	0.350823 -2.859539	-0.160720 1.504286	2.682982 1.326192	H H	4.372759 4.446365	-1.999196 -3.708941	-3.595730 -3.092488
C	-3.815889	1.054050	0.377667	С	2.266766	-3.388979	-4.797584
C	-4.868161	1.910168	-0.004971	Н	1.205313	-3.431237	-5.109982
H	-5.620565	1.549625	-0.723035	H	2.697952	-4.403613	-4.927941
C	-4.976695	3.203804	0.512514	Н	2.799349	-2.701963	-5.487420
H C	-5.809460 -4.002260	3.856611 3.668189	0.209140 1.402353	C C	0.381083 1.693472	1.583791 1.584060	-1.961064 -1.312093
Н	-4.073987	4.692533	1.799157	C	2.038167	2.708686	-0.511582
C	-2.943238	2.840154	1.821432	Н	3.003752	2.704984	0.011932
С	-3.776849	-0.354720	-0.194196	С	1.199137	3.814834	-0.407710
H	-2.816857	-0.805657	0.121053	Н	1.481144	4.661399	0.235125
C H	-3.809244 -2.931658	-0.353026 0.178153	-1.729848 -2.146673	C H	0.012893 -0.607417	3.866003 4.772207	-1.159666 -1.117462
H	-4.725400	0.130617	-2.125993	C	-0.410395	2.788168	-1.949232
Н	-3.787554	-1.387032	-2.123814	Č	2.814649	0.639222	-1.780534
С	-4.910013	-1.208541	0.399821	Н	2.388923	-0.376960	-1.886784
H	-4.839478	-1.252316	1.505264	C	3.273058	1.091849	-3.178638
H H	-4.871398 -5.904423	-2.245932 -0.787408	0.011077 0.143418	H H	2.436241 4.077607	1.066235 0.428877	-3.904966 -3.557514
C	-1.967804	3.371700	2.865106	Н	3.667385	2.128955	-3.146637
H	-1.131860	2.649932	2.926360	С	3.990832	0.540483	-0.807604
С	-1.370575	4.731059	2.473096	H	3.661539	0.282304	0.216985
H	-0.876691	4.676392	1.483167	H	4.570230	1.484929	-0.750389
H H	-0.614858 -2.140932	5.052248 5.528397	3.219105 2.428322	H C	4.692034 -1.658303	-0.248281 2.950440	-1.143948 -2.805409
C	-2.627567	3.426008	4.253927	Н	-2.069132	1.938215	-2.994532
H	-2.995749	2.426680	4.559346	С	-2.761716	3.774086	-2.131333
H	-3.491377	4.123255	4.261792	H	-2.960502	3.422611	-1.104082
H	-1.903678	3.770431	5.021043	H	-3.705544	3.692744	-2.706814
C C	1.854884 2.490845	-0.055611 1.197982	2.596157 2.877655	H C	-2.504694 -1.283345	4.852542 3.580975	-2.083535 -4.162630
C	3.894365	1.242068	2.968003	Н	-0.473591	3.030353	-4.681543
H	4.391404	2.196486	3.190059	H	-0.923056	4.620264	-4.015494
C	4.674920	0.090322	2.805428	Н	-2.164621	3.618274	-4.835683
H C	5.770588 4.054440	0.148470 -1.126029	2.894738 2.516905	Confo	ormation 30.		
Н	4.667148	-2.028040	2.369364		plicity: 5		
С	2.652675	-1.216657	2.397738	Charg			
С	1.681396	2.459815	3.165751		7-3c) = -3593.859560		
H C	0.833067 1.100893	2.461499 2.421261	2.448665 4.592830		N1-xTB) = -169.71534 N2-xTB) = -169.24126		
Н	0.431243	1.554222	4.744034		V-FF) = -24.04002482		
Н	0.519675	3.342041	4.802874		5/def2-TZVP) = -3593		rtree
H	1.919478	2.358179	5.339566		E - D3(BJ)/def2-TZVF		
C H	2.460533 2.985935	3.766697 3.803339	2.967757 1.993642		EO - D3(BJ)/def2-TZV Eh-3c) = -3588.82294		3187046 Hartree
Н	3.218769	3.921528	3.763410		5) = 168.20229 Kcal/		
Н	1.765450	4.628497	3.012202		7) = 59.27699  Kcal/m		
С	2.035853	-2.560096	2.039557	E(ωB9	97X-V/def2-TZVP) = -	3596.38265683669	4 Hartree
H	0.966826	-2.378890	1.810782	~			
C H	2.680219 2.615396	-3.144865 -2.429924	0.777393 -0.065105	Fe	dinates: -0.318772	-0.220240	-0.159804
H	2.163400	-4.072073	0.469300	C	-1.410219	1.440588	-0.732775
H	3.750057	-3.394441	0.933444	C	-1.344691	2.859027	-0.814902
C	2.102663	-3.560147	3.205276	С	-2.503296	3.613610	-1.121625
H	1.588738	-3.175379	4.107994	H	-2.414567	4.709454	-1.189796
H H	3.154840 1.623229	-3.778737 -4.519351	3.483697 2.919779	C H	-3.754872 -4.648789	3.007890 3.618343	-1.276690 -1.475565
C	0.076856	-0.864573	-1.737048	C	-3.855706	1.616662	-1.160762
С	-0.178139	-2.149315	-2.295685	Н	-4.831832	1.116019	-1.252398
C	-0.780968	-2.226664	-3.574130	C	-2.696125	0.852022	-0.928917
H C	-1.022446	-3.220677	-3.982268	C C	-0.123193	3.672603	-0.503715
Н	-1.002371 -1.439733	-1.085750 -1.186550	-4.357273 -5.362204	C	0.879624 1.956276	3.891575 4.742500	-1.487387 -1.177278
C	-0.594195	0.170561	-3.893577	Н	2.735665	4.928374	-1.930618
H	-0.659172	1.043346	-4.556355	С	2.052953	5.359213	0.077999
C	-0.073619	0.288969	-2.587334	H	2.907926	6.015544	0.303865
C C	0.390076 -0.274717	-3.462861 -4.390632	-1.797686 -0.944841	C H	1.053700 1.125386	5.150792 5.648554	1.035559 2.015529
_	V. L. I I I I I	1.000002	0.011011		1.120000	3.010007	2.010029

С	-0.053047	4.324036	0.758640	Н	0.487035	0.252831	5.617973
C	0.740654	3.276192	-2.877242	C	1.699961	1.837303	
							4.782740
H	0.218666	2.306140	-2.740334	H	1.618452	2.471514	5.678847
C	2.077063	2.998057	-3.576290	C	2.409582	2.284939	3.667042
Н	2.757310	2.391462	-2.946996	Н	2.878916	3.281766	3.678933
Н	2.604876	3.936103	-3.845964	C	2.528741	1.497666	2.502087
H	1.904963	2.447449	-4.523536	C	0.553414	-1.645489	3.639143
C	-0.156096	4.154689	-3.770399	H	0.206851	-1.865459	2.606334
H	-1.161416	4.289591	-3.327403	С	1.617128	-2.699607	4.002837
Н	-0.285138		-4.772103				3.286098
		3.694279		H	2.458470	-2.696429	
H	0.295242	5.159167	-3.909570	H	1.173934	-3.716617	4.007274
C	-1.169295	4.191875	1.792952	H	2.026581	-2.499625	5.014672
Н	-1.933040	3.512118	1.367998	С	-0.650433	-1.791070	4.579053
С	-0.683727	3.556269	3.099540	H	-1.406558	-0.997595	4.422424
H	-0.218069	2.570931	2.915037	H	-0.344892	-1.758059	5.645564
H	-1.528845	3.411700	3.803972	H	-1.141514	-2.772177	4.416470
Н	0.072259	4.186886	3.609696	C	3.344825	2.111299	1.359092
C	-1.862995	5.541833	2.039516	H	3.077775	3.189930	1.386674
H	-2.253662	5.974142	1.096273	C	4.859630	2.026485	1.632878
H	-1.166425	6.282920	2.483932	H	5.117101	2.413261	2.639182
H	-2.714121	5.419634	2.740995	Н	5.421455	2.620336	0.882215
C	-2.795639	-0.647203	-0.883609	H	5.215868	0.978965	1.566702
C	-2.882643	-1.340750	0.366167	C	3.033440	1.644141	-0.067559
C	-3.019325	-2.746491	0.332244	H	1.941353	1.596509	-0.248873
Н	-3.131141	-3.283346	1.285984	Н	3.470148	0.655352	-0.299506
С	-3.048197	-3.454914	-0.869180	H	3.451876	2.377666	-0.783980
H	-3.134797	-4.550479	-0.860331				
С	-2.975141	-2.767440	-2.086594	Confo	rmation 32.		
Н	-3.010420	-3.333590	-3.027413	Multir	olicity: 5		
				-			
C	-2.866242	-1.367795	-2.120997	Charge		222222	
C	-3.082530	-0.689083	1.741797	E(B97-	-3c) = -3593.85430	0309898 Hartree	
H	-2.890819	-1.510727	2.465481	E (GFN)	1-xTB) = $-169.7103$	64367265 Hartree	
С	-2.154218	0.461484	2.146202	F (CFN)	2-xTB) = $-169.2356$	88379871 Hartree	
					-FF) = $-24.0396904$		
Н	-1.073145	0.241645	1.970044				
H	-2.239734	0.648439	3.235894	E(M06)	/def2-TZVP) = -359	3.603649160272 Ha	rtree
H	-2.394834	1.405054	1.627103	E(PBE	- D3(BJ)/def2-TZV	P) = -3592.318681	547038 Hartree
С	-4.555725	-0.271597	1.915204		) - D3(BJ)/def2-TZ		
							JJ 17170 Hareree
H	-5.241938	-1.115217	1.704039		n-3c) = -3588.8206		
H	-4.810088	0.559867	1.227961	E(PM6)	) = 187.56521 Kcal	/mol	
H	-4.740152	0.075596	2.952486	E(PM7)	= 71.21472  Kcal/r	nol	
С	-2.921093	-0.629908	-3.458258		7X-V/def2-TZVP) =		8 Hartree
Н	-2.456109	0.366454	-3.303101	L (wb)	/M	3330.30012703337	o narcree
C	-2.167280	-1.333693	-4.594646	Coord	inates:		
H	-1.128375	-1.577722	-4.312750	Fe	-0.164081	0.233145	-0.039849
Н	-2.139576	-0.681329	-5.490653	С	-1.912397	-0.828594	-0.292444
				C	-2.307083	-2.102350	-0.803714
Н	-2.663628	-2.278661	-4.897067				
C	-4.384292	-0.398079	-3.885386	C	-3.642566	-2.550115	-0.651125
H	-4.951182	0.175317	-3.129713	H	-3.903362	-3.551007	-1.028300
H	-4.903239	-1.366899	-4.038906	С	-4.628932	-1.751245	-0.066475
Н	-4.425072	0.164955	-4.840358	Н	-5.661218	-2.120637	0.030997
C	1.359129	-1.254044	0.428188	C	-4.284108	-0.470555	0.375150
C	1.818175	-2.350451	-0.368311	H	-5.041839	0.192624	0.822024
C	3.143723	-2.829286	-0.274351	C	-2.949611	-0.023425	0.273374
Н	3.455029	-3.661742	-0.924140	C	-1.487227	-3.065261	-1.627626
		J. 001/42			-0.652411		
С	4.037873	0 000005	0 (57.004	С		-4.064365	-1.052667
H		-2.293065	0.657634				
	5.068058	-2.293065 -2.673611	0.657634 0.730728	C		-5.097507	-1.876260
C	5.068058	-2.673611	0.730728		-0.161888		-1.876260
С	5.068058 3.578233	-2.673611 -1.304022	0.730728 1.531161	H	-0.161888 0.476605	-5.872562	-1.876260 -1.422759
H	5.068058 3.578233 4.234251	-2.673611 -1.304022 -0.924400	0.730728 1.531161 2.329100	H C	-0.161888 0.476605 -0.464802	-5.872562 -5.159507	-1.876260 -1.422759 -3.240531
H C	5.068058 3.578233 4.234251 2.268722	-2.673611 -1.304022 -0.924400 -0.781695	0.730728 1.531161 2.329100 1.420453	H C H	-0.161888 0.476605 -0.464802 -0.075293	-5.872562 -5.159507 -5.982507	-1.876260 -1.422759 -3.240531 -3.858972
H	5.068058 3.578233 4.234251	-2.673611 -1.304022 -0.924400	0.730728 1.531161 2.329100 1.420453 -1.223519	H C	-0.161888 0.476605 -0.464802	-5.872562 -5.159507 -5.982507 -4.156005	-1.876260 -1.422759 -3.240531
H C	5.068058 3.578233 4.234251 2.268722	-2.673611 -1.304022 -0.924400 -0.781695	0.730728 1.531161 2.329100 1.420453	H C H	-0.161888 0.476605 -0.464802 -0.075293	-5.872562 -5.159507 -5.982507	-1.876260 -1.422759 -3.240531 -3.858972
H C C	5.068058 3.578233 4.234251 2.268722 0.914325	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216	0.730728 1.531161 2.329100 1.420453 -1.223519	H C H C	-0.161888 0.476605 -0.464802 -0.075293 -1.252590	-5.872562 -5.159507 -5.982507 -4.156005	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238
H C C C	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730	H C H C H	-0.161888 0.476605 -0.464802 -0.075293 -1.252590 -1.478147 -1.773699	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905
H C C C H	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164	H C H C H C	-0.161888 0.476605 -0.464802 -0.075293 -1.252590 -1.478147 -1.773699 -0.182711	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773
H C C C H C	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691	H C H C H C H	-0.161888 0.476605 -0.464802 -0.075293 -1.252590 -1.478147 -1.773699 -0.182711 0.342419	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645
H C C C C H C	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691 -3.366228	Н С Н С Н С Н С	-0.161888 0.476605 -0.464802 -0.075293 -1.252590 -1.478147 -1.773699 -0.182711 0.342419 -1.286732	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494
H C C C H C	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691	H C H C H C H	-0.161888 0.476605 -0.464802 -0.075293 -1.252590 -1.478147 -1.773699 -0.182711 0.342419	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645
Н С С С Н С Н	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963 -5.287496	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691 -3.366228 -1.384418	H C H C H C H C H	-0.161888 0.476605 -0.464802 -0.075293 -1.252590 -1.478147 -1.773699 -0.182711 0.342419 -1.286732 -2.079007	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016
Н С С С С Н С Н С	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832 -0.756760	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963 -5.287496 -6.190253	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691 -3.366228 -1.384418 -0.909141	H C H C C H C H H	-0.161888 0.476605 -0.464802 -0.075293 -1.252590 -1.478147 -1.773699 -0.182711 0.342419 -1.286732 -2.079007 -1.768191	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506 -3.014682	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016 1.521071
Н С С С С Н С Н С Н С	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832 -0.756760 0.367840	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963 -5.287496 -6.190253 -4.358239	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691 -3.366228 -1.384418 -0.909141 -0.600415	H C H C C H C H H H H	-0.161888 0.476605 -0.464802 -0.075293 -1.252590 -1.478147 -1.773699 -0.182711 0.342419 -1.286732 -2.079007 -1.768191 -0.854742	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506 -3.014682 -4.229497	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016 1.521071 2.463994
Н С С С С Н С Н С Н С Н С С С	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832 -0.756760 0.367840 1.356198	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963 -5.287496 -6.190253 -4.358239 -1.817529	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691 -3.366228 -1.384418 -0.909141 -0.600415 -3.386935	H C H C C H C H C H C	-0.161888 0.476605 -0.464802 -0.075293 -1.252590 -1.478147 -1.773699 -0.182711 0.342419 -1.286732 -2.079007 -1.768191 -0.854742 0.872481	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506 -3.014682 -4.229497 -2.962899	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016 1.521071 2.463994 0.601335
Н С С С С Н С Н С Н С	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832 -0.756760 0.367840	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963 -5.287496 -6.190253 -4.358239	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691 -3.366228 -1.384418 -0.909141 -0.600415	H C H C C H C H H H H	-0.161888 0.476605 -0.464802 -0.075293 -1.252590 -1.478147 -1.773699 -0.182711 0.342419 -1.286732 -2.079007 -1.768191 -0.854742	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506 -3.014682 -4.229497	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016 1.521071 2.463994
Н С С С С Н С Н С Н С Н С Н С Н С Н С Н	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832 -0.756760 0.367840 1.356198	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963 -5.287496 -6.190253 -4.358239 -1.817529 -1.879332	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691 -3.366228 -1.384418 -0.909141 -0.600415 -3.386935 -4.404625	H C H C H C H H H H H	-0.161888 0.476605 -0.464802 -0.075293 -1.252590 -1.478147 -1.773699 -0.182711 0.342419 -1.286732 -2.079007 -1.768191 -0.854742 0.872481	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506 -3.014682 -4.229497 -2.962899 -2.989762	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016 1.521071 2.463994 0.601335 -0.187667
Н ССССН СНСН ССН ССН ССН	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832 -0.756760 0.367840 1.356198 0.912370 2.879689	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963 -5.287496 -6.190253 -4.358239 -1.817529 -1.879332 -1.934056	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691 -3.366228 -1.384418 -0.909141 -0.600415 -3.386935 -4.404625 -3.577413	Н С Н С С Н С Н Н Н С Н Н Н Н Н Н Н Н Н	-0.161888 0.476605 -0.464802 -0.075293 -1.252590 -1.478147 -1.773699 -0.182711 0.342419 -1.286732 -2.079007 -1.768191 -0.854742 0.872481 1.649089 1.370199	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506 -3.014682 -4.229497 -2.962899 -2.989762 -3.058730	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016 1.521071 2.463994 0.601335 -0.187667 1.583243
H C C C C C H C H C H C H C H	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832 -0.756760 0.367840 1.356198 0.912370 2.879689 3.155482	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963 -5.287496 -6.190253 -4.358239 -1.817529 -1.879332 -1.934056 -2.919351	0.730728 1.531161 2.329100 1.420453 	H C H C C H C H H H H H H H H	-0.161888 0.476605 -0.464802 -0.075293 -1.252590 -1.478147 -1.773699 -0.182711 0.342419 -1.286732 -2.079007 -1.768191 -0.854742 0.872481 1.649089 1.370199 0.407636	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506 -3.014682 -4.229497 -2.962899 -2.989762 -3.058730 -1.950967	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016 1.521071 2.463994 0.601335 -0.187667 1.583243 0.571354
H C C C C H C H C H H H	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832 -0.756760 0.367840 1.356198 0.912370 2.879689 3.155482 3.415838	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963 -5.287496 -6.190253 -4.358239 -1.817529 -1.879332 -1.934056 -2.919351 -1.811348	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691 -3.366228 -1.384418 -0.909141 -0.600415 -3.386935 -4.404625 -3.577413 -4.003456 -2.617053	H C H C H C H H H C H C	-0.161888     0.476605     -0.464802     -0.075293     -1.252590     -1.478147     -1.773699     -0.182711     0.342419     -1.286732     -2.079007     -1.768191     -0.854742     0.872481     1.649089     1.370199     0.407636     -2.645206	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506 -3.014682 -4.229497 -2.962899 -2.989762 -3.058730 -1.950967 -2.054844	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016 1.521071 2.463994 0.601335 -0.187667 1.583243 0.571354 -3.701907
H C C C C C H C H C H C H C H	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832 -0.756760 0.367840 1.356198 0.912370 2.879689 3.155482	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963 -5.287496 -6.190253 -4.358239 -1.817529 -1.879332 -1.934056 -2.919351	0.730728 1.531161 2.329100 1.420453 	H C H C C H C H H H H H H H H	-0.161888 0.476605 -0.464802 -0.075293 -1.252590 -1.478147 -1.773699 -0.182711 0.342419 -1.286732 -2.079007 -1.768191 -0.854742 0.872481 1.649089 1.370199 0.407636	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506 -3.014682 -4.229497 -2.962899 -2.989762 -3.058730 -1.950967	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016 1.521071 2.463994 0.601335 -0.187667 1.583243 0.571354
H C C C C H C H C H H H H H	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832 -0.756760 0.367840 1.356198 0.912370 2.879689 3.155482 3.415838 3.241475	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963 -6.190253 -4.358239 -1.817529 -1.879332 -1.934056 -2.919351 -1.811348 -1.146041	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691 -3.366228 -1.384418 -0.909141 -0.600415 -3.386935 -4.404625 -3.577413 -4.003456 -2.617053 -4.269849	Н С Н С С Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н	-0.161888     0.476605     -0.464802     -0.075293     -1.252590     -1.478147     -1.773699     -0.182711     0.342419     -1.286732     -2.079007     -1.768191     -0.854742     0.872481     1.649089     1.370199     0.407636     -2.645206     -2.929056	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506 -3.014682 -4.229497 -2.962899 -2.989762 -3.058730 -1.950967 -2.054844 -1.319894	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016 1.521071 2.463994 0.601335 -0.187667 1.583243 0.571354 -3.701907 -2.924548
H C C C C H C H C C H C H C C H C C H C C H C C H C C H C C C C C C C C C C C C C C C C C C C C	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832 -0.756760 0.367840 1.356198 0.912370 2.879689 3.155482 3.415838 3.241475 0.976759	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963 -5.287496 -6.190253 -4.358239 -1.817529 -1.879332 -1.934056 -2.919351 -1.811348 -1.146041 -0.439357	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691 -3.366228 -1.384418 -0.909141 -0.600415 -3.386935 -4.404625 -3.577413 -4.003456 -2.617053 -4.269849 -2.829514	Н С Н С С Н С Н Н Н С Н С Н С Н С С Н С С Н С С Н С С Н С С Н С С Н С С Н С С Н С С Н С С Н С С Н С С Н С С Н С С Н С С С Н С С С С С Н С С С С С С С С С С С С С С С С С С С С	-0.161888     0.476605     -0.464802     -0.075293     -1.252590     -1.478147     -1.773699     -0.182711     0.342419     -1.286732     -2.079007     -1.768191     -0.854742     0.872481     1.649089     1.370199     0.407636     -2.645206     -2.929056     -1.867141	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506 -3.014682 -4.229497 -2.962899 -2.989762 -3.058730 -1.950967 -2.054844 -1.319894 -1.286918	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016 1.521071 2.463994 0.601335 -0.187667 1.583243 0.571354 -3.701907 -2.924548 -4.781268
H C C C C H C H C H C H H H H C H	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832 -0.756760 0.367840 1.356198 0.912370 2.879689 3.155482 3.415838 3.241475 0.976759 -0.112261	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963 -5.287496 -6.190253 -4.358239 -1.817529 -1.879332 -1.934056 -2.919351 -1.811348 -1.146041 -0.439357 -0.368946	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691 -3.366228 -1.384418 -0.909141 -0.600415 -3.386935 -4.404625 -3.577413 -4.003456 -2.617053 -4.269849 -2.829514 -2.612507	Н С Н С С Н С Н Н Н С Н С Н С Н	-0.161888 0.476605 -0.464802 -0.075293 -1.252590 -1.478147 -1.773699 -0.182711 0.342419 -1.286732 -2.079007 -1.768191 -0.854742 0.872481 1.649089 1.370199 0.407636 -2.645206 -2.929056 -1.867141 -0.956333	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506 -3.014682 -4.229497 -2.962899 -2.989762 -3.058730 -1.950967 -2.054844 -1.319894 -1.286918 -0.816800	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016 1.521071 2.463994 0.601335 -0.187667 1.583243 0.571354 -3.701907 -2.924548 -4.781268 -4.362716
H C C C C C H C H C H C H C H C H H C H H H H H H H H H H H H H H H H H H H H	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832 -0.756760 0.367840 1.356198 0.912370 2.879689 3.155482 3.415838 3.241475 0.976759 -0.112261 1.208617	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963 -5.287496 -6.190253 -4.358239 -1.817529 -1.879332 -1.934056 -2.919351 -1.811348 -1.146041 -0.439357 -0.368946 0.357148	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691 -3.366228 -1.384418 -0.909141 -0.600415 -3.386935 -4.404625 -3.577413 -4.003456 -2.617053 -4.269849 -2.829514 -2.612507 -3.562461	Н С Н С Н С Н Н Н С Н С Н Н Н С Н Н Н Н	-0.161888     0.476605     -0.464802     -0.075293     -1.252590     -1.478147     -1.773699     -0.182711     0.342419     -1.286732     -2.079007     -1.768191     -0.854742     0.872481     1.649089     1.370199     0.407636     -2.645206     -2.929056     -1.867141     -0.956333     -2.496396	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506 -3.014682 -4.229497 -2.962899 -2.989762 -3.058730 -1.950967 -2.054844 -1.319894 -1.286918 -0.816800 -0.482435	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016 1.521071 2.463994 0.601335 -0.187667 1.583243 0.571354 -3.701907 -2.924548 -4.781268 -4.362716 -5.215380
H C C C C H C H C H C H H H H C H	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832 -0.756760 0.367840 1.356198 0.912370 2.879689 3.155482 3.415838 3.241475 0.976759 -0.112261	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963 -5.287496 -6.190253 -4.358239 -1.817529 -1.879332 -1.934056 -2.919351 -1.811348 -1.146041 -0.439357 -0.368946	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691 -3.366228 -1.384418 -0.909141 -0.600415 -3.386935 -4.404625 -3.577413 -4.003456 -2.617053 -4.269849 -2.829514 -2.612507	Н С Н С С Н С Н Н Н С Н С Н С Н	-0.161888 0.476605 -0.464802 -0.075293 -1.252590 -1.478147 -1.773699 -0.182711 0.342419 -1.286732 -2.079007 -1.768191 -0.854742 0.872481 1.649089 1.370199 0.407636 -2.645206 -2.929056 -1.867141 -0.956333	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506 -3.014682 -4.229497 -2.962899 -2.989762 -3.058730 -1.950967 -2.054844 -1.319894 -1.286918 -0.816800	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016 1.521071 2.463994 0.601335 -0.187667 1.583243 0.571354 -3.701907 -2.924548 -4.781268 -4.362716
H C C C C H C H C H H H H H H H H	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832 -0.756760 0.367840 1.356198 0.912370 2.879689 3.155482 3.415838 3.241475 0.976759 -0.112261 1.208617 1.540983	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963 -5.287496 -6.190253 -4.358239 -1.817529 -1.879332 -1.934056 -2.919351 -1.811348 -1.146041 -0.439357 -0.368946 0.357148 -0.197442	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691 -3.366228 -1.384418 -0.909141 -0.600415 -3.386935 -4.404625 -3.577413 -4.003456 -2.617053 -4.269849 -2.829514 -2.612507 -3.562461 -1.906342	Н С Н С С Н С Н Н Н С Н С Н Н Н Н Н Н Н	-0.161888     0.476605     -0.464802     -0.075293     -1.252590     -1.478147     -1.773699     -0.182711     0.342419     -1.286732     -2.079007     -1.768191     -0.854742     0.872481     1.649089     1.370199     0.407636     -2.645206     -2.929056     -1.867141     -0.956333     -2.496396     -1.553184	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506 -3.014682 -4.229497 -2.962899 -2.989762 -3.058730 -1.950967 -2.054844 -1.319894 -1.286918 -0.816800 -0.482435 -1.950277	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016 1.521071 2.463994 0.601335 -0.187667 1.583243 0.571354 -3.701907 -2.924548 -4.781268 -4.362716 -5.215380 -5.614515
H C C C C H C H C C H H H H C C H H H H	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832 -0.756760 0.367840 1.356198 0.912370 2.879689 3.155482 3.415838 3.241475 0.976759 -0.112261 1.208617 1.540983 0.646025	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963 -5.287496 -6.190253 -4.358239 -1.817529 -1.879332 -1.934056 -2.919351 -1.811348 -1.146041 -0.439357 -0.368946 0.357148 -0.197442 -4.679281	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691 -3.366228 -1.384418 -0.909141 -0.600415 -3.386935 -4.404625 -3.577413 -4.003456 -2.617053 -4.269849 -2.829514 -2.612507 -3.562461 -1.906342 0.869116	Н С Н С С Н С Н Н Н С Н С Н Н Н С Н С Н	-0.161888     0.476605     -0.464802     -0.075293     -1.252590     -1.478147     -1.773699     -0.182711     0.342419     -1.286732     -2.079007     -1.768191     -0.854742     0.872481     1.649089     1.370199     0.407636     -2.645206     -2.929056     -1.867141     -0.956333     -2.496396     -1.553184     -3.946504	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506 -3.014682 -4.229497 -2.962899 -2.989762 -3.058730 -1.950967 -2.054844 -1.319894 -1.286918 -0.816800 -0.482435 -1.950277 -2.652860	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016 1.521071 2.463994 0.601335 -0.187667 1.583243 0.571354 -3.701907 -2.924548 -4.781268 -4.362716 -5.215380 -5.614515 -4.259293
H C C C C H C H C C H C H H H H C H	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832 -0.756760 0.367840 1.356198 0.912370 2.879689 3.155482 3.415838 3.241475 0.976759 -0.112261 1.208617 1.540983 0.646025 1.113062	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963 -5.287496 -6.190253 -4.358239 -1.817529 -1.879332 -1.934056 -2.919351 -1.811348 -1.146041 -0.439357 -0.368946 0.357148 -0.197442 -4.679281 -3.783819	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691 -3.366228 -1.384418 -0.909141 -0.600415 -3.386935 -4.404625 -3.577413 -4.003456 -2.617053 -4.269849 -2.829514 -2.612507 -3.562461 -1.906342 0.869116 1.320946	Н С Н С С Н С Н Н Н С Н С Н Н Н С Н	-0.161888     0.476605     -0.464802     -0.075293     -1.252590     -1.478147     -1.773699     -0.182711     0.342419     -1.286732     -2.079007     -1.768191     -0.854742     0.872481     1.649089     1.370199     0.407636     -2.645206     -2.929056     -1.867141     -0.956333     -2.496396     -1.553184     -3.946504     -4.533722	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506 -3.014682 -4.229497 -2.962899 -2.989762 -3.058730 -1.950967 -2.054844 -1.319894 -1.286918 -0.816800 -0.482435 -1.950277 -2.652860 -3.153117	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016 1.521071 2.463994 0.601335 -0.187667 1.583243 0.571354 -3.701907 -2.924548 -4.781268 -4.362716 -5.215380 -5.614515 -4.259293 -3.463731
H C C C C H C H C H H H H C C H C H C H	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832 -0.756760 0.367840 1.356198 0.912370 2.879689 3.155482 3.415838 3.241475 0.976759 -0.112261 1.208617 1.540983 0.646025 1.113062 -0.618547	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963 -5.287496 -6.190253 -4.358239 -1.817529 -1.879332 -1.934056 -2.919351 -1.811348 -1.146041 -0.439357 -0.368946 0.357148 -0.197442 -4.679281 -3.783819 -4.979769	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691 -3.366228 -1.384418 -0.909141 -0.600415 -3.386935 -4.404625 -3.577413 -4.003456 -2.617053 -4.269849 -2.829514 -2.612507 -3.562461 -1.906342 0.869116 1.320946 1.683760	Н С Н С С Н С Н Н Н С Н С Н Н Н С Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н	-0.161888     0.476605     -0.464802     -0.075293     -1.252590     -1.478147     -1.773699     -0.182711     0.342419     -1.286732     -2.079007     -1.768191     -0.854742     0.872481     1.649089     1.370199     0.407636     -2.645206     -2.929056     -1.867141     -0.956333     -2.496396     -1.553184     -3.946504     -4.533722     -3.742869	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506 -3.014682 -4.229497 -2.962899 -2.989762 -3.058730 -1.950967 -2.054844 -1.319894 -1.286918 -0.816800 -0.482435 -1.950277 -2.652860 -3.153117 -3.403312	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016 1.521071 2.463994 0.601335 -0.187667 1.583243 0.571354 -3.701907 -2.924548 -4.781268 -4.362716 -5.215380 -5.614515 -4.259293 -3.463731 -5.051406
H C C C C H C H C C H C H H H H C H	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832 -0.756760 0.367840 1.356198 0.912370 2.879689 3.155482 3.415838 3.241475 0.976759 -0.112261 1.208617 1.540983 0.646025 1.113062	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963 -5.287496 -6.190253 -4.358239 -1.817529 -1.879332 -1.934056 -2.919351 -1.811348 -1.146041 -0.439357 -0.368946 0.357148 -0.197442 -4.679281 -3.783819	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691 -3.366228 -1.384418 -0.909141 -0.600415 -3.386935 -4.404625 -3.577413 -4.003456 -2.617053 -4.269849 -2.829514 -2.612507 -3.562461 -1.906342 0.869116 1.320946	Н С Н С С Н С Н Н Н С Н С Н Н Н С Н	-0.161888     0.476605     -0.464802     -0.075293     -1.252590     -1.478147     -1.773699     -0.182711     0.342419     -1.286732     -2.079007     -1.768191     -0.854742     0.872481     1.649089     1.370199     0.407636     -2.645206     -2.929056     -1.867141     -0.956333     -2.496396     -1.553184     -3.946504     -4.533722	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506 -3.014682 -4.229497 -2.962899 -2.989762 -3.058730 -1.950967 -2.054844 -1.319894 -1.286918 -0.816800 -0.482435 -1.950277 -2.652860 -3.153117	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016 1.521071 2.463994 0.601335 -0.187667 1.583243 0.571354 -3.701907 -2.924548 -4.781268 -4.362716 -5.215380 -5.614515 -4.259293 -3.463731
H C C C C H C H C H H H C H H C H C H	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832 -0.756760 0.367840 1.356198 0.912370 2.879689 3.155482 3.415838 3.241475 0.976759 -0.112261 1.208617 1.540983 0.646025 1.113062 -0.618547 -1.292993	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963 -5.287496 -6.190253 -4.358239 -1.817529 -1.87529 -1.879332 -1.934056 -2.919351 -1.811348 -1.146041 -0.439357 -0.368946 0.357148 -0.197442 -4.679281 -3.783819 -4.979769 -4.104038	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691 -3.366228 -1.384418 -0.909141 -0.600415 -3.386935 -4.404625 -3.577413 -4.003456 -2.617053 -4.269849 -2.829514 -2.612507 -3.562461 -1.906342 0.869116 1.320946 1.683760 1.683760	Н С Н С С Н С Н Н Н С Н Н Н С Н Н Н Н Н	-0.161888     0.476605     -0.464802     -0.075293     -1.252590     -1.478147     -1.773699     -0.182711     0.342419     -1.286732     -2.079007     -1.768191     -0.854742     0.872481     1.649089     1.370199     0.407636     -2.645206     -2.929056     -1.867141     -0.956333     -2.496396     -1.553184     -3.946504     -4.533722     -3.742869     -4.581625	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506 -3.014682 -4.229497 -2.962899 -2.989762 -3.058730 -1.950967 -2.054844 -1.319894 -1.286918 -0.816800 -0.482435 -1.950277 -2.652860 -3.153117 -3.403312 -1.859613	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016 1.521071 2.463994 0.601335 -0.187667 1.583243 0.571354 -3.701907 -2.924548 -4.781268 -4.362716 -5.215380 -5.614515 -4.259293 -3.463731 -5.051406 -4.704976
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H C C C C H C H C C H C H H H C H C H H H H H H H H H H H H H H H H H H H H	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832 -0.756760 0.367840 1.356198 0.912370 2.879689 3.155482 3.415838 3.241475 0.976759 -0.112261 1.208617 1.540983 0.646025 1.113062 -0.618547 -1.292993 -0.350313 -1.186523	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.988394 -3.809978 -5.096795 -5.837963 -5.287496 -6.190253 -4.358239 -1.817529 -1.879332 -1.934056 -2.919351 -1.811348 -1.146041 -0.439357 -0.368946 0.357148 -0.197442 -4.679281 -3.783819 -4.979769 -4.104038 -5.222757 -5.843746	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691 -3.366228 -1.384418 -0.909141 -0.600415 -3.386935 -4.404625 -3.577413 -4.003456 -2.617053 -4.269849 -2.829514 -2.612507 -3.562461 -1.906342 0.869116 1.320946 1.683760 1.698574 2.732534 1.279826	НСНССНСИНННСНСНННСНННСС	-0.161888     0.476605     -0.464802     -0.075293     -1.252590     -1.478147     -1.773699     -0.182711     0.342419     -1.286732     -2.079007     -1.768191     -0.854742     0.872481     1.649089     1.370199     0.407636     -2.645206     -2.929056     -1.867141     -0.956333     -2.496396     -1.553184     -3.946504     -4.533722     -3.742869     -4.581625     -2.663473     -2.680431	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506 -3.014682 -4.229497 -2.962899 -2.989762 -3.058730 -1.950967 -2.054844 -1.319894 -1.286918 -0.816800 -0.482435 -1.950277 -2.652860 -3.153117 -3.403312 -1.859613 1.344286 2.506110	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016 1.521071 2.463994 0.601335 -0.187667 1.583243 0.571354 -3.701907 -2.924548 -4.781268 -4.362716 -5.215380 -5.614515 -4.259293 -3.463731 -5.051406 -4.704976 0.834564 0.005265
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H C C C C H C H C C H C H H H C H C H H H H C H H H H H H H H H H H H H H H H H H H H	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832 -0.75600 0.367840 1.356198 0.912370 2.879689 3.155482 3.415838 3.241475 0.976759 -0.112261 1.208617 1.540983 0.646025 1.113062 -0.618547 -1.292993 -0.350313 -1.186523 1.664538 2.602805 1.262031 1.918489	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963 -5.287496 -6.190253 -4.358239 -1.817529 -1.879332 -1.934056 -2.919351 -1.811348 -1.146041 -0.439357 -0.368946 0.357148 -0.197442 -4.679281 -3.783819 -4.979769 -4.104038 -5.222757 -5.843746 -5.826947 -5.586576 -6.769288 -6.015884	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691 -3.366228 -1.384418 -0.909141 -0.600415 -3.386935 -4.404625 -3.577413 -4.003456 -2.617053 -4.269849 -2.829514 -2.612507 -3.562461 -1.906342 0.869116 1.320946 1.688760 1.688760 1.698574 2.732534 1.279826 0.986122 0.449225 0.559611 2.049764	Н С Н С С Н С Н Н Н С Н С Н Н Н С Н Н Н С С С Н С Н	-0.161888     0.476605     -0.464802     -0.075293     -1.252590     -1.478147     -1.773699     -0.182711     0.342419     -1.286732     -2.079007     -1.768191     -0.854742     0.872481     1.649089     1.370199     0.407636     -2.645206     -2.929056     -1.867141     -0.956333     -2.496396     -1.553184     -3.946504     -4.533722     -3.742869     -4.581625     -2.663473     -2.680431     -2.540526     -2.554293     -2.330767	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506 -3.014682 -4.229497 -2.962899 -2.989762 -3.058730 -1.950967 -2.054844 -1.319894 -1.286918 -0.816800 -0.482435 -1.950277 -2.652860 -3.153117 -3.403312 -1.859613 1.344286 2.506110 3.770234 4.669474 3.902590 4.901035	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016 1.521071 2.463994 0.601335 -0.187667 1.583243 0.571354 -3.701907 -2.924548 -4.781268 -4.362716 -5.215380 -5.614515 -4.259293 -3.463731 -5.051406 -4.704976 0.834564 0.005265 0.620221 -0.015488 2.005053 2.457921
Н С С С С Н С Н С С Н С Н Н Н С Н С Н Н Н С Н Н Н С Н Н Н С Н Н Н С С Н Н Н Н С Н С Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С Л Н Н Н С Л Н Н Н Н	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832 -0.756760 0.367840 1.356198 0.912370 2.879689 3.155482 3.415838 3.241475 0.976759 -0.112261 1.208617 1.540983 0.646025 1.113062 -0.618547 -1.292993 -0.350313 -1.186523 1.664538 2.602805 1.262031 1.918489 1.921570	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963 -5.287496 -6.190253 -4.358239 -1.817529 -1.879332 -1.934056 -2.919351 -1.811348 -1.146041 -0.439357 -0.368946 0.357148 -0.197442 -4.679281 -3.783819 -4.979769 -4.104038 -5.222757 -5.843746 -5.826947 -5.586576 -6.769288 -6.015884 0.212665	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691 -3.366228 -1.384418 -0.909141 -0.600415 -3.386935 -4.404625 -3.577413 -4.003456 -2.617053 -4.269849 -2.829514 -2.612507 -3.562461 -1.906342 0.869116 1.320946 1.683760 1.698574 2.732534 1.279826 0.986122 0.449225 0.559611 2.049764 2.488354	Н С Н С С Н С Н Н Н С Н Н Н С Н Н Н С С С Н С Н С	-0.161888     0.476605     -0.464802     -0.075293     -1.252590     -1.478147     -1.773699     -0.182711     0.342419     -1.286732     -2.079007     -1.768191     -0.854742     0.872481     1.649089     1.370199     0.407636     -2.645206     -2.929056     -1.867141     -0.956333     -2.496396     -1.553184     -3.946504     -4.533722     -3.742869     -4.581625     -2.663473     -2.663473     -2.6680431     -2.5542936     -2.3330767     -2.446584	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506 -3.014682 -4.229497 -2.962899 -2.989762 -3.058730 -1.950967 -2.054844 -1.319894 -1.286918 -0.816800 -0.482435 -1.950277 -2.652860 -3.153117 -3.403312 -1.859613 1.344286 2.506110 3.770234 4.669474 3.902590 4.901035 2.761897	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016 1.521071 2.463994 0.601335 -0.187667 1.583243 0.571354 -3.701907 -2.924548 -4.781268 -4.362716 -5.215380 -5.614515 -4.259293 -3.463731 -5.051406 -4.704976 0.834564 0.005265 0.620221 -0.015488 2.005053 2.457921 2.818234
Н С С С С Н С Н С С Н С Н Н Н С Н С Н Н Н С С Н С Н Н Н С С С Н С С Н С Н Н Н С С Н Н Н С С С	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832 -0.756760 0.367840 1.356198 0.912370 2.879689 3.155482 3.415838 3.241475 0.976759 -0.112261 1.208617 1.540983 0.646025 1.113062 -0.618547 -1.292993 -0.350313 -1.186523 1.664538 2.602805 1.262031 1.918489 1.921570 1.161743	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963 -5.287496 -6.190253 -4.358239 -1.817529 -1.87529 -1.87529 -1.879332 -1.934056 -2.919351 -1.811348 -1.146041 -0.439357 -0.368946 0.357148 -0.197442 -4.679281 -3.783819 -4.979769 -4.104038 -5.222757 -5.843746 -5.826947 -5.586576 -6.769288 -6.015884 0.212665 -0.240624	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691 -3.366228 -1.384418 -0.909141 -0.600415 -3.386935 -4.404625 -3.577413 -4.003456 -2.617053 -4.269849 -2.829514 -2.612507 -3.562461 -1.906342 0.869116 1.320946 1.683760 1.683760 1.698574 2.732534 1.279826 0.986122 0.449225 0.559611 2.049764 2.488354 3.612865	НСНСНССНСНННСНННСНСНННСССНСНСН	-0.161888     0.476605     -0.464802     -0.075293     -1.252590     -1.478147     -1.73699     -0.182711     0.342419     -1.286732     -2.079007     -1.768191     -0.854742     0.872481     1.649089     1.370199     0.407636     -2.645206     -2.929056     -1.867141     -0.956333     -2.496396     -1.553184     -3.946504     -4.533722     -3.742869     -4.581625     -2.663473     -2.680431     -2.540526     -2.554293     -2.425936     -2.330767     -2.446584     -2.370270	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506 -3.014682 -4.229497 -2.962899 -2.989762 -3.058730 -1.950967 -2.054844 -1.319894 -1.286918 -0.816800 -0.482435 -1.950277 -2.652860 -3.153117 -3.403312 -1.859613 1.344286 2.506110 3.770234 4.669474 3.902590 4.901035 2.761897 2.874994	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016 1.521071 2.463994 0.601335 -0.187667 1.583243 0.571354 -3.701907 -2.924548 -4.781268 -4.362716 -5.215380 -5.614515 -4.259293 -3.463731 -5.051406 -4.704976 0.834564 0.005265 0.620221 -0.015488 2.005053 2.457921 2.818234 3.908106
Н С С С С Н С Н С С Н С Н Н Н С Н С Н Н Н С Н Н Н С Н Н Н С Н Н Н С С Н Н Н Н С Н С Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С С Н Н Н Н С Л Н Н Н С Л Н Н Н Н	5.068058 3.578233 4.234251 2.268722 0.914325 0.751337 0.042283 -0.072280 -0.501165 -1.045446 -0.341832 -0.756760 0.367840 1.356198 0.912370 2.879689 3.155482 3.415838 3.241475 0.976759 -0.112261 1.208617 1.540983 0.646025 1.113062 -0.618547 -1.292993 -0.350313 -1.186523 1.664538 2.602805 1.262031 1.918489 1.921570	-2.673611 -1.304022 -0.924400 -0.781695 -3.196216 -2.993605 -3.958394 -3.809978 -5.096795 -5.837963 -5.287496 -6.190253 -4.358239 -1.817529 -1.879332 -1.934056 -2.919351 -1.811348 -1.146041 -0.439357 -0.368946 0.357148 -0.197442 -4.679281 -3.783819 -4.979769 -4.104038 -5.222757 -5.843746 -5.826947 -5.586576 -6.769288 -6.015884 0.212665	0.730728 1.531161 2.329100 1.420453 -1.223519 -2.621190 -3.365730 -4.451164 -2.760691 -3.366228 -1.384418 -0.909141 -0.600415 -3.386935 -4.404625 -3.577413 -4.003456 -2.617053 -4.269849 -2.829514 -2.612507 -3.562461 -1.906342 0.869116 1.320946 1.683760 1.698574 2.732534 1.279826 0.986122 0.449225 0.559611 2.049764 2.488354	Н С Н С С Н С Н Н Н С Н Н Н С Н Н Н С С С Н С Н С	-0.161888     0.476605     -0.464802     -0.075293     -1.252590     -1.478147     -1.773699     -0.182711     0.342419     -1.286732     -2.079007     -1.768191     -0.854742     0.872481     1.649089     1.370199     0.407636     -2.645206     -2.929056     -1.867141     -0.956333     -2.496396     -1.553184     -3.946504     -4.533722     -3.742869     -4.581625     -2.663473     -2.663473     -2.6680431     -2.5542936     -2.3330767     -2.446584	-5.872562 -5.159507 -5.982507 -4.156005 -4.185689 -3.109974 -4.059315 -5.030160 -4.008389 -4.756506 -3.014682 -4.229497 -2.962899 -2.989762 -3.058730 -1.950967 -2.054844 -1.319894 -1.286918 -0.816800 -0.482435 -1.950277 -2.652860 -3.153117 -3.403312 -1.859613 1.344286 2.506110 3.770234 4.669474 3.902590 4.901035 2.761897	-1.876260 -1.422759 -3.240531 -3.858972 -3.810238 -4.887596 -3.024905 0.397773 0.533645 1.466494 1.264016 1.521071 2.463994 0.601335 -0.187667 1.583243 0.571354 -3.701907 -2.924548 -4.781268 -4.362716 -5.215380 -5.614515 -4.259293 -3.463731 -5.051406 -4.704976 0.834564 0.005265 0.620221 -0.015488 2.005053 2.457921 2.818234

C	-3.032636	2.526869	-1.485132		-3c) = -3593.86363		
H C	-2.752323 -2.291197	3.549103 1.546870	-1.820604 -2.400357		1-xTB) = $-169.708$ 9 2-xTB) = $-169.225$ 7		
Н	-2.291197	1.477809	-2.400357		-FF) = $-24.126324$		
H	-2.355184	1.882174	-3.455313			93.609934844182 Ha	rtree
Н	-2.708727	0.527208	-2.342426			VP) = -3592.330664	
C	-4.557284	2.412929	-1.683947			ZVP) = -3592.62461	
H	-5.101800	3.164320	-1.078068		h-3c) = -3588.8233		
H	-4.919795	1.406766	-1.394277	E(PM6	) = 151.96419 Kca	l/mol	
H	-4.819446	2.572068	-2.750373		) = 55.64619 Kcal,		
C	-2.664509	0.248087	3.154593	E(ωB9	7X-V/def2-TZVP) =	-3596.37699765089	7 Hartree
H	-3.422513	-0.422735	2.700129				
C	-1.330801	-0.507188	3.173184		inates:	0 504550	0 000050
H	-1.002060	-0.796215	2.152509	Fe	-0.156784	0.504572	-0.386650
H H	-1.411848 -0.540933	-1.441452 0.118080	3.764633 3.622414	C C	0.423675 1.228397	-0.946465 -2.098916	-1.685348 -1.902727
C	-3.115958	0.548115	4.589244	C	0.834961	-3.030941	-2.890923
Н	-4.057842	1.132277	4.615744	Н	1.427625	-3.951050	-3.014557
Н	-2.342906	1.110229	5.153260	C	-0.257574	-2.789203	-3.736509
Н	-3.286520	-0.400904	5.136018	Н	-0.521856	-3.521962	-4.514126
С	1.840243	0.478776	0.370793	С	-0.976196	-1.593457	-3.629695
C	2.591570	0.449364	1.592925	H	-1.761730	-1.365485	-4.360515
С	4.000249	0.355034	1.565366	C	-0.645899	-0.676454	-2.607912
H	4.545968	0.335210	2.521009	C	2.566034	-2.378007	-1.261117
С	4.711581	0.346828	0.359821	С	2.679433	-3.052099	-0.018396
H	5.810214	0.280376	0.360237	C	3.952612	-3.444186	0.441959
C	4.007955	0.488338	-0.837380	H	4.037372	-3.974773	1.402985
H	4.548747	0.570871	-1.792207	C	5.103077	-3.194597	-0.311765
С	2.595323	0.552755	-0.839090	H C	6.088828	-3.520891	0.053930
C C	2.001886 1.970123	0.711312 -0.280909	2.951819 3.970930	Н	4.992171 5.898792	-2.515819 -2.306457	-1.530393 -2.118147
C	1.470328	0.061984	5.243760	С	3.741957	-2.092318	-2.018346
Н	1.470320	-0.703464	6.033710	C	1.450943	-3.457515	0.780208
C	1.003275	1.351593	5.516307	Н	0.576221	-3.005625	0.274161
Н	0.591701	1.593507	6.508409	C	1.480591	-2.928326	2.221364
C	1.095317	2.342602	4.530520	Н	1.523038	-1.821537	2.241396
H	0.783927	3.371210	4.765852	H	2.355101	-3.315613	2.783964
С	1.627886	2.055083	3.260060	H	0.570373	-3.233133	2.774346
C	2.501954	-1.693018	3.747475	С	1.278182	-4.986077	0.729109
H	2.671863	-1.810516	2.657564	H	1.196179	-5.343120	-0.317480
C	1.513287	-2.782235	4.194468	H	0.365785	-5.303951	1.272469
H	0.522348	-2.655376	3.719223	H	2.142535	-5.504638	1.193130
H	1.363178	-2.772952	5.293540	С	3.683989	-1.364498	-3.358959
H	1.896273	-3.788724	3.927502	H	2.676884	-0.911211	-3.440346
C	3.856845	-1.886843	4.453982	C	4.709946	-0.224205	-3.460533
H H	4.609597 4.260702	-1.148801 -2.901617	4.114400 4.258184	H H	4.655536 4.528267	0.456412 0.374621	-2.588752 -4.376695
Н	3.749243	-1.770308	5.552526	Н	5.749311	-0.607776	-3.522819
C	1.989688	3.197530	2.313608	C	3.843119	-2.341665	-4.537261
Н	2.043492	2.773699	1.293615	Н	3.056127	-3.120027	-4.525915
C	0.985357	4.350144	2.277645	Н	4.827294	-2.853371	-4.496255
Н	-0.021656	3.998077	1.989750	H	3.778711	-1.804144	-5.506100
H	1.308078	5.112710	1.539648	C	-1.339220	0.633749	-2.349913
H	0.901585	4.868839	3.255503	C	-0.492695	1.806592	-2.157062
C	3.399006	3.711282	2.668046	C	-1.087573	2.948557	-1.546445
H	4.148615	2.896551	2.637768	H	-0.444376	3.823746	-1.365762
H	3.412008	4.147714	3.688686	C	-2.445490	3.001116	-1.248570
H	3.720651	4.496672	1.952970	H	-2.867819	3.894247	-0.765949
C C	1.939683 2.054621	0.792967	-2.171422 -3.206433	C H	-3.283652	1.940617	-1.641138
C	1.543375	-0.181477 0.112972	-4.484644	С	-4.367361 -2.769462	2.029146 0.771015	-1.483775 -2.215902
Н	1.620344	-0.641067	-5.282546	C	0.857102	2.068316	-2.865683
C	0.945344	1.346299	-4.757877	Н	0.793477	3.149465	-3.120444
Н	0.549725	1.559077	-5.762837	C	2.077108	1.923098	-1.946860
С	0.859241	2.314034	-3.750972	Н	1.943133	2.496998	-1.008901
H	0.405706	3.287550	-3.982431	H	2.994643	2.305511	-2.438371
C	1.350731	2.068504	-2.454830	H	2.250053	0.859509	-1.683984
С	2.755717	-1.519622	-2.993054	С	1.030284	1.336415	-4.200548
H	2.986468	-1.607773	-1.912291	H	0.146173	1.472512	-4.855074
C	1.856883	-2.701816	-3.368940	H	1.185524	0.250092	-4.069817
H	0.898101	-2.665234	-2.821484	H	1.917151	1.740652	-4.729953
H	2.349969	-3.663994	-3.125096	C	-3.721948	-0.281809	-2.764588
H C	1.620930 4.087223	-2.717937 -1.580067	-4.452750 -3.763243	H C	-3.228719 -5.070749	-1.270396 -0.356946	-2.657345 -2.042854
Н	4.772023	-0.756195	-3.480403	Н	-4.946370	-0.463539	-0.951139
H	3.918005	-1.509268	-4.857981	H	-5.646934	-1.230711	-2.408820
Н	4.607860	-2.539902	-3.566473	Н	-5.692902	0.541147	-2.237018
C	1.347284	3.194606	-1.418732	C	-3.956866	-0.012728	-4.267733
Н	1.074254	2.736815	-0.442918	Н	-3.012718	0.104818	-4.835192
С	2.757070	3.796208	-1.265155	H	-4.529379	0.928833	-4.397762
H	3.501527	3.035405	-0.964271	H	-4.541975	-0.834683	-4.729364
H	2.756214	4.595473	-0.496407	С	-0.438306	0.589948	1.597255
H	3.090217	4.243395	-2.224734	С	-1.411868	-0.169940	2.318846
C	0.333423	4.309818	-1.693956	C	-1.166040	-0.536480	3.660844
H	-0.684795	3.914650	-1.866876	H	-1.912913	-1.150583	4.188910
H H	0.618647 0.285077	4.921536 4.992759	-2.575032 -0.823234	C H	-0.015448 0.166307	-0.102483 -0.405193	4.333026 5.375456
11	0.2030//	7.224133	0.023234	н С	0.858009	0.781611	3.690131
Confor	mation 6.			Н	1.703614	1.220538	4.241252
	licity: 5			C	0.648905	1.145417	2.340898
Charge				C	-2.800362	-0.488744	1.816426
-							

С	-3.137356	-1.759607	1.281793	Н	-4.649537	-0.611819	-3.449664
Ċ	-4.490814	-2.079456	1.056409	C	-2.553702	-0.123866	-3.155136
Н	-4.750356	-3.071959	0.656978	C	0.458904	-1.994857	-4.738190
С	-5.507245	-1.163637	1.343239	Н	1.162123	-1.453509	-4.074360
H	-6.560856	-1.431169	1.169626	C	0.803436	-1.608103	-6.186963
С	-5.173281	0.102172	1.838253	H	0.712772	-0.516120	-6.346104
H	-5.973403	0.824681	2.059102	H	0.123000	-2.110993	-6.905407
С	-3.833964	0.458392	2.084801	H	1.842474	-1.905746	-6.438334
С	-2.079019	-2.825174	1.046488	С	0.686188	-3.498487	-4.509256
Н	-1.095213	-2.329879	1.171154	Н	0.445291	-3.793386	-3.469022
C	-2.130624	-3.412534	-0.371545	Н	1.745820	-3.762447	-4.704690
				H		-4.120125	-5.185234
H	-1.941055	-2.633692	-1.135448		0.063707		
H	-3.112909	-3.879612	-0.590045	С	-2.879478	1.089848	-2.299038
H	-1.359004	-4.197685	-0.500130	H	-1.913820	1.488282	-1.930737
C	-2.197927	-3.921018	2.120475	С	-3.541561	2.175579	-3.166315
H	-2.103180	-3.495633	3.139488	H	-2.895982	2.460206	-4.021677
H	-1.410696	-4.691063	1.995661	H	-3.749128	3.087427	-2.571068
H	-3.181517	-4.431267	2.059519	H	-4.507640	1.820230	-3.580829
С	-3.532675	1.807084	2.730320	С	-3.743941	0.750917	-1.075185
Н	-2.452748	2.000171	2.585549	Н	-3.228878	0.043727	-0.397729
C	-4.300653	2.970405	2.087480	Н	-4.714785	0.299674	-1.367032
Н	-4.137990	3.002548	0.993242	H	-3.966809	1.663119	-0.486386
H							
	-3.964312	3.936955	2.515791	С	2.718224	0.167062	-0.462969
H	-5.393088	2.900920	2.268769	С	2.539765	-1.228427	-0.062598
С	-3.789254	1.755023	4.247243	С	2.978317	-1.605791	1.238570
H	-3.177805	0.968905	4.730698	H	2.806201	-2.636698	1.575995
H	-4.856738	1.538827	4.461740	С	3.648713	-0.711510	2.066192
H	-3.532588	2.724792	4.721576	H	3.968729	-1.023345	3.071040
C	1.529542	2.217675	1.754869	С	3.958775	0.579314	1.601299
С	2.918521	1.989856	1.544997	H	4.551197	1.243989	2.243579
С	3.725317	3.039595	1.060556	С	3.518460	1.044776	0.355720
Н	4.798068	2.860587	0.894223	C	2.285158	-2.337097	-1.106416
C	3.184753	4.294517	0.776856	Н	1.418475	-2.044045	-1.731947
Н	3.825393	5.100532	0.770050	C	3.508767	-2.422755	-2.036720
		4.527142					-2.570921
С	1.821843		1.002716	H	3.679600	-1.467521	
H	1.411541	5.526964	0.804892	H	3.360790	-3.217393	-2.796192
С	0.979567	3.519451	1.508473	Н	4.425207	-2.663242	-1.458525
C	3.577628	0.647678	1.837587	С	1.961576	-3.701110	-0.493809
H	2.770255	-0.093093	2.006538	H	1.133673	-3.644819	0.237651
С	4.419264	0.148157	0.658042	H	2.840533	-4.148080	0.015125
H	3.813395	0.067434	-0.263335	H	1.654582	-4.406711	-1.291166
H	4.824196	-0.858442	0.871087	C	3.854952	2.468395	-0.081377
H	5.279949	0.815980	0.448101	H	4.195996	2.418195	-1.134256
С	4.431271	0.713340	3.117128	С	2.605699	3.356806	-0.029580
Н	3.839184	1.032319	3.997465	Н	1.784913	2.952872	-0.648384
H	5.266107	1.435194	2.997735	H	2.828337	4.380489	-0.392458
H	4.872216	-0.279769	3.341280	H	2.239249	3.433877	1.010567
C	-0.462398	3.861652	1.885444	С	4.995713	3.115941	0.713780
H	-1.095677	3.024662	1.521454	H	5.910429	2.489681	0.726258
С	-0.615513	3.942940	3.417683	H	4.700246	3.319477	1.763785
H	-0.353082	2.989669	3.912214	H	5.256657	4.091750	0.257987
H	-1.661200	4.191435	3.691602	C	-0.789921	0.199170	1.564624
H	0.041992	4.736949	3.828487	С	-1.293616	1.486772	1.932946
С	-0.998077	5.158085	1.264551	C	-2.597009	1.606440	2.463219
Н	-0.854375	5.203361	0.167614	Н	-2.973630	2.607465	2.727625
Н	-0.512652	6.055217	1.702029	C	-3.393166	0.475947	2.693232
H	-2.084122	5.247903	1.466459		-4.409891	0.586909	3.099924
п	-2.004122	3.24/903	1.400459	H			
				С	-2.856889	-0.797311	2.468767
	nation 9.			H	-3.429227	-1.696889	2.743279
	icity: 5			С	-1.559890	-0.946227	1.926568
Charge:				C	-0.463034	2.746327	1.968213
E(B97-3	3c) = -3593.86519	9182437 Hartree		C	-0.645218	3.797663	1.030158
E(GFN1-	-xTB) = $-169.7101$	01482010 Hartree		С	0.002833	5.031287	1.239061
E (GFN2-	-xTB) = $-169.2248$	17520193 Hartree		H	-0.144392	5.846662	0.514173
	$^{\circ}$ F) = -24.1327528			С	0.829093	5.237764	2.346793
		3.612487956287 на	rtree	H	1.326639	6.208287	2.496271
		P) = -3592.333150		C	1.023535	4.196528	3.261701
		VP) = -3592.62620			1.665998	4.360030	4.140240
		82696111 Hartree		C	0.385254	2.952159	3.097743
	= 152.41249 Kcal			C	-1.560324	3.649405	-0.177495
						2.595846	
	= 53.08478 Kcal/		6 Hawt	H	-1.901255		-0.194658
F(0B)/X	-v/αerz-TZVP) =	-3596.37891512363	o martree	C	-0.825818	3.928361	-1.499969
~				H	-0.015068	3.194245	-1.674977
Coordin		0		H	-0.375267	4.941777	-1.513206
Fe	0.577094	-0.169639	0.162694	H	-1.520853	3.865096	-2.359072
С	0.666207	0.170487	-1.829836	С	-2.805635	4.539620	-0.023316
С	-0.018708	0.348229	-3.061099	H	-3.359661	4.299899	0.906406
C	0.574513	1.157036	-4.057097	Н	-3.500318	4.406811	-0.877750
H	0.013029	1.354796	-4.983969	H	-2.529276	5.613545	0.019603
C	1.888420	1.633338	-3.925771	С	0.513452	1.907086	4.200253
H	2.341913	2.219452	-4.739610	Н	0.152692	0.948636	3.781870
C	2.650667	1.289666	-2.802544	C	1.958887	1.686507	4.664618
Н	3.718442	1.548938	-2.768714	Н	2.612643	1.415507	3.813069
C	2.038590	0.586743	-1.742113	Н	2.002219	0.862966	5.406540
C	-1.217469	-0.457327	-3.493004	Н	2.385347	2.585933	5.155358
C							
	-0.959900	-1.557111	-4.368584	C	-0.407204	2.270828	5.379139
C	-2.047126	-2.259375	-4.921521	H	-1.462422	2.351335	5.050894
H	-1.855150	-3.099149	-5.606852	H	-0.113705	3.244307	5.824341
C	-3.367258	-1.924486	-4.598060	H	-0.354864	1.499434	6.174820
H	-4.205457	-2.489484	-5.033811	C	-1.021617	-2.355219	1.869839
С	-3.611741	-0.874408	-3.707462	C	-1.523295	-3.273517	0.906582

С	-1.215755	-4.643287	1.031407	Н	-0.674043	1.677329	4.528708
Н	-1.618861	-5.355562	0.296644	С	-1.980425	-1.509550	3.853700
C	-0.390005	-5.104548	2.058383	Н	-1.895119	-2.242817	3.027201
Н							
	-0.156072	-6.176823	2.144051	H	-3.036654	-1.180101	3.896484
C	0.160848	-4.190764	2.965752	H	-1.768522	-2.033953	4.808100
H	0.827464	-4.560455	3.757156	C	-2.508342	2.015167	-0.728295
C	-0.143285	-2.817829	2.900878	C	-2.496344	2.235409	-2.139242
C	-2.359823	-2.808336	-0.278011	C	-3.714622	2.136045	-2.837522
Н	-2.216163	-1.711071	-0.365878	H	-3.721268	2.302062	-3.923466
C	-1.864974	-3.430120	-1.588714	C	-4.914059	1.832829	-2.185142
Н		-3.227466	-1.740624	Н	-5.852737	1.765152	-2.755657
	-0.787606						
H	-2.414510	-3.006628	-2.447472	C	-4.910332	1.609958	-0.805874
H	-2.011610	-4.529612	-1.611985	H	-5.854611	1.367539	-0.294904
C	-3.862822	-3.068168	-0.086535	C	-3.723391	1.688016	-0.052964
H	-4.260530	-2.542354	0.802599	C	-1.222102	2.606806	-2.891444
H	-4.065675	-4.152581	0.037545	H	-0.392404	2.063721	-2.397892
Н	-4.426430	-2.713275	-0.973671	C	-0.913225	4.111510	-2.789714
C			3.961971	Н	0.026531		
	0.415101	-1.871885				4.345931	-3.330015
H	0.655407	-0.920214	3.442288	H	-0.784549	4.444706	-1.743688
C	-0.634330	-1.563780	5.047553	Н	-1.729654	4.714665	-3.239692
H	-1.526623	-1.059851	4.632072	C	-1.237152	2.171680	-4.362943
H	-0.203860	-0.902635	5.827339	H	-1.492112	1.099491	-4.473674
H	-0.965345	-2.500795	5.541642	H	-0.234761	2.319483	-4.809140
С	1.703765	-2.376347	4.625466	H	-1.953651	2.769387	-4.965244
Н	2.456764	-2.705249	3.883463	C	-3.799689	1.450195	1.454434
		-3.229354	5.308264	Н	-2.762348		
H	1.509462					1.389955	1.839645
H	2.155893	-1.569736	5.236466	С	-4.509594	0.130685	1.803737
				H	-5.556448	0.121566	1.439067
ONE	ם א כו			H	-4.546611	-0.002846	2.903286
ONE	IAS			H	-3.994835	-0.754014	1.380457
				С	-4.503329	2.617443	2.172812
Conform	nation 12.			Н	-4.029096	3.590825	1.949893
	icity: 3			Н	-4.480237	2.468893	3.272242
Charge:				H	-5.567253	2.688130	1.864553
	3c) = -3245.80740			C	0.685078	-0.349302	-2.903933
E(M06/d	lef2-TZVP) = -324	15.833553992144 Hai	rtree	C	1.328920	-0.071296	-4.138315
E(PBE -	<ul> <li>D3(BJ)/def2-TZ\</li> </ul>	(7P) = -3244.5466965	525168 Hartree	H	2.102130	0.707132	-4.185382
E(PBE0	- D3(BJ)/def2-T2	EVP) = -3244.79427	7672185 Hartree	С	0.971302	-0.745537	-5.312318
E (PBEh-	-3c) = $-3241.1225$	784359298 Hartree		H	1.496290	-0.493541	-6.248399
	= -144.03455 Kca			C	-0.049503	-1.714964	-5.336228
	= -168.29481 Kca			C	-0.710610	-1.967737	-4.115404
			E 11				
		-3246.87854583249	o Hartree	H	-1.534825	-2.699663	-4.087772
		257451535 Hartree		C	-0.356489	-1.312637	-2.933312
E(GFN2-	-xTB) = $-162.8423$	394260921 Hartree		H	-0.912143	-1.512962	-2.008761
E (GFN-F	(F) = -22.3294157	705169 Hartree		C	-0.413562	-2.458582	-6.596059
				H	-0.025400	-1.946412	-7.498692
Coordin	nates:			H	-1.512576	-2.560952	-6.708411
V	-0.120290	0.464668	-0.061726	Н	0.005194	-3.488890	-6.597809
0	0.294920	-2.666341	0.201537	С	2.127884	1.157053	-1.632775
0	-1.899268	-3.336947	0.535816	С	2.026449	2.427028	-1.015805
N	0.762403	0.846123	1.666870	H	1.036634	2.812922	-0.735170
N	-1.286121	2.079985	0.028479	C	3.164242	3.206607	-0.759095
N	0.984390	0.337146	-1.714138	H	3.041091	4.176166	-0.250247
N	-1.406749	-0.905059	0.212079	С	4.444823	2.786430	-1.158639
H	-2.409831	-0.696484	0.165737	C	4.537031	1.546069	-1.832968
C	0.847573	2.108425		Н			
			2.171137		5.524760	1.189511	-2.168617
С	0.075944	3.186209	1.701326	С	3.417265	0.743219	-2.059499
H	0.265409	4.154179	2.184760	H	3.530633	-0.233317	-2.549292
С	-0.997257	3.165850	0.776787	C	5.677590	3.603751	-0.867862
С	1.824741	2.381028	3.291854	H	6.291280	3.133155	-0.068838
H	1.650289	1.715012	4.159952	H	5.419027	4.625385	-0.527353
Н	1.760760	3.431307	3.628477	H	6.330164	3.694889	-1.760387
Н	2.860844	2.178600	2.950770	C	0.353765	-4.087379	0.496224
C			0.659345	C			
	-1.804220	4.441130			-1.143805	-4.544462 -4.235321	0.242732
H	-2.619531	4.360213	-0.080383	C	0.784696		1.957192
H	-1.140416	5.278841	0.362864	H	1.744065	-3.704684	2.105329
H	-2.239826	4.715153	1.640872	Н	0.920964	-5.297163	2.241487
C	1.263348	-0.218053	2.503114	H	0.048062	-3.773831	2.642451
С	2.593520	-0.697240	2.376504	C	1.379049	-4.733122	-0.432531
С	3.076121	-1.605823	3.339112	H	1.188751	-4.469110	-1.488970
Н	4.112384	-1.968038	3.256871	Н	1.365200	-5.836745	-0.328729
C	2.272577	-2.047958	4.393592	Н	2.394504	-4.376959	-0.170609
Н	2.675008	-2.742833	5.146283	C	-1.415643	-4.899219	-1.224871
C	0.940899	-1.623439	4.465728	H	-2.509543	-4.987933	-1.373657
H	0.296764	-2.000544	5.274310	H	-0.944447	-5.860222	-1.509136
С	0.406612	-0.724139	3.525564	H	-1.037655	-4.109946	-1.904019
C	3.501155	-0.297256	1.223970	С	-1.632578	-5.660682	1.160235
H	2.987336	0.499120	0.651887	H	-1.586292	-5.360756	2.223080
С	4.852332	0.267999	1.688300	Н	-1.024321	-6.577193	1.022991
Н	4.722071	1.131710	2.371545	Н	-2.685420	-5.907920	0.919877
Н	5.437224	0.614870	0.812768	В	-1.031662	-2.270614	0.335518
H	5.461528	-0.492061	2.220143		1.001002	2.2/0013	3.333310
				0			
C	3.689919	-1.506746	0.289512		rmation 14.		
H	4.108545	-2.371921	0.845641		plicity: 3		
H	4.390662	-1.263364	-0.532118	Charge			
H	2.721714	-1.817620	-0.149530	E(B97-	-3c) = -3245.807559	768978 Hartree	
С	-1.054632	-0.303039	3.633694		/def2-TZVP) = -3245		rtree
Н	-1.327446	0.142556	2.657229		- D3(BJ)/def2-TZVE		
C	-1.272837	0.765429	4.719448		) - D3(BJ)/def2-TZV		
Н	-0.995814	0.378815	5.722679		n-3c) = -3241.12174		marcree
н Н	-2.340139	1.068980	4.756281		(1-30) = -3241.12174 (1-30) = -149.80649  Kcal		
11	2.J4U1J7	1.000300	7./JUZOT	□ ( E M O )	, - 149.00043 MCdl	., mo±	

E (ωB97X		-3246.878271518955	Hartree	C H	-1.209572 -2.153514	3.954317 3.909950	-2.346868 -2.914423
	-xTB) = $-165.4445-xTB$ ) = $-162.8404$			C H	-0.569783 -1.011673	2.756078 1.805831	-2.011339 -2.341700
	$^{\circ}$ F) = -22.3281087			C	-1.351432	6.492679	-2.371714
				H	-0.821892	7.372733	-1.957323
Coordin V	nates: -0.143516	0.063693	-0.495559	H H	-2.395808 -1.405605	6.520002 6.623976	-1.995678 -3.473690
Ö	1.270747	-2.881901	2.293573	C	2.559140	1.395906	-0.665890
0	1.029832	-0.600079	2.607399	C	3.442253	1.946417	-1.627775
N N	-1.882254 -0.963366	0.610287 -0.765383	0.236333 -2.117671	H C	3.026190 4.826134	2.510843 1.775713	-2.473924 -1.518869
N	1.157776	1.526591	-0.796353	Н	5.480862	2.208901	-2.292783
N	0.474086	-1.504231	0.379142	С	5.399867	1.050351	-0.453821
H C	0.586779 -2.967546	-2.338918 0.854256	-0.208641 -0.550486	C H	4.517260 4.929877	0.511735 -0.049782	0.503694 1.358462
C	-3.083770	0.382172	-1.868678	C	3.130628	0.685183	0.413408
H	-4.010980	0.648243	-2.394089	H	2.474262	0.280407	1.194812
C C	-2.200281 -4.089515	-0.471740 1.700116	-2.573781 0.004800	C H	6.894007 7.342581	0.893167 1.730790	-0.325584 0.252611
Н	-4.462395	1.316497	0.974472	Н	7.390363	0.883740	-1.316710
H	-4.933069	1.761209	-0.706279	H	7.162852	-0.044192	0.201177
H C	-3.715787 -2.707467	2.727923 -1.024984	0.198118 -3.888150	C C	1.988394 1.426180	-2.570088 -1.134541	3.515753 3.897406
Н	-1.948798	-1.628477	-4.416116	C	3.481255	-2.554943	3.162215
Н	-3.024140	-0.194732	-4.551381	H	3.751568	-3.531689	2.715976
H C	-3.605369 -2.077164	-1.653000 0.690890	-3.719918 1.660803	H H	4.117538 3.705392	-2.387262 -1.770089	4.052977 2.413500
C	-2.720745	-0.408789	2.302324	C	1.699046	-3.658955	4.544915
С	-3.068225	-0.282108	3.658297	H	0.612531	-3.790649	4.699702
H	-3.587370	-1.112927	4.160258	H	2.169471	-3.416556	5.518836
C H	-2.759984 -3.048606	0.876803 0.960531	4.382574 5.441454	H C	2.113748 0.177275	-4.624153 -1.189835	4.193457 4.779739
C	-2.057717	1.913206	3.758989	Н	-0.269954	-0.179308	4.828645
H	-1.785637	2.810755	4.335684	H	0.418989	-1.521797	5.808419
C C	-1.700419 -3.050735	1.842514 -1.692407	2.398240 1.546439	H C	-0.588614 2.456783	-1.867331 -0.186447	4.357162 4.508218
Н	-2.480436	-1.657258	0.597190	Н	3.300944	-0.000628	3.819129
C	-2.587769	-2.945202	2.306614	H	2.856245	-0.593650	5.458696
H H	-1.492072 -2.836053	-2.940793 -3.857035	2.467993 1.727457	H B	1.976630 0.895139	0.788128 -1.668834	4.726025 1.724686
Н	-3.086266	-3.041791	3.293006	Б	0.055155	1.000034	1.724000
С	-4.544871	-1.789376	1.191218		mation 17.		
H H	-5.173041 -4.745946	-1.818330 -2.715484	2.106273 0.613336	Multip Charge	licity: 3		
Н	-4.879397	-0.932665	0.574914		3c) = -3245.80153	0001250 #	
				E (D) /-	30)3243.00133	9281332 Hartree	
C	-0.911047	2.977002	1.768271	E(M06/	def2-TZVP) = -324	5.829049263117 Ha	
H	-0.819017	2.977002 2.752789	1.768271 0.689134	E(M06/ E(PBE	def2-TZVP) = -324 - D3(BJ)/def2-TZV	5.829049263117 HaP) = $-3244.540307$	955796 Hartree
		2.977002	1.768271	E(M06/ E(PBE E(PBE0	def2-TZVP) = -324 - D3(BJ)/def2-TZV	5.829049263117 Ha. P) = $-3244.540307$ VP) = $-3244.78794$	955796 Hartree
H C H H	-0.819017 0.508390 0.481497 1.120244	2.977002 2.752789 3.018729 3.266349 3.789061	1.768271 0.689134 2.359534 3.441903 1.849961	E (M06/ E (PBE E (PBE0 E (PBEh E (PM6)	def2-TZVP) = -324 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' -3c) = -3241.1162 = -148.93650 Kca	5.829049263117 Ha P) = -3244.540307 VP) = -3244.78794 37118545 Hartree 1/mo1	955796 Hartree
Н С Н Н	-0.819017 0.508390 0.481497 1.120244 1.012928	2.977002 2.752789 3.018729 3.266349 3.789061 2.039307	1.768271 0.689134 2.359534 3.441903 1.849961 2.249786	E (M06/ E (PBE E (PBE0 E (PBEh E (PM6) E (PM7)	def2-TZVP) = -324 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZ -3c) = -3241.1162 = -148.93650 Kca = -167.99316 Kca	5.829049263117 Ha P) = -3244.540307 VP) = -3244.78794 37118545 Hartree 1/mol	955796 Hartree 4505697 Hartree
H C H H	-0.819017 0.508390 0.481497 1.120244	2.977002 2.752789 3.018729 3.266349 3.789061	1.768271 0.689134 2.359534 3.441903 1.849961	E (M06/ E (PBE E (PBE0 E (PBEh E (PM6) E (PM7) E (ωB97	def2-TZVP) = -324 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZ -3c) = -3241.1162 = -148.93650 Kca = -167.99316 Kca	5.829049263117 Ha P) = -3244.540307 VP) = -3244.78794 37118545 Hartree 1/mol 1/mol -3246.87209338705	955796 Hartree 4505697 Hartree
H C H H C H H	-0.819017 0.508390 0.481497 1.120244 1.012928 -1.613571 -2.638438 -1.043382	2.977002 2.752789 3.018729 3.266349 3.789061 2.039307 4.337945 4.304616 5.108317	1.768271 0.689134 2.359534 3.441903 1.849961 2.249786 1.886947 1.464555 1.329530	E (M06/ E (PBE E (PBE0 E (PBEh E (PM6) E (PM7) E (ωB97 E (GFN1 E (GFN2	def2-TZVP) = -324 - D3 (BJ)/def2-TZV - D3 (BJ)/def2-TZV -3c) = -3241.1162 = -148.93650 Kca = -167.99316 Kca X-V/def2-TZVP) = -XTB) = -165.4384 -XTB) = -162.8352	5.829049263117 Ha P) = -3244.540307 WP) = -3244.78794 37118545 Hartree 1/mol 1/mol -3246.87209338705 39133982 Hartree 64001613 Hartree	955796 Hartree 4505697 Hartree
Н С Н Н С Н Н	-0.819017 0.508390 0.481497 1.120244 1.012928 -1.613571 -2.638438 -1.043382 -1.695927	2.977002 2.752789 3.018729 3.266349 3.789061 2.039307 4.337945 4.304616 5.108317 4.671912	1.768271 0.689134 2.359534 3.441903 1.849961 2.249786 1.886947 1.464555 1.329530 2.942514	E (M06/ E (PBE E (PBE0 E (PBEh E (PM6) E (PM7) E (ωB97 E (GFN1 E (GFN2	def2-TZVP) = -324 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' -3c) = -3241.1162 = -148.93650 Kca = -167.99316 Kca X-V/def2-TZVP) = -xTB) = -165.4384	5.829049263117 Ha P) = -3244.540307 WP) = -3244.78794 37118545 Hartree 1/mol 1/mol -3246.87209338705 39133982 Hartree 64001613 Hartree	955796 Hartree 4505697 Hartree
H C H H C H H	-0.819017 0.508390 0.481497 1.120244 1.012928 -1.613571 -2.638438 -1.043382	2.977002 2.752789 3.018729 3.266349 3.789061 2.039307 4.337945 4.304616 5.108317	1.768271 0.689134 2.359534 3.441903 1.849961 2.249786 1.886947 1.464555 1.329530	E (M06/ E (PBE E (PBE0 E (PBEh E (PM6) E (PM7) E (ωB97 E (GFN1 E (GFN2	def2-TZVP) = -324 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZ - 3c) = -3241.1162 = -148.93650 Kca = -167.99316 Kca X-V/def2-TZVP) = -xTB) = -165.4384 -xTB) = -162.8352 FF) = -22.3224418	5.829049263117 Ha P) = -3244.540307 WP) = -3244.78794 37118545 Hartree 1/mol 1/mol -3246.87209338705 39133982 Hartree 64001613 Hartree	955796 Hartree 4505697 Hartree
H C H H C H H C C C	-0.819017 0.508390 0.481497 1.120244 1.012928 -1.613571 -2.638438 -1.043382 -1.695927 -0.160709 0.865545 1.621730	2.977002 2.752789 3.018729 3.266349 3.789061 2.039307 4.337945 4.304616 5.108317 4.671912 -1.755856 -1.350134 -2.353095	1.768271 0.689134 2.359534 3.441903 1.849961 2.249786 1.886947 1.464555 1.329530 2.942514 -2.784115 -3.691197 -4.326468	E (M06/ E (PBE E (PBE0 E (PBE0 E (PM6) E (PM7) E (ωB97 E (GFN1 E (GFN2 E (GFN- Coordi V	def2-TZVP) = -324 - D3 (BJ)/def2-TZV - D3 (BJ)/def2-TZV -3c) = -3241.1162 = -148.93650 Kca = -167.99316 Kca X-V/def2-TZVP) = -XTB) = -165.4384 -XTB) = -162.8352 FF) = -22.3224418 mates: 0.127637	5.829049263117 Ha P) = -3244.540307 VP) = -3244.78794 37118545 Hartree 1/mol 1/mol -3246.87209338705 39133982 Hartree 64001613 Hartree 39424 Hartree	955796 Hartree 4505697 Hartree 8 Hartree 0.105026
H C H H C H H C C C H	-0.819017 0.508390 0.481497 1.120244 1.012928 -1.613571 -2.638438 -1.043382 -1.695927 -0.160709 0.865545 1.621730 2.411565	2.977002 2.752789 3.018729 3.266349 3.789061 2.039307 4.337945 4.304616 5.108317 4.671912 -1.755856 -1.350134 -2.353095 -2.061420	1.768271 0.689134 2.359534 3.441903 1.849961 2.249786 1.886947 1.464555 1.329530 2.942514 -2.784115 -3.691197 -4.326468 -5.031820	E (M06/ E (PBE E (PBE0) E (PBE0) E (PM6) E (PM7) E (GB97 E (GFN1 E (GFN2 Coordi V	def2-TZVP) = -324 - D3 (BJ)/def2-TZV - D3 (BJ)/def2-TZV - D3 (BJ)/def2-TZ' -3c) = -3241.1162 = -148.93650 Kca = -167.99316 Kca X-V/def2-TZVP) = -xTB) = -165.4384 -xTB) = -162.8352 FF) = -22.3224418 mates: 0.127637 -2.083691	5.829049263117 Ha P) = -3244.540307 VP) = -3244.78794 37118545 Hartree 1/mol 1/mol -3246.87209338705 39133982 Hartree 64001613 Hartree 39424 Hartree	955796 Hartree 4505697 Hartree 8 Hartree 0.105026 1.787176
H C H H C H H C C C	-0.819017 0.508390 0.481497 1.120244 1.012928 -1.613571 -2.638438 -1.043382 -1.695927 -0.160709 0.865545 1.621730	2.977002 2.752789 3.018729 3.266349 3.789061 2.039307 4.337945 4.304616 5.108317 4.671912 -1.755856 -1.350134 -2.353095	1.768271 0.689134 2.359534 3.441903 1.849961 2.249786 1.886947 1.464555 1.329530 2.942514 -2.784115 -3.691197 -4.326468	E (M06/ E (PBE E (PBE0 E (PBE0 E (PM6) E (PM7) E (ωB97 E (GFN1 E (GFN2 E (GFN- Coordi V	def2-TZVP) = -324 - D3 (BJ)/def2-TZV - D3 (BJ)/def2-TZV -3c) = -3241.1162 = -148.93650 Kca = -167.99316 Kca X-V/def2-TZVP) = -XTB) = -165.4384 -XTB) = -162.8352 FF) = -22.3224418 mates: 0.127637	5.829049263117 Ha P) = -3244.540307 VP) = -3244.78794 37118545 Hartree 1/mol 1/mol -3246.87209338705 39133982 Hartree 64001613 Hartree 39424 Hartree	955796 Hartree 4505697 Hartree 8 Hartree 0.105026
Н С Н Н С Н Н С С С Н С Н С Н С Н С Н С	-0.819017 0.508390 0.481497 1.120244 1.012928 -1.613571 -2.638438 -1.043382 -1.695927 -0.160709 0.865545 1.621730 2.411565 1.393402 1.997026 0.405276	2.977002 2.752789 3.018729 3.266349 3.789061 2.039307 4.337945 4.304616 5.108317 4.671912 -1.755856 -1.350134 -2.353095 -2.061420 -3.712112 -4.474651 -4.093170	1.768271 0.689134 2.359534 3.441903 1.849961 2.249786 1.886947 1.464555 1.329530 2.942514 -2.784115 -3.691197 -4.326468 -5.031820 -4.083053 -4.598113 -3.172158	E (M06/ E (PBE E (PBE0 E (PBE0) E (PM6) E (PM7) E (GFN1 E (GFN2 E (GFN- Coordi V O O N N	def2-TZVP) = -324 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' -3c) = -3241.1162 -3c) = -3241.1162 = -148.93650 Kca = -167.99316 Kca X-V/def2-TZVP) = -xTB) = -165.4384 -xTB) = -162.8352 FF) = -22.3224418  nates:	5.829049263117 Ha P) = -3244.540307 VP) = -3244.78794 37118545 Hartree 1/mol -3246.87209338705 39133982 Hartree 64001613 Hartree 39424 Hartree  0.418946 -2.896228 -3.075856 0.254494 1.743630	955796 Hartree 4505697 Hartree 8 Hartree 0.105026 1.787176 0.205300 -0.239374 1.583545
Н С Н Н С Н С С С Н С Н С Н С Н	-0.819017 0.508390 0.481497 1.120244 1.012928 -1.613571 -2.638438 -1.043382 -1.695927 -0.160709 0.865545 1.621730 2.411565 1.393402 1.997026 0.405276 0.235840	2.977002 2.752789 3.018729 3.266349 3.789061 2.039307 4.337945 4.304616 5.108317 4.671912 -1.755856 -1.350134 -2.353095 -2.061420 -3.712112 -4.474651 -4.093170 -5.161653	1.768271 0.689134 2.359534 3.441903 1.849961 2.249786 1.886947 1.464555 1.329530 2.942514 -2.784115 -3.691197 -4.326468 -5.031820 -4.083053 -4.083053 -4.598113 -3.172158 -2.970772	E (M06/ E (PBE E (PBE0) E (PBE0) E (PM6) E (PM7) E (GB97 E (GFN1 E (GFN2 Coordi V O O N N	def2-TZVP) = -324 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV = -148.93650 Kca = -167.99316 Kca X-V/def2-TZVP) = -465.4384 -XTB) = -162.4384 -XTB) = -162.8352 FF) = -22.3224418  nates:	5.829049263117 Ha P) = -3244.540307 WP) = -3244.78794 37118545 Hartree 1/mol 1/mol -3246.87209338705 39133982 Hartree 64001613 Hartree 39424 Hartree  0.418946 -2.896228 -3.075856 0.254494 1.743630 1.099925	955796 Hartree 4505697 Hartree 8 Hartree 0.105026 1.787176 0.205300 -0.239374 1.583545 -1.451740
Н С Н Н С С С С Н С Н С С С Н С С С Н С С С С С С С С С С С С С С С С С С С С	-0.819017 0.508390 0.481497 1.120244 1.012928 -1.613571 -2.638438 -1.043382 -1.695927 -0.160709 0.865545 1.621730 2.411565 1.393402 1.997026 0.405276	2.977002 2.752789 3.018729 3.266349 3.789061 2.039307 4.337945 4.304616 5.108317 4.671912 -1.755856 -1.350134 -2.353095 -2.061420 -3.712112 -4.474651 -4.093170 -5.161653 -3.137962 0.121656	1.768271 0.689134 2.359534 3.441903 1.849961 2.249786 1.886947 1.464555 1.329530 2.942514 -2.784115 -3.691197 -4.326468 -5.031820 -4.083053 -4.598113 -3.172158	E (M06/ E (PBE E (PBE0 E (PBE0 E (PM6)) E (PM7) E (GFN1 E (GFN2 E (GFN- Coordi V O O N N N N H	def2-TZVP) = -324 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' -3c) = -3241.1162 -3c) = -3241.1162 = -148.93650 Kca = -167.99316 Kca X-V/def2-TZVP) = -xTB) = -165.4384 -xTB) = -162.8352 FF) = -22.3224418  nates:	5.829049263117 Ha P) = -3244.540307 VP) = -3244.78794 37118545 Hartree 1/mol -3246.87209338705 39133982 Hartree 64001613 Hartree 39424 Hartree  0.418946 -2.896228 -3.075856 0.254494 1.743630	955796 Hartree 4505697 Hartree 8 Hartree 0.105026 1.787176 0.205300 -0.239374 1.583545
Н С Н Н С С С С Н С Н С С Н С Н С Н С Н	-0.819017 0.508390 0.481497 1.120244 1.012928 -1.613571 -2.638438 -1.043382 -1.695927 -0.160709 0.865545 1.621730 2.411565 1.393402 1.997026 0.405276 0.235840 -0.382087 1.140300 1.031265	2.977002 2.752789 3.018729 3.266349 3.789061 2.039307 4.337945 4.304616 5.108317 4.671912 -1.755856 -1.350134 -2.353095 -2.061420 -3.712112 -4.474651 -4.093170 -5.161653 -3.137962 0.121656 0.668086	1.768271 0.689134 2.359534 3.441903 1.849961 2.249786 1.886947 1.464555 1.329530 2.942514 -2.784115 -3.691197 -4.326468 -5.031820 -4.083053 -4.598113 -3.172158 -2.970772 -2.501196 -3.994593 -3.034626	E (M06/ E (PBE C) PBE D) E (PBE D) E (PBE D) E (PMT) E (WB97 E) GFN1 E (GFN2 E) GFN- Coordi V O O N N N N N N N N N N N N N N N N N	def2-TZVP) = -324 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZ -3c) = -3241.1162 = -148.93650 Kca = -167.99316 Kca X-V/def2-TZVP) = -XTB) = -165.4384 -XTB) = -162.8352 FF) = -22.3224418  nates:  0.127637 -2.083691 -0.399281 2.101772 0.367103 -0.829279 -0.916974 -1.500420 3.025810	5.829049263117 Ha P) = -3244.540307 VP) = -3244.78794 37118545 Hartree 1/mol -3246.87209338705 39133982 Hartree 64001613 Hartree  0.418946 -2.896228 -3.075856 0.254494 1.743630 1.099925 -0.820014 -0.372342 1.121182	955796 Hartree 4505697 Hartree 8 Hartree 0.105026 1.787176 0.205300 -0.239374 1.583545 -1.451740 1.112620 1.833367 0.223751
Н С Н Н Н С С С Н С Н С С Н С С Н С С С Н С С С С С С С С С С С С С С С С С С С С	-0.819017 0.508390 0.481497 1.120244 1.012928 -1.613571 -2.638438 -1.043382 -1.695927 -0.160709 0.865545 1.621730 2.411565 1.393402 1.997026 0.405276 0.235840 -0.382087 1.140300 1.031265 0.122463	2.977002 2.752789 3.018729 3.266349 3.789061 2.039307 4.337945 4.304616 5.108317 4.671912 -1.755856 -1.350134 -2.353095 -2.061420 -3.712112 -4.474651 -4.093170 -5.161653 -3.137962 0.121656 0.668086 0.718363	1.768271 0.689134 2.359534 3.441903 1.849961 2.249786 1.886947 1.464555 1.329530 2.942514 -2.784115 -3.691197 -4.326468 -5.031820 -4.083053 -4.598113 -3.172158 -2.970772 -2.501196 -3.994593 -3.034626 -4.984164	E (M06/ E (PBE E (PBE0) E (PBE0) E (PM6) E (PM7) E (GB97) E (GFN1 E (GFN2 Coordi V O O N N N N N H C C	def2-TZVP) = -324 - D3 (BJ)/def2-TZV = -148.93650 Kca = -167.99316 Kca X-V/def2-TZVP) = -165.4384 -XTB) = -165.4384 -XTB) = -162.3322 FF) = -22.3224418  nates:	5.829049263117 Ha P) = -3244.540307 WP) = -3244.78794 37118545 Hartree 1/mol 1/mol -3246.87209338705 39133982 Hartree 64001613 Hartree 39424 Hartree  0.418946 -2.896228 -3.075856 0.254494 1.743630 1.099925 -0.820014 -0.372342 1.121182 2.163901	955796 Hartree 4505697 Hartree 8 Hartree 0.105026 1.787176 0.205300 -0.239374 1.583545 -1.451740 1.112620 1.833367 0.223751 1.127033
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Н С Н Н Н С С С Н С Н С С Н С Н Н Н С Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н	-0.819017 0.508390 0.481497 1.120244 1.012928 -1.613571 -2.638438 -1.043382 -1.695927 -0.160709 0.865545 1.621730 2.411565 1.393402 1.997026 0.405276 0.235840 -0.382087 1.140300 1.031265 0.122463 0.360285 -0.911430 0.147225 2.563862 3.331066 2.738458 2.725783	2.977002 2.752789 3.018729 3.266349 3.789061 2.039307 4.337945 4.304616 5.108317 4.671912 -1.755856 -1.350134 -2.353095 -2.061420 -3.712112 -4.474651 -4.093170 -5.161653 -3.137962 0.121656 0.668086 0.718363 1.783792 0.681044 0.175689 0.380021 -0.033554 1.470823 -0.045054	1.768271 0.689134 2.359534 3.441903 1.849961 2.249786 1.886947 1.464555 1.329530 2.942514 -2.784115 -3.691197 -4.326468 -5.031820 -4.083053 -4.598113 -3.172158 -2.970772 -2.501196 -3.994593 -3.034626 -4.984164 -5.178473 -4.598358 -5.952404 -4.504935 -3.821970 -4.585961 -5.517810	E (M06/ E (PBE) E (PBE) E (PBE) E (PM6) E (PM7) E (GFN1 E (GFN1 Coordi V O O N N N N H C C C H H C	def2-TZVP) = -324 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' - 3c) = -3241.1162 = -148.93650 Kca = -167.99316 Kca X-V/def2-TZVP) = -xTB) = -165.4384 -xTB) = -162.8352 FF) = -22.3224418  nates:	5.829049263117 Ha P) = -3244.78794 37118545 Hartree 1/mol 1/mol -3246.87209338705 39133982 Hartree 64001613 Hartree 0.418946 -2.896228 -3.075856 0.254494 1.743630 1.099925 -0.820014 -0.372342 1.121182 2.163901 2.817458 2.439037 0.995150 0.198101 0.7771097 1.954252 3.607116	955796 Hartree 4505697 Hartree  8 Hartree  0.105026 1.787176 0.205300 -0.239374 1.583545 -1.451740 1.112620 1.833367 0.223751 1.127033 1.390029 1.796011 -0.180437 -0.926642 0.711811 -0.593966 2.757513
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Н С Н Н Н С С С Н С Н С С Н С Н Н Н С Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н	-0.819017 0.508390 0.481497 1.120244 1.012928 -1.613571 -2.638438 -1.043382 -1.695927 -0.160709 0.865545 1.621730 2.411565 1.393402 1.997026 0.405276 0.235840 -0.382087 1.140300 1.031265 0.122463 0.360285 -0.911430 0.147225 2.563862 3.331066 2.738458 2.725783	2.977002 2.752789 3.018729 3.266349 3.789061 2.039307 4.337945 4.304616 5.108317 4.671912 -1.755856 -1.350134 -2.353095 -2.061420 -3.712112 -4.474651 -4.093170 -5.161653 -3.137962 0.121656 0.668086 0.718363 1.783792 0.681044 0.175689 0.380021 -0.033554 1.470823 -0.045054	1.768271 0.689134 2.359534 3.441903 1.849961 2.249786 1.886947 1.464555 1.329530 2.942514 -2.784115 -3.691197 -4.326468 -5.031820 -4.083053 -4.598113 -3.172158 -2.970772 -2.501196 -3.994593 -3.034626 -4.984164 -5.178473 -4.598358 -5.952404 -4.504935 -3.821970 -4.585961 -5.517810	E (M06/ E (PBE) E (PBE) E (PBE) E (PM6) E (PM7) E (GFN1 E (GFN1 Coordi V O O N N N N H C C C H H C	def2-TZVP) = -324 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' - 3c) = -3241.1162 = -148.93650 Kca = -167.99316 Kca X-V/def2-TZVP) = -xTB) = -165.4384 -xTB) = -162.8352 FF) = -22.3224418  nates:	5.829049263117 Ha P) = -3244.78794 37118545 Hartree 1/mol 1/mol -3246.87209338705 39133982 Hartree 64001613 Hartree 0.418946 -2.896228 -3.075856 0.254494 1.743630 1.099925 -0.820014 -0.372342 1.121182 2.163901 2.817458 2.439037 0.995150 0.198101 0.7771097 1.954252 3.607116	955796 Hartree 4505697 Hartree  8 Hartree  0.105026 1.787176 0.205300 -0.239374 1.583545 -1.451740 1.112620 1.833367 0.223751 1.127033 1.390029 1.796011 -0.180437 -0.926642 0.711811 -0.593966 2.757513
Н С Н Н Н С С С Н С Н С С Н С Н Н Н С Н Н Н С Н С Н	-0.819017 0.508390 0.481497 1.120244 1.012928 -1.613571 -2.638438 -1.043382 -1.695927 -0.160709 0.865545 1.621730 2.411565 1.393402 1.997026 0.405276 0.235840 -0.382087 1.140300 1.031265 0.122463 0.360285 -0.911430 0.147225 2.563862 3.331066 2.738458 2.725783 -1.449150 -1.809674 -0.893400 -0.543098	2.977002 2.752789 3.018729 3.266349 3.789061 2.039307 4.337945 4.304616 5.108317 4.671912 -1.755856 -1.350134 -2.353095 -2.061420 -3.712112 -4.474651 -4.093170 -5.161653 -3.137962 0.121656 0.668086 0.718363 1.783792 0.681044 0.175689 0.380021 -0.033554 1.470823 -0.045054 -3.625793 -2.743369 -4.639453 -5.567199	1.768271 0.689134 2.359534 3.441903 1.849961 2.249786 1.886947 1.464555 1.329530 2.942514 -2.784115 -3.691197 -4.326468 -5.031820 -4.083053 -4.598113 -3.172158 -2.970772 -2.501196 -3.994593 -3.034626 -4.984164 -5.178473 -4.598358 -5.952404 -4.504935 -3.821970 -4.585961 -5.517810 -1.521920 -0.956269 -0.504863 -1.001413	E (M06/ E (PBE) E (PBE) E (PBE) E (PM7) E (GFM7) E (GFN1- Coordi V O O N N N N H C C C H H C C H H H C H H C	def2-TZVP) = -324 - D3 (BJ)/def2-TZV - D3 (BJ)/def2-TZV - D3 (BJ)/def2-TZV - D3 (BJ)/def2-TZ' -3c) = -3241.1162 = -148.93650 Kca = -167.99316 Kca X-V/def2-TZVP) = -xTB) = -165.4384 -xTB) = -162.8352 FF) = -22.3224418  mates:	5.829049263117 Ha P) = -3244.78794 37118545 Hartree 1/mol 1/mol -3246.87209338705 39133982 Hartree 64001613 Hartree 39424 Hartree 0.418946 -2.896228 -3.075856 0.254494 1.743630 1.099925 -0.820014 -0.372342 1.121182 2.163901 2.817458 2.439037 0.995150 0.198101 0.771097 1.954252 3.607116 3.367038 4.455919 3.946901 -0.793270	955796 Hartree 4505697 Hartree  8 Hartree  0.105026 1.787176 0.205300 -0.239374 1.583545 -1.451740 1.112620 1.833367 0.223751 1.127033 1.390029 1.796011 -0.180437 -0.926642 0.711811 -0.593966 2.757513 3.702771 2.304025 2.986820 -1.166622
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Н С Н Н Н С С С Н С Н С С Н С Н Н Н С Н Н Н С Н С Н Н Н С Н Н Н С Н	-0.819017 0.508390 0.481497 1.120244 1.012928 -1.613571 -2.638438 -1.043382 -1.695927 -0.160709 0.865545 1.621730 2.411565 1.393402 1.997026 0.405276 0.235840 -0.382087 1.140300 1.031265 0.122463 0.360285 -0.911430 0.147225 2.563862 3.331066 2.738458 2.725783 -1.449150 -1.809674 -0.893400 -0.543098 -1.686626 -0.052094 -2.654463 -3.092232	2.977002 2.752789 3.018729 3.266349 3.789061 2.039307 4.337945 4.304616 5.108317 4.671912 -1.755856 -1.350134 -2.353095 -2.061420 -3.712112 -4.474651 -4.093170 -5.161653 -3.137962 0.121656 0.668086 0.718363 1.783792 0.681044 0.175689 0.380021 -0.033554 1.470823 -0.045054 -3.625793 -2.743369 -4.639453 -5.567199 -4.933215 -4.233342 -4.241677 -3.546618	1.768271 0.689134 2.359534 3.441903 1.849961 2.249786 1.886947 1.464555 1.329530 2.942514 -2.784115 -3.691197 -4.326468 -5.031820 -4.083053 -4.598113 -3.172158 -2.970772 -2.501196 -3.994593 -3.034626 -4.984164 -5.178473 -4.598358 -5.952404 -4.504935 -3.821970 -4.585961 -5.517810 -1.521920 -0.956269 -0.504863 -1.001413 0.210301 0.089715 -2.256845 -2.996624	E (M06/ E (PBE) E (PBE) E (PBE) E (PM6) E (PM7) E (GFN1 E (GFN2 E (GFN- Coordi V O O N N N N H C C H H C C H H C C H H C C C H H C C C H H C C C H H C C C C C C C C C C C C C C C C C C C C	def2-TZVP) = -324 - D3 (BJ)/def2-TZVP - D3 (BJ)/def2-TZV = -148.93650 Kca = -167.99316 Kca X-V/def2-TZVP) = -xTB) = -165.4384 - TB) = -165.4384 - TB) = -162.8352 FF) = -22.3224418  mates:	5.829049263117 Ha P) = -3244.78794 37118545 Hartree 1/mol 1/mol -3246.87209338705 39133982 Hartree 64001613 Hartree 39424 Hartree 0.418946 -2.896228 -3.075856 0.254494 1.743630 1.099925 -0.820014 -0.372342 1.121182 2.163901 2.817458 2.439037 0.995150 0.198101 0.771097 1.954252 3.607116 3.367038 4.455919 3.946901 -0.793270 -0.525978 -1.586228 -1.384374 -2.886358	955796 Hartree 4505697 Hartree  8 Hartree  0.105026 1.787176 0.205300 -0.239374 1.583545 -1.451740 1.112620 1.833367 0.223751 1.127033 1.390029 1.796011 -0.180437 -0.926642 0.711811 -0.593966 2.757513 3.702771 2.304025 2.986820 -1.166622 -2.572455 -3.478252 -4.556611 -3.033485
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Н С Н Н Н С С С Н С Н С Н С Н Н Н С Н Н Н С Н Н Н С Н Н Н С С Н	-0.819017 0.508390 0.481497 1.120244 1.012928 -1.613571 -2.638438 -1.043382 -1.695927 -0.160709 0.865545 1.621730 2.411565 1.393402 1.997026 0.405276 0.235840 -0.382087 1.140300 1.031265 0.122463 0.360285 -0.911430 0.147225 2.563862 3.331066 2.738458 2.725783 -1.449150 -1.809674 -0.893400 -0.543098 -1.686626 -0.052094 -2.654463 -3.092232 -3.449750 -2.358048 0.633391 1.200809 2.142573	2.977002 2.752789 3.018729 3.266349 3.789061 2.039307 4.337945 4.304616 5.108317 4.671912 -1.755856 -1.350134 -2.353095 -2.061420 -3.712112 -4.474651 -4.093170 -5.161653 -3.137962 0.121656 0.668086 0.718363 1.783792 0.681044 0.175689 0.380021 -0.033554 1.470823 -0.045054 -3.625793 -2.743369 -4.639453 -5.567199 -4.933215 -4.233342 -4.241677 -3.546618 -4.517837 -5.163128 2.745777 4.003641 4.037569	1.768271 0.689134 2.359534 3.441903 1.849961 2.249786 1.886947 1.464555 1.329530 2.942514 -2.784115 -3.691197 -4.326468 -5.031820 -4.083053 -4.598113 -3.172158 -2.970772 -2.501196 -3.994593 -3.034626 -4.984164 -5.178473 -4.598358 -5.952404 -4.504935 -3.821970 -4.585961 -5.517810 -1.521920 -0.956269 -0.504863 -1.001413 0.210301 0.089715 -2.256845 -2.996624 -1.533914 -2.800315 -1.261235 -0.931911 -0.366287	E (M06/ E (PBE) E (PBE) E (PBE) E (PM6) E (PM7) E (GFN2 E (GFN2 C O O T D O O N N N N N N N N N N N N N N N N N	def2-TZVP) = -324 - D3 (BJ)/def2-TZV - D3 (BJ)/def2-TZV - D3 (BJ)/def2-TZV - 320 = -3241.1162 = -148.93650 Kca = -167.99316 Kca X-V/def2-TZVP) = -27816 Kca X-V/def2-TZVP) = -165.4384 -XTB) = -162.8352 FF) = -22.3224418  nates:  0.127637 -2.083691 -0.399281 2.101772 0.367103 -0.829279 -0.916974 -1.500420 3.025810 2.721714 3.564436 1.510282 4.478498 4.640948 5.098349 4.848360 0.976646 0.944724 2.524641 2.444764 2.358642 2.539423 2.462165 2.799843 2.910325 2.937060 3.174567 2.793622 2.129993	5.829049263117 Ha P) = -3244.540307 WP) = -3244.78794 37118545 Hartree 1/mol -3246.87209338705 39133982 Hartree 64001613 Hartree 39424 Hartree 0.418946 -2.896228 -3.075856 0.254494 1.743630 1.099925 -0.820014 -0.372342 1.121182 2.163901 2.817458 2.439037 0.995150 0.198101 0.771097 1.954252 3.607116 3.367038 4.455919 3.946901 -0.793270 -0.525978 -1.586228 -1.384374 -2.886358 -3.710838 -3.121715 -4.137211 -2.096978 0.876465	955796 Hartree 4505697 Hartree 8 Hartree  0.105026 1.787176 0.205300 -0.239374 1.583545 -1.451740 1.112620 1.833367 0.223751 1.127033 1.390029 1.796011 -0.180437 -0.926642 0.711811 -0.593966 2.757513 3.702771 2.304025 2.986820 -1.166622 -2.5772455 -3.478252 -4.556611 -3.033485 -3.754025 -1.664456 -1.3033485 -3.754025 -1.664456 -1.308055 -0.704803 -3.124611
Н С Н Н Н С С С Н С Н С С Н С Н Н Н С Н Н Н С Н Н Н С Н Н Н С С Н С Н	-0.819017 0.508390 0.481497 1.120244 1.012928 -1.613571 -2.638438 -1.043382 -1.695927 -0.160709 0.865545 1.621730 2.411565 1.393402 1.997026 0.405276 0.235840 -0.382087 1.140300 1.031265 0.122463 0.360285 -0.9114330 0.147225 2.563862 3.331066 2.738458 2.725783 -1.449150 -1.809674 -0.893400 -0.543098 -1.686626 -0.052094 -2.654463 -3.092232 -3.449750 -2.358048 0.633391 1.200809 2.142573 0.563866 1.027262	2.977002 2.752789 3.018729 3.266349 3.789061 2.039307 4.337945 4.304616 5.108317 4.671912 -1.755856 -1.350134 -2.353095 -2.061420 -3.712112 -4.474651 -4.093170 -5.161653 -3.137962 0.121656 0.668086 0.718363 1.783792 0.681044 0.175689 0.380021 -0.033554 1.470823 -0.045054 -3.625793 -2.743369 -4.639453 -5.567199 -4.933215 -4.233342 -4.241677 -3.546618 -4.517837 -5.163128 2.745777 4.003641 4.037569 5.194598 6.154097	1.768271 0.689134 2.359534 3.441903 1.849961 2.249786 1.886947 1.464555 1.329530 2.942514 -2.784115 -3.691197 -4.326468 -5.031820 -4.083053 -4.598113 -3.172158 -2.970772 -2.501196 -3.994593 -3.034626 -4.984164 -5.178473 -4.598388 -5.952404 -5.517810 -1.521920 -0.956269 -0.504863 -1.001413 0.210301 0.089715 -2.256845 -2.996624 -1.533914 -2.800315 -1.261235 -0.931911 -0.366287 -1.297548 -1.015033	E (M06/ E (PBE) E (PBE) E (PBE) E (PM6) E (PM7) E (GFN7) E (GFN2) E (GFN- COORD N N N N N N H C C H H C C H H C C H H C C H C C H C C H C C C H C C C C C C C C C C C C C C C C C C C C	def2-TZVP) = -324 - D3 (BJ)/def2-TZV = -3241.1162 = -148.93650 Kca = -167.99316 Kca X-V/def2-TZVP) = -26.4384 -XTB) = -165.4384 -XTB) = -162.4384 -XTB) = -162.33224418  nates:	5.829049263117 Ha P) = -3244.78794 37118545 Hartree 1/mol 1/mol -3246.87209338705 39133982 Hartree 64001613 Hartree 39424 Hartree 0.418946 -2.896228 -3.075856 0.254494 1.743630 1.099925 -0.820014 -0.372342 1.121182 2.163901 2.817458 2.439037 0.995150 0.198101 0.771097 1.954252 3.607116 3.367038 4.455919 3.946901 -0.793270 -0.525978 -1.586228 -1.384374 -2.886358 -3.710838 -3.121715 -4.137211 -2.096978 0.876465 1.493846 1.518286	955796 Hartree 4505697 Hartree 8 Hartree  0.105026 1.787176 0.205300 -0.239374 1.583545 -1.451740 1.112620 1.833367 0.223751 1.127033 1.390029 1.796011 -0.180437 -0.926642 0.711811 -0.593966 2.757513 3.702771 2.304025 2.986820 -1.166622 -2.572455 -3.478252 -4.556611 -3.033485 -3.754025 -1.664456 -1.308055 -0.704803 -3.124611 -2.304296 -3.571972
Н С Н Н Н С С С Н С Н С Н С Н Н Н С Н Н Н С Н Н Н С Н Н Н С С Н С Н С Н С Н Н Н С Н Н Н С Н Н Н С С Н С	-0.819017 0.508390 0.481497 1.120244 1.012928 -1.613571 -2.638438 -1.043382 -1.695927 -0.160709 0.865545 1.621730 2.411565 1.393402 1.997026 0.405276 0.235840 -0.382087 1.140300 1.031265 0.122463 0.360285 -0.911430 0.147225 2.563862 3.331066 2.738458 2.725783 -1.449150 -1.809674 -0.893400 -0.543098 -1.686626 -0.052094 -2.654463 -3.092232 -3.449750 -2.358048 0.633391 1.200809 2.142573 0.563866	2.977002 2.752789 3.018729 3.266349 3.789061 2.039307 4.337945 4.304616 5.108317 4.671912 -1.755856 -1.350134 -2.353095 -2.061420 -3.712112 -4.474651 -4.093170 -5.161653 -3.137962 0.121656 0.668086 0.718363 1.783792 0.681044 0.175689 0.380021 -0.033554 1.470823 -0.045054 -3.625793 -2.743369 -4.639453 -5.567199 -4.933215 -4.233342 -4.241677 -3.546618 -4.517837 -5.163128 2.745777 4.003641 4.037569 5.194598	1.768271 0.689134 2.359534 3.441903 1.849961 2.249786 1.886947 1.464555 1.329530 2.942514 -2.784115 -3.691197 -4.326468 -5.031820 -4.083053 -4.598113 -3.172158 -2.970772 -2.501196 -3.994593 -3.034626 -4.984164 -5.178473 -4.598358 -5.952404 -5.517810 -1.521920 -0.956269 -0.504863 -1.001413 0.210301 0.089715 -2.256845 -2.996624 -1.533914 -2.800315 -1.261235 -0.931911 -0.366287 -1.297548	E (M06/ E (PBE) E (PBE) E (PBE) E (PM6) E (PM7) E (GFN1 E (GFN2 E (GFN- COORDIN N N N N N N N C C H H C C H H H C C H H C C H H C C H H C C H H C C H H C C C H H C C C H H C C C H H C C C C C C C C C C C C C C C C C C C C	def2-TZVP) = -324 - D3 (BJ)/def2-TZV = -148.93650 Kca = -167.99316 Kca X-V/def2-TZVP) = -165.4384 -XTB) = -165.4384 -XTB) = -162.3352 FF) = -22.3224418  nates:	5.829049263117 Ha P) = -3244.540307 WP) = -3244.78794 37118545 Hartree 1/mol 1/mol -3246.87209338705 39133982 Hartree 64001613 Hartree 39424 Hartree  0.418946 -2.896228 -3.075856 0.254494 1.743630 1.099925 -0.820014 -0.372342 1.121182 2.163901 2.817458 2.439037 0.995150 0.198101 0.771097 1.954252 3.607116 3.367038 4.455919 3.946901 -0.793270 -0.525978 -1.586228 -1.384374 -2.886358 -3.710838 -3.121715 -4.137211 -2.096978 0.876465 1.493846	955796 Hartree 4505697 Hartree 8 Hartree  0.105026 1.787176 0.205300 -0.239374 1.583545 -1.451740 1.112620 1.833367 0.223751 1.127033 1.390029 1.796011 -0.180437 -0.926642 0.711811 -0.593966 2.757513 3.702771 2.304025 2.986820 -1.166622 -2.572455 -3.478252 -4.556611 -3.033485 -3.754025 -1.664456 -1.308055 -0.704803 -3.124611 -2.304296

Н	3.280915	2.555658	-3.922807	В	-1.132993	-2.219760	1.023094
H	3.908662	0.946902	-4.410492	D	1.132333	2.213700	1.023034
C	1.123939	0.924804	-4.284227	Conf	formation 22.		
Н	1.537105	0.463401	-5.205308		iplicity: 3		
Н	0.876735	1.978008	-4.522123		ge: 0		
Н	0.178291	0.407826	-4.036914		97-3c) = -3245.80104	8785473 Hartree	
C	3.153282	-2.510726	0.725630		16/def2-TZVP) = -324		rtree
Н	2.819778	-3.568186	0.723030		BE - D3(BJ)/def2-TZV		
C	2.487097	-1.787998	1.895320		BEO - D3(BJ)/def2-TZ		
Н	2.487097	-0.764459	2.049754		BEh-3c) = -3241.1159		1027074 Hardies
H	2.677538	-2.355523	2.829633		(6) = -146.90124  Kca		
Н	1.393200	-1.721451	1.757035		17) = -168.32908 Kca		
п С			0.897916				2 11
Н	4.686453 5.178979	-2.533844 -3.130848	0.104849		397X-V/def2-TZVP) = -100000000000000000000000000000000000		3 naitiee
н	4.957267		1.880188		N2-xTB) = -163.4364 N2-xTB) = -162.8363		
		-2.973389	0.860916		N-FF) = -22.3240613		
H	5.112852	-1.511910		E (GF	N-FF) = -22.3240613	3030/ Hartree	
C C	-0.700503	1.899541	2.545004 2.326571	0			
	-1.761977	2.817702			dinates:	0 250105	0 114517
C	-2.759787	2.945025	3.312850	V	0.278278	0.358105	0.114517
H	-3.580613	3.660589	3.150195	0	-0.887803	-2.586994	-1.359183
C	-2.728395	2.183744	4.484441	0	0.525673	-3.944014	-0.121773
H	-3.517402	2.298471	5.243156	N	0.151133	1.388990	-1.589309
C	-1.690883	1.264069	4.680042	N	2.103959	1.047927	0.570175
H	-1.672993	0.653247	5.595071	N	-1.143101	0.859788	1.353299
C	-0.667834	1.098753	3.729131	N	0.713678	-1.495733	0.194741
C	-1.860809	3.650073	1.060316	H	1.467253	-1.726457	0.857007
H	-0.989438	3.394858	0.430265	C	0.950375	2.432439	-1.899505
C	-1.802985	5.161699	1.330637	C	2.094899	2.771532	-1.149803
H	-1.781417	5.717900	0.371121	H	2.650254	3.648551	-1.511367
H	-0.899188	5.443823	1.907586	C	2.679396	2.101747	-0.049930
H	-2.686533	5.511002	1.904902	C	0.656643	3.300900	-3.103891
C	-3.120147	3.283760	0.260059	H	-0.189902	2.918878	-3.700403
H	-3.165512	2.191480	0.087825	H	1.549967	3.368447	-3.756008
H	-3.113519	3.788819	-0.726897	H	0.416929	4.332977	-2.776742
H	-4.045112	3.583486	0.795851	C	4.009518	2.651721	0.423709
C	0.446553	0.090517	3.982392	H	4.417413	2.096770	1.285963
H	0.919887	-0.094980	3.002175	H	3.888997	3.715790	0.712568
C	-0.075686	-1.258551	4.501789	H	4.754699	2.626031	-0.396256
H	-0.477820	-1.181165	5.533415	С	-0.948758	0.984292	-2.424892
H	0.753011	-1.995189	4.532787	С	-2.260187	1.496706	-2.158832
H	-0.871147	-1.672846	3.852125	С	-3.353445	0.959168	-2.861856
C	1.527625	0.647713	4.925954	H	-4.363041	1.340164	-2.647916
H	2.001235	1.562741	4.522123	С	-3.178467	-0.039139	-3.825593
Н	2.329795	-0.103624	5.078904	H	-4.046082	-0.463051	-4.353720
H	1.100462	0.896116	5.920324	С	-1.886368	-0.473354	-4.129306
C	-1.683072	0.086034	-1.962544	H	-1.739408	-1.228377	-4.918571
C	-3.092230	0.226365	-2.033431	С	-0.747961	0.026124	-3.462830
H	-3.556388	1.171510	-1.720820	С	-2.503823	2.667455	-1.212767
C	-3.893339	-0.830205	-2.473484	H	-1.604194	2.781540	-0.580393
H	-4.986269	-0.693523	-2.511672	С	-2.685575	3.974858	-2.010213
С	-3.338304	-2.073519	-2.854917	H	-1.832895	4.183468	-2.682049
С	-1.942205	-2.211770	-2.769305	H	-2.794064	4.833952	-1.316636
Н	-1.468713	-3.164867	-3.051640	H	-3.599808	3.927068	-2.638214
C	-1.126083	-1.156130	-2.338100	С	-3.707964	2.478168	-0.278378
Н	-0.036955	-1.299294	-2.292652	H	-4.667307	2.505716	-0.836377
С	-4.219628	-3.201916	-3.327586	H	-3.733185	3.296317	0.467889
H	-4.721149	-2.953240	-4.286969	H	-3.661510	1.523767	0.276207
H	-5.022628	-3.421866	-2.593306	С	0.593326	-0.452903	-4.029515
H	-3.639790	-4.132552	-3.483486	Н	0.385059	-1.482849	-4.387559
C	-0.771689	2.374250	-2.019842	С	1.798489	-0.570157	-3.093771
С	-1.586466	2.799336	-3.100102	H	2.240747	0.413410	-2.842371
H	-2.312891	2.102850	-3.539268	H	2.589946	-1.164744	-3.594786
C	-1.462085	4.088479	-3.633494	H	1.538912	-1.077884	-2.147456
H	-2.115004	4.377532	-4.473366	C	0.957615	0.370435	-5.282645
С	-0.527837	5.019617	-3.137500	H	0.125884	0.390841	-6.014668
C	0.307722	4.583556	-2.087337	H	1.848866	-0.062147	-5.782597
H	1.075851	5.264231	-1.685425	Н	1.198545	1.418388	-5.016911
С	0.199872	3.299463	-1.546731	C	2.868939	0.275750	1.519193
H	0.895675	2.996803	-0.749074	С	2.640677	0.428972	2.917216
C	-0.432490	6.418974	-3.690509	C	3.381754	-0.361116	3.815373
H	-1.055764	7.132310	-3.107220	Н	3.212894	-0.240692	4.895423
H	-0.782205	6.468576	-4.741044	C	4.322312	-1.292591	3.362691
H	0.607654	6.801865	-3.658896	Н	4.889650	-1.903494	4.081154
C	-2.174067	-4.239452	1.254450	C	4.530772	-1.444937	1.988713
C	-0.754076	-4.430495	0.578045	Н	5.266018	-2.182059	1.631049
C	-3.320928	-4.244720	0.236140	C	3.820766	-0.678250	1.044732
H	-4.241127	-3.885060	0.736601	C	1.646811	1.448035	3.445776
H	-3.515026	-5.258104	-0.167609	Н	0.897329	1.597221	2.649638
H	-3.102787	-3.559775	-0.606060	C	2.307218	2.814393	3.697566
C	-2.474368	-5.202514	2.400134	H	1.548533	3.548543	4.036733
H	-1.745552	-5.092825	3.224019	H	2.775007	3.218571	2.779943
H	-2.460343	-6.253798	2.048173	Н	3.095301	2.737223	4.476105
H	-3.482439	-4.991326	2.807886	С	0.890289	0.979003	4.695427
С	0.303591	-4.929506	1.570793	H	0.530857	-0.063053	4.583903
H	1.299135	-4.884273	1.088137	H	0.012122	1.633877	4.866624
H	0.118972	-5.976725	1.879619	H	1.519982	1.021647	5.608738
H	0.332668	-4.291336	2.476055	С	4.117808	-0.887382	-0.436783
С	-0.749131	-5.299828	-0.676630	H	3.394326	-0.275895	-1.007010
H	-1.431018	-4.900617	-1.448832	С	3.931412	-2.352279	-0.871148
H	-1.049774	-6.340194	-0.439651	H	4.655093	-3.023358	-0.363867
H	0.272742	-5.321936	-1.104823	H	4.100445	-2.451884	-1.962804

Н	2.911702	-2.719114	-0.650015	С	1.865564	1.105367	4.148258
C	5.535156	-0.404446	-0.798413	Н	1.947534	2.031759	4.737673
H	5.705145	0.646789	-0.497904	С	1.602614	-0.105750	4.798338
H	5.704206	-0.481189	-1.892267	Н	1.468151	-0.131960	5.890575
H	6.308229	-1.022499	-0.295938	C	1.535686	-1.285002	4.050489
C	-1.973936	-0.251861	1.663260	Н	1.365019	-2.244258	4.562217
C	-2.031214	-0.806535	2.964104	С	1.709709	-1.282725	2.652867
Н		-0.352857	3.763176	C	2.374345	2.510455	2.115198
	-1.429333						
С	-2.835126	-1.918301	3.232642	H	2.450899	2.350006	1.024200
H	-2.860805	-2.328678	4.255042	С	1.285255	3.569318	2.343510
C	-3.609407	-2.530505	2.221984	H	0.315813	3.249209	1.916133
C	-3.534910	-1.983560	0.927280	Н	1.567631	4.526362	1.860439
H	-4.127639	-2.429572	0.113059	H	1.138659	3.773496	3.423797
C	-2.734897	-0.867175	0.645821	C	3.741755	3.027370	2.598881
H	-2.695980	-0.467525	-0.377672	H	3.725672	3.261241	3.683722
С	-4.449167	-3.748398	2.512879	Н	4.015785	3.958074	2.060654
Н	-4.852192	-3.732142	3.545012	Н	4.547127	2.286081	2.428710
H	-3.850230	-4.680382	2.412805	С	1.767476	-2.611403	1.913806
H	-5.302038	-3.833979	1.810674	H	1.746336	-2.391557	0.831018
C	-1.343287	2.098449	1.968303	С	0.580958	-3.532976	2.225470
Č	-0.526139	3.201157	1.594922	Н	0.571589	-3.845803	3.290587
H	0.260340	3.068498	0.835615	H	0.642796	-4.450685	1.608010
С	-0.696484	4.461021	2.175303	H	-0.386203	-3.045830	2.001984
H	-0.034115	5.283230	1.858869	С	3.093677	-3.340067	2.203722
С	-1.690568	4.704787	3.146258	Н	3.971878	-2.697889	1.997743
C				Н			
	-2.511054	3.615457	3.502462		3.176305	-4.248096	1.571929
H	-3.307136	3.763712	4.250594	H	3.154368	-3.653743	3.267038
С	-2.352958	2.345547	2.933942	C	0.189454	1.437976	-3.057600
H	-3.027956	1.532132	3.232121	C	-0.077814	2.841412	-3.096085
С	-1.893783	6.075026	3.742206	C	-0.897074	3.320838	-4.144953
H	-2.641257	6.665128	3.167229	Н	-1.086245	4.404247	-4.203676
H	-0.953681	6.662351	3.747567	C	-1.455518	2.481674	-5.105769
H	-2.264614	6.016113	4.785328	H	-2.082906	2.895935	-5.909355
С	-1.061061	-3.929910	-1.875730	С	-1.207735	1.106748	-5.037424
C	-0.458921	-4.825168	-0.714158	Н	-1.651241	0.442324	-5.791518
С	-0.253863	-4.032335	-3.175422	С	-0.390915	0.561337	-4.033562
H	-0.623454	-3.267671	-3.884860	C	0.411328	3.961056	-2.152645
H	-0.361143	-5.025894	-3.652595	H	0.801563	4.739465	-2.847829
Н	0.821717	-3.840280	-2.992394	C	1.525233	3.674396	-1.144671
С	-2.543291	-4.156002	-2.160918	Н	1.736932	4.600372	-0.573665
H	-3.158186	-3.986212	-1.259227	H	2.474240	3.352382	-1.608483
H	-2.724707	-5.186934	-2.526089	H	1.214835	2.899279	-0.423360
H	-2.880577	-3.444687	-2.940742	С	-0.777293	4.613355	-1.407402
C	-1.485582	-5.147526	0.379057	Н	-1.614397	4.863173	-2.087229
H	-0.952856	-5.577197	1.249775	H	-0.445736	5.551076	-0.916688
H	-2.244085	-5.878418	0.035569	H	-1.176870	3.956040	-0.609527
H	-1.999528	-4.226316	0.715902	С	-0.124174	-0.941576	-4.024364
С	0.239929	-6.098684	-1.182069	Н	-0.084435	-1.243094	-2.959801
Н	1.093212	-5.872880	-1.847741	C	1.225385	-1.320979	-4.662694
H	-0.465524	-6.763928	-1.719711	H	1.282408	-0.957141	-5.710407
H	0.631178	-6.651499	-0.305393	H	1.341112	-2.423169	-4.669961
В	0.123948	-2.640013	-0.404967	H	2.087215	-0.913351	-4.105214
				С	-1.237017	-1.762801	-4.690929
Confor	mation 23.			Н	-2.244232	-1.466384	-4.338163
-	licity: 3			H	-1.090290	-2.837845	-4.462051
Charge	: 0			H	-1.220754	-1.664297	-5.796535
E(B97-	3c) = -3245.79322	5753192 Hartree		С	0.308462	-2.880824	-1.125236
	def2-TZVP) = -324		rtree	C	-0.159756	-4.219513	-1.102412
	- D3(BJ)/def2-TZV			Н	-1.168649	-4.431577	-0.723254
	- D3(BJ)/def2-TZ		0643286 Hartree		0.656595	-5.275557	-1.527979
E (PBEh	-3c) = -3241.1067	49211474 Hartree		H	0.257431	-6.302332	-1.487006
E(PM6)	= -142.86329 Kca	l/mol		C	1.970996	-5.069069	-1.991411
	= -161.26403 Kca			C	2.436049	-3.736692	-2.012923
	X-V/def2-TZVP) =		7 !!>*+**	Н	3.455925	-3.520912	-2.371168
			, 1101 0166				
	-xTB) = $-165.4331$			С	1.631829	-2.671542	-1.601260
E (GFN2	-xTB) = $-162.8275$	17342368 Hartree		H	2.044342	-1.652616	-1.654842
E (GFN-	FF) = -22.3151093	70906 Hartree		C	2.839578	-6.208449	-2.461794
				Н	2.389809	-7.190567	-2.216448
Coordi	nates:			Н	3.848122	-6.173156	-1.999471
		0 000007	0 427446				
V	0.327300	0.008867	-0.437446	H	2.992625	-6.180505	-3.562584
0	-1.581615	0.880722	2.419084	С	-1.830554	-1.965264	-0.427888
0	-2.554424	2.687223	1.348706	C	-2.402338	-1.716140	0.836841
N	2.027873	0.036468	0.561627	Н	-1.765187	-1.373348	1.663783
N	1.086611	0.871045	-2.078513	C	-3.779748	-1.883444	1.041190
N	-0.436301	-1.795015	-0.646340	Н	-4.196024	-1.704654	2.045400
N	-0.902330	1.361129	0.070924	С	-4.640620	-2.298401	0.007820
H	-1.166695	1.972223	-0.713379	C	-4.061173	-2.549925	-1.254313
C	3.238468	0.169524	-0.038345	Н	-4.701463	-2.877649	-2.089385
C	3.396343	0.550653	-1.386775	C	-2.689069	-2.390207	-1.469451
H	4.434344	0.607588	-1.740210	Н	-2.259719	-2.602078	-2.456358
С	2.415074	0.955895	-2.322358	C	-6.124755	-2.443142	0.230069
С	4.494955	-0.149462	0.738290	H	-6.674074	-1.548159	-0.135425
Н	4.385190	0.066250	1.816556	Н	-6.367293	-2.559173	1.304807
H	5.363697	0.406748	0.340758	H	-6.537841	-3.317421	-0.312434
H	4.716726	-1.234071	0.646733	С	-2.443090	1.507980	3.405222
С	2.906400	1.559414	-3.621290	C	-3.380146	2.428161	2.511501
		1.237289	-4.487319	C	-1.559391	2.304543	4.369000
H	2.300017						
			-3.798414	H	-0.788943	1.626206	4.782050
H	3.964821	1.293873	-3.798414 -3.587880	H H	-0.788943 -2 150500	1.626206 2.725097	4.782050 5.205794
H H	3.964821 2.834089	1.293873 2.666893	-3.587880	Н	-2.150500	2.725097	5.205794
H H C	3.964821 2.834089 1.923841	1.293873 2.666893 -0.036544	-3.587880 1.996939	H H	-2.150500 -1.037903	2.725097 3.131070	5.205794 3.853557
H H	3.964821 2.834089	1.293873 2.666893	-3.587880	Н	-2.150500	2.725097	5.205794

	2 722402	0.050000	2 500000		0.050505	1 046000	0 071000
H	-3.733423	-0.259962	3.502299	H	3.958527	-1.246280	-2.871223
H	-3.879402	0.844300	4.911669	H	2.774732	0.027458	-2.457516
H	-2.432572	-0.202060	4.730061	C	0.753815	-0.749933	-4.209495
С	-4.635261	1.701625	2.009761	H	-0.043520	-1.390449	-4.635975
H	-5.125394	2.331247	1.241823	H	1.094299	-0.044717	-4.995859
H	-5.362491	1.513475	2.824112	Н	0.301970	-0.169951	-3.382710
Н	-4.372727	0.734954	1.537020	C	0.425882	-3.649260	0.883946
C	-3.760069	3.761285	3.150494	Н	0.897507	-2.721624	1.250982
				C			
H	-2.866678	4.369548	3.381443		1.097339	-4.814916	1.625409
H	-4.334322	3.602255	4.085143	H	0.629946	-5.790186	1.374686
H	-4.395506	4.340142	2.451736	H	1.011341	-4.666962	2.721257
В	-1.648927	1.632782	1.252787	H	2.176855	-4.889694	1.381326
				C	-1.070012	-3.558669	1.221846
Confor	mation 27.			H	-1.540678	-2.700597	0.702812
Multip	licity: 3			Н	-1.204079	-3.421834	2.314571
Charge				Н	-1.612057	-4.480497	0.923932
	3c) = -3245.78140	320/910 Hartroo		C	0.372272	-0.927428	3.043158
	,	5.813225579809 Hai		C			
	,				1.687646	-1.457685	2.977869
		(P) = -3244.5218403		H	2.275761	-1.323037	2.058688
		VP) = -3244.769945	5125457 Hartree	C	2.263639	-2.121287	4.064607
E (PBEh	-3c) = -3241.0945	02843497 Hartree		H	3.284774	-2.522432	3.959973
E(PM6)	= -146.60975 Kca	1/mol		С	1.579766	-2.272254	5.287919
E(PM7)	= -160.53152 Kca	1/mol		С	0.291818	-1.704586	5.368920
		-3246.85386309183	4 Hartree	Н	-0.269376	-1.776555	6.315101
	-xTB) = $-165.4270$			C	-0.303103	-1.046164	4.286114
	-xTB) = $-162.8190$			Н	-1.301564	-0.606328	4.409112
	FF) = -22.3090549			C			
E (GFN-	FF) = -22.3090549	20//8 Hartree			2.206976	-2.967402	6.470058
				H	3.117725	-3.525965	6.177356
Coordi:				H	1.505618	-3.685963	6.942443
V	0.552269	-0.058340	0.119855	H	2.502669	-2.243730	7.260597
0	-2.893716	-0.936093	-2.348666	С	-1.453969	0.294747	1.930496
0	-2.544982	1.253399	-1.686648	С	-1.626629	1.621078	1.472511
N	2.061006	1.296096	0.183168	Н	-0.746024	2.217629	1.189939
N	1.799844	-1.500427	-0.571222	C	-2.900514	2.204840	1.407359
N	-0.154360	-0.272287	1.925447	Н	-2.992862	3.236866	1.035598
N	-0.771146	-0.473674	-1.205268	С	-4.045995	1.508351	1.826604
H	-0.621983	-1.444838	-1.521017	C	-3.874032	0.172799	2.260789
C	3.372794	0.982894	0.156292	H	-4.757264	-0.411742	2.565781
С	3.841294	-0.347423	0.075008	С	-2.616167	-0.431495	2.298927
H	4.924979	-0.476658	0.193327	H	-2.521387	-1.479261	2.611714
С	3.128577	-1.501389	-0.311985	С	-5.412468	2.145821	1.826656
Č	4.427742	2.068102	0.146200	Н	-6.154364	1.518661	1.288809
Н	4.714046	2.284433	-0.904848	Н	-5.397917	3.143430	1.346915
Н	5.342723	1.731708	0.668713	H	-5.797321	2.276434	2.860557
H	4.078255	3.015961	0.591203	С	-4.165698	-0.264843	-2.493608
C	3.915645	-2.780732	-0.487583	С	-3.734784	1.256736	-2.519238
H	3.904226	-3.124571	-1.540814	C	-5.007632	-0.615486	-1.259555
H	3.460128	-3.599661	0.104626	H	-5.077255	-1.717802	-1.178028
H	4.965266	-2.646982	-0.169698	H	-6.034074	-0.203282	-1.325621
С	1.640675	2.668902	0.281032	H	-4.527750	-0.234798	-0.336905
С	1.185582	3.299672	-0.920362	С	-4.844265	-0.766401	-3.765223
C	0.722335	4.624976	-0.868666	Н	-4.180281	-0.670205	-4.643759
Н	0.368060	5.105685	-1.791719	H	-5.781858	-0.208888	-3.964215
				H			
C	0.716850	5.340904	0.331715		-5.100843	-1.838035	-3.650555
H	0.360911	6.381827	0.360260	С	-3.330266	1.722583	-3.924150
С	1.175374	4.721184	1.494506	Н	-2.879153	2.731412	-3.863096
H	1.177977	5.285863	2.440572	H	-4.206563	1.778529	-4.599120
C	1.638834	3.385831	1.520389	H	-2.583054	1.038041	-4.371577
С	1.230269	2.588596	-2.268139	С	-4.753067	2.220041	-1.918444
H	1.238137	1.497481	-2.066046	H	-4.960594	1.975597	-0.862792
С	-0.003572	2.873286	-3.131497	H	-5.704451	2.193418	-2.487187
Н	-0.932838	2.672529	-2.567111	Н	-4.358720	3.254854	-1.958140
Н	0.000102	2.217715	-4.025198	В	-2.029511	-0.041208	-1.713954
Н	-0.022306	3.920213	-3.500037	2	2.023011	0.011200	1.710301
11	-0.022300	3.920213		0			
~	0 501160	2 022150	2 021754				
C	2.521162	2.932159	-3.031754		mation 30.		
H	2.580932	4.023568	-3.224846	Multip	olicity: 3		
H H	2.580932 2.545370	4.023568 2.408778	-3.224846 -4.008933	Multip Charge	plicity: 3 e: 0		
H H H	2.580932 2.545370 3.428001	4.023568 2.408778 2.638707	-3.224846 -4.008933 -2.469515	Multip Charge E(B97-	elicity: 3 e: 0 e3c) = -3245.778887		
H H	2.580932 2.545370	4.023568 2.408778	-3.224846 -4.008933	Multip Charge E(B97-	plicity: 3 e: 0		rtree
H H H	2.580932 2.545370 3.428001	4.023568 2.408778 2.638707	-3.224846 -4.008933 -2.469515	Multip Charge E(B97- E(M06/	elicity: 3 e: 0 e3c) = -3245.778887	.807028098133 На	
H H H C H	2.580932 2.545370 3.428001 2.018737 2.487877	4.023568 2.408778 2.638707 2.908164	-3.224846 -4.008933 -2.469515 2.936758	Multip Charge E(B97- E(M06/ E(PBE	dlicity: 3 :: 0 3c) = -3245.778887 def2-TZVP) = -3245 - D3(BJ)/def2-TZVP	.807028098133 Ha ) = $-3244.519852$	550107 Hartree
Н Н С Н С	2.580932 2.545370 3.428001 2.018737 2.487877 3.021805	4.023568 2.408778 2.638707 2.908164 3.808444 1.766840	-3.224846 -4.008933 -2.469515 2.936758 3.393138 3.125388	Multip Charge E(B97- E(M06/ E(PBE E(PBE0	plicity: 3 :: 0 :: 0 :3c) = -3245.778887 def2-TZVP) = -3245 - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP	(0.807028098133) Ha (0.807028098133) Ha (0.80702809813) Ha (0.8070280980) Ha (0.807028009813) Ha (0.80702800980) Ha (0.80702800980) Ha (0.807028000980) Ha (0.80702800000000000000000000000000000000	550107 Hartree
H H C H C	2.580932 2.545370 3.428001 2.018737 2.487877 3.021805 2.638657	4.023568 2.408778 2.638707 2.908164 3.808444 1.766840 0.804575	-3.224846 -4.008933 -2.469515 2.936758 3.393138 3.125388 2.748215	Multip Charge E(B97- E(M06/ E(PBE E(PBE0 E(PBEh	plicity: 3 2: 0 3c) = -3245.778887 def2-TZVP) = -3245 - D3 (BJ)/def2-TZVP - D3 (BJ)/def2-TZVP - 3c) = -3241.09352	.807028098133 Ha ) = -3244.519852 P) = -3244.76770 1830369 Hartree	550107 Hartree
H H C H C H	2.580932 2.545370 3.428001 2.018737 2.487877 3.021805 2.638657 3.204889	4.023568 2.408778 2.638707 2.908164 3.808444 1.766840 0.804575 1.631300	-3.224846 -4.008933 -2.469515 2.936758 3.393138 3.125388 2.748215 4.210479	Multip Charge E(B97- E(M06/ E(PBE E(PBE0 E(PBE0 E(PM6)	plicity: 3 2: 0 3c) = -3245.778887 def2-TZVP) = -3245 - D3 (BJ)/def2-TZVP 0 - D3 (BJ)/def2-TZV 1-3c) = -3241.09352 = -136.19646 Kcal	.807028098133 Ha b) = -3244.519852 p) = -3244.76770 1830369 Hartree /mol	550107 Hartree
H H C H C H H H	2.580932 2.545370 3.428001 2.018737 2.487877 3.021805 2.638657 3.204889 3.998950	4.023568 2.408778 2.638707 2.908164 3.808444 1.766840 0.804575 1.631300 1.972807	-3.224846 -4.008933 -2.469515 2.936758 3.393138 3.125388 2.748215 4.210479 2.653222	Multip Charge E (B97- E (M06/ E (PBE E (PBE) E (PBE) E (PM6) E (PM7)	Dicity: 3 :: 0 3c) = -3245.778887 def2-TZVP) = -3245 - D3(BJ)/def2-TZVP 1- D3(BJ)/def2-TZVP 1-3c) = -3241.09352 = -136.19646 Kcal = -154.29838 Kcal	.807028098133 Ha b) = -3244.519852 p) = -3244.76770 1830369 Hartree /mol /mol	550107 Hartree 4867240 Hartree
Н Н С Н С Н Н Н	2.580932 2.545370 3.428001 2.018737 2.487877 3.021805 2.638657 3.204889 3.998950 0.748946	4.023568 2.408778 2.638707 2.908164 3.808444 1.766840 0.804575 1.631300 1.972807 2.616397	-3.224846 -4.008933 -2.469515 2.936758 3.393138 3.125388 2.748215 4.210479 2.653222 3.763590	Multip Charge E (B97- E (M06/ E (PBE E (PBE) E (PBE) E (PM6) E (PM7) E (\omega B97	Dlicity: 3 :: 0 3c) = -3245.778887 def2-TZVP) = -3245 - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZV :-3c) = -3241.09352 = -136.19646 Kcal = -154.29838 Kcal (X-V/def2-TZVP) = -	.807028098133 Ha ) = -3244.519852 P) = -3244.76770 1830369 Hartree /mol /mol 3246.85188749789	550107 Hartree 4867240 Hartree
Н Н С Н С Н Н С Н	2.580932 2.545370 3.428001 2.018737 2.487877 3.021805 2.638657 3.204889 3.998950 0.748946 0.012480	4.023568 2.408778 2.638707 2.908164 3.808444 1.766840 0.804575 1.631300 1.972807 2.616397 3.441043	-3.224846 -4.008933 -2.469515 2.936758 3.393138 3.125388 2.748215 4.210479 2.653222 3.763590 3.699459	Multip Charge E (B97- E (M06/ E (PBE E (PBE) E (PM6) E (PM7) E (\omega B97 E (GFN1	Dlicity: 3 :: 0 :: 0 :3c) = -3245.778887 def2-TZVP) = -3245 - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZV :-3c) = -3241.09352 = -136.19646 Kcal = -154.29838 Kcal X-V/def2-TZVP) = - :-xTB) = -165.42319	.807028098133 Ha ) = -3244.519852 P) = -3244.76770 1830369 Hartree /mol /mol 3246.85188749789 8959961 Hartree	550107 Hartree 4867240 Hartree
Н Н С Н С Н Н С Н Н Н Н Н	2.580932 2.545370 3.428001 2.018737 2.487877 3.021805 2.638657 3.204889 3.99850 0.748946 0.012480 1.014187	4.023568 2.408778 2.638707 2.908164 3.808444 1.766840 0.804575 1.631300 1.972807 2.616397 3.441043 2.465864	-3.224846 -4.008933 -2.469515 2.936758 3.393138 3.125388 2.748215 4.210479 2.653222 3.763590 3.699459 4.829673	Multip Charge E (B97- E (M06/ E (PBE E (PBE) E (PBE) E (PM6) E (PM7) E (GFN1 E (GFN1	Dlicity: 3 0: 0 3c) = -3245.778887 def2-TZVP) = -3245 - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP - 3c) = -3241.09352 = -136.19646 Kcal = -154.29838 Kcal X-V/def2-TZVP) = - -xTB) = -165.42319 (-xTB) = -162.81602	.807028098133 Ha ) = -3244.519852 P) = -3244.76770 1830369 Hartree /mol /mol 3246.85188749789 8959961 Hartree 7443892 Hartree	550107 Hartree 4867240 Hartree
Н Н С Н С Н Н Н Н Н	2.580932 2.545370 3.428001 2.018737 2.487877 3.021805 2.638657 3.204889 3.998950 0.748946 0.012480 1.014187 0.259258	4.023568 2.408778 2.638707 2.908164 3.808444 1.766840 0.804575 1.631300 1.972807 2.616397 3.441043 2.465864 1.693503	-3.224846 -4.008933 -2.469515 2.936758 3.393138 3.125388 2.748215 4.210479 2.653222 3.763590 3.699459 4.829673 3.408002	Multip Charge E (B97- E (M06/ E (PBE E (PBE) E (PBE) E (PM6) E (PM7) E (GFN1 E (GFN1	Dlicity: 3 :: 0 :: 0 :3c) = -3245.778887 def2-TZVP) = -3245 - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZV :-3c) = -3241.09352 = -136.19646 Kcal = -154.29838 Kcal X-V/def2-TZVP) = - :-xTB) = -165.42319	.807028098133 Ha ) = -3244.519852 P) = -3244.76770 1830369 Hartree /mol /mol 3246.85188749789 8959961 Hartree 7443892 Hartree	550107 Hartree 4867240 Hartree
Н Н С Н С Н Н С Н Н С Н С Н С Н С С Н С С Н С С С С Н С С С С С Н С С С С С С С С С С С С С С С С С С С С	2.580932 2.545370 3.428001 2.018737 2.487877 3.021805 2.638657 3.204889 3.998950 0.748946 0.012480 1.014187 0.259258 1.285995	4.023568 2.408778 2.638707 2.908164 3.808444 1.766840 0.804575 1.631300 1.972807 2.616397 3.441043 2.465864 1.693503 -2.630688	-3.224846 -4.008933 -2.469515 2.936758 3.393138 3.125388 2.748215 4.210479 2.653222 3.763590 3.699459 4.829673 3.408002 -1.315272	Multip Charge E (B97- E (M06/ E (PBE E (PBE) E (PM6) E (PM7) E (GFN1 E (GFN2 E (GFN2	Dicity: 3 :: 0 :: 0 :	.807028098133 Ha ) = -3244.519852 P) = -3244.76770 1830369 Hartree /mol /mol 3246.85188749789 8959961 Hartree 7443892 Hartree	550107 Hartree 4867240 Hartree
Н Н С Н С Н Н Н С Н Н С С С Н С С С Н С С С С С С С С С С С С С С С С С С С С	2.580932 2.545370 3.428001 2.018737 2.487877 3.021805 2.638657 3.204889 3.998950 0.748946 0.012480 1.014187 0.259258 1.285995 1.418910	4.023568 2.408778 2.638707 2.908164 3.808444 1.766840 0.804575 1.631300 1.972807 2.616397 3.441043 2.465864 1.693503 -2.630688 -2.684351	-3.224846 -4.008933 -2.469515 2.936758 3.393138 3.125388 2.748215 4.210479 2.653222 3.763590 3.699459 4.829673 3.408002 -1.315272 -2.739264	Multip Charge E (B97- E (M06/ E (PBE E (PBEC) E (PBEC) E (PM7) E (GFN1 E (GFN2 E (GFN-	Dicity: 3 :: 0 3c) = -3245.778887 def2-TZVP) = -3245 - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP D3(BJ)/def2-TZVP 136.19646 Kcal 154.29838 Kcal (X-V/def2-TZVP) = - -xTB) = -165.42319 -xTB) = -162.81602 FF) = -22.30942928 .nates:	.807028098133 Ha ) = -3244.519852 P) = -3244.76770 1830369 Hartree /mol /mol 3246.85188749789 8959961 Hartree 7443892 Hartree 3128 Hartree	550107 Hartree 4867240 Hartree 3 Hartree
Н Н С Н С Н Н С Н Н С Н С Н С Н С С Н С С Н С С С С Н С С С С С Н С С С С С С С С С С С С С С С С С С С С	2.580932 2.545370 3.428001 2.018737 2.487877 3.021805 2.638657 3.204889 3.998950 0.748946 0.012480 1.014187 0.259258 1.285995	4.023568 2.408778 2.638707 2.908164 3.808444 1.766840 0.804575 1.631300 1.972807 2.616397 3.441043 2.465864 1.693503 -2.630688	-3.224846 -4.008933 -2.469515 2.936758 3.393138 3.125388 2.748215 4.210479 2.653222 3.763590 3.699459 4.829673 3.408002 -1.315272	Multip Charge E (B97- E (M06/ E (PBE E (PBE) E (PM6) E (PM7) E (GFN1 E (GFN2 E (GFN2	Dicity: 3 :: 0 :: 0 :	.807028098133 Ha ) = -3244.519852 P) = -3244.76770 1830369 Hartree /mol /mol 3246.85188749789 8959961 Hartree 7443892 Hartree	550107 Hartree 4867240 Hartree
Н Н С Н С Н Н Н С Н Н С С С Н С С С Н С С С С С С С С С С С С С С С С С С С С	2.580932 2.545370 3.428001 2.018737 3.021805 2.638657 3.204889 3.998950 0.748946 0.012480 1.014187 0.259258 1.285995 1.418910 0.932301	4.023568 2.408778 2.638707 2.908164 3.808444 1.766840 0.804575 1.631300 1.972807 2.616397 3.441043 2.465864 1.693503 -2.630688 -2.684351 -3.834074	-3.224846 -4.008933 -2.469515 2.936758 3.393138 3.125388 2.748215 4.210479 2.653222 3.763590 3.699459 4.829673 3.408002 -1.315272 -2.739264	Multip Charge E (B97- E (M06/ E (PBE E (PBEC) E (PBEC) E (PM7) E (GFN1 E (GFN2 E (GFN-	Dicity: 3 :: 0 3c) = -3245.778887 def2-TZVP) = -3245 - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP D3(BJ)/def2-TZVP 136.19646 Kcal 154.29838 Kcal (X-V/def2-TZVP) = - -xTB) = -165.42319 -xTB) = -162.81602 FF) = -22.30942928 .nates:	.807028098133 Ha ) = -3244.519852 P) = -3244.76770 1830369 Hartree /mol /mol 3246.85188749789 8959961 Hartree 7443892 Hartree 3128 Hartree	550107 Hartree 4867240 Hartree 3 Hartree -0.373391
Н Н Н С Н Н Н С Н Н С С С С Н	2.580932 2.545370 3.428001 2.018737 3.021805 2.638657 3.204889 3.998950 0.748946 0.012480 1.014187 0.259258 1.285995 1.418910 0.932301 1.038082	4.023568 2.408778 2.638707 2.908164 3.808444 1.766840 0.804575 1.631300 1.972807 2.616397 3.441043 2.465864 1.693503 -2.630688 -2.684351 -3.834074 -3.884956	-3.224846 -4.008933 -2.469515 2.936758 3.393138 3.125388 2.748215 4.210479 2.653222 3.763590 3.699459 4.829673 3.408002 -1.315272 -2.739264 -3.399028 -4.494639	Multip Charge E(B97- E(M06/ E(PBE) E(PBE) E(PM6) E(PM7) E(GFN1 E(GFN2 Coordi V	Dlicity: 3 :: 0 :: 0 :: 0 :: 0 :: 0 :: 0 :: 0 :	.807028098133 Ha ) = -3244.519852 P) = -3244.76770 1830369 Hartree /mol /mol 3246.85188749789 8959961 Hartree 7443892 Hartree 3128 Hartree -0.191725 1.211190	550107 Hartree 4867240 Hartree 3 Hartree -0.373391 2.580084
Н Н Н С Н Н Н С С С Н С	2.580932 2.545370 3.428001 2.018737 2.487877 3.021805 2.638657 3.204889 3.998950 0.748946 0.012480 1.014187 0.259258 1.285995 1.418910 0.932301 1.038082 0.320026	4.023568 2.408778 2.638707 2.908164 3.808444 1.766840 0.804575 1.631300 1.972807 2.616397 3.441043 2.465864 1.693503 -2.630688 -2.684351 -3.834074 -3.884956 -4.890434	-3.224846 -4.008933 -2.469515 2.936758 3.393138 3.125388 2.748215 4.210479 2.653222 3.763590 3.699459 4.829673 3.408002 -1.315272 -2.739264 -3.399028 -4.494639 -2.720572	Multip Charge E (B97- E (M06A) E (PBE E (PBEC E (PBEC) E (PM7) E (GFN1 E (GFN2 E (GFN2 V O O	Dicity: 3 :: 0 :3c) = -3245.778887 def2-TZVP) = -3245 - D3(BJ)/def2-TZVP 1- D3(BJ)/def2-TZVP 1-3c) = -3241.09352 = -136.19646 Kcal = -154.29838 Kcal  X-V/def2-TZVP) = - XTB) = -165.42319  XTB) = -162.81602 	.807028098133 Ha ) = -3244.519852 P) = -3244.76770 1830369 Hartree /mol /mol 3246.85188749789 8959961 Hartree 7443892 Hartree 3128 Hartree -0.191725 1.211190 3.148733	550107 Hartree 4867240 Hartree 3 Hartree -0.373391 2.580084 2.253464
Н Н Н С Н Н Н С С С Н С Н	2.580932 2.545370 3.428001 2.018737 2.487877 3.021805 2.638657 3.204889 3.998950 0.748946 0.012480 1.014187 0.259258 1.285995 1.418910 0.932301 1.038082 0.320026 -0.044187	4.023568 2.408778 2.638707 2.908164 3.808444 1.766840 0.804575 1.631300 1.972807 2.616397 3.441043 2.465864 1.693503 -2.630688 -2.684351 -3.834074 -3.884956 -4.890434 -5.769269	-3.224846 -4.008933 -2.469515 2.936758 3.393138 3.125388 2.748215 4.210479 2.653222 3.763590 3.699459 4.829673 3.408002 -1.315272 -2.739264 -3.399028 -4.494639 -2.720572 -3.273656	Multip Charge E (B87- E (M066) E (PBE E (PBE) E (PM6) E (PM7) E (GFN1 E (GFN2 Coordi V O N	Dicity: 3 :: 0 3c) = -3245.778887 def2-TZVP) = -3245 - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP - 136.19646 Kcal = -154.29838 Kcal (X-V/def2-TZVP) =xTB) = -165.42319 -xTB) = -162.81602 -FF) = -22.30942928  nates:	.807028098133 Ha ) = -3244.519852 P) = -3244.76770 1830369 Hartree /mol /mol 3246.85188749789 8959961 Hartree 7443892 Hartree 3128 Hartree -0.191725 1.211190 3.148733 -0.228420	550107 Hartree 4867240 Hartree 3 Hartree -0.373391 2.580084 2.253464 -0.782217
Н Н Н С Н С Н Н Н С С С Н С Н С Н С	2.580932 2.545370 3.428001 2.018737 3.021805 2.638657 3.204889 3.998950 0.748946 0.012480 1.014187 0.259258 1.285995 1.418910 0.932301 1.038082 0.320026 -0.044187 0.169456	4.023568 2.408778 2.638707 2.908164 3.808444 1.766840 0.804575 1.631300 1.972807 2.616397 3.441043 2.465864 1.693503 -2.630688 -2.684351 -3.834074 -3.884956 -4.890434 -5.769269 -4.808426	-3.224846 -4.008933 -2.469515 2.936758 3.393138 3.125388 2.748215 4.210479 2.653222 3.763590 3.699459 4.829673 3.408002 -1.315272 -2.739264 -3.399028 -4.494639 -2.720572 -3.273656 -1.334860	Multip Charge E (B87- E (M66- E (PBE- E (PBE- E (PBE- E (PM6)) E (GFN1- E (GFN2- E (GFN- Coordi V O O N	Dicity: 3 :: 0 3c) = -3245.778887 def2-TZVP) = -3245 - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP3c) = -3241.09352 = -136.19646 Kcal = -154.29838 Kcal (X-V/def2-TZVP) =xTB) = -165.42319 -xTB) = -165.42319 -xTB) = -162.81602 -FF) = -22.30942928  .nates:	.807028098133 Ha ) = -3244.519852 P) = -3244.76770 1830369 Hartree /mol /mol 3246.85188749789 8959961 Hartree 7443892 Hartree 3128 Hartree -0.191725 1.211190 3.148733 -0.228420 0.265676	550107 Hartree 4867240 Hartree 3 Hartree -0.373391 2.580084 2.253464 -0.782217 -2.242153
Н Н Н С Н С Н С С С Н С Н С Н С Н	2.580932 2.545370 3.428001 2.018737 3.021805 2.638657 3.204889 3.998950 0.748946 0.012480 1.014187 0.259258 1.285995 1.418910 0.932301 1.038082 0.320026 -0.044187 0.169456 -0.322308	4.023568 2.408778 2.638707 2.908164 3.808444 1.766840 0.804575 1.631300 1.972807 2.616397 3.441043 2.465864 1.693503 -2.630688 -2.684351 -3.834074 -3.884956 -4.890434 -5.769269 -4.808426 -5.626023	-3.224846 -4.008933 -2.469515 2.936758 3.393138 3.125388 2.748215 4.210479 2.653222 3.763590 3.699459 4.829673 3.408002 -1.315272 -2.739264 -3.399028 -4.494639 -2.720572 -3.273656 -1.334860 -0.785925	Multip Charge E (B87- E (M06/ E (PBEC E (PBEC E (PBEC) E (PM7) E (GFN1 E (GFN2 C (GFN- C Oordi V O O N N	Dicity: 3 :: 0 :3c) = -3245.778887 def2-TZVP) = -3245 - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP3c) = -3241.09352 = -136.19646 Kcal = -154.29838 Kcal X-V/def2-TZVP) =xTB) = -165.42319 :xTB) = -162.81602 :FF) = -22.30942928  .nates:	.807028098133 Ha ) = -3244.519852 P) = -3244.76770 1830369 Hartree /mol 3246.85188749789 8959961 Hartree 7443892 Hartree 3128 Hartree -0.191725 1.211190 3.148733 -0.228420 0.265676 -1.786924	550107 Hartree 4867240 Hartree 3 Hartree -0.373391 2.580084 2.253464 -0.782217 -2.242153 0.294937
Н Н Н С Н Н Н С С С Н С Н С Н С Н С Н С	2.580932 2.545370 3.428001 2.018737 2.487877 3.021805 2.638657 3.204889 3.998950 0.748946 0.012480 1.014187 0.259258 1.285995 1.418910 0.932301 1.038082 0.320026 -0.044187 0.169456 -0.322308 0.643106	4.023568 2.408778 2.638707 2.908164 3.808444 1.766840 0.804575 1.631300 1.972807 2.616397 3.441043 2.465864 1.693503 -2.630688 -2.684351 -3.884956 -4.890434 -5.769269 -4.808426 -5.626023 -3.695159	-3.224846 -4.008933 -2.469515 2.936758 3.393138 3.125388 2.748215 4.210479 2.653222 3.763590 3.699459 4.829673 3.408002 -1.315272 -2.739264 -3.399028 -4.494639 -2.720572 -3.273656 -1.334860 -0.785925 -0.617943	Multip Charge E (B97- E (M06A) E (PBE E (PBE) E (PMT) E (GFN1 E (GFN2 E (GFN- Coordi V O O N N	Dicity: 3 :: 0 3c) = -3245.778887 def2-TZVP) = -3245 - D3(BJ)/def2-TZVP 1- D3(BJ)/def2-TZVP 1- D3(BJ)/def2-TZVP 1- 3c) = -3241.09352 = -136.19646 Kcal = -154.29838 Kcal X-V/def2-TZVP) = - 1-XTB) = -165.42319 1-XTB) = -162.81602 1-XTB) = -22.30942928 1.018082 0.667283 -0.558059 1.964531 -0.595333 -0.988544 -0.577431	.807028098133 Ha ) = -3244.519852 P) = -3244.76770 1830369 Hartree /mol /mol 3246.85188749789 8959961 Hartree 3128 Hartree 3128 Hartree -0.191725 1.211190 3.148733 -0.228420 0.265676 -1.786924 1.415832	550107 Hartree 4867240 Hartree 3 Hartree -0.373391 2.580084 2.253464 -0.782217 -2.242153 0.294937 0.463457
Н Н Н С Н С Н Н Н Н С С С Н С Н С Н С С	2.580932 2.545370 3.428001 2.018737 2.487877 3.021805 2.638657 3.204889 3.998950 0.748946 0.012480 1.014187 0.259258 1.285995 1.418910 0.932301 1.038082 0.320026 -0.044187 0.169456 -0.322308 0.643106 1.937179	4.023568 2.408778 2.638707 2.908164 3.808444 1.766840 0.804575 1.631300 1.972807 2.616397 3.441043 2.465864 1.693503 -2.630688 -2.684351 -3.834074 -3.884956 -4.890434 -5.769269 -4.808426 -5.626023 -3.695159 -1.593957	-3.224846 -4.008933 -2.469515 2.936758 3.393138 3.125388 2.748215 4.210479 2.653222 3.763590 3.699459 4.829673 3.408002 -1.315272 -2.739264 -3.399028 -4.494639 -2.720572 -3.273656 -1.334860 -0.785925 -0.617943 -3.691078	Multip Charge E (B87- E (M06A) E (PBE E (PBEA) E (PMEA) E (GFM1) E (GFN2 E (GFN- Coordi V O O N N N N H	Dicity: 3 1: 0 3c) = -3245.778887 def2-TZVP) = -3245 - D3(BJ)/def2-TZVP 1- D3(BJ)/def2	.807028098133 Ha ) = -3244.76770 1830369 Hartree /mol /mol 3246.85188749789 8959961 Hartree 3128 Hartree 3128 Hartree -0.191725 1.211190 3.148733 -0.228420 0.265676 -1.786924 1.415832 1.971428	550107 Hartree 4867240 Hartree 3 Hartree -0.373391 2.580084 2.253464 -0.782217 -2.242153 0.294937 0.463457 -0.017838
Н Н Н С Н С Н Н Н С С С Н С Н С С С Н	2.580932 2.545370 3.428001 2.018737 2.487877 3.021805 2.638657 3.204889 3.998950 0.748946 0.012480 1.014187 0.259258 1.285995 1.418910 0.932301 1.038082 0.320026 -0.044187 0.169456 -0.322308 0.643106 1.937179 2.323250	4.023568 2.408778 2.638707 2.908164 3.808444 1.766840 0.804575 1.631300 1.972807 2.616397 3.441043 2.465864 1.693503 -2.630688 -2.684351 -3.834074 -3.884956 -4.890434 -5.769269 -4.808426 -5.626023 -3.695159 -1.593957 -2.164279	-3.224846 -4.008933 -2.469515 2.936758 3.393138 3.125388 2.748215 4.210479 2.653222 3.763590 3.699459 4.829673 3.408002 -1.315272 -2.739264 -3.399028 -4.494639 -2.720572 -3.273656 -1.334860 -0.785925 -0.617943 -3.691078 -4.564399	Multip Charge E (B87- E (M966) E (PBED E (PBED E (PMED) E (GFN1) E (GFN2) E (GFN1) Coordid V O O N N N N H C	Dicity: 3 :: 0 3c) = -3245.778887 def2-TZVP) = -3245 - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP136.19646 Kcal = -154.29838 Kcal (X-V/def2-TZVP) =xTB) = -165.42319 -xTB) = -162.81602 -FF) = -22.30942928  .nates:	.807028098133 Ha ) = -3244.76770 1830369 Hartree /mol /mol 3246.85188749789 8959961 Hartree 7443892 Hartree 3128 Hartree -0.191725 1.211190 3.148733 -0.228420 0.265676 -1.786924 1.415832 1.971428 -0.639132	550107 Hartree 4867240 Hartree 3 Hartree  -0.373391 2.580084 2.253464 -0.782217 -2.242153 0.294937 0.463457 -0.017838 -2.027745
Н Н Н С Н С Н Н Н С С С Н С Н С С С Н С С С С С С С С С С С С С С С С С С С С	2.580932 2.545370 3.428001 2.018737 3.021805 2.638657 3.204889 3.998950 0.748946 0.012480 1.014187 0.259258 1.285995 1.418910 0.932301 1.038082 0.320026 -0.044187 0.169456 -0.322308 0.643106 1.937179 2.333250 3.083716	4.023568 2.408778 2.638707 2.908164 3.808444 1.766840 0.804575 1.631300 1.972807 2.616397 3.441043 2.465864 1.693503 -2.630688 -2.684351 -3.834074 -3.884956 -4.890434 -5.769269 -4.808426 -5.626023 -3.695159 -1.593957 -2.164279 -0.681724	-3.224846 -4.008933 -2.469515 2.936758 3.393138 3.125388 2.748215 4.210479 2.653222 3.763590 3.699459 4.829673 3.408002 -1.315272 -2.739264 -3.399028 -4.494639 -2.720572 -3.273656 -1.334860 -0.785925 -0.617943 -3.691078 -4.564399 -3.245243	Multip Charge E (B87- E (M96-) E (PBE- E (PBE- E (PBE- E (PM6)) E (GFN1- E (GFN2- Coordi V O O N N N N H C C	Dicity: 3 :: 0 3c) = -3245.778887 def2-TZVP) = -3245 - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - 136.19646 Kcal = -154.29838 Kcal (X-V/def2-TZVP) =xTB) = -165.42319 -xTB) = -165.42319 -xTB) = -162.81602 -FF) = -22.30942928  .nates:	.807028098133 Ha ) = -3244.519852 P) = -3244.76770 1830369 Hartree /mol /mol 3246.85188749789 8959961 Hartree 7443892 Hartree 3128 Hartree -0.191725 1.211190 3.148733 -0.228420 0.265676 -1.786924 1.415832 1.971428 -0.639132 -0.614111	550107 Hartree 4867240 Hartree 3 Hartree  -0.373391 2.580084 2.253464 -0.782217 -2.242153 0.294937 0.463457 -0.017838 -2.027745 -3.151840
Н Н Н С Н С Н Н Н С С С Н С Н С С С Н	2.580932 2.545370 3.428001 2.018737 2.487877 3.021805 2.638657 3.204889 3.998950 0.748946 0.012480 1.014187 0.259258 1.285995 1.418910 0.932301 1.038082 0.320026 -0.044187 0.169456 -0.322308 0.643106 1.937179 2.323250	4.023568 2.408778 2.638707 2.908164 3.808444 1.766840 0.804575 1.631300 1.972807 2.616397 3.441043 2.465864 1.693503 -2.630688 -2.684351 -3.834074 -3.884956 -4.890434 -5.769269 -4.808426 -5.626023 -3.695159 -1.593957 -2.164279	-3.224846 -4.008933 -2.469515 2.936758 3.393138 3.125388 2.748215 4.210479 2.653222 3.763590 3.699459 4.829673 3.408002 -1.315272 -2.739264 -3.399028 -4.494639 -2.720572 -3.273656 -1.334860 -0.785925 -0.617943 -3.691078 -4.564399	Multip Charge E (B87- E (M966) E (PBED E (PBED E (PMED) E (GFN1) E (GFN2) E (GFN1) Coordid V O O N N N N H C	Dicity: 3 :: 0 3c) = -3245.778887 def2-TZVP) = -3245 - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP - D3(BJ)/def2-TZVP136.19646 Kcal = -154.29838 Kcal (X-V/def2-TZVP) =xTB) = -165.42319 -xTB) = -162.81602 -FF) = -22.30942928  .nates:	.807028098133 Ha ) = -3244.76770 1830369 Hartree /mol /mol 3246.85188749789 8959961 Hartree 7443892 Hartree 3128 Hartree -0.191725 1.211190 3.148733 -0.228420 0.265676 -1.786924 1.415832 1.971428 -0.639132	550107 Hartree 4867240 Hartree 3 Hartree  -0.373391 2.580084 2.253464 -0.782217 -2.242153 0.294937 0.463457 -0.017838 -2.027745

С	0.184492	-0.051594	-3.297779	C 0.8	843217	-6.815748	-1.908964
С	3.731648	-1.146218	-2.293224		853669	-7.049493	-1.508177
H	4.425064	-0.937589	-1.461238		927422	-6.781281	-3.012975
H	4.143388	-0.706404	-3.222212	н 0.1	188713	-7.671168	-1.643185
H	3.691833	-2.245073	-2.440129	C 0.9	939681	2.038913	3.739827
С	-0.275261	0.195278	-4.719492		207448	3.140901	3.660271
H	-1.348123	0.445563	-4.786522		349520	2.612625	3.577348
H	-0.071333	-0.695078	-5.346141	н 3.0	058882	1.778702	3.416218
H	0.303214	1.033015	-5.160286	Н 2.6	666601	3.181331	4.473256
		0.118887			416901		
С	3.022095		0.150176			3.276631	2.695835
C	3.673882	1.391276	0.013074	C 0.8	883850	1.153566	4.984397
C	4.735698	1.705240	0.887669	н -0.0	064877	0.589370	5.047546
Н	5.230598	2.682384	0.770964		998663	1.759371	5.905440
С	5.171679	0.831023	1.881615		713576	0.420174	4.952675
H	6.004686	1.103813	2.546667	C -1.4	474887	2.749665	4.429956
С	4.535049	-0.403072	2.002402	н -2.2	279563	3.467268	4.177078
Н	4.873113	-1.117463	2.769451		320312	2.769741	5.526429
C	3.477751	-0.795015	1.154559	H -1.8	824505	1.741032	4.137342
C	3.318801	2.553669	-0.927658	C 0.2	238050	4.545344	4.060384
H	4.251236	3.157655	-0.950841	н 1.0	054332	4.911396	3.411558
С	2.992882	2.275712	-2.398102		585088	4.564762	5.112841
H	3.745532	1.617916	-2.873366	н -0.6	613876	5.247001	3.965988
H	2.995672	3.237538	-2.951263	в -0.1	165765	1.926714	1.724347
H	2.000036	1.818014	-2.541501				
С	2.248991	3.447768	-0.282204	Conformation 3			
H	1.292186	2.905892	-0.163056	Multiplicity:	3		
H	2.067962	4.345783	-0.906616	Charge: 0			
Н	2.569270	3.793538	0.719531	E(B97-3c) = -3	2015 70740044	12277	
				, ,			
C	2.932925	-2.193799	1.452703	E(M06/def2-TZV	JP) = -3245.8	314781131296 Ha	rtree
H	3.699805	-2.642182	2.120514	E(PBE - D3(BJ)	/def2-TZVP)	= -3244.527681	.443584 Hartree
C	2.829909	-3.150033	0.259147				9788862 Hartree
							J. JUJUL MAILLEE
H	2.072636	-2.839392	-0.480713	E(PBEh-3c) = -			
H	2.532526	-4.158371	0.609766	E(PM6) = -134.	.93475 Kcal/m	nol	
H	3.806520	-3.245353	-0.255055	E(PM7) = -161.	13247 Kcal/m	101	
C			2.289188				· C II
	1.649193	-2.116885				246.86011602816	об нагигее
H	1.795218	-1.484306	3.185573	E(GFN1-xTB) =	-165.4306641	14686 Hartree	
H	1.329897	-3.127990	2.612367	E(GFN2-xTB) =	-162.8292810	041310 Hartree	
Н	0.814055	-1.681748	1.709564	E(GFN-FF) = -2			
				E(GEN-FE) = -2	12.3131230307	//4 naitiee	
С	-1.864662	0.919267	-2.458421				
C	-3.063685	0.147582	-2.556394	Coordinates:			
C	-4.272432	0.820451	-2.816744	V 0.0	071462	-0.468708	0.213491
Н							
	-5.198958	0.236499	-2.902998		377560	2.491289	-0.791239
C	-4.325648	2.209279	-2.968497	0 2.2	274583	2.284208	-2.107296
H	-5.283656	2.708486	-3.178608	N 0.3	334851	0.095048	2.126806
С	-3.154215	2.956114	-2.834644	N 0.6	657887	-2.347032	0.482424
H	-3.195480	4.050888	-2.937173		707564	-0.422865	-0.646674
С	-1.914526	2.341600	-2.571160	N 1.3	397113	0.266668	-0.917281
С	-3.074035	-1.371154	-2.411318	Н 2.0	058941	-0.330129	-1.422402
Н	-2.288071	-1.619277	-1.672086		439896	-0.833910	3.120349
C	-2.734337	-2.091260	-3.729360	C 0.4	451033	-2.225936	2.896747
H	-2.744494	-3.189547	-3.577398	н 0.4	443728	-2.843366	3.804626
H	-1.733580	-1.825963	-4.114362		603664	-2.947931	1.688439
H	-3.476912	-1.842383	-4.516532		552321	-0.378354	4.559478
C	-4.400376	-1.915001	-1.861756	н 1.4	437612	0.269738	4.707328
H	-4.699058	-1.404217	-0.925908	н 0.6	632270	-1.244902	5.239766
H	-4.297979	-2.996628	-1.643238		321762	0.230910	4.856156
H	-5.227328	-1.816803	-2.595646		721668	-4.448888	1.815290
С	-0.683243	3.232437	-2.443936	н 1.1	113864	-4.917822	0.895267
H	0.136168	2.605091	-2.044510	н -0.2	278480	-4.882733	2.023235
C	-0.905648	4.394956	-1.460916		376349	-4.720234	2.665865
H	-1.719479	5.068876	-1.797442		627622	1.460871	2.509212
H	0.012025	5.009760	-1.381476	C 2.0	003140	1.846146	2.553366
H	-1.154398	4.044821	-0.439896	C 2.3	349176	3.095908	3.099905
C	-0.235000	3.781469	-3.810321		411087	3.379331	3.156222
H	-0.032362	2.973099	-4.537932		375282	3.977656	3.571294
H	0.692459	4.380227	-3.701404		660060	4.947791	4.005498
H	-1.013582	4.439015	-4.250166	C 0.0	028984	3.619661	3.459542
С	-1.942535	-1.776285	1.341268		749911	4.320700	3.798901
C	-1.780202	-0.979459	2.495196		383555	2.376740	2.934823
H	-0.869198	-0.379670	2.617505		130451	0.940776	2.063416
C	-2.759975	-0.963238	3.498444	Н 2.6	662055	0.113694	1.495601
Н	-2.599058	-0.336661	4.391370		073920	1.672327	1.093974
						2.033476	
C	-3.930409	-1.739512	3.412830		537113		0.195759
С	-4.078449	-2.551275	2.267125		872648	0.986523	0.748016
H	-4.978614	-3.178466	2.159469	Н 4.5	575685	2.538525	1.571990
C	-3.112856	-2.573414	1.257881		928656	0.328511	3.228592
H	-3.253786	-3.219816	0.381237		374266	1.119196	3.867593
C	-4.983870	-1.713989	4.491158	H 4.7	757339	-0.298922	2.842313
H	-4.674957	-1.082547	5.347069	Н 3.2	299441	-0.315346	3.872708
Н	-5.196422	-2.731898	4.880542		897923	2.175261	2.838106
H	-5.946731	-1.311990	4.109363		327608	3.074837	3.329647
C	-0.625140	-3.033399	-0.249004	C -2.4	477106	0.975852	3.600511
Č	-0.189451	-3.130298	-1.592240		114514	0.010304	3.208577
H	-0.220046	-2.245740	-2.239348		581270	0.966536	3.499545
C	0.282736	-4.339557	-2.120585		241924	1.035807	4.682537
H	0.620466	-4.363057	-3.169398	C -2.3	361392	2.220344	1.376073
C	0.318558	-5.516728	-1.351741		058558	3.168688	0.892038
С	-0.142126	-5.425820	-0.018417		464646	2.122362	1.311519
H	0 101000	-6.326959	0.616641	H -1.9	918810	1.398974	0.785032
	-0.131002	0.320333	0.010011				
C	-0.131002 -0.594824	-4.223012	0.527892	C 1.0	027291	-3.061444	-0.716389
	-0.594824	-4.223012	0.527892		027291		
C H						-3.061444 -3.637316	-0.716389 -1.537748

С	0.351291	-4.158196	-2.796795	V	0.332629	-0.340136	0.038918
H	-0.440046	-4.582405	-3.432097	0	-1.318444	2.287809	-0.505452
C	1.675121	-4.162022	-3.243974	Ö	-2.259129	1.751296	-2.556145
							-0.057536
Н	1.930954	-4.565513	-4.235245	N	2.098685	0.603033	
С	2.675532	-3.690894	-2.393436	N	1.056994	-2.112095	-0.466313
H	3.728456	-3.753898	-2.712531	N	-0.687980	-0.513994	1.719852
C	2.398159	-3.148450	-1.118459	N	-0.759149	0.092619	-1.444920
С	-1.437873	-3.805148	-1.069827	Н	-1.003850	-0.601079	-2.158097
H	-1.586781	-3.159027	-0.184860	С	3.281031	-0.079403	-0.062398
C	-1.700510	-5.264468	-0.644241	Ċ	3.373228	-1.483010	-0.110923
Н	-2.716734	-5.355867	-0.208818	Н	4.389891	-1.890100	-0.030609
Н	-0.973274	-5.629152	0.103746	С	2.361578	-2.440949	-0.364598
H	-1.644129	-5.945209	-1.519385	С	4.583416	0.690944	-0.016491
С	-2.478904	-3.401776	-2.124409	H	4.685882	1.366812	-0.887782
Н	-2.312004	-2.378096	-2.504250	H	5.446124	0.000933	-0.003772
H	-3.493129	-3.433942	-1.681418	Н	4.629772	1.338770	0.878885
H	-2.472251	-4.095431	-2.991018	С	2.812674	-3.878361	-0.490106
С	3.666271	-2.760278	-0.333104	Н	2.044728	-4.521736	-0.954950
Н	4.374703	-3.575381	-0.600955	Н	3.032417	-4.285923	0.518999
C	3.619015	-2.749028	1.197234	Н	3.748261	-3.947317	-1.077895
				C			
H	2.993397	-1.934410	1.602555		2.186923	2.006211	-0.395375
Н	4.647068	-2.600359	1.585989	С	2.299132	2.326148	-1.784180
H	3.248892	-3.706032	1.608969	С	2.567380	3.654461	-2.161125
C	4.311513	-1.463484	-0.859910	Н	2.675737	3.896413	-3.229274
H	4.377717	-1.455139	-1.966065	C	2.697389	4.666422	-1.206994
H	5.340672	-1.358205	-0.459093	Н	2.917254	5.700077	-1.513812
H	3.742191	-0.570705	-0.542184	С	2.518790	4.352966	0.143525
С	-1.811129	0.239455	-1.897663	Н	2.588667	5.149792	0.900973
C	-1.043529	-0.206490	-2.998765	C	2.260048	3.038853	0.587284
Н	-0.378716	-1.072492	-2.866648	C	2.159619	1.269811	-2.879241
С	-1.128322	0.430644	-4.241870	H	1.731737	0.367602	-2.402083
H	-0.518124	0.055293	-5.078903	С	1.176126	1.714454	-3.973797
С	-1.986323	1.530996	-4.448524	H	0.173595	1.935721	-3.559465
C	-2.746332	1.975847	-3.347220	H	1.053093	0.911509	-4.727546
H	-3.420596	2.838809	-3.471394	Н	1.536440	2.613848	-4.514123
С	-2.657564	1.354405	-2.095201	С	3.513545	0.873551	-3.494592
Н	-3.251604	1.734203	-1.253075	Н	4.026544	1.751615	-3.940071
C	-2.051381	2.232950	-5.780890	Н	3.366779	0.124879	-4.300769
Н		1.530707	-6.622452	H	4.192851	0.424025	-2.745644
	-1.887590						
Н	-1.266264	3.017597	-5.857005	C	2.038066	2.875526	2.092533
Н	-3.027806	2.733623	-5.933790	H	2.252350	3.880824	2.515844
С	-2.853491	-0.924536	-0.020198	С	2.982689	1.907261	2.817891
C	-2.725537	-1.551806	1.247834	H	2.869930	0.867774	2.463920
H	-1.742066	-1.609617	1.739717	Н	2.753550	1.902292	3.902754
С	-3.820651	-2.126200	1.898512	Н	4.042014	2.213929	2.701561
H	-3.661525	-2.603561	2.879168	С	0.564022	2.580460	2.399813
С	-5.112323	-2.103821	1.334147	Н	-0.100565	3.355723	1.973150
Č	-5.241111	-1.486321	0.073368	Н	0.396970	2.528299	3.495443
Н	-6.229754	-1.461991	-0.413939	Н	0.250093	1.612413	1.969419
C	-4.151717	-0.913671	-0.594134	C	0.083026	-3.067778	-0.929661
	-4.302149		-1.590602		-0.615713		
H		-0.477836		C		-3.910465	-0.017489
С	-6.301064	-2.685245	2.056824	C	-1.608373	-4.770067	-0.528971
H	-6.797004	-1.929321	2.705077	H	-2.154295	-5.422104	0.169431
H	-6.007730	-3.529040	2.713348	C	-1.906895	-4.816427	-1.893316
H	-7.069455	-3.055479	1.348614	H	-2.689633	-5.493338	-2.267941
C	0.727336	3.843248	-1.190205	C	-1.195662	-4.002228	-2.782605
С	1.725310	3.596717	-2.401983	Н	-1.420213	-4.051316	-3.857961
C	1.395421	4.518199	0.010262	С	-0.195251	-3.123091	-2.330372
Н	0.724492	4.438391	0.886107	C	-0.295572	-3.967473	1.470732
Н		5.589277			0.379598	-3.122662	
	1.600789		-0.183629	H			1.703132
Н	2.345057	4.019025	0.278500	С	0.437572	-5.274005	1.833628
С	-0.552051	4.585292	-1.567629	Н	0.735716	-5.258298	2.901953
Н	-1.147080	4.014289	-2.303208	Н	1.348662	-5.431195	1.226822
H	-0.317626	5.584984	-1.985138	H	-0.220413	-6.154778	1.679020
Н	-1.175575	4.730823	-0.663376	C	-1.542263	-3.821992	2.356493
С	1.008043	3.488237	-3.751836	Н	-2.120024	-2.911090	2.114928
H	1.728663	3.124779	-4.510531	Н	-1.242052	-3.754391	3.420562
Н	0.610324	4.465717	-4.088324	Н	-2.220300	-4.695111	2.253597
Н	0.174354	2.763724	-3.696656	C	0.599976	-2.297300	-3.339776
C	2.875888	4.595285	-2.490883	Н	1.002705	-1.421768	-2.792811
			-1.578216				
Н	3.499540	4.584707		С	-0.255065	-1.770743	-4.502439
Н	2.493895	5.624129	-2.646959	H	-0.624806	-2.591311	-5.150698
H	3.524674	4.336239	-3.350592	H	0.347323	-1.098899	-5.145611
В	1.366500	1.643533	-1.275010	Н	-1.135899	-1.194784	-4.153013
				C	1.801481	-3.091988	-3.883693
Confo	rmation 33.			H	2.483661	-3.413880	-3.075603
Multi	plicity: 3			Н	2.387859	-2.473847	-4.594638
Charo				Н	1.460559	-4.001620	-4.420704
	(-3c) = -3245.801500	718708 Hartree		C	-2.054956	-0.136401	1.689812
	5/def2-TZVP) = -3245		rtree	C	-2.569634	0.908159	2.491335
	- D3(BJ)/def2-TZVP				-1.893530	1.450295	3.166018
	: - D3(B3)/de12-12VP :0 - D3(BJ)/def2-TZV				-3.924912	1.450295	2.432319
			Sellibu Corotec				
	2h-3c) = -3241.11632			H	-4.297304	2.073409	3.072644
	= -142.54922 Kcal			C	-4.820757	0.597469	1.566616
	() = -168.05699  Kcal			С	-4.299630	-0.433976	0.757122
	97X-V/def2-TZVP) = -		1 Hartree	H	-4.970024	-0.972020	0.067847
	11-xTB) = $-165.44194$			С	-2.950300	-0.799183	0.817787
	12-xTB) = $-162.84126$			H	-2.569811	-1.613242	0.183917
E (GFN	I-FF) = -22.32419641	6754 Hartree		C	-6.269371	1.003826	1.472963
				H	-6.600074	1.555495	2.374714
Coord	linates:			H	-6.933262	0.125357	1.343597

H C	-6.442097					1.344870	-1.588713
С		1.668659	0.597916	H	4.567299		
	-0.077636	-0.877305	2.923754	C	3.883411	1.783358	0.371272
C	1.307465	-1.194554	2.925835	Н	3.033534	1.644228	1.062436
H	1.890588	-1.131788	1.993746	H	4.030394	2.876295	0.263779
C	1.963200	-1.610305	4.088151	H	4.797863	1.369134	0.842323
H	3.038593	-1.845707	4.033258	C	2.499501	1.813884	-1.783530
С	1.285246	-1.730794	5.318280	H	2.394346	1.369515	-2.792216
C	-0.091980	-1.427970		H	2.682471	2.901943	-1.892298
			5.315158				
H	-0.665859	-1.527518	6.251302	H	1.533313	1.690143	-1.261652
С				С			
	-0.764183	-1.015791	4.158587		-2.336188	-0.640195	2.344414
H	-1.844134	-0.821854	4.203839	C	-3.111235	0.556407	2.512354
C	2.001910	-2.134572	6.581931	С	-4.511800	0.461435	2.593582
H	2.327915	-1.247834	7.169291	H	-5.102442	1.378427	2.719688
							2.530154
H	2.911115	-2.729931	6.364036	С	-5.167508	-0.769334	
H	1.351060	-2.737600	7.247199	H	-6.264406	-0.824902	2.597408
		3.498529					
C	-1.971549		-0.971176	С	-4.406949	-1.928017	2.395051
С	-2.943387	2.949032	-2.099681	H	-4.913867	-2.905554	2.360808
C							
	-0.884994	4.426959	-1.519721	С	-2.996220	-1.912273	2.302287
H	-0.118975	4.590487	-0.738212	C	-2.473145	1.934531	2.660812
Н	-1.299325	5.409964	-1.818200	Н	-1.580326	1.948032	2.007437
H	-0.372135	3.979382	-2.392031	C	-2.008466	2.200086	4.104221
С	-2.683195	4.152813	0.210213	H	-1.538245	3.201559	4.174615
H	-3.328769	3.429683	0.740784	H	-1.262608	1.463506	4.448809
H	-3.298090	5.011123	-0.127439	H	-2.868019	2.167270	4.806429
H	-1.933892	4.532691	0.932429	C	-3.382892	3.084449	2.207127
С	-4.301428	2.503138	-1.546554	H	-3.763051	2.934788	1.178128
H	-4.840204	1.940044	-2.333706	H	-2.814536	4.034845	2.225122
H	-4.928068	3.364091	-1.241369	H	-4.249122	3.221364	2.887590
H	-4.167245	1.833607	-0.676011	C	-2.405689	-3.323058	2.119516
С	-3.131115	3.886078	-3.289155	H	-3.160954	-3.973580	2.611125
H	-2.172123	4.097598	-3.796549	C	-1.079967	-3.674718	2.798507
Н	-3.581199	4.846640	-2.967088	H	-0.222677	-3.103837	2.402116
H	-3.812334	3.418804	-4.027358	H	-0.864985	-4.750422	2.634444
В	-1.434852	1.340672	-1.515828	H	-1.128911	-3.515202	3.891480
ii.	1.404007	1.0400/2	1.01000				
				C	-2.407895	-3.743307	0.638061
Conform	mation 34.			H	-3.382078	-3.525627	0.156590
Multipl	licity: 3			H	-2.222190	-4.833186	0.547984
Charge:	. ∩			H	-1.621766	-3.222600	0.063230
_							
E(B97-3	3c) = -3245.77871	.1502396 Hartree		C	-0.996124	2.693349	-0.835606
E (M06/c	def2-TZVP) = -324	5.806681454457 Ha	rtree	C	-1.123156	2.131989	-2.126320
	,						
E ( PRE -	- D3(BJ)/deI2-TZV	$^{\prime}P) = -3244.520070$	438693 Hartree	H	-0.554796	1.228809	-2.382088
E(PBE0	- D3(BJ)/def2-TZ	SVP) = -3244.76750	5271749 Hartree	С	-1.938432	2.732567	-3.093650
E (PREU-	-3c) = -3241.0928	75854910 Hartree		H	-2.006642	2.271301	-4.093154
E(PM6)	= -136.36198 Kca	l/mol		C	-2.648942	3.922019	-2.837611
	= -152.75292 Kca			C	-2.494650	4.495790	-1.558865
E (ωB97)	X-V/def2-TZVP) =	-3246.85162709803	4 Hartree	H	-3.022498	5.433228	-1.318758
	-xTB) = $-165.4211$			С		3.901401	-0.580505
					-1.690712		
E (GFN2-	-xTB) = $-162.8142$	03654987 Hartree		H	-1.587793	4.381739	0.401580
E (CEN_I	FF) = -22.3095080	32722 Hartron		С	-3.546273	4.542350	-3.878275
E (GEM-1	FF) = -22.3093000	JZ/ZZ Haitiee					
				H	-3.158996	4.375665	-4.903723
Coordin	nates.			H	-3.655955	5.634672	-3.726647
V	-0.091688	0.118184	0.473959	H	-4.568220	4.104798	-3.844495
0	-1.575977	-2.180524	-2.849755	С	0.598603	2.893886	0.979488
0	0.241233	-0.747144	-2.815797	C	1.172477	4.109618	0.519081
N	1.727055	-0.648182	0.770843	H			
					0 0/13312	4 460412	
N					0.943312	4.460412	-0.496632
N	-0.898487	-0.530795	2.213503	C	0.943312 2.032920	4.460412 4.850779	
	-0.898487	-0.530795			2.032920	4.850779	-0.496632 1.331831
	-0.898487 -0.204260	-0.530795 2.075068	0.162540	Н	2.032920 2.462254	4.850779 5.786243	-0.496632 1.331831 0.936645
N	-0.898487	-0.530795			2.032920	4.850779	-0.496632 1.331831
N	-0.898487 -0.204260 -1.080398	-0.530795 2.075068 -0.953724	0.162540 -0.739662	H C	2.032920 2.462254 2.386052	4.850779 5.786243 4.426796	-0.496632 1.331831 0.936645 2.633100
N H	-0.898487 -0.204260 -1.080398 -1.968041	-0.530795 2.075068 -0.953724 -1.322479	0.162540 -0.739662 -0.377191	H C C	2.032920 2.462254 2.386052 1.822585	4.850779 5.786243 4.426796 3.220090	-0.496632 1.331831 0.936645 2.633100 3.084980
N H C	-0.898487 -0.204260 -1.080398 -1.968041 2.155775	-0.530795 2.075068 -0.953724 -1.322479 -0.862204	0.162540 -0.739662 -0.377191 2.047981	H C C H	2.032920 2.462254 2.386052 1.822585 2.067849	4.850779 5.786243 4.426796 3.220090 2.847677	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743
N H C	-0.898487 -0.204260 -1.080398 -1.968041 2.155775	-0.530795 2.075068 -0.953724 -1.322479 -0.862204	0.162540 -0.739662 -0.377191 2.047981	H C C H	2.032920 2.462254 2.386052 1.822585 2.067849	4.850779 5.786243 4.426796 3.220090 2.847677	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743
N H C C	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507	0.162540 -0.739662 -0.377191 2.047981 3.179482	Н С С Н С	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045
N H C C H	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070	H C C H C	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290
N H C C H	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593	0.162540 -0.739662 -0.377191 2.047981 3.179482	H C C H C	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290
N H C C H C	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362 -0.097853	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593 -0.768926	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070 3.275219	H C C H C H	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524 3.309445	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655 5.247528	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290 3.497230
N H C C H C	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362 -0.097853 3.625107	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593 -0.768926 -1.121780	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070 3.275219 2.302743	Н С С Н С Н С	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524 3.309445 2.814577	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655 5.247528 6.175471	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290 3.497230 3.857392
N H C C H C	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362 -0.097853	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593 -0.768926	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070 3.275219	H C C H C H	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524 3.309445	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655 5.247528	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290 3.497230
N H C C H C C H	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362 -0.097853 3.625107 4.046227	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593 -0.768926 -1.121780 -1.864052	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070 3.275219 2.302743 1.599025	H C C H C H C H	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524 3.309445 2.814577 4.215043	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655 5.247528 6.175471 5.565335	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290 3.497230 3.857392 2.939983
N H C C H C H H	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362 -0.097853 3.625107 4.046227 3.794038	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593 -0.768926 -1.121780 -1.864052 -1.470162	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070 3.275219 2.302743 1.599025 3.337421	H C C H C H C H H	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524 3.309445 2.814577 4.215043 3.641112	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655 5.247528 6.175471 5.565335 4.681837	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290 3.497230 3.857392 2.933983 4.389919
N H C C H C C H	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362 -0.097853 3.625107 4.046227	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593 -0.768926 -1.121780 -1.864052	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070 3.275219 2.302743 1.599025	H C C H C H C H	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524 3.309445 2.814577 4.215043	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655 5.247528 6.175471 5.565335	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290 3.497230 3.857392 2.939983
N H C C H C H H H	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362 -0.097853 3.625107 4.046227 3.794038 4.199464	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593 -0.768926 -1.121780 -1.864052 -1.470162 -0.185949	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070 3.275219 2.302743 1.599025 3.337421 2.149689	H C C H C H C H C	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524 3.309445 2.814577 4.215043 3.641112 -1.210651	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655 5.247528 6.175471 5.565335 4.681837 -1.976065	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290 3.497230 3.857392 2.939983 4.389919 -4.238440
N H C C H C H C C H C C	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362 -0.097853 3.625107 4.046227 3.794038 4.199464 -0.665792	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593 -0.768926 -1.121780 -1.864052 -1.470162 -0.185949 -0.983758	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070 3.275219 2.302743 1.599025 3.337421 2.149689 4.663552	H C C H C H C H C C H C C	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524 3.309445 2.814577 4.215043 3.641112 -1.210651 0.246921	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655 5.247528 6.175471 5.565335 4.681837 -1.976065 -1.348040	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290 3.497230 3.857392 2.939983 4.389919 -4.238440 -4.136213
N H C C H C H H H	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362 -0.097853 3.625107 4.046227 3.794038 4.199464	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593 -0.768926 -1.121780 -1.864052 -1.470162 -0.185949	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070 3.275219 2.302743 1.599025 3.337421 2.149689	H C C H C H C H C	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524 3.309445 2.814577 4.215043 3.641112 -1.210651	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655 5.247528 6.175471 5.565335 4.681837 -1.976065	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290 3.497230 3.857392 2.939983 4.389919 -4.238440
N H C C H C H H H	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362 -0.097853 3.625107 4.046227 3.794038 4.199464 -0.665792 -1.769101	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593 -0.768926 -1.121780 -1.864052 -1.470162 -0.185949 -0.983758 -0.964181	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070 3.275219 2.302743 1.599025 3.337421 2.149689 4.663552 4.679859	H C C H C H H H C C	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524 3.309445 2.814577 4.215043 3.641112 -1.210651 0.246921 -2.243216	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.5555655 5.247528 6.175471 5.565335 4.681837 -1.976065 -1.348040 -1.007284	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290 3.497230 3.857392 2.939983 4.389919 -4.238440 -4.136213 -4.828908
N H C C H C H H H H H H	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362 -0.097853 3.625107 4.046227 3.794038 4.199464 -0.665792 -1.769101 -0.288978	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593 -0.768926 -1.121780 -1.864052 -1.470162 -0.185949 -0.983758 -0.964181 -0.196514	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070 3.275219 2.302743 1.599025 3.337421 2.149689 4.663552 4.679859 5.347659	H C C H C H H H C C H	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524 3.309445 2.814577 4.215043 3.641112 -1.210651 0.246921 -2.243216 -3.253919	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655 5.247528 6.175471 5.565335 4.681837 -1.976065 -1.348040 -1.007284 -1.439036	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290 3.497230 3.857392 2.939983 4.389919 -4.238440 -4.136213 -4.828908 -4.693104
N H C C H C H H H H	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362 -0.097853 3.625107 4.046227 3.794038 4.199464 -0.665792 -1.769101	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593 -0.768926 -1.121780 -1.864052 -1.470162 -0.185949 -0.983758 -0.964181	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070 3.275219 2.302743 1.599025 3.337421 2.149689 4.663552 4.679859	H C C H C H H H C C	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524 3.309445 2.814577 4.215043 3.641112 -1.210651 0.246921 -2.243216	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655 5.247528 6.175471 5.565335 4.681837 -1.976065 -1.348040 -1.007284 -1.439036 -0.832335	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290 3.497230 3.857392 2.939983 4.389919 -4.238440 -4.136213 -4.828908
N H C C H C H H H H	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362 -0.097853 3.625107 4.046227 3.794038 4.199464 -0.665792 -1.769101 -0.288978 -0.320038	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593 -0.768926 -1.121780 -1.864052 -1.470162 -0.185949 -0.983758 -0.964181 -0.196514 -1.951845	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070 3.275219 2.302743 1.599025 3.337421 2.149689 4.663552 4.679859 5.347659 5.075059	Н С С Н С Н Н С С С Н Н С С Н Н С Н Н С Н Н С Н Н С С Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524 3.309445 2.814577 4.215043 3.641112 -1.210651 0.246921 -2.243216 -3.253919 -2.079392	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655 5.247528 6.175471 5.565335 4.681837 -1.976065 -1.348040 -1.007284 -1.439036 -0.832335	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290 3.497230 3.857392 2.939983 4.389919 -4.238440 -4.136213 -4.828908 -4.693104 -5.910203
N H C C H H C H H C H C	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362 -0.097853 3.625107 4.046227 3.794038 4.199464 -0.665792 -1.769101 -0.288978 -0.320038 2.569476	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593 -0.768926 -1.121780 -1.864052 -1.470162 -0.185949 -0.983758 -0.964181 -0.196514 -1.951845 -1.166190	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070 3.275219 2.302743 1.599025 3.337421 2.149689 4.663552 4.679859 5.347659 5.075059 -0.289991	Н С С Н С Н С Н С С Н Н С С Н Н Н С С Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524 3.309445 2.814577 4.215043 3.641112 -1.210651 0.246921 -2.243216 -3.253919 -2.079392 -2.222315	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655 5.247528 6.175471 5.565335 4.681837 -1.976065 -1.348040 -1.007284 -1.439036 -0.832335 -0.032631	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290 3.497230 3.857392 2.939983 4.389919 -4.238440 -4.136213 -4.828908 -4.693104 -5.910203 -4.303504
N H C C H H H H C H C C	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362 -0.097853 3.625107 4.046227 3.794038 4.199464 -0.665792 -1.769101 -0.288978 -0.320038 2.569476 2.501292	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593 -0.768926 -1.121780 -1.864052 -1.470162 -0.185949 -0.983758 -0.964181 -0.196514 -1.951845 -1.166190 -2.576371	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070 3.275219 2.302743 1.599025 3.337421 2.149689 4.663552 4.679859 5.347659 5.075059 -0.289991 -0.523046	Н С С Н С Н Н Н Н С С Н Н Н Н С С Н Н С С С Н Н С С С С С С С С С С С С С С С С С С С С	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524 3.309445 2.814577 4.215043 3.641112 -1.210651 0.246921 -2.243216 -3.253919 -2.079392 -2.222315 -1.271550	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655 5.247528 6.175471 5.565335 4.681837 -1.976065 -1.348040 -1.007284 -1.439036 -0.832335 -0.032631 -3.317945	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290 3.497230 3.857392 2.939983 4.389919 -4.238440 -4.136213 -4.828908 -4.693104 -5.910203 -4.303504 -4.963227
N H C C H H H H C H C C	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362 -0.097853 3.625107 4.046227 3.794038 4.199464 -0.665792 -1.769101 -0.288978 -0.320038 2.569476 2.501292	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593 -0.768926 -1.121780 -1.864052 -1.470162 -0.185949 -0.983758 -0.964181 -0.196514 -1.951845 -1.166190 -2.576371	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070 3.275219 2.302743 1.599025 3.337421 2.149689 4.663552 4.679859 5.347659 5.075059 -0.289991 -0.523046	Н С С Н С Н Н Н Н С С Н Н Н Н С С Н Н С С С Н Н С С С С С С С С С С С С С С С С С С С С	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524 3.309445 2.814577 4.215043 3.641112 -1.210651 0.246921 -2.243216 -3.253919 -2.079392 -2.222315 -1.271550	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655 5.247528 6.175471 5.565335 4.681837 -1.976065 -1.348040 -1.007284 -1.439036 -0.832335 -0.032631 -3.317945	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290 3.497230 3.857392 2.939983 4.389919 -4.238440 -4.136213 -4.828908 -4.693104 -5.910203 -4.303504 -4.963227
N H C C H H H C H H C C	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362 -0.097853 3.625107 4.046227 3.794038 4.199464 -0.665792 -1.769101 -0.288978 -0.320038 2.569476 2.501292 3.409377	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593 -0.768926 -1.121780 -1.864052 -1.470162 -0.185949 -0.983758 -0.964181 -0.196514 -1.951845 -1.166190 -2.576371 -3.175070	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070 3.275219 2.302743 1.599025 3.337421 2.149689 4.663552 4.679859 5.347659 5.075059 -0.289991 -0.523046 -1.413741	Н С С Н С Н Н Н С С С Н Н Н Н С Н	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524 3.309445 2.814577 4.215043 3.641112 -1.210651 0.246921 -2.243216 -3.253919 -2.079392 -2.222315 -1.271550 -0.645612	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655 5.247528 6.175471 5.565335 4.681837 -1.976065 -1.348040 -1.007284 -1.439036 -0.832335 -0.032631 -3.317945 -4.078484	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290 3.497230 3.857392 2.939983 4.389919 -4.238440 -4.136213 -4.828908 -4.693104 -5.910203 -4.963327 -4.461648
N H C C H H C H H C H H C H H H C H	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362 -0.097853 3.625107 4.046227 3.794038 4.199464 -0.665792 -1.769101 -0.288978 -0.320038 2.569476 2.501292 3.409377 3.371540	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593 -0.768926 -1.121780 -1.864052 -1.470162 -0.185949 -0.983758 -0.964181 -0.196514 -1.951845 -1.166190 -2.576371 -3.175070 -4.264264	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070 3.275219 2.302743 1.599025 3.337421 2.149689 4.663552 4.679859 5.347659 5.075059 -0.289991 -0.523046 -1.413741 -1.564896	Н С С Н С Н Н С С С Н С Н С С Н С С Н С С С С С С С С С С С С С С С С С С С С	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524 3.309445 2.814577 4.215043 3.641112 -1.210651 0.246921 -2.243216 -3.253919 -2.079392 -2.222315 -1.271550 0.645612 -0.930824	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655 5.247528 6.175471 5.565335 4.681837 -1.976065 -1.348040 -1.007284 -1.439036 -0.832335 -0.032631 -3.317945 -4.078484 -3.215117	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290 3.497230 3.857392 2.939983 4.389919 -4.238440 -4.136213 -4.828908 -4.693104 -5.910203 -4.963227 -4.461648 -6.012976
N H C C H H H C H H C C	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362 -0.097853 3.625107 4.046227 3.794038 4.199464 -0.665792 -1.769101 -0.288978 -0.320038 2.569476 2.501292 3.409377	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593 -0.768926 -1.121780 -1.864052 -1.470162 -0.185949 -0.983758 -0.964181 -0.196514 -1.951845 -1.166190 -2.576371 -3.175070	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070 3.275219 2.302743 1.599025 3.337421 2.149689 4.663552 4.679859 5.347659 5.075059 -0.289991 -0.523046 -1.413741	Н С С Н С Н Н Н С С С Н Н Н Н С Н	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524 3.309445 2.814577 4.215043 3.641112 -1.210651 0.246921 -2.243216 -3.253919 -2.079392 -2.222315 -1.271550 -0.645612	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655 5.247528 6.175471 5.565335 4.681837 -1.976065 -1.348040 -1.007284 -1.439036 -0.832335 -0.032631 -3.317945 -4.078484	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290 3.497230 3.857392 2.939983 4.389919 -4.238440 -4.136213 -4.828908 -4.693104 -5.910203 -4.963327 -4.461648
N H C C H H C C H H C C H C C H C C H C C H C C H C C C C C C C C C C C C C C C C C C C C	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362 -0.097853 3.625107 4.046227 3.794038 4.199464 -0.665792 -1.769101 -0.288978 -0.320038 2.569476 2.501292 3.409377 3.371540 4.353729	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593 -0.768926 -1.121780 -1.864052 -1.470162 -0.185949 -0.983758 -0.964181 -0.196514 -1.951845 -1.166190 -2.576371 -3.175070 -4.264264 -2.416599	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070 3.275219 2.302743 1.599025 3.337421 2.149689 4.663552 4.679859 5.347659 5.075059 -0.289991 -0.523046 -1.413741 -1.564896 -2.107311	Н С С С Н С Н Н С С С С Н Н Н Н С Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524 3.309445 2.814577 4.215043 3.641112 -1.210651 0.246921 -2.243216 -3.253919 -2.079392 -2.222315 -1.271550 -0.645612 -0.930824 -2.315530	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655 5.247528 6.175471 5.565335 4.681837 -1.976065 -1.348040 -1.007284 -1.439036 -0.832335 -0.032631 -3.317945 -4.078484 -3.215117 -3.688122	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290 3.497230 3.857392 2.939983 4.389919 -4.238440 -4.136213 -4.828908 -4.693104 -5.910203 -4.903227 -4.461648 -6.012976 -4.975215
N H C C H H C H H C C H H H C C H H H C C H H C C H H C C H H C C H H H H H H H H H H H H H H H H H H H H	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362 -0.097853 3.625107 4.046227 3.794038 4.199464 -0.665792 -1.769101 -0.288978 -0.320038 2.569476 2.501292 3.409377 3.371540 4.353729 5.064932	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593 -0.768926 -1.121780 -1.864052 -1.470162 -0.185949 -0.983758 -0.964181 -0.196514 -1.951845 -1.166190 -2.576371 -3.175070 -4.264264 -2.416599 -2.897330	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070 3.275219 2.302743 1.599025 3.337421 2.149689 4.663552 4.679859 5.347659 5.075059 -0.289991 -0.523046 -1.413741 -1.564896 -2.107311 -2.795834	Н С С Н С Н Н Н С С С Н Н Н Н С С Н Н Н С С Н Н С С Н Н С С Н Н С С С Н Н Н С С Н Н С Н С Н С Н Н С Н С Н Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С В С Н С В С В	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524 3.309445 2.814577 4.215043 3.641112 -1.210651 0.246921 -2.243216 -3.253919 -2.079392 -2.222315 -1.271550 -0.645612 -0.930824 -2.315530 1.363636	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655 5.247528 6.175471 5.565335 4.681837 -1.976065 -1.348040 -1.007284 -1.439036 -0.832335 -0.032631 -3.317945 -4.078484 -3.215117 -3.688122 -2.393499	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290 3.497230 3.857392 2.939983 4.389919 -4.23840 -4.136213 -4.828908 -4.693104 -5.910203 -4.303504 -4.963227 -4.461648 -6.012976 -4.975215 -4.168416
N H C C H H C H H C C H H H C C H H H C C H H C C H H C C H H C C H H H H H H H H H H H H H H H H H H H H	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362 -0.097853 3.625107 4.046227 3.794038 4.199464 -0.665792 -1.769101 -0.288978 -0.320038 2.569476 2.501292 3.409377 3.371540 4.353729 5.064932	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593 -0.768926 -1.121780 -1.864052 -1.470162 -0.185949 -0.983758 -0.964181 -0.196514 -1.951845 -1.166190 -2.576371 -3.175070 -4.264264 -2.416599 -2.897330	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070 3.275219 2.302743 1.599025 3.337421 2.149689 4.663552 4.679859 5.347659 5.075059 -0.289991 -0.523046 -1.413741 -1.564896 -2.107311 -2.795834	Н С С Н С Н Н Н С С С Н Н Н Н С С Н Н Н С С Н Н С С Н Н С С Н Н С С С Н Н Н С С С Н Н С Н С Н С Н Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С В С В	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524 3.309445 2.814577 4.215043 3.641112 -1.210651 0.246921 -2.243216 -3.253919 -2.079392 -2.222315 -1.271550 -0.645612 -0.930824 -2.315530 1.363636	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655 5.247528 6.175471 5.565335 4.681837 -1.976065 -1.348040 -1.007284 -1.439036 -0.832335 -0.032631 -3.317945 -4.078484 -3.215117 -3.688122 -2.393499	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290 3.497230 3.857392 2.939983 4.389919 -4.23840 -4.136213 -4.828908 -4.693104 -5.910203 -4.303504 -4.963227 -4.461648 -6.012976 -4.975215 -4.168416
N H C C H H H H C C H H H C C H H C C H C C H C C H C C C H C C C C C C C C C C C C C C C C C C C C	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362 -0.097853 3.625107 4.046227 3.794038 4.199464 -0.665792 -1.769101 -0.288978 -0.320038 2.569476 2.501292 3.409377 3.371540 4.353729 5.064932 4.368055	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593 -0.768926 -1.121780 -1.864052 -1.470162 -0.185949 -0.983758 -0.964181 -0.196514 -1.951845 -1.166190 -2.576371 -3.175070 -4.264264 -2.416599 -2.897330 -1.032636	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070 3.275219 2.302743 1.599025 3.337421 2.149689 4.663552 4.679859 5.075059 -0.289991 -0.523046 -1.413741 -1.564896 -2.107311 -2.795834 -1.924909	Н С С Н С Н Н Н С С С Н Н Н Н С Н Н Н С Н	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524 3.309445 2.814577 4.215043 3.641112 -1.210651 0.246921 -2.243216 -3.253919 -2.079392 -2.222315 -1.271550 -0.645612 -0.930824 -2.315530 1.363636 2.315698	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655 5.247528 6.175471 5.565335 4.681837 -1.976065 -1.348040 -1.007284 -1.439036 -0.832335 -0.032631 -3.317945 -4.078484 -3.215117 -3.688122 -2.393499 -1.909772	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290 3.497230 3.857392 2.939983 4.389919 -4.238440 -4.136213 -4.828908 -4.693104 -5.910203 -4.303504 -4.963227 -4.461648 -6.012976 -4.975215 -4.168416 -3.879768
N H C C H H C H H C C H H C C H C H C H	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362 -0.097853 3.625107 4.046227 3.794038 4.199464 -0.665792 -1.769101 -0.288978 -0.320038 2.569476 2.501292 3.409377 3.371540 4.353729 5.064932 4.368055 5.092502	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593 -0.768926 -1.121780 -1.864052 -1.470162 -0.185949 -0.983758 -0.964181 -0.196514 -1.951845 -1.166190 -2.576371 -3.175070 -4.264264 -2.416599 -2.897330 -1.032636 -0.419374	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070 3.275219 2.302743 1.599025 3.337421 2.149689 4.663552 4.679859 5.075059 -0.289991 -0.523046 -1.413741 -1.564896 -2.107311 -2.795834 -1.924909 -2.483741	Н С С Н С Н Н Н С С С Н Н Н С С Н Н Н Н	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524 3.309445 2.814577 4.215043 3.641112 -1.210651 0.246921 -2.243216 -3.253919 -2.079392 -2.222315 -1.271550 -0.645612 -0.930824 -2.315530 1.363636 2.315698 1.481076	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655 5.247528 6.175471 5.565335 4.681837 -1.976065 -1.348040 -1.007284 -1.439036 -0.832335 -0.032631 -3.317945 -4.078484 -3.215117 -3.688122 -2.393499 -1.909772 -2.832897	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290 3.497230 3.857392 2.939983 4.389919 -4.238440 -4.136213 -4.828908 -4.693104 -5.910203 -4.303504 -4.963227 -4.461648 -6.012976 -4.975215 -4.168416 -3.879768 -5.178470
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N H C C H H H C C C H C H C C H C C H C C H C C H C C H C C H C C C C C C C C C C C C C C C C C C C C	-0.898487 -0.204260 -1.080398 -1.968041 2.155775 1.315311 1.830362 -0.097853 3.625107 4.046227 3.794038 4.199464 -0.665792 -1.769101 -0.288978 -0.320038 2.569476 2.501292 3.409377 3.371540 4.353729 5.064932 4.368055 5.092502 3.498939 1.508644 0.751622 0.764623	-0.530795 2.075068 -0.953724 -1.322479 -0.862204 -0.834507 -0.977593 -0.768926 -1.121780 -1.864052 -1.470162 -0.185949 -0.983758 -0.964181 -0.196514 -1.951845 -1.166190 -2.576371 -3.175070 -4.264264 -2.416599 -2.897330 -1.032636 -0.419374 -0.372690 -3.484051 -2.831645 -4.413262	0.162540 -0.739662 -0.377191 2.047981 3.179482 4.139070 3.275219 2.302743 1.599025 3.337421 2.149689 4.663552 4.679859 5.347659 5.075059 -0.289991 -0.523046 -1.413741 -1.564896 -2.107311 -2.795834 -1.924909 -2.483741 -1.029048 0.196317 0.672974 -0.776435	Н С С Н С Н Н Н С С С Н Н Н С С Н Н Н С С Н Н Н Н С Н Н Н Н С Н Н Н Н С Н Н Н С Н Н Н С Н Н Н С Н Н	2.032920 2.462254 2.386052 1.822585 2.067849 0.939258 0.510524 3.309445 2.814577 4.215043 3.641112 -1.210651 0.246921 -2.243216 -3.253919 -2.079392 -2.222315 -1.271550 -0.645612 -0.930824 -2.315530 1.363636 2.315698 1.481076 1.179754 0.538070 -0.155582 0.464954	4.850779 5.786243 4.426796 3.220090 2.847677 2.478403 1.555655 5.247528 6.175471 5.565335 4.681837 -1.976065 -1.348040 -1.007284 -1.439036 -0.832335 -0.032631 -3.317945 -4.078484 -3.215117 -3.688122 -2.393499 -1.909772 -2.832897 -3.210789 -0.250021 0.604116 -0.642577	-0.496632 1.331831 0.936645 2.633100 3.084980 4.092743 2.289045 2.700290 3.497230 3.857392 2.939983 4.389919 -4.238440 -4.136213 -4.828908 -4.693104 -5.910203 -4.303504 -4.963227 -4.461648 -6.012976 -4.975215 -4.168416 -3.879768 -5.178470 -3.446460 -5.158991 -5.053107 -6.192996
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Charg	e: 0			N	-4.426615	-0.097347	1.314330
	-3c) = -6287.33453	9666292 Hartree		Н	-3.768084	-0.645966	0.749374
	,	7.327396830854 Hartre	20	C	-5.394274	0.470653	0.510656
		P) = -6285.1475112918		0	-5.449589	0.127638	-0.677083
		(VP) = -6285.322362667	7313 Hartree	С	-6.367847	1.485302	1.028823
E (PBE	h-3c) = -6277.9248	60852325 Hartree		C	-7.705966	1.333028	0.576981
E(PM6	) = 262.06750  Kcal	/mol		Н	-7.934052	0.444703	-0.029007
E (PM7	) = 121.09013 Kcal	/mol		С	-8.682052	2.268378	0.862154
		-6289.218225469356 Ha	artree	Н	-9.717992	2.132052	0.517297
	1-xTB) = $-298.8471$		110100	C	-8.337678	3.433177	1.599826
				C			
	2-xTB) = $-290.6857$				-9.288281	4.444479	1.918478
E (GFN	-FF) = $-36.5452506$	44598 Hartree		H	-10.330544	4.317002	1.585489
				C	-8.897116	5.563877	2.633166
Coord	inates:			H	-9.611228	6.360492	2.889339
Cu	0.165046	-1.124304	-0.702265	С	-7.538697	5.662560	3.037916
N	1.120164	0.207456	-1.893151	Н	-7.198806	6.540945	3.616444
N	-0.423841	0.395384	0.496491	N	-6.624102	4.746882	2.760969
N	-0.834468	-2.448053	0.471405	C	-6.979267	3.641580	2.051562
N	0.844072	-2.654649	-1.846764	C	-5.975119	2.646633	1.730494
C	1.831796	-0.080461	-3.038626	0	-4.669847	2.729625	2.032493
C	2.307309	1.145040	-3.650903	C	-4.019330	3.870931	2.606050
H	2.878579	1.194429	-4.584260	Н	-4.192832	4.784232	2.010564
С	1.907869	2.174738	-2.837686	Н	-2.945572	3.615803	2.574588
Н	2.079228	3.248970	-2.962553	Н	-4.354435	4.044946	3.644910
	1.195360						
С		1.576172	-1.725618	С	0.017272	-6.057789	-0.347452
С	0.718944	2.299478	-0.616339	С	1.226077	-6.611435	0.173568
C	-0.007775	1.709709	0.437758	C	1.298651	-7.990576	0.464859
C	-0.497413	2.436137	1.593073	H	2.228655	-8.384396	0.892646
H	-0.282799	3.488320	1.807502	С	0.192963	-8.813471	0.214336
С	-1.267452	1.559096	2.313902	Н	0.263820	-9.887705	0.443410
Н	-1.813866	1.730163	3.246754	C	-0.991592	-8.286058	-0.322867
С	-1.214248	0.290433	1.620002	H	-1.853267	-8.939052	-0.525295
C	-1.889737	-0.862609	2.062245	С	-1.071357	-6.912240	-0.594921
C	-1.678017	-2.143884	1.522572	H	-1.994884	-6.477950	-1.006605
С	-2.236118	-3.357396	2.084113	N	2.312276	-5.743882	0.357987
Н	-2.939203	-3.389739	2.923495	Н	2.155228	-4.788180	0.027819
C	-1.668215	-4.403393	1.401580	C	3.572491	-5.982679	0.874970
H	-1.811471	-5.476596	1.562193	0	3.934094	-7.031389	1.399050
С	-0.813330	-3.824516	0.381569	C	4.502560	-4.806413	0.668885
C	-0.075033	-4.578640	-0.554721	С	4.873707	-4.408458	-0.647946
C	0.670740	-4.003888	-1.604196	H	4.413538	-4.918662	-1.508116
С	1.421123	-4.782107	-2.571752	С	5.818119	-3.414827	-0.852979
H	1.436145	-5.876757	-2.613601	Н	6.119277	-3.125761	-1.870886
C	2.076158	-3.887011	-3.378593	C	6.400682	-2.746560	0.262006
Н	2.745482	-4.093734	-4.219857	C	7.362749	-1.704570	0.125890
С	1.704501	-2.560884	-2.922080	H	7.714334	-1.418616	-0.877492
С	2.181944	-1.367775	-3.497749	С	7.819183	-1.046374	1.255980
C	1.026736	3.755774	-0.501302	H	8.546036	-0.224647	1.180618
C	-0.016477	4.726959	-0.519152	C	7.307345	-1.433540	2.524078
С	0.289700	6.077712	-0.238928	Н	7.641638	-0.901425	3.433672
Н	-0.528362	6.806752	-0.214367	N	6.433967	-2.414224	2.702172
C	1.614138	6.460814	0.007626	C	5.987338	-3.088225	1.602922
H	1.834091	7.518303	0.220028	С	5.031864	-4.151423	1.784888
С	2.654335	5.518274	-0.025520	0	4.529945	-4.473121	3.003570
H	3.695206	5.821209	0.161600	С	5.433398	-4.972549	3.995134
С	2.352660	4.173534	-0.277033	H	5.857729	-5.944404	3.662819
H	3.148386	3.414689	-0.273943	Н	4.827757	-5.136753	4.905817
N	-1.308116	4.297874	-0.850779	H	6.237465	-4.240252	4.206010
H	-1.401504	3.402550	-1.353357	С	3.256289	-1.468496	-4.533473
C	-2.506096	4.893612	-0.515139	C	4.596707	-1.132290	-4.165882
0	-2.579713	5.910953	0.183967	C	5.631262	-1.243446	-5.120409
C	-3.753325	4.245270	-1.069130	H	6.650084	-0.974775	-4.817367
С	-4.959649	4.940293	-0.760330	С	5.337792	-1.680115	-6.419255
H	-4.847270	5.845384	-0.146370	Н	6.154353	-1.760752	-7.152900
С	-6.197098	4.501831	-1.184406	С	4.026163	-2.014770	-6.789106
H	-7.115577	5.036170	-0.899050	Н	3.802915	-2.355341	-7.810896
С	-6.285625	3.358608	-2.025234	С	2.996043	-1.908369	-5.842179
C	-7.517013	2.875589	-2.549325	Н	1.959849	-2.160609	-6.113697
Н	-8.452845	3.372672	-2.250339	N	4.807791	-0.682789	-2.856407
C	-7.516853	1.803040	-3.423981	H	4.007380	-0.761628	-2.214791
H	-8.452173	1.405359	-3.845204	С	5.882541	0.004766	-2.338213
С	-6.268545	1.230228	-3.791074	0	6.973830	0.107742	-2.910005
H	-6.240256	0.399406	-4.519680	C	5.621596	0.725026	-1.034793
N	-5.105894	1.635942	-3.311455	С	6.547705	1.765611	-0.738457
C	-5.088097	2.656354	-2.411961	H	7.375371	1.890394	-1.451779
Č	-3.821497	3.069296	-1.850715	C	6.420634	2.572345	0.375594
0	-2.670687	2.390766	-2.091340	Н	7.146012	3.374768	0.578402
	-2.613967	0.971969	-2.346598		5.310224	2.398602	1.248167
C				C			
H	-3.446379	0.445668	-1.842606	С	5.041331	3.260025	2.349819
H	-1.638180	0.646680	-1.936708	H	5.751438	4.070050	2.579299
H	-2.669953	0.773557	-3.431685	C	3.884640	3.088652	3.091527
С	-2.935364	-0.660227	3.114037	H	3.641023	3.752265	3.934045
C	-4.216189	-0.193852	2.695847	С	2.997257	2.036918	2.732984
C	-5.203778	0.080364	3.663606	Н	2.053305	1.894870	3.289323
Н	-6.198742	0.418076	3.345060	N	3.226830	1.193966	1.739305
	-4.921024		5.023399	C	4.356633	1.345991	0.993694
C		-0.098314					
H	-5.702597	0.123089	5.765946	C	4.565412	0.469739	-0.134763
С	-3.667046	-0.571502	5.442151	0	3.736387	-0.564508	-0.409682
H	-3.455049	-0.719325	6.511148	С	3.057091	-1.324547	0.601673
C	-2.683728	-0.854724	4.482157	Н	3.681496	-1.421488	1.509750
H	-1.690611	-1.217263	4.787711	H	2.895062	-2.320134	0.148643

H	2.096370	-0.850217	0.875961	C	0.928076	-7.108192	2.182819
				Н	1.378990	-7.765527	2.941248
Conform	mation 10.			С	1.055685	-5.717178	2.293746
Multip:	licity: 2			H	1.601213	-5.275777	3.138744
Charge				N	-0.785153	-4.525653	-0.697528
_	3c) = -6287.34021	4950242 Hartree		Н	-0.607043	-3.531438	-0.526460
		7.333843592487 Hai	rtree	C	-1.532603	-4.826697	-1.823544
,		P) = -6285.1507037		0	-1.798056	-5.967544	-2.197920
		VP) = -6285.330952		C	-2.036103	-3.615525	-2.564912
	-3c) = -6277.9409		LOTOTOT HATCICE	C	-2.813064	-2.612029	-1.915314
	= 241.98631 Kcal			Н	-2.979537	-2.683840	-0.828153
	= 118.77608 Kcal			С	-3.395146	-1.583213	-2.640861
		-6289.231338142972	z Hartree	H	-4.033874	-0.829751	-2.154917
	-xTB) = $-298.8511$			С	-3.192491	-1.502700	-4.050127
	-xTB) = $-290.6782$			С	-3.746687	-0.464098	-4.851537
E (GFN-	FF) = -36.5452629	04680 Hartree		Н	-4.378237	0.310671	-4.390711
				С	-3.464800	-0.433749	-6.207403
Coordi				H	-3.869273	0.363746	-6.848243
Cu	0.970674	0.068310	1.805932	С	-2.640577	-1.450630	-6.761895
N	2.373890	1.400704	1.233409	Н	-2.407237	-1.437437	-7.842943
N	2.221537	-1.457550	1.333613	N	-2.115348	-2.442389	-6.058188
N	-0.525622	-1.257833	2.117820	C	-2.379116	-2.487090	-4.720065
N	-0.286385	1.604701	2.254749	C	-1.800453	-3.547031	-3.942964
С	2.217522	2.757378	1.082544	0	-0.927496	-4.427770	-4.504085
С	3.456893	3.351766	0.610528	С	-1.471694	-5.398891	-5.404275
Н	3.596610	4.415069	0.388018	Н	-2.155641	-6.076101	-4.850794
С	4.375334	2.336787	0.543796	Н	-0.612512	-5.981740	-5.786219
Н	5.423731	2.389810	0.231061	Н	-1.990519	-4.905862	-6.251203
C	3.686878	1.122178	0.945568	C	-3.690185	0.376674	3.437626
C	4.301710	-0.145216	1.031839	C	-4.714038	0.834796	2.556796
C	3.585419	-1.353266	1.172228	C	-6.058958	0.835709	2.988246
C	4.173507	-2.678465	1.095187	H	-6.831396	1.172423	2.287215
H	5.242252	-2.894299	1.007011	С	-6.376710	0.402720	4.281991
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Charge:	c) = $-6287.35894$	14014061 11		H	3.181953	0.550700	-4.372400
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C	4.484179	-0.535194	-2.430879	H	-0.834025	-4.986896	5.985297
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H H	-4.352660 -4.277426	-2.568332 -3.376541	0.256812	H C	-5.889407	1.665947 0.035759	-5.961402 -4.535348
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Confor	mation 17.			C	-4.820524	-0.582024	-3.606289
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Coordi				H	-5.315450	8.978797	-1.718740
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C	3.310237	-3.361333	-0.129132	H	-0.437644	6.173355	-6.308973
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H	-4.985004	1.067752	1.399596	0	-4.465079	3.640067	1.811437
C C	-3.082547	-0.159064 -0.335469	1.264468	C C	-2.205086 -1.258581	4.062802 3.200643	1.129933
C	-2.787822 -1.731670	-1.134144	2.632641 3.109451	Н	-1.276503	2.129746	0.745456
C	-1.518697	-1.461600	4.506967	C	-0.398011	3.654852	-0.489372
Н	-2.142554	-1.115185	5.336769	Н	0.282022	2.966386	-1.011444
С	-0.417499	-2.275592	4.559874	С	-0.426914	5.026571	-0.874648
H	0.044994	-2.735573	5.439628	С	0.404234	5.558449	-1.901161
C	0.083515	-2.389156	3.203884	Н	1.060824	4.876846	-2.459364
С	1.322170	-2.972415	2.872842	C	0.324406	6.908327	-2.202927
C	2.819394	-3.065425	-2.982978	H	0.954110	7.354537	-2.987272
C	2.843013	-4.398858	-3.479223	C H	-0.593927	7.717471	-1.479997
C H	3.829866 3.830755	-4.761826 -5.772059	-4.421984 -4.849208	n N	-0.669848 -1.394147	8.796503 7.259599	-1.710011 -0.529122
C	4.795497	-3.834125	-4.829651	C	-1.333547	5.934119	-0.226754
Н	5.558095	-4.142576	-5.560707	C	-2.235538	5.429649	0.789794
C	4.783334	-2.521117	-4.334495	0	-3.026134	6.377402	1.328857
Н	5.537401	-1.791104	-4.663004	С	-3.615851	6.254809	2.614170
C	3.785823	-2.144678	-3.424304	H	-4.583635	5.717074	2.569495
H	3.748164	-1.117571	-3.030979	Н	-3.761569	7.288846	2.982169
N	1.836141	-5.275204	-3.046733	H	-2.946967	5.710249	3.316735
H	0.985658	-4.831304	-2.682173	С	2.148000	-3.591793	3.953491
C	1.745346	-6.656584	-3.020898	С	2.789898	-2.801608	4.953339
0 C	0.669886 2.974904	-7.201061 -7.478798	-2.779195 -3.297313	C H	3.604485 4.098758	-3.439841 -2.817457	5.918592 6.672288
C	2.888634	-8.461134	-4.319344	C	3.768017	-4.830106	5.896316
Н	1.945145	-8.535733	-4.879942	Н	4.404930	-5.303513	6.659111
C	3.950201	-9.302602	-4.603475	C	3.135542	-5.615004	4.920765
Н	3.879577	-10.052499	-5.405626	Н	3.262810	-6.707539	4.907679
C	5.151355	-9.197676	-3.849690	C	2.335664	-4.987237	3.956851
С	6.297165	-10.002299	-4.110195	Н	1.832566	-5.580581	3.178401
Н	6.248610	-10.754887	-4.913081	N	2.579715	-1.414632	4.934382
C	7.449783	-9.824368	-3.364185	H	1.929333	-1.042794	4.225190
H	8.350643	-10.428710	-3.546656	С	3.043297	-0.474403	5.826046
C H	7.449574 8.361305	-8.831654 -8.664657	-2.346266 -1.743731	0 C	3.820237 2.520312	-0.724517 0.940012	6.751745 5.646230
n N	6.403788	-8.073178	-2.058747	C	2.976677	1.846827	6.649745
C	5.256933	-8.232841	-2.777799	Н	3.646870	1.421731	7.410529
C	4.121652	-7.387654	-2.489165	C	2.620860	3.178521	6.652033
0	4.098485	-6.457260	-1.509897	Н	3.005575	3.864357	7.422114
С	4.784309	-6.643551	-0.267464	С	1.740685	3.679236	5.653170
H	4.760615	-7.706099	0.046513	С	1.331076	5.040491	5.602640

	1 510544	5 544416	6 055106	_	0.00000	0 111000	5 551604
H	1.719744	5.744416	6.355186	С	0.978398	0.111872	5.551684
C	0.459019	5.453669	4.610932	0	1.395309	1.241267	6.148290
H	0.131067	6.499947	4.526268	С	2.558804	1.945706	5.745557
C	-0.029068	4.485494	3.694894	H	3.392041	1.248613	5.505620
H	-0.742142	4.784606	2.908568	H	2.849307	2.569676	6.611787
N	0.315916	3.203784	3.711133	Н	2.367823	2.577269	4.855828
C	1.220941	2.786170	4.646679	C	5.477486	1.737847	-3.233639
C	1.664886	1.412902	4.634588	С	5.293641	3.091428	-2.826178
0	1.215452	0.558084	3.664136	C	6.343513	4.021098	-2.993195
C	1.524354	0.867698	2.289982	H	6.185997	5.052273	-2.655239
H	1.063926	1.828622	1.991996	C	7.551654	3.607546	-3.569694
Н	1.094370	0.038779	1.698455	Н	8.361232	4.342668	-3.695101
Н	2.624784	0.899788	2.143284	C	7.739414	2.279308	-3.982559
11	2.024/04	0.033700	2.143204	Н	8.690461	1.963147	-4.435753
	mation 22.						
				С	6.700847	1.352649	-3.807349
_	licity: 2			H	6.828747	0.304214	-4.116413
Charge	: 0			N	4.050922	3.436519	-2.277242
E(B97-	3c) = -6287.329015	5287301 Hartree		H	3.367703	2.675474	-2.238871
E(M06/	def2-TZVP) = -628	7.318642663349 Hai	rtree	С	3.605271	4.656801	-1.795555
E (PBE	- D3(BJ)/def2-TZV	P) = -6285.142703	178262 Hartree	0	4.299352	5.660773	-1.687817
	- D3(BJ)/def2-TZV			Č	2.126627	4.641790	-1.478648
	-3c) = -6277.9267	,	0040105 Hartree	C			
					1.197011	4.395349	-2.523093
	= 254.54567 Kcal,			Н	1.582099	4.122691	-3.518374
	= 114.14864 Kcal			С	-0.169042	4.514735	-2.316496
E(ωB97	X-V/def2-TZVP) = -	-6289.2133333313693	3 Hartree	H	-0.881782	4.350678	-3.139433
E (GFN1	-xTB) = $-298.8458$	11164812 Hartree		С	-0.650809	4.892273	-1.033690
E (GFN2	-xTB) = $-290.6833$	98326237 Hartree		C	-2.029762	5.139207	-0.775408
	FF) = -36.53695353			Н	-2.755605	5.025718	-1.595672
E (GEN	11) - 30:3303333	11415 Hartree		C	-2.440434	5.526512	0.488619
0							
Coordi				Н	-3.498547	5.729555	0.710117
Cu	1.764629	-1.413395	-2.297578	C	-1.457560	5.653130	1.506759
N	1.382508	-2.792965	-0.850867	H	-1.761694	5.939269	2.530257
N	3.524999	-0.961011	-1.405539	N	-0.165540	5.440434	1.311102
N	2.121231	-0.004759	-3.715360	С	0.268090	5.081742	0.069365
N	0.001077	-1.862165	-3.187042	Č	1.686811	4.936158	-0.173406
	0.295713	-3.640541	-0.780992	0		5.113137	0.743051
C					2.653677		
C	0.363552	-4.439548	0.426138	С	2.490965	4.795272	2.130631
H	-0.366512	-5.204616	0.710437	Н	1.823318	5.512812	2.640106
C	1.483618	-4.035104	1.106733	H	3.512920	4.843883	2.552930
H	1.859329	-4.400961	2.067884	H	2.100037	3.764174	2.254106
С	2.122802	-3.016741	0.292614	C	-0.852721	0.497387	-6.043270
C	3.327723	-2.372352	0.632402	Č	-2.092141	1.118122	-5.718124
C	3.986678	-1.450298	-0.201678	C	-2.901024	1.646899	-6.745792
С	5.274151	-0.862937	0.115899	Н	-3.864005	2.099700	-6.483397
H	5.870326	-1.100337	1.004406	С	-2.478727	1.575731	-8.078802
C	5.580142	-0.003280	-0.909932	H	-3.121292	1.992481	-8.869048
H	6.468319	0.625025	-1.032909	C	-1.249762	0.983059	-8.409096
С	4.477476	-0.066445	-1.848375	H	-0.921211	0.924903	-9.457256
С	4.382452	0.746436	-2.995065	С	-0.447205	0.449993	-7.391902
C	3.254841	0.774592	-3.837605	Н	0.506448	-0.041572	-7.636326
C							
	3.096095	1.719136	-4.926356	N	-2.493256	1.178038	-4.369897
H	3.855580	2.444390	-5.238150	Н	-1.752698	1.023255	-3.680940
С	1.837855	1.525534	-5.436483	С	-3.791344	0.918877	-3.919989
H	1.348842	2.062934	-6.255114	0	-4.747524	0.797248	-4.674575
C	1.247385	0.428239	-4.691116	С	-3.908413	0.859824	-2.420881
С	-0.021181	-0.120990	-4.968111	С	-3.407299	1.930689	-1.636824
С	-0.557187	-1.231618	-4.281653	Н	-2.833575	2.722018	-2.142263
C	-1.819740	-1.857733	-4.626382	С	-3.652676	2.014250	-0.275333
Н	-2.470362	-1.555008	-5.453598	Н	-3.267157	2.853611	0.319632
C	-2.026722	-2.859483	-3.715920	C	-4.440363	1.013479	0.350639
H	-2.877664	-3.542849	-3.640600	С	-4.827289	1.094860	1.719933
C	-0.887892	-2.853998	-2.817908	H	-4.485930	1.954500	2.317144
C	-0.770509	-3.703675	-1.701722	С	-5.621468	0.107096	2.272665
C	3.889631	-2.620362	1.993947	H	-5.936766	0.146708	3.324668
C	3.740156	-1.620104	2.992701	C	-5.996408	-0.994166	1.455186
С	4.158056	-1.882687	4.312072	Н	-6.588319	-1.822469	1.883828
Н	4.032810	-1.103953	5.077083	N	-5.654440	-1.111780	0.182726
C	4.722825	-3.119671	4.644210	C	-4.907492	-0.131236	-0.399119
Н	5.040226	-3.310586	5.680162	C	-4.600668	-0.211071	-1.810904
C	4.902412	-4.101126	3.656452 3.910509	0	-4.927942	-1.222013	-2.631175
H	5.362577	-5.067400		С	-5.464280	-2.477974	-2.214733
С	4.489304	-3.845725	2.341170	H	-4.831470	-2.956722	-1.443487
H	4.612301	-4.611239	1.560440	H	-5.474762	-3.095437	-3.133868
N	3.175396	-0.370281	2.644007	H	-6.486860	-2.374978	-1.808054
Н	3.516439	0.074299	1.784220	C	-1.855657	-4.707730	-1.474391
С	2.189622	0.359929	3.287156	С	-2.805348	-4.549064	-0.421559
0	1.961419	1.523345	2.943615	C	-3.816689	-5.524335	-0.252550
C	1.363095	-0.386603	4.293025	Н	-4.531052	-5.391710	0.567255
C	0.825802	-1.636464	3.841727	C	-3.884717	-6.625370	-1.114660
H	1.094824	-1.982460	2.833669	H	-4.681548	-7.370097	-0.965834
C	-0.043433	-2.389614	4.599233	С	-2.958795	-6.784493	-2.156710
H	-0.458223	-3.330330	4.208522	H	-3.014852	-7.651340	-2.831428
C	-0.439343	-1.920504	5.883552	C	-1.953500	-5.823074	-2.326872
С	-1.331177	-2.638321	6.727784	Н	-1.213354	-5.928696	-3.134440
H	-1.729702	-3.605542	6.384034	N	-2.698085	-3.417228	0.396212
C	-1.694799	-2.101986	7.951886	Н	-2.042958	-2.679262	0.103898
Н	-2.384075	-2.629703	8.627878	C	-3.319272	-3.183454	1.607165
п С	-1.158624	-0.837561	8.321056	0	-4.146440	-3.956109	2.102651
Н	-1.441545	-0.387009	9.290698	C	-2.911887	-1.932702	2.351076
N	-0.319123	-0.140889	7.568568	C	-3.434861	-1.867322	3.674300
C	0.050042	-0.657706	6.365476	Н	-4.054744	-2.721033	3.982753

С	-3.177914	-0.811785	4 522045	С	2.062683	0 216169	7.122055
			4.522945			-0.216168	
H	-3.565078	-0.802300	5.552598	H	2.473612	0.809774	7.108960
С	-2.393848	0.279238	4.064515	N	1.741935	-0.738421	5.947774
C	-2.083221	1.401122	4.883645	C	1.244091	-2.006774	5.908326
H	-2.422900	1.407152	5.930684	C	0.889871	-2.572118	4.629882
С	-1.346128	2.450412	4.362885	0	1.012766	-1.897456	3.471909
H	-1.076379	3.321392	4.977554	С	0.439587	-0.585518	3.329839
С	-0.927288	2.375580	3.007635	H	-0.558377	-0.562969	3.809539
H	-0.353705	3.206376	2.564236	H	0.320665	-0.439481	2.240691
N	-1.180546	1.340063	2.222294	Н	1.105856	0.193464	3.743875
C	-1.875543	0.281594	2.717879	C	-4.232613	-1.820066	-2.025113
C	-2.111488	-0.870075	1.872270	C	-5.187396	-2.377921	-1.123424
0	-1.624316	-0.987654	0.611228	С	-6.476172	-2.714974	-1.596029
С	-0.666400	-0.118040	-0.015919	Н	-7.186851	-3.166703	-0.894863
Н			-0.221723	C	-6.815063	-2.479019	-2.934363
	-1.105882	0.873036					
H	-0.404239	-0.637334	-0.956798	H	-7.823893	-2.746169	-3.284666
H	0.233525	0.013041	0.613544	C	-5.889358	-1.911503	-3.823595
				Н	-6.159432	-1.731632	-4.874753
~							
	mation 26.			C	-4.605366	-1.589052	-3.361948
Multip	licity: 2			H	-3.856194	-1.163628	-4.046716
Charge	e: 0			N	-4.795784	-2.553333	0.209844
F/B97-	3c) = -6287.31867	0069100 Hartree		Н	-3.899157	-2.133383	0.499393
	,						
	def2-TZVP) = -628			C	-5.407463	-3.303801	1.187616
E (PBE	- D3(BJ)/def2-TZV	P) = -6285.132064	212398 Hartree	0	-6.447708	-3.945287	1.015521
E(PBEC	- D3(BJ)/def2-TZ	VP) = -6285.30636	7682145 Hartree	С	-4.728163	-3.304957	2.542547
F (DBFh	(-3c) = -6277.9130	89849062 Hartree		C	-5.258313	-4.263274	3.457431
	= 266.17446 Kcal			H	-6.045158	-4.922769	3.063977
E(PM7)	= 138.11293 Kcal	/mol		C	-4.826192	-4.344420	4.764176
E (GB97	X-V/def2-TZVP) = -	-6289 20317574683	4 Hartree	H	-5.240841	-5.098700	5.450445
	, ,			C			
	-xTB) = $-298.8253$				-3.851369	-3.426383	5.246413
	-xTB) = $-290.6696$			С	-3.393772	-3.423572	6.593154
E (GFN-	FF) = $-36.5198773$	67473 Hartree		H	-3.794635	-4.172719	7.294117
				C	-2.464666	-2.481891	7.002391
C	natas.			Н	-2.090080		
	nates:					-2.448503	8.035508
Cu	0.270814	-0.816000	-0.240811	C	-1.995829	-1.542047	6.047541
N	1.778401	-1.921312	0.543756	Н	-1.262496	-0.773168	6.350086
N	-0.748985	-2.509735	-0.670652	N	-2.381814	-1.523388	4.780118
N	-1.219292	0.296347	-1.046881	C	-3.293748	-2.441150	4.353349
N	1.292135	0.890775	0.201939	C	-3.720884	-2.423576	2.974227
С	2.917334	-1.446658	1.159822	0	-3.105887	-1.602308	2.070439
C	3.773790	-2.551358	1.543316	C	-3.190715	-0.175033	2.219485
H	4.750472	-2.443180	2.025624	H	-4.222912	0.172392	1.996964
С	3.123723	-3.699622	1.172729	H	-2.490918	0.244406	1.472804
Н	3.464910	-4.735001	1.276558	Н	-2.887862	0.129187	3.238344
С	1.862863	-3.297700	0.581245	С	-0.439105	4.022295	-1.104667
C	0.868426	-4.198484	0.159927	C	-0.392302	4.524246	-2.437120
С	-0.349733	-3.804678	-0.425008	С	-0.545716	5.910713	-2.655920
С	-1.391443	-4.731507	-0.822987	Н	-0.444764	6.315234	-3.669776
Н	-1.341859			C			
		-5.818790	-0.714089		-0.799913	6.777577	-1.587279
C	-2.421534	-3.979611	-1.320457	H	-0.922102	7.852850	-1.786814
H	-3.379618	-4.323378	-1.723664	С	-0.878978	6.287147	-0.275337
C	-2.018993	-2.591373	-1.202897	Н	-1.080315	6.966247	0.566109
С	-2.849300	-1.508685	-1.554295	С	-0.683566	4.919142	-0.046392
С	-2.453941	-0.160296	-1.466637	H	-0.728031	4.514727	0.975961
С	-3.298028	0.959267	-1.832199	N	-0.143546	3.616338	-3.483558
Н	-4.336845	0.869789	-2.167038	Н	0.321112	2.739199	-3.215784
C	-2.544565	2.095171	-1.670197	C	-0.485794	3.635963	-4.819075
H	-2.822790	3.137007	-1.856740	0	-0.131088	2.727536	-5.573407
С	-1.253207	1.670566	-1.173834	С	-1.259390	4.801942	-5.377959
Č	-0.226402	2.569359	-0.819471	C	-0.614292	5.605663	-6.355001
~							
C	0.946958	2.182988	-0.142638	H	0.429435	5.370320	-6.611758
C	1.935521	3.113688	0.368790	C	-1.271660	6.656953	-6.971308
Н	1.912795	4.197817	0.219999	H	-0.762235	7.282390	-7.719735
C	2.852434	2.372763	1.068496	C	-2.624176	6.935999	-6.632780
H	3.736678	2.722249	1.611788	С	-3.352367	8.020552	-7.199831
C	2.462465	0.984163	0.929124	H	-2.859500	8.659010	-7.950013
C	3.230150	-0.095768	1.405338	C	-4.655388	8.261398	-6.798693
C	1.098957	-5.658082	0.368618	Н	-5.240154	9.093965	-7.216891
C							
	1.203770	-6.239854	1.661490	C	-5.231148	7.403937	-5.821381
C	1.483078	-7.616991	1.787691	H	-6.266898	7.582286	-5.478490
H	1.554251	-8.049900	2.797514	N	-4.597911	6.376124	-5.279073
C	1.650744	-8.427328	0.659844	C	-3.315685	6.117013	-5.662069
H	1.869425	-9.498522	0.783411	С	-2.608882	5.013430	-5.056838
C	1.524575	-7.868435	-0.621113	0	-3.143824	4.181575	-4.135028
H	1.649798	-8.493429	-1.517618	С	-4.520268	3.790266	-4.176554
C	1.250891	-6.501526	-0.753229	Н	-5.167314	4.527506	-3.667131
H	1.173094	-6.048874	-1.752932	H	-4.560652	2.808749	-3.666718
N	1.108962	-5.481066	2.853061	H	-4.871454	3.677407	-5.221538
H	1.809988	-5.687201	3.567786	C	4.456162	0.188899	2.213790
C	0.173156	-4.520125	3.207534	Ċ	5.643260	0.692058	1.604242
0	-0.795147	-4.207276	2.530094	C	6.791838	0.909740	2.400176
С	0.494116	-3.915982	4.559452	H	7.697143	1.288007	1.911911
С	0.384305	-4.698763	5.739730	C	6.751674	0.642559	3.774810
Н	0.049321	-5.744161	5.650386	Н	7.655365	0.820229	4.378147
С	0.651405	-4.160728	6.989826	C	5.583983	0.154767	4.381734
H	0.537332	-4.766572	7.901496	H	5.554647	-0.051302	5.462343
С	1.095063	-2.814060	7.097100	С	4.444783	-0.073404	3.596286
C	1.431381	-2.202409	8.338516	Н	3.519754	-0.453332	4.057888
Н	1.317036	-2.781013	9.269090	N	5.599011	0.958819	0.230583
С	1.908868	-0.902182	8.358864	H	4.701814	0.786356	-0.251250
Н	2.180391	-0.405844	9.302185	C	6.553881	1.552305	-0.563563

0	7.695242	1.830245	-0.183839	С	-5.699342	-7.408663	-6.070657
C	6.105931	1.912407	-1.968558	H	-6.440825	-8.222204	-6.029682
C	7.080121	2.629770	-2.725483	C	-5.316368	-6.848689	-7.277420
H	8.044451	2.800290	-2.225265	H	-5.736189	-7.198838	-8.231982
С	6.832345	3.077117	-4.006969	С	-4.360418	-5.796667	-7.259867
H	7.604471	3.619085	-4.574450	H	-4.045632	-5.326325	-8.209570
C	5.556556	2.861069	-4.600223	N	-3.802113	-5.328691	-6.155022
C	5.208585	3.337683	-5.895376	С	-4.159009	-5.867547	-4.954913
Н	5.966611	3.872358	-6.489658	C	-3.572346	-5.344204	-3.742400
C	3.927200	3.132176	-6.378136	0	-2.647734	-4.357917	-3.710357
H	3.625375	3.487731	-7.374646	C	-1.679936	-4.178616	-4.749054
C	2.984687	2.455430	-5.554606	H	-1.306801	-5.153754	-5.120527
Н	1.942183	2.315761	-5.891533	Н	-0.846678	-3.620884	-4.279618
N	3.274207	1.985881	-4.347719	H	-2.097824	-3.615242	-5.602729
C	4.538613	2.155008	-3.863576	C	-3.016969	1.295492	5.394284
C	4.852948	1.642414	-2.551794	С	-3.605941	2.497219	4.892968
0	3.911074	0.956397	-1.838352	C	-4.462635	3.258557	5.716608
C				Н			
	3.295433	-0.212753	-2.415756		-4.902671	4.175406	5.306234
H	2.705972	0.067088	-3.307662	C	-4.729860	2.830417	7.023780
H	2.637956	-0.617943	-1.625566	H	-5.400209	3.431660	7.656856
H	4.072517	-0.963096	-2.676102	С	-4.153082	1.655197	7.529738
				Н	-4.366429	1.325929	8.557416
~ -							
	mation 3.			C	-3.299243	0.898782	6.712210
Multip	licity: 2			H	-2.838669	-0.026252	7.090415
Charge	: 0			N	-3.293092	2.851940	3.576365
E (B97-	3c) = -6287.33530	5010298 Hartree		Н	-2.633134	2.219771	3.097631
		7.332416021612 Ha	x+x00		-3.861808		
				С		3.801322	2.757361
		P) = -6285.148760		0	-4.669803	4.655455	3.125630
E(PBE0	- D3(BJ)/def2-TZ	VP) = -6285.32472	6779480 Hartree	С	-3.508206	3.628926	1.290880
	-3c) = -6277.9303			С	-4.413422	4.240213	0.373818
	= 239.99018 Kcal			Н	-5.195099	4.878082	0.812415
	= 115.73053 Kcal			С	-4.329876	4.017423	-0.987781
E(ωB972	X-V/def2-TZVP) = 0	-6289.22330564620	9 Hartree	H	-5.042114	4.493974	-1.679078
E (GFN1-	-xTB) = $-298.8500$	32310286 Hartree		С	-3.344575	3.130593	-1.508425
	-xTB) = $-290.6872$			С	-3.250039	2.782880	-2.886196
	FF) = -36.5480239			Н	-3.951299	3.237279	-3.603755
E (GEN-1	FF) = =30.3400239	91346 naitiee					
				С	-2.296214	1.866463	-3.296436
Coordi	nates:			H	-2.204517	1.564439	-4.349706
Cu	0.069978	-0.934022	2.242479	С	-1.430282	1.302015	-2.319083
N	-0.110109	-1.710096	0.383162	Н	-0.679531	0.548470	-2.617964
N	-1.931641	-0.699416	2.351605	N	-1.463478	1.622249	-1.035547
N	0.283768	-0.039429	4.047402	C	-2.393762	2.521657	-0.611075
N	2.065958	-1.325237	2.204614	C	-2.458847	2.840844	0.790269
C	0.908565	-2.160676	-0.432491	0	-1.510213	2.287436	1.613615
С	0.384153	-2.490014	-1.744386	С	-0.502411	3.195756	2.102184
Н	0.983296	-2.882464	-2.573651	Н	0.063887	3.623930	1.251229
С	-0.964502	-2.239516	-1.706015	H	0.181186	2.600000	2.734609
H	-1.712838	-2.390049	-2.490304	H	-0.955575	4.005201	2.713347
С	-1.265152	-1.775098	-0.366355	С	3.904299	0.077713	5.210880
C	-2.570415	-1.500498	0.090439	C	4.999141	0.855305	4.748206
C	-2.859456	-1.043741	1.392031	С	6.137209	1.016135	5.562417
C	-4.201136	-0.795112	1.888048	H	6.970275	1.628320	5.185610
H	-5.122713	-1.010329	1.337577	С	6.197829	0.433873	6.834757
С	-4.064600	-0.248319	3.138865	H	7.095535	0.569273	7.456531
H	-4.849183	0.081673	3.828515	С	5.103124	-0.299598	7.317371
C	-2.641358			Н		-0.750788	8.320316
		-0.163644	3.404910		5.134184		
C	-2.091554	0.511235	4.516269	C	3.972040	-0.471575	6.508215
С	-0.709299	0.591813	4.770339	H	3.122424	-1.073021	6.864839
С	-0.124811	1.346192	5.863988	N	4.987348	1.472745	3.473869
Н	-0.691008	1.961102	6.571142	Н	5.737206	1.264860	2.804077
C	1.228374	1.135996	5.810491	С	4.042262	2.381741	3.055820
H	2.010691	1.558755	6.447806	0	3.092378	2.732295	3.762020
C	1.471746	0.254415	4.685544	C	4.243758	2.980775	1.684781
С	2.740787	-0.239425	4.332633	С	3.527824	4.192327	1.458989
C	2.981037	-1.039860	3.197574	Н	2.967811	4.591339	2.317095
C	4.266369	-1.619926	2.864085	С	3.503491	4.811230	0.226294
H	5.157161	-1.576249	3.499656	H	2.942037	5.744276	0.071072
С	4.129271	-2.212648	1.634015	C	4.187572	4.219707	-0.871598
Н	4.883190	-2.746560	1.046741	C	4.163104	4.771492	-2.183393
C	2.757209	-2.001858	1.218071	Н	3.585308	5.691912	-2.361715
C	2.252984	-2.347011	-0.052424	С	4.840687	4.138447	-3.211463
C	-3.708191	-1.650170	-0.868852	H	4.823487	4.531358	-4.238071
С	-4.136043	-2.932212	-1.322139	C	5.548269	2.942027	-2.917685
C	-5.237801	-3.015995	-2.201566	Н	6.072454	2.398667	-3.724097
Н	-5.609114	-3.998535	-2.516135	N	5.602817	2.401303	-1.710394
C	-5.878754	-1.856749	-2.653234	С	4.937597	3.001745	-0.685021
H	-6.731415	-1.952006	-3.342628	С	4.974361	2.398148	0.628582
С	-5.458550	-0.591047	-2.217188	0	5.724513	1.303084	0.913908
H	-5.964844	0.321918	-2.563552	С	5.974825	0.236228	-0.017681
C	-4.388696	-0.502126	-1.318115	Н	5.062150	-0.002253	-0.594838
H	-4.055883	0.477328	-0.947733	H	6.251744	-0.629726	0.611286
N	-3.470244	-4.056807	-0.814021	Н	6.783798	0.499301	-0.720666
H	-2.903727	-3.885409	0.024971	C	3.200528	-2.950680	-1.043218
С	-3.412092	-5.386400	-1.193143	C	3.695236	-2.199382	-2.151408
0	-2.884500	-6.212533	-0.449802	C	4.603191	-2.803741	-3.051384
C	-4.015086	-5.830530	-2.499506	Н	4.969800	-2.207516	-3.894532
С	-4.955021	-6.894251	-2.436633	C	5.008208	-4.129943	-2.856472
H	-5.219765	-7.283056	-1.442481	H	5.715432	-4.582340	-3.568440
C	-5.517243	-7.432677	-3.580335	C	4.524199	-4.878333	-1.773184
H	-6.254115	-8.247557	-3.519627	Н	4.839140	-5.921916	-1.625643
С	-5.138333	-6.926966	-4.853622	С	3.625107	-4.281753	-0.877878
-	= = = = = =			-	/	. = . =	

Н	3.227727	-4.851793	-0.024635	Н	2.900826	-0.470820	1.174417
N	3.244370	-0.880488	-2.300375	C	2.972244	-0.421266	3.305842
H	2.659525	-0.501932	-1.543004	H	1.958796	-0.001063	3.392452
С	3.429102	-0.017652	-3.361245	С	3.742418	-0.658668	4.476790
0	4.146564	-0.269242	-4.334415	С	3.267359	-0.385893	5.790341
C	2.626331	1.265362	-3.324978	H	2.270308	0.064123	5.917756
С	2.498981	1.899292	-4.591156	С	4.060681	-0.703045	6.880671
H	3.000068	1.399117	-5.432354	H	3.723565	-0.511584	7.910046
С	1.786546	3.069622	-4.759998	С	5.331965	-1.299094	6.646603
Н	1.681169	3.532430	-5.752938	Н	5.971854	-1.572873	7.505375
C	1.190107	3.694364	-3.632703	N	5.816886	-1.559522	5.441587
С	0.459417	4.911539	-3.736427	С	5.057289	-1.237644	4.355612
					5.577673		
H	0.333389	5.371069	-4.729514	C		-1.543453	3.044837
C	-0.075193	5.497241	-2.602113	0	6.743417	-2.215369	2.918858
H	-0.648299	6.434680	-2.651211	С	7.957624	-1.520810	3.217395
C	0.136654	4.852783	-1.354277	H	8.126679	-0.730243	2.456871
H	-0.274738	5.299883	-0.430316	H	8.766757	-2.271381	3.146690
N	0.803259	3.718285	-1.215597	H	7.935978	-1.100677	4.243244
С	1.326450	3.111387	-2.316388	С	-2.627771	-4.122773	-1.841618
C	2.037542	1.855222	-2.181562	С	-2.005476	-5.365688	-1.534514
0	2.222865	1.198211	-1.017973	С	-2.482351	-6.555468	-2.118107
C	1.539189		0.227133	Н	-1.967908	-7.497677	
		1.451606					-1.893122
H	1.842385	2.423842	0.642076	С	-3.594408	-6.520438	-2.969272
H	1.874235	0.635794	0.891373	H	-3.959786	-7.456029	-3.419622
						-5.305790	
H	0.442456	1.411627	0.076391	С	-4.244754		-3.238022
				H	-5.118793	-5.276903	-3.905676
Confor	mation 30.			C	-3.762268	-4.114279	-2.678495
	olicity: 2			H	-4.238704	-3.155424	-2.927989
Charge	e: 0			N	-0.913944	-5.367969	-0.645455
E (B97-	-3c) = -6287.335183	1890482 Hartree		H	-0.892554	-4.660822	0.102065
	•		x+x00				-0.877230
	def2-TZVP) = -628			C	0.288244	-6.000618	
E (PBE	- D3(BJ)/def2-TZVI	P) = -6285.146661	.111422 Hartree	0	0.460705	-6.791432	-1.807923
E (PREC	- D3(BJ)/def2-TZ	$P_1 = -6285 32566$	0216599 Hartree	C	1.418727	-5.651597	0.067176
			JOZIOJJJ HAICIEE				
	1-3c) = -6277.93114			С	2.654549	-6.291753	-0.241269
E(PM6)	= 274.06109 Kcal,	/mol		H	2.645416	-6.939359	-1.129969
E. (PM7)	= 124.90508 Kcal	/mol		С	3.792098	-6.105903	0.517499
	'X-V/def2-TZVP) = -		8 Hartree	H	4.739238	-6.597309	0.248058
E (GFN1	-xTB) = $-298.83588$	38980236 Hartree		С	3.731391	-5.310689	1.695333
F (CEN2	2-xTB) = $-290.6710$	57223873 Hartree		С	4.829562	-5.163856	2.589528
E (GFN-	-FF) = -36.5423696	/6091 Hartree		H	5.800639	-5.609627	2.324517
				С	4.658804	-4.479033	3.779171
Coordi	.nates:			Н	5.490043	-4.329092	4.482438
Cu	-0.528735	0.006191	-0.045052	C	3.381370	-3.922532	4.059695
N	1.295766	0.865926	-0.179446	H	3.218277	-3.389102	5.012986
N	0.017308	-1.428416	-1.366172	N	2.349855	-3.984674	3.232587
N	-2.354582	-0.839779	0.091952	C	2.495818	-4.658631	2.055761
N	-1.047221	1.388506	1.352926	С	1.357345	-4.780016	1.174281
C	1.780578	1.933413	0.555729	Ō	0.183226	-4.136286	1.434827
C	3.096934	2.301938	0.077868	С	0.149498	-2.798648	1.958163
H	3.697460	3.125442	0.477211	H	0.261552	-2.799830	3.055979
C	3.413376			Н			1.649783
		1.430641	-0.936371		-0.828521	-2.382179	
H	4.329820	1.389651	-1.534851	H	0.963247	-2.187361	1.517703
С	2.296882	0.520206	-1.071150	С	-4.830389	1.499248	1.668259
Č			-1.898779	Č			0.469056
	2.308114	-0.623405			-5.488877	1.918568	
C	1.236219	-1.528507	-2.008587	С	-6.808825	2.402797	0.513297
C	1.270156	-2.723179	-2.828062	H	-7.302324	2.680517	-0.426620
H	2.122323	-3.042577	-3.436290	C	-7.460650	2.507424	1.750733
C	0.049272	-3.329501	-2.691965	H	-8.492826	2.887818	1.784263
H	-0.299773	-4.250067	-3.170117	С	-6.811377	2.139412	2.940069
С	-0.721283	-2.525069	-1.761702	H	-7.330522	2.229130	3.905684
С	-2.030180	-2.850316	-1.334554	C	-5.501798	1.632707	2.893540
С	-2.784617	-2.026943	-0.476818	H	-4.998617	1.303415	3.815201
С	-4.161105	-2.280865	-0.099496	N	-4.753375	1.801171	-0.718251
H	-4.734829	-3.166800	-0.387317	H	-3.753257	1.658775	-0.561190
C	-4.575197	-1.204815	0.643502	С	-5.169159	1.428990	-1.985385
Н	-5.556889		1.093951		-6.331405	1.473700	-2.379281
		-1.024523		0			
C	-3.434489	-0.321662	0.770271	C	-3.996080	0.941538	-2.806245
C	-3.472738	0.899098	1.482810	С	-2.767206	1.669637	-2.811160
C							
	-2.320739	1.633736	1.823244	H	-2.726187	2.634186	-2.274695
С	-2.301610	2.730492	2.770569	C	-1.664292	1.202616	-3.504800
Н	-3.182045	3.131010	3.283793	Н	-0.719425	1.767167	-3.505380
С	-0.989426	3.103991	2.912860	C	-1.737762	-0.014162	-4.238542
H	-0.571978	3.877380	3.566173	C	-0.643847	-0.552772	-4.971025
C	-0.222426	2.310478	1.969320	H	0.316989	-0.014382	-4.974751
С	1.118736	2.577885	1.624132	С	-0.802982	-1.747004	-5.653316
С	3.585830	-0.942926	-2.609238	H	0.026247	-2.198658	-6.217062
C	4.702594	-1.407569	-1.856202	С	-2.065912	-2.399246	-5.600958
С	5.939619	-1.627905	-2.495362	Н	-2.209580	-3.356495	-6.134325
H	6.793878	-1.954928	-1.891232	N	-3.110179	-1.934783	-4.931701
C	6.056812	-1.416169	-3.875538	C	-2.968700	-0.763453	-4.249913
H	7.026700	-1.592381	-4.364853	C	-4.091916	-0.273183	-3.492342
С	4.953352	-0.995678	-4.634422	0	-5.199648	-1.051441	-3.352505
H	5.049284	-0.839753	-5.719078	С	-6.119137	-1.052394	-4.448664
C	3.726422	-0.761573	-3.996316	H	-6.568373	-0.042993	-4.559489
H	2.857469	-0.406525	-4.571059	H	-6.912675	-1.777647	-4.188379
N	4.520702	-1.623770	-0.478189	Н	-5.617884	-1.374990	-5.384895
H	3.545826	-1.729553	-0.190748	C	1.881553	3.617998	2.385576
C	5.437746	-1.373751	0.533655	Č	1.561816	5.006445	2.299157
0	6.635511	-1.198112	0.323958	C	2.326430	5.945234	3.029403
C	4.816438	-1.243397	1.903190	H	2.060397	7.005242	2.948277
Č	3.504095	-0.706621	2.061391	C	3.394533	5.514545	3.825746
	J.JU4U9J	-U./UUUZI	∠.∪∪⊥391	C	J.J94JJJ	J.JI4J4J	3.043/40
C							

Н	3.978201	6.261181	4.385567	С	-5.437868	-4.519883	2.629429
C	3.726973	4.153992	3.906511	0	-6.324894	-5.374165	2.606005
H	4.569985	3.815681	4.526869	С	-5.514583	-3.271404	3.468527
C	2.971245	3.220954	3.184179	C	-5.296998	-2.029695	2.787832
H	3.222353	2.151281	3.227666	H	-4.981147	-2.059811	1.734380
N	0.491464	5.377876	1.476464	С	-5.529624	-0.804770	3.379221
Н	0.005563	4.617786	0.974813	Н	-5.379118	0.125486	2.810948
C	-0.107769	6.609667	1.340888	C	-6.000383	-0.752704	4.721702
0	0.287400	7.643288	1.884991	С	-6.281164	0.466522	5.400205
C	-1.352308	6.629438	0.474771	H	-6.140839	1.420270	4.867030
С	-2.090315	7.850600	0.520964	С	-6.724217	0.433199	6.712004
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С	-3.257398	8.027233	-0.194335	С	-6.877577	-0.832595	7.341765
H	-3.815118	8.974414	-0.135300	H	-7.223361	-0.880895	8.391260
С	-3.756485	6.977549	-1.017098	N	-6.626464	-1.989591	6.748441
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C	-3.026083	5.739599	-1.102662	C	-3.980001	1.814134	-0.219789
C	-1.818684	5.585349	-0.336786	С	-4.211276	2.036612	-1.611040
0	-1.175294	4.371049	-0.367808	С	-5.300034	2.849539	-2.006012
C	-0.396986	4.080821	-1.539655	Н	-5.469416	3.002235	-3.077810
H	-1.022189	4.157524	-2.451114	С	-6.129449	3.435058	-1.041548
H	-0.033577	3.044427	-1.412592	H	-6.970809	4.062698	-1.372863
H	0.469345	4.773290	-1.613196	С	-5.899930	3.232725	0.327740
				Н	-6.553938	3.694363	1.082099
C	: 6						
	ation 6.			С	-4.825801	2.424117	0.724645
Multipl	icity: 2			Н	-4.623451	2.249694	1.792803
Charge:	0			N	-3.335252	1.439788	-2.525982
		27227346 Hartree		Н	-2.540280	0.897713	-2.147927
		37.318295915039 Hai	rtroo	C	-3.398875	1.443207	-3.903724
	,						
		IP) = -6285.1368735		0	-4.287454	2.000012	-4.553602
E(PBE0	- D3(BJ)/def2-T2	ZVP) = -6285.312063	3486670 Hartree	C	-2.283832	0.703033	-4.618895
E (PBEh-	3c) = -6277.9160	003702228 Hartree		С	-2.431286	0.645149	-6.038004
	= 257.39815 Kcal			Н	-3.338361	1.112421	-6.447852
				C			
	= 133.22851 Kcal				-1.481561	0.061039	-6.850969
		-6289.206697843812	2 Hartree	H	-1.613429	0.037409	-7.943565
E (GFN1-	xTB) = -298.8253	323984688 Hartree		С	-0.313548	-0.519043	-6.279006
E (GFN2-	xTB) = -290.6644	148258978 Hartree		С	0.709046	-1.137787	-7.051815
	F) = -36.528459			Н	0.609171	-1.164655	-8.148380
В (ОПТ Т	1, 30.320133	, oo lol nalelee		C			
					1.807895	-1.693756	-6.417110
Coordin				H	2.617658	-2.174732	-6.985155
Cu	-0.237623	-1.069419	1.286095	C	1.868863	-1.638945	-4.998351
N	0.064409	-3.073261	1.425940	H	2.731595	-2.082335	-4.466882
N	-2.035995	-1.394530	0.420936	N	0.939064	-1.074722	-4.243168
			1.230431		-0.139446		
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N	1.617973	-0.739924	2.036499	C	-1.144134	0.131010	-4.027601
С	1.169510	-3.711399	1.952379	0	-1.001009	0.128051	-2.669250
С	0.990788	-5.149617	1.889553	С	0.113547	0.874799	-2.125672
Н	1.722619	-5.884974	2.238954	Н	1.073870	0.497054	-2.517945
С	-0.234812	-5.372165	1.315792	H	0.073049	0.713206	-1.034907
H	-0.721938	-6.328143	1.097575	H	0.002900	1.952396	-2.357898
C	-0.794982	-4.070534	1.009094	С	2.526223	2.952985	2.095351
C	-2.021169	-3.881594	0.344517	C	2.975127	3.690133	0.965608
C	-2.561859		0.046467		3.818367	4.804611	1.148582
		-2.613965		С			
С	-3.830688	-2.423824	-0.629598	H	4.231564	5.311871	0.267108
H	-4.447919	-3.230577	-1.039096	С	4.167800	5.223498	2.438629
С	-4.083789	-1.075821	-0.621609	Н	4.822285	6.099441	2.561927
Н	-4.955844	-0.546885	-1.019967	C	3.711598	4.516108	3.561068
C	-2.956238	-0.441911	0.035360	H	3.988284	4.839496	4.575510
С	-2.852943	0.948070	0.243063	С	2.910573	3.380200	3.381678
C	-1.729341	1.567891	0.823592	H	2.554921	2.806578	4.250704
С	-1.573346	3.003089	0.956753	N	2.599908	3.271303	-0.336076
Н	-2.348913	3.738300	0.717186	Н	2.616985	2.261458	-0.537291
C	-0.297650	3.221591	1.416033	С	2.099053	4.029632	-1.368207
H	0.192428	4.173237	1.647572	0	1.791339	3.528821	-2.452560
С	0.325313	1.923027	1.556394	C	1.850054	5.504842	-1.148525
С	1.671324	1.738579	1.927370	С	0.563357	5.947895	-0.739052
C	2.253212	0.478640	2.159361	Н	-0.200753	5.196526	-0.493871
С	3.612305	0.287762	2.632124	С	0.265712	7.299158	-0.676027
H	4.335595	1.091381	2.803380	H	-0.731876	7.639900	-0.359947
С	3.774830	-1.057821	2.831995	С	1.252206	8.263811	-1.023457
Н	4.657793	-1.590029	3.201691	C	1.021411	9.666621	-0.949842
C	2.532424	-1.692648	2.435839	H	0.031733	10.030292	-0.631112
С	2.340878	-3.087164	2.425048	C	2.040131	10.548474	-1.269770
С	-2.831707	-5.089082	-0.008531	Н	1.893175	11.637384	-1.219441
Č	-3.987998	-5.411023	0.762510	C	3.297557	10.016509	-1.667095
C	-4.760559		0.426029	Н			
		-6.543933			4.126045	10.703440	-1.919424
H	-5.647463	-6.769482	1.029711	N	3.555611	8.721012	-1.760852
С	-4.383726	-7.344763	-0.660074	C	2.563226	7.835793	-1.455905
H	-4.996422	-8.223710	-0.912210	С	2.829931	6.424064	-1.532929
C	-3.243019	-7.042441	-1.419553	0	4.046793	5.905888	-1.860650
H	-2.953010	-7.676443	-2.270290	C	4.699263	6.324270	-3.065599
С	-2.475012	-5.916913	-1.086772	H	4.033801	6.153542	-3.939230
H	-1.581910	-5.656514	-1.674686	Н	5.592399	5.678936	-3.161289
N	-4.300805	-4.565563	1.836786	H	4.987674	7.390846	-3.013189
Н	-3.622955	-3.815617	1.996996	C	3.458703	-3.970281	2.882523
	022700	2.01001/	,,,,,,,,	Ü	2.100.00	1.3.0201	2.002020

C C							
	4.602989	-4.185940	2.057722	С	-4.534166	-1.142185	-3.402043
	5.608016	-5.081819	2.492038	Н	-3.803668	-0.370931	-3.692541
Н	6.470560	-5.249281	1.837274	N	-5.252622	-3.197760	-0.405676
С	5.484709	-5.732472	3.725828	H	-4.652819	-2.656713	0.231368
H	6.279462	-6.423834	4.045270	С	-5.508426	-4.485683	0.022124
C	4.369848	-5.513972	4.549144	0	-6.222152	-5.277795	-0.596493
H	4.279016	-6.024434	5.519236	C	-4.748547	-4.928461	1.259516
С	3.364784	-4.637426	4.117066	C	-4.818510	-6.328036	1.511903
Н	2.475982	-4.456732	4.740297	Н		-6.897426	0.843871
					-5.481149		
N	4.681032	-3.481389	0.848527	С	-4.092962	-6.938820	2.515872
H	3.947480	-2.778397	0.658446	H	-4.163537	-8.023919	2.684627
C	5.678702	-3.516559	-0.100925	С	-3.209766	-6.163933	3.316476
0	6.645046	-4.282585	-0.064897	C	-2.360734	-6.729337	4.311215
C	5.557651	-2.496136	-1.217905	Н	-2.419268	-7.811143	4.510045
C	6.665751	-2.473972	-2.118253	С	-1.462180	-5.924596	4.991671
H	7.458164	-3.211852	-1.926442	H	-0.783211	-6.338060	5.751784
C	6.731046	-1.589733	-3.175711	C	-1.421436	-4.538386	4.676934
Н	7.585924	-1.604878	-3.869300	Н	-0.689707	-3.878815	5.177697
С	5.698560	-0.627847	-3.367912	N	-2.217294	-3.967948	3.786234
C	5.716451	0.338829	-4.412359	С	-3.111602	-4.738640	3.104638
H	6.550244	0.335402	-5.132313	C	-3.942906	-4.122097	2.095501
C	4.695057	1.269775	-4.495131	0	-3.941620	-2.787213	1.862908
H	4.676111	2.033662	-5.286340	Ċ	-3.607343	-1.781956	2.828624
С	3.663314	1.245935	-3.515940	H	-4.043811	-2.025661	3.816579
H	2.870806	2.014885	-3.519328	H	-4.052005	-0.849258	2.432053
N	3.599526	0.349754	-2.538005	H	-2.512017	-1.682403	2.937333
С	4.578902	-0.597932	-2.461471	С	-2.503660	4.507643	0.612621
C	4.504667	-1.588052	-1.416386	C	-2.151052	5.121446	-0.628362
0	3.404365	-1.598157	-0.598495	С	-2.412066	6.501168	-0.806052
C	2.182520	-2.061869	-1.210707	H	-2.101953	6.970796	-1.745371
H	1.927208	-1.486121	-2.121188	С	-3.039153	7.242141	0.202063
H	1.390628	-1.922536	-0.453570	Н	-3.234452	8.312268	0.033310
H	2.265945		-1.447970	C			
н	2.203943	-3.144797	-1.44/9/0		-3.418203	6.638197	1.409879
				H	-3.918060	7.219414	2.198793
Conforma	tion 8.			C	-3.141185	5.278935	1.603417
Multipli	citv: 2			Н	-3.416816	4.784719	2.547265
Charge:	4			N	-1.581685	4.328664	-1.640882
_		DE 400000 H					
		05406908 Hartree		H	-1.581171	3.307811	-1.502912
	,	37.343554937966 Ha		C	-1.082791	4.749520	-2.855677
E(PBE -	D3(BJ)/def2-TZV	IP) = -6285.165369	469711 Hartree	0	-0.929773	5.938082	-3.158338
E(PBE0 -	D3(BJ)/def2-T2	ZVP) = -6285.34067	2448954 Hartree	C	-0.756543	3.678100	-3.878095
		632264553 Hartree		C	-0.378099	4.192517	-5.154898
	259.34585 Kcal			Н	-0.327425	5.288397	-5.228765
	116.68290 Kcal			С	-0.084169	3.377249	-6.229690
E(ωB97X-	V/def2-TZVP) =	-6289.23606214673	4 Hartree	H	0.221445	3.803726	-7.197185
E(GFN1-x	TB) = -298.855	723892688 Hartree		С	-0.226343	1.967341	-6.102143
E (GFN2-x	TB) = -290.6864	196946523 Hartree		С	0 004000	1.061191	-7.181596
	12) 230.000	100110020 11010100					
	\36 5700439	216002 Hartron			-0.024998		
	) = -36.5700438	316992 Hartree		H	0.310866	1.454371	-8.154053
E (GFN-FF		316992 Hartree		H C	0.310866 -0.272179	1.454371 -0.289521	-8.154053 -7.000513
		316992 Hartree		H	0.310866	1.454371	-8.154053
E (GFN-FF		316992 Hartree -0.188219	1.239497	H C	0.310866 -0.272179	1.454371 -0.289521	-8.154053 -7.000513
E (GFN-FF Coordina Cu	tes: -1.115358	-0.188219		H C H C	0.310866 -0.272179 -0.133158 -0.735100	1.454371 -0.289521 -1.013149 -0.727325	-8.154053 -7.000513 -7.817017 -5.729751
E (GFN-FF Coordina Cu N	tes: -1.115358 -1.474296	-0.188219 -1.895579	0.218181	H C H C	0.310866 -0.272179 -0.133158 -0.735100 -0.979207	1.454371 -0.289521 -1.013149 -0.727325 -1.792873	-8.154053 -7.000513 -7.817017 -5.729751 -5.567730
E(GFN-FF Coordina Cu N	tes: -1.115358 -1.474296 -2.608213	-0.188219 -1.895579 0.728450	0.218181 0.217924	H C H C H	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988	-8.154053 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429
E (GFN-FF Coordina Cu N N	tes: -1.115358 -1.474296 -2.608213 -0.675700	-0.188219 -1.895579 0.728450 1.556791	0.218181 0.217924 2.172303	H C H C H N C	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517	-8.154053 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483
E (GFN-FF Coordina Cu N	tes: -1.115358 -1.474296 -2.608213 -0.675700 0.312550	-0.188219 -1.895579 0.728450 1.556791 -1.119838	0.218181 0.217924 2.172303 2.325356	H C H C H	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309	-8.154053 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595
E (GFN-FF Coordina Cu N N	tes: -1.115358 -1.474296 -2.608213 -0.675700	-0.188219 -1.895579 0.728450 1.556791	0.218181 0.217924 2.172303	H C H C H N C	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517	-8.154053 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483
E (GFN-FF Coordina Cu N N N C	tes: -1.115358 -1.474296 -2.608213 -0.675700 0.312550 -0.757526	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906	0.218181 0.217924 2.172303 2.325356 0.302943	H C H C H N C C	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749	-8.154053 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205
E (GFN-FF Coordina Cu N N N C C	tes: -1.115358 -1.474296 -2.608213 -0.675700 0.312550 -0.757526 -1.236457	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966	H C H C H N C C O C	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855	-8.154053 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205 -2.012330
E (GFN-FF Coordina Cu N N N C C C C	tes: -1.115358 -1.474296 -2.608213 -0.675700 0.312550 -0.757526 -1.236457 -0.829031	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152	H C H C H N C C O C H	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242	-8.154053 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205 -2.012330 -2.272618
E (GFN-FF Coordina Cu N N N C C C C	tes: -1.115358 -1.474296 -2.608213 -0.675700 0.312550 -0.757526 -1.236457 -0.829031 -2.274510	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116 -3.408827	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152 -1.343691	H C H C H N C C O C H H	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612 -0.387455	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242 0.693450	-8.154053 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205 -2.012330 -2.272618 -0.916266
E (GFN-FF Coordina Cu N N N C C C H C	tes: -1.115358 -1.474296 -2.608213 -0.675700 0.312550 -0.757526 -1.236457 -0.829031 -2.274510 -2.895637	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152 -1.343691 -2.151776	H C H C H N C C O C H H H H H	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612 -0.387455 0.578803	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242 0.693450 0.511042	-8.154053 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205 -2.012330 -2.272616 -0.916266 -2.437030
E (GFN-FF Coordina Cu N N N C C C C	tes: -1.115358 -1.474296 -2.608213 -0.675700 0.312550 -0.757526 -1.236457 -0.829031 -2.274510	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116 -3.408827	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152 -1.343691	H C H C H N C C O C H H	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612 -0.387455	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242 0.693450	-8.154053 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205 -2.012330 -2.272618 -0.916266
E (GFN-FF Coordina Cu N N N C C C H C	tes: -1.115358 -1.474296 -2.608213 -0.675700 0.312550 -0.757526 -1.236457 -0.829031 -2.274510 -2.895637	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116 -3.408827 -3.810034	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152 -1.343691 -2.151776	H C H C H N C C O C H H H H H	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612 -0.387455 0.578803	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242 0.693450 0.511042	-8.154053 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205 -2.012330 -2.272616 -0.916266 -2.437030
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E (GFN-FF Coordina Cu N N N C C C H C C H C C H C C H	tes: -1.115358 -1.474296 -2.608213 -0.675700 0.312550 -0.757526 -1.236457 -0.829031 -2.274510 -2.895637 -2.424706 -3.441578 -3.511195 -4.461927 -5.310097	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116 -3.408827 -3.810034 -2.088635 -1.180111 0.141488 1.132589 0.922741	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152 -1.343691 -2.151776 -0.760679 -1.127351 -0.646388 -1.115196 -1.774859	Н С Н С Н С С С С С Н Н Н С С С Н С	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612 -0.387455 0.578803 1.878896 3.067697 3.870761 4.784729 3.495537	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242 0.693450 0.511042 1.103382 1.884706 2.110696 2.702310 1.590012	-8.154053 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205 -2.012330 -2.272618 -0.916266 -2.437030 4.984036 4.854510 5.998792 5.877444 7.242763
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E (GFN-FF Coordina Cu N N N C C H C C H C C C C C C C C C C C	tes:     -1.115358     -1.474296     -2.608213     -0.675700     0.312550     -0.757526     -1.236457     -0.829031     -2.274510     -2.895637     -2.424706     -3.441578     -3.511195     -4.461927     -5.310097     -4.063057     -4.513745     -2.896769     -2.166476     -1.149603     -0.517374	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116 -3.408827 -3.810034 -2.088635 -1.180111 0.141488 1.132589 0.922741 2.338393 3.327042 2.076184 3.079083 2.808461 3.817871	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152 -1.343691 -2.151776 -0.760679 -1.127351 -0.646388 -1.115196 -1.774859 -0.596025 -0.735993 0.223949 0.892324 1.832176 2.661663	Н С Н С Н С С С С Н С Н С Н С Н С Н И	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612 -0.387455 0.578803 1.878896 3.067697 3.870761 4.784729 3.495537 4.135588 2.322380 2.024719 1.530929 0.610202 3.382032	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242 0.693450 0.511042 1.103382 1.884706 2.110696 2.702310 1.590012 1.782081 0.833818 0.429110 0.595454 -0.001667 2.412512	-8.154053 -7.000513 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205 -2.012330 -2.272618 -0.916266 -2.437030 4.984036 4.854510 5.998792 5.877444 7.242763 8.117782 7.381642 8.360265 6.250597 6.333340 3.594787
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E (GFN-FF Coordina Cu N N N C C H C C H C C C C H C C C H C C C H C C C H C C C C H C C C C H C C C C H C C C C C H C C C C C C H C C C C C C C C C C C C C C C C C C C C	tes:     -1.115358     -1.474296     -2.608213     -0.675700     0.312550     -0.757526     -1.236457     -0.829031     -2.274510     -2.895637     -2.424706     -3.441578     -3.511195     -4.461927     -5.310097     -4.063057     -4.513745     -2.896769     -2.166476     -1.149603     -0.517374     -0.693664     0.289774     0.908941     0.908941     0.216647	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116 -3.408827 -3.810034 -2.088635 -1.180111 0.141488 1.132589 0.922741 2.338393 3.327042 2.076184 3.079083 2.808461 3.817871 4.895101 3.153476 3.574016 1.746191	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152 -1.343691 -2.151776 -0.760679 -1.127351 -0.646388 -1.115196 -1.774859 -0.596025 -0.735993 0.223949 0.892324 1.832176 2.661663 2.585285 3.548544 4.347873 3.210968	Н С Н С Н Л С С О С Н Н Н С С С Н С Н С Н С Н М Н С О С	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612 -0.387455 0.578803 1.878896 3.067697 3.870761 4.784729 3.495537 4.135588 2.322380 2.024719 1.530929 0.610202 3.382032 2.734988 4.387497 5.277647 4.329057	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242 0.693450 0.511042 1.103382 1.884706 2.110696 2.702310 1.590012 1.782081 0.833818 0.429110 0.595454 -0.001667 2.412512 2.202220 3.301961 3.642219 3.920051	-8.154053 -7.000513 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205 -2.012330 -2.272618 -0.916266 -2.437030 4.984036 4.854510 5.998792 5.877444 7.242763 8.117782 7.381642 8.360265 6.250597 6.333440 3.594787 2.821670 3.270113 4.054956 1.886536
E (GFN-FF Coordina Cu N N N C C C H C C C C C C C H C C C C C	tes:     -1.115358     -1.474296     -2.608213     -0.675700     0.312550     -0.757526     -1.236457     -0.829031     -2.274510     -2.895637     -2.424706     -3.441578     -3.511195     -4.461927     -5.310097     -4.063057     -4.513745     -2.896769     -2.166476     -1.149603     -0.517374     -0.693664     0.289774     0.908941     0.216647     1.011076	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116 -3.408827 -3.810034 -2.088635 -1.180111 0.141488 1.132589 0.922741 2.338393 3.327042 2.076184 3.079083 2.808461 3.817871 4.895101 3.153476 3.574016 1.746191 0.750842	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152 -1.343691 -2.151776 -0.760679 -1.127351 -0.646388 -1.115196 -1.774859 -0.596025 -0.735993 0.223949 0.892324 1.832176 2.661663 2.585285 3.548544 4.347873 3.210968 3.814571	Н С Н С Н И С С О С Н Н Н С С С Н С Н С Н И Н С О С С	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612 -0.387455 0.578803 1.878896 3.067697 3.870761 4.784729 3.495537 4.135588 2.322380 2.024719 1.530929 0.610202 3.382032 2.734988 4.387497 5.277647 4.329057 5.321766	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242 0.693450 0.511042 1.103382 1.884706 2.110696 2.702310 1.590012 1.782081 0.833818 0.429110 0.595454 -0.001667 2.412512 2.202220 3.301961 3.642219 3.920051 4.916268	-8.154053 -7.000513 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205 -2.012330 -2.272618 -0.916266 -2.437030 4.984036 4.854510 5.998792 5.877444 7.242763 8.117782 7.381642 8.360265 6.250597 6.333340 3.594787 2.821670 3.270113 4.054956 1.886536 1.658067
E (GFN-FF Coordina Cu N N N C C H C C H C C C H C C C H C C C C	tes:     -1.115358     -1.474296     -2.608213     -0.675700     0.312550     -0.757526     -1.236457     -0.829031     -2.274510     -2.895637     -2.424706     -3.441578     -3.511195     -4.461927     -5.310097     -4.063057     -4.513745     -2.896769     -2.166476     -1.149603     -0.517374     -0.693664     0.289774     0.908941     0.216647     1.011076     1.047147	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116 -3.408827 -3.810034 -2.088635 -1.180111 0.141488 1.132589 0.922741 2.338393 3.327042 2.076184 3.079083 2.808461 3.817871 4.895101 3.153476 3.574016 1.746191 0.750842 -0.587236	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152 -1.343691 -2.151776 -0.760679 -1.127351 -0.646388 -1.115196 -1.774859 -0.596025 -0.735993 0.223949 0.892324 1.832176 2.661663 2.585285 3.548544 4.347873 3.210968 3.814571 3.367486	Н С Н С Н Л С С О С Н Н Н С С С Н С Н С Н С Н Л Н С О С С Н	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612 -0.387455 0.578803 1.878896 3.067697 3.870761 4.784729 3.495537 4.135588 2.322380 2.024719 1.530929 0.610202 3.382032 2.734988 4.387497 5.277647 4.329057 5.321766 6.031303	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242 0.693450 0.511042 1.103382 1.884706 2.110696 2.702310 1.590012 1.782081 0.833818 0.429110 0.595454 -0.001667 2.412512 2.202220 3.301961 3.642219 3.920051 4.916268 5.079494	-8.154053 -7.000513 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205 -2.012330 -2.272618 -0.916266 -2.437030 4.984036 4.854510 5.998792 5.877444 7.242763 8.117782 7.381642 8.360265 6.250597 6.333440 3.594787 2.821670 3.270113 4.054956 1.886536 1.658067 2.481889
E (GFN-FF Coordina Cu N N N C C C H C C C C C C C H C C C C C	tes:     -1.115358     -1.474296     -2.608213     -0.675700     0.312550     -0.757526     -1.236457     -0.829031     -2.274510     -2.895637     -2.424706     -3.441578     -3.511195     -4.461927     -5.310097     -4.063057     -4.513745     -2.896769     -2.166476     -1.149603     -0.517374     -0.693664     0.289774     0.908941     0.216647     1.011076	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116 -3.408827 -3.810034 -2.088635 -1.180111 0.141488 1.132589 0.922741 2.338393 3.327042 2.076184 3.079083 2.808461 3.817871 4.895101 3.153476 3.574016 1.746191 0.750842	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152 -1.343691 -2.151776 -0.760679 -1.127351 -0.646388 -1.115196 -1.774859 -0.596025 -0.735993 0.223949 0.892324 1.832176 2.661663 2.585285 3.548544 4.347873 3.210968 3.814571	Н С Н С Н И С С О С Н Н Н С С С Н С Н С Н И Н С О С С	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612 -0.387455 0.578803 1.878896 3.067697 3.870761 4.784729 3.495537 4.135588 2.322380 2.024719 1.530929 0.610202 3.382032 2.734988 4.387497 5.277647 4.329057 5.321766	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242 0.693450 0.511042 1.103382 1.884706 2.110696 2.702310 1.590012 1.782081 0.833818 0.429110 0.595454 -0.001667 2.412512 2.202220 3.301961 3.642219 3.920051 4.916268	-8.154053 -7.000513 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205 -2.012330 -2.272618 -0.916266 -2.437030 4.984036 4.854510 5.998792 5.877444 7.242763 8.117782 7.381642 8.360265 6.250597 6.333340 3.594787 2.821670 3.270113 4.054956 1.886536 1.658067
E (GFN-FF Coordina Cu N N N C C H C C H C C C H C C C H C C C C	tes:     -1.115358     -1.474296     -2.608213     -0.675700     0.312550     -0.757526     -1.236457     -0.829031     -2.274510     -2.895637     -2.424706     -3.441578     -3.511195     -4.461927     -5.310097     -4.063057     -4.513745     -2.896769     -2.166476     -1.149603     -0.517374     -0.693664     0.289774     0.908941     0.216647     1.011076     1.047147	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116 -3.408827 -3.810034 -2.088635 -1.180111 0.141488 1.132589 0.922741 2.338393 3.327042 2.076184 3.079083 2.808461 3.817871 4.895101 3.153476 3.574016 1.746191 0.750842 -0.587236 -1.597225	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152 -1.343691 -2.151776 -0.760679 -1.127351 -0.646388 -1.115196 -1.774859 -0.596025 -0.735993 0.223949 0.892324 1.832176 2.661663 2.585285 3.548544 4.347873 3.210968 3.814571 3.367486	н с н с н и с с о с н н н с с с н с н с н с н и н с о с с н с	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612 -0.387455 0.578803 1.878896 3.067697 3.870761 4.784729 3.495537 4.135588 2.322380 2.024719 1.530929 0.610202 3.382032 2.734988 4.387497 5.277647 4.329057 5.321766 6.031303	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242 0.693450 0.511042 1.103382 1.884706 2.110696 2.702310 1.590012 1.782081 0.833818 0.429110 0.595454 -0.001667 2.412512 2.202220 3.301961 3.642219 3.920051 4.916268 5.079494	-8.154053 -7.000513 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205 -2.012330 -2.272618 -0.916266 -2.437030 4.984036 4.854510 5.998792 5.877444 7.242763 8.117782 7.381642 8.360265 6.250597 6.333440 3.594787 2.821670 3.270113 4.054956 1.886536 1.658067 2.481889
E (GFN-FF Coordina Cu N N N C C C H C C C C H C C C C H C C C C	tes:     -1.115358     -1.474296     -2.608213     -0.675700     0.312550     -0.757526     -1.236457     -0.829031     -2.274510     -2.895637     -2.424706     -3.441578     -3.511195     -4.461927     -5.310097     -4.063057     -4.513745     -2.896769     -2.166476     -1.149603     -0.517374     -0.693664     0.289774     0.908941     0.216647     1.011076     1.047147     1.934884     2.633267	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116 -3.408827 -3.810034 -2.088635 -1.180111 0.141488 1.132589 0.922741 2.338393 3.327042 2.076184 3.079083 2.808461 3.817871 4.895101 3.153476 3.574016 1.746191 0.750842 -0.587236 -1.597225 -1.435071	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152 -1.343691 -2.151776 -0.760679 -1.127351 -0.646388 -1.115196 -1.774859 -0.596025 -0.735993 0.223949 0.892324 1.832176 2.661663 2.585285 3.548544 4.347873 3.210968 3.814571 3.367486 3.911454 4.738435	Н С Н С Н И С С О С Н Н Н С С С Н С Н С Н С Н И Н С О С С Н С Н	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612 -0.387455 0.578803 1.878896 3.067697 3.870761 4.784729 3.495537 4.135588 2.322380 2.024719 1.530929 0.610202 3.382032 2.734988 4.387497 5.277647 4.329057 5.321766 6.031303 5.389959 6.166324	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242 0.693450 0.511042 1.103382 1.884706 2.110696 2.702310 1.590012 1.782081 0.833818 0.429110 0.595454 -0.001667 2.412512 2.202220 3.301961 3.642219 3.920051 4.916268 5.079494 5.637931 6.404041	-8.154053 -7.000513 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205 -2.012330 -2.272618 -0.916266 -2.437030 4.984036 4.854510 5.998792 5.877444 7.242763 8.117782 7.381642 8.360265 6.250597 6.333440 3.594787 2.821670 3.270113 4.054956 1.886536 1.658067 2.481889 0.483798 0.335575
E (GFN-FF Coordina Cu N N N C C H C C H C C C C H C C C C H C C C C H C C C C C H C C C C C H C C C C C C C C C C C C C C C C C C C C	tes:     -1.115358     -1.474296     -2.608213     -0.675700     0.312550     -0.757526     -1.236457     -0.829031     -2.274510     -2.895637     -2.424706     -3.441578     -3.511195     -4.461927     -5.310097     -4.063057     -4.513745     -2.896769     -2.166476     -1.149603     -0.517374     -0.693664     0.289774     0.908941     0.216647     1.011076     1.047147     1.934884     2.633267     1.732466	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116 -3.408827 -3.810034 -2.088635 -1.180111 0.141488 1.132589 0.922741 2.338393 3.327042 2.076184 3.079083 2.808461 3.817871 4.895101 3.153476 3.574016 1.746191 0.750842 -0.587236 -1.597225 -1.435071 -2.740392	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152 -1.343691 -2.151776 -0.760679 -1.127351 -0.646388 -1.115196 -1.774859 -0.596025 -0.735993 0.223949 0.892324 1.832176 2.661663 2.585285 3.548544 4.347873 3.210968 3.814571 3.367486 3.911454 4.738435 3.180059	Н С Н С Н И С С О С Н Н Н С С С Н С Н С Н С Н И Н С О С С Н С Н С	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612 -0.387455 0.578803 1.878896 3.067697 3.870761 4.784729 3.495537 4.135588 2.322380 2.024719 1.530929 0.610202 3.382032 2.734988 4.387497 5.277647 4.329057 5.321766 6.031303 5.389959 6.166324 4.421262	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242 0.693450 0.511042 1.103382 1.884706 2.110696 2.702310 1.590012 1.782081 0.833818 0.429110 0.595454 -0.001667 2.412512 2.202220 3.301961 3.642219 3.920051 4.916268 5.079494 5.637931 6.404041 5.420465	-8.154053 -7.000513 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205 -2.012330 -2.272618 -0.916266 -2.437030 4.984036 4.854510 5.998792 5.877444 7.242763 8.117782 7.381642 8.360265 6.250547 6.3333440 3.594787 2.821670 3.270113 4.054956 1.886536 1.658067 2.481889 0.483798 0.483795 0.335575 -0.533548
E (GFN-FF Coordina Cu N N N C C H C C H C C C H C C H C C H C C H C C H C H C C H C C H C H C C C H C H C C C H C H C C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C C C H C C C C H C C C C C H C C C C C C C C C C C C C C C C C C C C	tes:     -1.115358     -1.474296     -2.608213     -0.675700     0.312550     0.757526     -1.236457     -0.829031     -2.274510     -2.895637     -2.424706     -3.441578     -3.511195     -4.461927     -5.310097     -4.063057     -4.513745     -2.896769     -2.166476     -1.149603     -0.517374     -0.693664     0.289774     0.908941     0.216647     1.01076     1.047147     1.934884     2.633267     1.732466     2.224797	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116 -3.408827 -3.810034 -2.088635 -1.180111 0.141488 1.132589 0.922741 2.338393 3.327042 2.076184 3.079083 2.808461 3.817871 4.895101 3.153476 3.574016 1.746191 0.750842 -0.587236 -1.597225 -1.435071 -2.740392 -3.712539	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152 -1.343691 -2.151776 -0.760679 -1.127351 -0.646388 -1.115196 -1.774859 -0.596025 -0.735993 0.223949 0.892324 1.832176 2.661663 2.585285 3.548544 4.347873 3.210968 3.814571 3.367486 3.911454 4.738435 3.180059 3.288434	н с н с н и с с о с н н н с с с н с н с н с н и н с о с с н с н с с	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612 -0.387455 0.578803 1.878896 3.067697 3.870761 4.784729 3.495537 4.135588 2.322380 2.024719 1.530929 0.610202 3.382032 2.734988 4.387497 5.277647 4.329057 5.321766 6.031303 5.389959 6.166324 4.421262 4.379038	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242 0.693450 0.511042 1.103382 1.884706 2.110696 2.702310 1.590012 1.782081 0.833818 0.429110 0.595454 -0.001667 2.412512 2.202220 3.301961 3.642219 3.920051 4.916268 5.079494 5.637931 6.404041 5.420465 6.185966	-8.154053 -7.000513 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205 -2.012330 -2.272618 -0.916266 -2.437030 4.984036 4.854510 5.998792 5.877444 7.242763 8.117782 7.381642 8.360265 6.250597 6.333440 3.594787 2.821670 3.270113 4.054956 1.886536 1.658067 2.481889 0.483798 0.335575 -0.533548 -1.733456
E (GFN-FF Coordina Cu N N N C C H C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C C H C C C C C H C C C C C C C C C C C C C C C C C C C C	tes:     -1.115358     -1.474296     -2.608213     -0.675700     0.312550     -0.757526     -1.236457     -0.829031     -2.274510     -2.895637     -2.424706     -3.441578     -3.511195     -4.461927     -5.310097     -4.063057     -4.513745     -2.896769     -2.166476     -1.149603     -0.517374     -0.693664     -0.289774     0.908941     0.216647     1.011076     1.047147     1.934884     2.633267     1.732466     2.224797     0.722366	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116 -3.408827 -3.810034 -2.088635 -1.180111 0.141488 1.132589 0.922741 2.338393 3.327042 2.076184 3.079083 2.808461 3.817871 4.895101 3.153476 3.574016 1.746191 0.750842 -0.587236 -1.597225 -1.435071 -2.740392 -3.712539 -2.430935	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152 -1.343691 -2.151776 -0.760679 -1.127351 -0.646388 -1.115196 -1.774859 -0.596025 -0.735993 0.223949 0.892324 1.832176 2.661663 2.585285 3.548544 4.347873 3.210968 3.814571 3.367486 3.911454 4.738435 3.180059 3.288434 2.189561	н с н с н и с с о с н н н с с с н с н с н с н и н с о с с н с н с н	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612 -0.387455 0.578803 1.878896 3.067697 3.870761 4.784729 3.495537 4.135588 2.322380 2.024719 1.530929 0.610202 3.382032 2.734988 4.387497 5.277647 4.329057 5.321766 6.031303 5.389959 6.166324 4.421262 4.379038 5.149428	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242 0.693450 0.511042 1.103382 1.884706 2.110696 2.702310 1.590012 1.782081 0.833818 0.429110 0.595454 -0.001667 2.412512 2.202220 3.301961 3.642219 3.920051 4.916268 5.079494 5.637931 6.404041 5.420465 6.185966 6.954906	-8.154053 -7.000513 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205 -2.012330 -2.272618 -0.916266 -2.437030 4.984036 4.854510 5.998792 5.877444 7.242763 8.117782 7.381642 8.360265 6.250597 6.333440 3.594787 2.821670 3.270113 4.054956 1.886536 1.658067 2.481889 0.483798 0.335575 -0.533548 -1.733456 -1.733456 -1.733456 -1.733456
E (GFN-FF Coordina Cu N N N C C H C C H C C C H C C H C C H C C H C C H C H C C H C C H C H C C C H C H C C C H C H C C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C C C H C C C C H C C C C C H C C C C C C C C C C C C C C C C C C C C	tes:     -1.115358     -1.474296     -2.608213     -0.675700     0.312550     0.757526     -1.236457     -0.829031     -2.274510     -2.895637     -2.424706     -3.441578     -3.511195     -4.461927     -5.310097     -4.063057     -4.513745     -2.896769     -2.166476     -1.149603     -0.517374     -0.693664     0.289774     0.908941     0.216647     1.01076     1.047147     1.934884     2.633267     1.732466     2.224797	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116 -3.408827 -3.810034 -2.088635 -1.180111 0.141488 1.132589 0.922741 2.338393 3.327042 2.076184 3.079083 2.808461 3.817871 4.895101 3.153476 3.574016 1.746191 0.750842 -0.587236 -1.597225 -1.435071 -2.740392 -3.712539	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152 -1.343691 -2.151776 -0.760679 -1.127351 -0.646388 -1.115196 -1.774859 -0.596025 -0.735993 0.223949 0.892324 1.832176 2.661663 2.585285 3.548544 4.347873 3.210968 3.814571 3.367486 3.911454 4.738435 3.180059 3.288434	н с н с н и с с о с н н н с с с н с н с н с н и н с о с с н с н с с	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612 -0.387455 0.578803 1.878896 3.067697 3.870761 4.784729 3.495537 4.135588 2.322380 2.024719 1.530929 0.610202 3.382032 2.734988 4.387497 5.277647 4.329057 5.321766 6.031303 5.389959 6.166324 4.421262 4.379038	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242 0.693450 0.511042 1.103382 1.884706 2.110696 2.702310 1.590012 1.782081 0.833818 0.429110 0.595454 -0.001667 2.412512 2.202220 3.301961 3.642219 3.920051 4.916268 5.079494 5.637931 6.404041 5.420465 6.185966	-8.154053 -7.000513 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205 -2.012330 -2.272618 -0.916266 -2.437030 4.984036 4.854510 5.998792 5.877444 7.242763 8.117782 7.381642 8.360265 6.250597 6.333440 3.594787 2.821670 3.270113 4.054956 1.886536 1.658067 2.481889 0.483798 0.335575 -0.533548 -1.733456
E (GFN-FF Coordina Cu N N C C C H C C C H C C C C H C C C C H C C C C C C C C C C C C C C C C C C C C	tes:     -1.115358     -1.474296     -2.608213     -0.675700     0.312550     -0.757526     -1.236457     -0.829031     -2.274510     -2.895637     -2.424706     -3.441578     -3.511195     -4.461927     -5.310097     -4.063057     -4.513745     -2.896769     -2.166476     -1.149603     -0.517374     -0.693664     -0.289774     0.908941     0.216647     1.011076     1.047147     1.934884     2.633267     1.732466     2.224797     0.722366	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116 -3.408827 -3.810034 -2.088635 -1.180111 0.141488 1.132589 0.922741 2.338393 3.327042 2.076184 3.079083 2.808461 3.817871 4.895101 3.153476 3.574016 1.746191 0.750842 -0.587236 -1.597225 -1.435071 -2.740392 -3.712539 -2.430935	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152 -1.343691 -2.151776 -0.760679 -1.127351 -0.646388 -1.115196 -1.774859 -0.596025 -0.735993 0.223949 0.892324 1.832176 2.661663 2.585285 3.548544 4.347873 3.210968 3.814571 3.367486 3.911454 4.738435 3.180059 3.288434 2.189561	н с н с н и с с о с н н н с с с н с н с н с н и н с о с с н с н с н	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612 -0.387455 0.578803 1.878896 3.067697 3.870761 4.784729 3.495537 4.135588 2.322380 2.024719 1.530929 0.610202 3.382032 2.734988 4.387497 5.277647 4.329057 5.321766 6.031303 5.389959 6.166324 4.421262 4.379038 5.149428	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242 0.693450 0.511042 1.103382 1.884706 2.110696 2.702310 1.590012 1.782081 0.833818 0.429110 0.595454 -0.001667 2.412512 2.202220 3.301961 3.642219 3.920051 4.916268 5.079494 5.637931 6.404041 5.420465 6.185966 6.954906	-8.154053 -7.000513 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205 -2.012330 -2.272618 -0.916266 -2.437030 4.984036 4.854510 5.998792 5.877444 7.242763 8.117782 7.381642 8.360265 6.250597 6.333440 3.594787 2.821670 3.270113 4.054956 1.886536 1.658067 2.481889 0.483798 0.335575 -0.533548 -1.733456 -1.733456 -1.733456 -1.733456
E (GFN-FF Coordina Cu N N N C C H C C C H C C C C H C C C C H C C C C C H C C C C C C C C C C C C C C C C C C C C	tes:     -1.115358     -1.474296     -2.608213     -0.675700     0.312550     -0.757526     -1.236457     -0.829031     -2.274510     -2.895637     -2.424706     -3.441578     -3.511195     -4.461927     -5.310097     -4.063057     -4.513745     -2.896769     -2.166476     -1.149603     -0.517374     -0.693664     0.289774     0.908941     0.216647     1.011076     1.047147     1.934884     2.633267     1.732466     2.224797     0.722366     0.262997     -4.473851	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116 -3.408827 -3.810034 -2.088635 -1.180111 0.141488 1.132589 0.922741 2.338393 3.327042 2.076184 3.079083 2.808461 3.817871 4.895101 3.153476 3.574016 1.746191 0.750842 -0.587236 -1.597225 -1.435071 -2.740392 -3.712539 -2.430935 -3.351252 -1.658218	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152 -1.343691 -2.151776 -0.760679 -1.127351 -0.646388 -1.115196 -1.774859 -0.596025 -0.735993 0.223949 0.892324 1.832176 2.661663 2.585285 3.548544 4.347873 3.210968 3.814571 3.367486 3.911454 4.738435 3.180059 3.288434 2.189561 1.226770 -2.094792	Н С Н С Н И С С О С Н Н Н С С С Н С Н С Н С Н И Н С О С С Н С Н С Н С Н	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612 -0.387455 0.578803 1.878896 3.067697 3.870761 4.784729 3.495537 4.135588 2.322380 2.024719 1.530929 0.610202 3.382032 2.734988 4.387497 5.277647 4.329057 5.321766 6.031303 5.389959 6.166324 4.421262 4.379038 5.149428 3.363523 3.289577	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242 0.693450 0.511042 1.103382 1.884706 2.110696 2.702310 1.590012 1.782081 0.833818 0.429110 0.595454 -0.001667 2.412512 2.202220 3.301961 3.642219 3.92051 4.916268 5.079494 5.637931 6.404041 5.420465 6.185966 6.954906 5.973551 6.559675	-8.154053 -7.000513 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205 -2.012330 -2.272618 -0.916266 -2.437030 4.984036 4.854510 5.998792 5.877444 7.242763 8.117782 7.381642 8.360256 6.250597 6.333440 3.594787 2.821670 3.270113 4.054956 1.886536 1.658067 2.481889 0.483798 0.483798 0.483798 0.335575 -0.533548 -1.733456 -1.903137
E (GFN-FF Coordina Cu N N N C C H C C H C C C H C C C H C C C C	tes:     -1.115358     -1.474296     -2.608213     -0.675700     0.312550     -0.757526     -1.236457     -0.829031     -2.274510     -2.895637     -2.424706     -3.441578     -3.511195     -4.461927     -5.310097     -4.063057     -4.513745     -2.896769     -2.166476     -1.149603     -0.517374     -0.693664     0.289774     0.908941     0.216647     1.011076     1.047147     1.934884     2.633267     1.732466     2.224797     0.722366     0.262997     -4.473851     -5.377093	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116 -3.408827 -3.810034 -2.088635 -1.180111 0.141488 1.132589 0.922741 2.338393 3.327042 2.076184 3.079083 2.808461 3.817871 4.895101 3.153476 3.574016 1.746191 0.750842 -0.587236 -1.57225 -1.435071 -2.740392 -3.712539 -2.430935 -3.351252 -1.658218 -2.693949	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152 -1.343691 -2.151776 -0.760679 -1.127351 -0.646388 -1.115196 -1.774859 -0.596025 -0.735993 0.223949 0.892324 1.832176 2.661663 2.585285 3.548544 4.347873 3.210968 3.814571 3.367486 3.911454 4.738435 3.180059 3.288434 2.189561 1.226770 -2.094792 -1.707872	Н С Н С Н И С С О С Н Н Н С С С Н С Н С Н С Н И Н С О С С Н С Н С Н С Н С	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612 -0.387455 0.578803 1.878896 3.067697 3.870761 4.784729 3.495537 4.135588 2.322380 2.024719 1.530929 0.610202 3.382032 2.734988 4.387497 5.277647 4.329057 5.321766 6.031303 5.389959 6.166324 4.421262 4.379038 5.149428 3.363523 3.289577 2.389611	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242 0.693450 0.511042 1.103382 1.884706 2.110696 2.702310 1.590012 1.782081 0.833818 0.429110 0.595454 -0.001667 2.412512 2.202220 3.301961 3.642219 3.920051 4.916268 5.079494 5.637931 6.404041 5.420465 6.185966 6.954906 5.973551 6.559675 4.979932	-8.154053 -7.000513 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205 -2.012330 -2.272618 -0.916266 -2.437030 -4.984036 -4.854510 -5.998792 -5.877444 -7.242763 -8.117782 -7.381642 -8.360265 -6.250597 -6.333440 -3.594787 -2.821670 -3.270113 -4.054956 -1.86536 -1.658067 -2.481889 -0.483798 -0.335575 -0.533548 -1.733456 -1.903138 -2.649597 -3.577317 -2.360929
E (GFN-FF Coordina Cu N N N C C H C C H C C C H C C C H C C C C	tes:     -1.115358     -1.474296     -2.608213     -0.675700     0.312550     -0.757526     -1.236457     -0.829031     -2.274510     -2.895637     -2.424706     -3.441578     -3.511195     -4.461927     -5.310097     -4.063057     -4.513745     -2.896769     -2.166476     -1.149603     -0.517374     -0.693664     0.289774     0.908941     0.216647     1.011076     1.047147     1.934884     2.633267     1.732466     2.224797     0.722366     0.262997     -4.473851     -5.377093     -6.314683	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116 -3.408827 -3.810034 -2.088635 -1.180111 0.141488 1.132589 0.922741 2.338393 3.327042 2.076184 3.079083 2.808461 3.817871 4.895101 3.153476 3.574016 1.746191 0.750842 -0.587236 -1.597225 -1.435071 -2.740392 -3.712539 -2.430935 -3.351252 -1.658218 -2.693949 -3.185641	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152 -1.343691 -2.151776 -0.760679 -1.127351 -0.646388 -1.115196 -1.774859 -0.596025 -0.735993 0.223949 0.892324 1.832176 2.661663 2.585285 3.548544 4.347873 3.210968 3.814571 3.367486 3.911454 4.738435 3.180059 3.288434 2.189561 1.226770 -2.094792 -1.707872 -2.640438	н с н с н и с с о с н н н с с с н с н с н с н и н с о с с н с н с н с н с н	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612 -0.387455 0.578803 1.878896 3.067697 3.870761 4.784729 3.495537 4.135588 2.322380 2.024719 1.530929 0.610202 3.382032 2.734988 4.387497 5.277647 4.329057 5.321766 6.031303 5.389959 6.166324 4.421262 4.379038 5.149428 3.363523 3.289577 2.389611 1.563948	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242 0.693450 0.511042 1.103382 1.884706 2.110696 2.702310 1.590012 1.782081 0.833818 0.429110 0.595454 -0.001667 2.412512 2.202220 3.301961 3.642219 3.920051 4.916268 5.079494 5.637931 6.404041 5.420465 6.185966 6.954906 5.973551 6.559675 4.979932 4.806841	-8.154053 -7.000513 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205 -2.012330 -2.272618 -0.916266 -2.437030 -4.984036 -4.854510 -5.998792 -5.877444 -7.242763 -8.117782 -7.381642 -8.360265 -6.250597 -6.333440 -3.594787 -2.821670 -3.270113 -4.054956 -1.865367 -2.481889 -0.483798 -0.335575 -0.533548 -1.7733456 -1.903138 -2.649597 -3.5777317 -2.360929 -3.070800
E (GFN-FF Coordina Cu N N C C H C C H C C C H C C C H C C C H C C C C H C C C C H C C C C H C C C C C H C C C C C C C C C C C C C C C C C C C C	tes:     -1.115358     -1.474296     -2.608213     -0.675700     0.312550     -0.757526     -1.236457     -0.829031     -2.274510     -2.895637     -2.424706     -3.441578     -3.511195     -4.461927     -5.310097     -4.063057     -4.513745     -2.896769     -2.166476     -1.149603     -0.517374     -0.693664     0.289774     0.908941     0.216647     1.011076     1.047147     1.934884     2.633267     1.732466     2.224797     0.722366     0.262997     -4.473851     -5.377093     -6.314683     -6.988390	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116 -3.408827 -3.810034 -2.088635 -1.180111 0.141488 1.132589 0.922741 2.338393 3.327042 2.076184 3.079083 2.808461 3.817871 4.895101 3.153476 3.574016 1.746191 0.750842 -0.587236 -1.597225 -1.435071 -2.740392 -3.712539 -2.430935 -3.351252 -1.658218 -2.693949 -3.185641 -3.992416	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152 -1.343691 -2.151776 -0.760679 -1.127351 -0.646388 -1.115196 -1.774859 -0.596025 -0.735993 0.223949 0.892324 1.832176 2.661663 2.585285 3.548544 4.347873 3.210968 3.814571 3.367486 3.911454 4.738435 3.180059 3.288434 2.189561 1.226770 -2.094792 -1.707872 -2.640438 -2.329133	н с н с н и с с о с н н н с с с н с н с н с н и н с о с с н с н с н с н и и н с о с с н с н с н с н и	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612 -0.387455 0.578803 1.878896 3.067697 3.870761 4.784729 3.495537 4.135588 2.322380 2.024719 1.530929 0.610202 3.382032 2.734988 4.387497 5.277647 4.329057 5.321766 6.031303 5.389959 6.166324 4.421262 4.379038 5.149428 3.363523 3.289577 2.389611 1.563948 2.405092	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242 0.693450 0.511042 1.103382 1.884706 2.110696 2.702310 1.590012 1.782081 0.833818 0.429110 0.595454 -0.001667 2.412512 2.202220 3.301961 3.642219 3.920051 4.916268 5.079494 5.637931 6.404041 5.420465 6.185966 6.954906 5.973551 6.559675 4.979932 4.886841 4.230847	-8.154053 -7.000513 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.012330 -2.272618 -0.916266 -2.437030 4.984036 4.854510 5.998792 5.877444 7.242763 8.117782 7.381642 8.360265 6.250597 6.333440 3.594787 2.821670 3.270113 4.054956 1.886536 1.658067 2.481889 0.483798 0.335575 -0.533548 -1.733456 -1.903138 -2.649597 -3.577317 -2.360299 -3.070800 -1.268742
E (GFN-FF Coordina Cu N N C C C H C C C C H C C C C H C C C C	tes:     -1.115358     -1.474296     -2.608213     -0.675700     0.312550     -0.757526     -1.236457     -0.829031     -2.274510     -2.895637     -2.424706     -3.441578     -3.511195     -4.461927     -5.310097     -4.063057     -4.513745     -2.896769     -2.166476     -1.149603     -0.517374     -0.693664     0.289774     0.908941     0.216647     1.011076     1.047147     1.934884     2.633267     1.732466     2.224797     0.722366     0.262997     -4.473851     -5.377093     -6.314683	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116 -3.408827 -3.810034 -2.088635 -1.180111 0.141488 1.132589 0.922741 2.338393 3.327042 2.076184 3.079083 2.808461 3.817871 4.895101 3.153476 3.574016 1.746191 0.750842 -0.587236 -1.597225 -1.435071 -2.740392 -3.712539 -2.430935 -3.351252 -1.658218 -2.693949 -3.185641	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152 -1.343691 -2.151776 -0.760679 -1.127351 -0.646388 -1.115196 -1.774859 -0.596025 -0.735993 0.223949 0.892324 1.832176 2.661663 2.585285 3.548544 4.347873 3.210968 3.814571 3.367486 3.911454 4.738435 3.180059 3.288434 2.189561 1.226770 -2.094792 -1.707872 -2.640438	н с н с н и с с о с н н н с с с н с н с н с н и н с о с с н с н с н с н и и с	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612 -0.387455 0.578803 1.878896 3.067697 3.870761 4.784729 3.495537 4.135588 2.322380 2.024719 1.530929 0.610202 3.382032 2.734988 4.387497 5.277647 4.329057 5.321766 6.031303 5.389959 6.166324 4.421262 4.379038 5.149428 3.363523 3.289577 2.389611 1.563948	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242 0.693450 0.511042 1.103382 1.884706 2.110696 2.702310 1.590012 1.782081 0.833818 0.429110 0.595454 -0.001667 2.412512 2.202220 3.301961 3.642219 3.920051 4.916268 5.079494 5.637931 6.404041 5.420465 6.185966 6.954906 5.973551 6.559675 4.979932 4.806841	-8.154053 -7.000513 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205 -2.012330 -2.272618 -0.916266 -2.437030 -4.984036 -4.854510 -5.998792 -5.877444 -7.242763 -8.117782 -7.381642 -8.360265 -6.250597 -6.333440 -3.594787 -2.821670 -3.270113 -4.054956 -1.865367 -2.481889 -0.483798 -0.335575 -0.533548 -1.7733456 -1.903138 -2.649597 -3.5777317 -2.360929 -3.070800
E (GFN-FF Coordina Cu N N C C H C C H C C C H C C C H C C C H C C C C H C C C C H C C C C H C C C C C H C C C C C C C C C C C C C C C C C C C C	tes:     -1.115358     -1.474296     -2.608213     -0.675700     0.312550     -0.757526     -1.236457     -0.829031     -2.274510     -2.895637     -2.424706     -3.441578     -3.511195     -4.461927     -5.310097     -4.063057     -4.513745     -2.896769     -2.166476     -1.149603     -0.517374     -0.693664     0.289774     0.908941     0.216647     1.011076     1.047147     1.934884     2.633267     1.732466     2.224797     0.722366     0.262997     -4.473851     -5.377093     -6.314683     -6.988390	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116 -3.408827 -3.810034 -2.088635 -1.180111 0.141488 1.132589 0.922741 2.338393 3.327042 2.076184 3.079083 2.808461 3.817871 4.895101 3.153476 3.574016 1.746191 0.750842 -0.587236 -1.597225 -1.435071 -2.740392 -3.712539 -2.430935 -3.351252 -1.658218 -2.693949 -3.185641 -3.992416	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152 -1.343691 -2.151776 -0.760679 -1.127351 -0.646388 -1.115196 -1.774859 -0.596025 -0.735993 0.223949 0.892324 1.832176 2.661663 2.585285 3.548544 4.347873 3.210968 3.814571 3.367486 3.911454 4.738435 3.180059 3.288434 2.189561 1.226770 -2.094792 -1.707872 -2.640438 -2.329133	н с н с н и с с о с н н н с с с н с н с н с н и н с о с с н с н с н с н и и н с о с с н с н с н с н и	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612 -0.387455 0.578803 1.878896 3.067697 3.870761 4.784729 3.495537 4.135588 2.322380 2.024719 1.530929 0.610202 3.382032 2.734988 4.387497 5.277647 4.329057 5.321766 6.031303 5.389959 6.166324 4.421262 4.379038 5.149428 3.363523 3.289577 2.389611 1.563948 2.405092	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242 0.693450 0.511042 1.103382 1.884706 2.110696 2.702310 1.590012 1.782081 0.833818 0.429110 0.595454 -0.001667 2.412512 2.202220 3.301961 3.642219 3.920051 4.916268 5.079494 5.637931 6.404041 5.420465 6.185966 6.954906 5.973551 6.559675 4.979932 4.886841 4.230847	-8.154053 -7.000513 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.012330 -2.272618 -0.916266 -2.437030 4.984036 4.854510 5.998792 5.877444 7.242763 8.117782 7.381642 8.360265 6.250597 6.333440 3.594787 2.821670 3.270113 4.054956 1.886536 1.658067 2.481889 0.483798 0.335575 -0.533548 -1.733456 -1.903138 -2.649597 -3.577317 -2.360299 -3.070800 -1.268742
E (GFN-FF Coordina Cu N N N C C H C C H C C C H C C C H C C C H C C C H C C C C H C C C C H C C C C C C C C C C C C C C C C C C C C	tes:     -1.115358     -1.474296     -2.608213     -0.675700     0.312550     -0.757526     -1.236457     -0.829031     -2.274510     -2.895637     -2.424706     -3.441578     -3.511195     -4.461927     -5.310097     -4.063057     -4.513745     -2.896769     -2.166476     -1.149603     -0.517374     -0.693664     0.289774     0.908941     0.216647     1.011076     1.047147     1.934884     2.633267     1.732466     2.224797     0.722366     0.262997     -4.473851     -5.377093     -6.314683     -6.988390     -6.3553787     -7.091210	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116 -3.408827 -3.810034 -2.088635 -1.180111 0.141488 1.132589 0.922741 2.338393 3.327042 2.076184 3.079083 2.808461 3.817871 4.895101 3.153476 3.574016 1.746191 0.750842 -0.587236 -1.597225 -1.435071 -2.740392 -3.712539 -2.430935 -3.351252 -1.658218 -2.693949 -3.185641 -3.992416 -2.651921 -3.043501	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152 -1.343691 -2.151776 -0.760679 -1.127351 -0.646388 -1.115196 -1.774859 -0.596025 -0.735993 0.223949 0.892324 1.832176 2.661663 2.585285 3.548544 4.347873 3.210968 3.814571 3.367486 3.911454 4.738435 3.180059 3.288434 2.189561 1.226770 -2.094792 -1.707872 -2.640438 -2.329133 -3.936101 -4.653289	н с н с н и с с о с н н н с с с н с н с н с н и н с о с с н с н с н с н и и с с	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612 -0.387455 0.578803 1.878896 3.067697 3.870761 4.784729 3.495537 4.135588 2.322380 2.024719 1.530929 0.610202 3.382032 2.734988 4.387497 5.277647 4.329057 5.321766 6.031303 5.389959 6.166324 4.421262 4.379038 5.149428 3.363523 3.289577 2.389611 1.563948 2.405092 3.395020 3.394709	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242 0.693450 0.511042 1.103382 1.884706 2.110696 2.702310 1.590012 1.782081 0.833818 0.429110 0.595454 -0.001667 2.412512 2.202220 3.301961 3.642219 3.920051 4.916268 5.079494 5.637931 6.404041 5.420465 6.185966 6.954906 5.973551 6.559675 4.979932 4.806841 4.230847 4.420930 3.637167	-8.154053 -7.000513 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205 -2.012330 -2.272618 -0.916266 -2.437030 4.984036 4.854510 5.998792 5.877444 7.242763 8.117782 7.381642 8.360265 6.250597 6.333440 3.594787 2.821670 3.270113 4.054956 1.886536 1.658067 2.481889 0.483798 0.335575 -0.533548 -1.733456 -1.903138 -2.649597 -3.577317 -2.360929 -3.070800 -1.268742 -0.350762
E (GFN-FF Coordina Cu N N C C C H C C C C H C C C C H C C C C	tes:     -1.115358     -1.474296     -2.608213     -0.675700     0.312550     -0.757526     -1.236457     -0.829031     -2.274510     -2.895637     -2.424706     -3.441578     -3.511195     -4.461927     -5.310097     -4.063057     -4.513745     -2.896679     -2.166476     -1.149603     -0.517374     -0.693664     0.289774     0.908941     0.216647     1.011076     1.047147     1.934884     2.633267     1.732466     2.224797     0.722366     0.262997     -4.473851     -5.377093     -6.314683     -6.988390     -6.353787	-0.188219 -1.895579 0.728450 1.556791 -1.119838 -3.070906 -4.018077 -5.024116 -3.408827 -3.810034 -2.088635 -1.180111 0.141488 1.132589 0.922741 2.338393 3.327042 2.076184 3.079083 2.808461 3.817871 4.895101 3.153476 3.574016 1.746191 0.750842 -0.587236 -1.597225 -1.435071 -2.740392 -3.712539 -2.430935 -3.351252 -1.658218 -2.693949 -3.185641 -3.992416 -2.651921	0.218181 0.217924 2.172303 2.325356 0.302943 -0.683966 -0.829152 -1.343691 -2.151776 -0.760679 -1.127351 -0.646388 -1.115196 -1.774859 -0.596025 -0.735993 0.223949 0.892324 1.832176 2.661663 2.585285 3.548544 4.347873 3.210968 3.814571 3.367486 3.911454 4.738435 3.180059 3.288434 2.189561 1.226770 -2.094792 -1.707872 -2.640438 -2.329133 -3.936101	н с н с н и с с о с н н н с с с н с н с н с н и н с о с с н с н с н с н и и с	0.310866 -0.272179 -0.133158 -0.735100 -0.979207 -0.902877 -0.635910 -0.821322 -1.101725 -0.440719 -1.034612 -0.387455 0.578803 1.878896 3.067697 3.870761 4.784729 3.495537 4.135588 2.322380 2.024719 1.530929 0.610202 3.382032 2.734988 4.387497 5.277647 4.329057 5.321766 6.031303 5.389959 6.166324 4.421262 4.379038 5.149428 3.363523 3.289577 2.389611 1.563948 2.405092 3.395020	1.454371 -0.289521 -1.013149 -0.727325 -1.792873 0.077988 1.405517 2.281309 1.786749 0.584855 -0.305242 0.693450 0.511042 1.103382 1.884706 2.110696 2.702310 1.590012 1.782081 0.833818 0.429110 0.595454 -0.001667 2.412512 2.202220 3.301961 3.642219 3.920051 4.916268 5.079494 5.637931 6.404041 5.420465 6.185966 6.954906 5.973551 6.559675 4.979932 4.806841 4.230847 4.230847	-8.154053 -7.000513 -7.000513 -7.817017 -5.729751 -5.567730 -4.692429 -4.839483 -3.701595 -2.474205 -2.012330 -2.272618 -0.916266 -2.437030 4.984036 4.854510 5.998792 5.877444 7.242763 8.117782 7.381642 8.360265 6.250597 6.333440 3.594787 2.821670 3.270113 4.054956 1.886536 1.658067 2.481889 0.483798 0.335575 -0.533548 -1.73456 -1.903138 -2.649597 -3.577317 -2.360929 -3.070929 -3.070920 -1.268742 -0.350762

H H	0.998701						
H		2.400744	-0.343623	С	-1.092907	-3.214314	0.783151
	1.560893	0.935751	0.575788	C	-2.183131	-3.832719	1.418722
H	2.588280	1.661371	-0.731263	Н	-2.665277	-4.698942	0.940785
С	0.928283	-4.690032	1.189143	С	-2.674618	-3.359422	2.643971
C	2.240611	-4.801890	0.646130	H	-3.532834	-3.853815	3.123322
С	2.925974	-6.034752	0.718524	С	-2.078672	-2.243039	3.243743
Н	3.949463	-6.093443	0.329564	Н	-2.476937	-1.864038	4.197997
С	2.290924	-7.148801	1.284356	С	-0.975833	-1.597765	2.656057
H	2.833177	-8.105492	1.331489	C	-0.613132	-3.678816	-0.587723
С	0.979363	-7.059334	1.776537	H	0.438447	-3.343113	-0.697071
Н	0.481587	-7.938789	2.211013	С	-0.625362	-5.202756	-0.763506
C	0.307747	-5.829247	1.727992	H	-0.051469	-5.711087	0.038114
H	-0.710342	-5.734123	2.128407	H	-0.173847	-5.481907	-1.737306
N	2.770327	-3.658463	0.031287	H	-1.655244	-5.615730	-0.754432
							-1.695381
H	2.096916	-2.915603	-0.206133	С	-1.424791	-2.980018	
C	4.073503	-3.391125	-0.317861	H	-1.424387	-1.879253	-1.552275
0	5.021505	-4.147014	-0.097143	H	-2.485913	-3.303907	-1.673070
Č	4.298596	-2.053067	-0.995682	Н	-1.012546	-3.207702	-2.700471
C	5.646157	-1.583940	-0.973741	С	-0.336040	-0.394138	3.339617
H	6.376799	-2.216314	-0.449332	H	0.525045	-0.085790	2.711777
С	6.013675	-0.396970	-1.575909	С	0.204931	-0.744657	4.736665
Н	7.051465	-0.035581	-1.518867	Н	0.921386	-1.589939	4.704334
C	5.048726	0.373293	-2.285533	H	-0.614092	-1.029566	5.429401
C	5.343336	1.618384	-2.910725	H	0.727184	0.127277	5.181858
H	6.364348	2.024989	-2.840411	С	-1.301606	0.800334	3.408217
C				Н			2.398229
	4.345280	2.299647	-3.587634		-1.641727	1.092919	
H	4.535545	3.272292	-4.064145	H	-0.806957	1.678021	3.872733
C	3.047091	1.722371	-3.646623	H	-2.200137	0.561071	4.014516
H	2.235955	2.241975	-4.188384	С	1.174559	1.876320	-1.651735
N	2.726965	0.575728	-3.064707	С	0.390023	1.838635	-2.843087
C	3.691297	-0.099342	-2.373395	С	-0.022344	3.057228	-3.411869
С	3.325716	-1.303662	-1.675302	H	-0.618200	3.043825	-4.337474
0	2.001337	-1.665878	-1.623224	C	0.314093	4.283293	-2.824751
C	1.435077	-2.235191	-2.817888	H	-0.007865	5.226254	-3.291348
H	1.446520	-1.494639	-3.641538	С	1.041830	4.304319	-1.624104
H	0.391788	-2.502968	-2.567304	H	1.275612	5.269853	-1.151860
H	1.994186		-3.108377	C	1.465153	3.118241	-1.005481
п	1.994100	-3.150607	-3.1003//				
				C	0.012649	0.513546	-3.497332
<b>OTTITI</b>	777 (7			H	0.310699	-0.294118	-2.789282
QUH	VAS			С	-1.502568	0.385515	-3.721623
				H	-2.056482	0.495518	-2.768256
Conform	mation 16.			H	-1.747881	-0.610454	-4.143190
Multip	licity: 4			H	-1.878955	1.150379	-4.431337
Charge	. 0			С	0.797339	0.281416	-4.799678
	3c) = -3413.53958	1.COO.4FE H		Н	1.892094		
						0.322485	-4.631543
		3.225808808773 Ha		H	0.545428	1.053379	-5.556394
E (PBE -	<ul> <li>D3(BJ)/def2-TZV</li> </ul>	P) = -3412.100375	520925 Hartree	H	0.554114	-0.710172	-5.233486
E (PREO	- D3(BJ)/def2-T7	(VP) = -3412.31477	8635724 Hartree	С	2.142590	3.121774	0.359763
	-3c) = -3408.8771		0000721 Hartree	Н	2.824451	2.247832	0.392045
E(PM6)	= 95.08553 Kcal/	mol		С	1.086748	2.904244	1.461021
E(PM7)	= 109.71159 Kcal						
E (0B973		/mol		H		2.755085	2.450708
	X-V/def2-TZVP) =		5 Hartree		1.565106	2.755085	
E (CEN1		-3415.59789474214	5 Hartree	H	1.565106 0.458676	2.755085 2.015674	1.242523
	-xTB) = $-148.5414$	-3415.59789474214 13151347 Hartree	5 Hartree	H H	1.565106 0.458676 0.400275	2.755085 2.015674 3.772277	1.242523 1.528369
E (GFN2-	-xTB) = $-148.5414-xTB$ ) = $-147.3205$	-3415.59789474214 13151347 Hartree 08912646 Hartree	5 Hartree	H H C	1.565106 0.458676 0.400275 2.987664	2.755085 2.015674 3.772277 4.369369	1.242523 1.528369 0.637582
E (GFN2-	-xTB) = $-148.5414$	-3415.59789474214 13151347 Hartree 08912646 Hartree	15 Hartree	H H	1.565106 0.458676 0.400275	2.755085 2.015674 3.772277	1.242523 1.528369
E (GFN2-	-xTB) = $-148.5414-xTB$ ) = $-147.3205$	-3415.59789474214 13151347 Hartree 08912646 Hartree	5 Hartree	H H C H	1.565106 0.458676 0.400275 2.987664 3.736366	2.755085 2.015674 3.772277 4.369369 4.546598	1.242523 1.528369 0.637582 -0.161547
E (GFN2-	-xTB) = $-148.5414-xTB$ ) = $-147.3205FF$ ) = $-20.5044518$	-3415.59789474214 13151347 Hartree 08912646 Hartree	5 Hartree	Н Н С Н Н	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473	1.242523 1.528369 0.637582 -0.161547 1.597171
E (GFN2- E (GFN-l	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates:	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree		Н Н С Н Н	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908
E (GFN2- E (GFN-1 Coordin	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates: -0.135033	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree	-0.336980	H H C H H H	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474
E (GFN2- E (GFN-) Coordin Co	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates: -0.135033 0.588906	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree		H H C H H H C	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908
E (GFN2- E (GFN-) Coordin Co	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates: -0.135033 0.588906	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree 0.030378 -1.427145	-0.336980 0.766997	H H C H H H C	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072
E (GFN-1 Coordin Co N	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates: -0.135033 0.588906 1.528759	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree 0.030378 -1.427145 0.658613	-0.336980 0.766997 -1.025825	H H C H H H C C	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656
E (GFN2-E (GFN-I) Coordin Co N N C	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates: -0.135033 0.588906 1.528759 2.536625	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree 0.030378 -1.427145 0.658613 -2.876839	-0.336980 0.766997 -1.025825 1.670887	H H C H H H C C C	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154
E (GFN2- E (GFN-1 Coordin Co N N C	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates: -0.135033 0.588906 1.528759 2.536625 1.893502	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree 0.030378 -1.427145 0.658613 -2.876839 -1.747278	-0.336980 0.766997 -1.025825 1.670887 0.789058	H H C H H C C C C	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655
E (GFN2- E (GFN-) Coordin Co N C C C	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896	H H C H H C C C C H C	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303
E (GFN2- E (GFN-1 Coordin Co N N C	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates: -0.135033 0.588906 1.528759 2.536625 1.893502	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree 0.030378 -1.427145 0.658613 -2.876839 -1.747278	-0.336980 0.766997 -1.025825 1.670887 0.789058	H H C H H C C C C	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655
E (GFN2- E (GFN-l Coordin Co N C C C C	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038	H H C H H C C C C H C H	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166
E (GFN2- E (GFN-l Coordin Co N N C C C C	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254	H H C H H C C C C H C C H C C H C	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322
E (GFN2-E (GFN-I) Coordin Co N C C C C C C C C C C C	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056 4.018328	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112	H H H H N C C C H C H C H	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935
E (GFN2-E (GFN-I) Coordin Co N C C C C C H C C C C	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056 4.018328 1.579016	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329 -3.766697	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112 2.486729	H H C H H C C C H C H C H C H C H C H C	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291 -3.971107	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233 4.233247	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935 1.744368
E (GFN2-E (GFN-I) Coordin Co N C C C C C C C C C C	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056 4.018328	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112	H H H H N C C C H C H C H	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935
E (GFN2-E (GFN-I) Coordin Co N C C C C C C C C H C C C C H	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056 4.018328 1.579016 2.194663	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329 -3.766697 -4.483149	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112 2.486729 3.068471	H H C H H N C C C H C H C H C H	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291 -3.971107 -4.678956	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233 4.233247 4.592638	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935 1.744368 2.507192
E (GFN2-E (GFN-E) Coordin Co N C C C C C C C C H C C C H C C C H H H	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056 4.018328 1.579016 2.194663 0.897053	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329 -3.766697 -4.483149 -4.354052	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112 2.486729 3.068471 1.847111	H H C H H N C C C H C H C H C H C H C H	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291 -3.971107 -4.678956 -3.982537	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233 4.233247 4.592638 2.883281	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935 1.744368 2.507192 1.365476
E(GFN2-E(GFN-ICO) COORDING CO N CC CC CC CC H CC CC H H	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056 4.018328 1.579016 2.194663 0.897053 0.997000	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329 -3.766697 -4.483149 -4.354052 -3.202667	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112 2.486729 3.068471 1.847111 3.202346	H H H H H C C C H C H C H C H C H C H C	1.565106 0.458676 0.40275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291 -3.971107 -4.678956 -3.982537 -4.694742	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233 4.233247 4.592638 2.883281 2.184780	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935 1.744368 2.507192 1.365476 1.830251
E (GFN2-E (GFN-I) COORDIN CO N C C C C C C C H C C C C H C C C C C C	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056 4.018328 1.579016 2.194663 0.897053 0.957000 3.339372	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329 -3.766697 -4.483149 -4.354052 -3.202667 -3.840727	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112 2.486729 3.068471 1.847111 3.202346 0.760715	H H H H H C C C C H C H C H C H C H C H	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291 -3.971107 -4.678956 -3.982537 -4.694742 -4.269168	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233 4.233247 4.592638 2.883281 2.184780 0.181803	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935 1.744368 2.507192 1.365476 1.830251 -0.138137
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E (GFN2-E (GFN-I) COORDIN CO N C C C C C H C C C H C C C H H C C H H H	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056 4.018328 1.579016 2.194663 0.897053 0.957000 3.339372 3.768705	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329 -3.766697 -4.483149 -4.354052 -3.202667 -3.840727 -4.657273	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112 2.486729 3.068471 1.847111 3.202346 0.760715 1.376458	Н Н С Н Н Н С С С Н С Н С Н С Н С С С Н С С С С С С С С С С С С С С С С С С С С	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291 -3.971107 -4.678956 -3.982537 -4.694742 -4.269168 -4.273260	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233 4.233247 4.592638 2.883281 2.184780 0.181803 -1.209661	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935 1.744368 2.507192 1.365476 1.830251 -0.138137 0.102714
E (GFN2-E (GFN-I) Coordin Co N C C C C C H C C C H C C C H H H H	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056 4.018328 1.579016 2.194663 0.897053 0.957000 3.339372 3.768705 4.177696	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329 -3.766697 -4.483149 -4.354052 -3.202667 -3.840727 -4.657273 -3.350321	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112 2.486729 3.068471 1.847111 3.202346 0.760715 1.376458 0.230561	H H H H H N C C C H C H C H C H C H C H	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291 -3.971107 -4.678956 -3.982537 -4.694742 -4.269168 -4.273260 -3.349446	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233 4.233247 4.592638 2.883281 2.184780 0.181803 -1.209661 -1.682231	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935 1.744368 2.507192 1.365476 1.830251 -0.138137 0.102714 0.462453
E(GFN2-E(GFN-ICO) COORDINATE COORDINATE CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056 4.018328 1.579016 2.194663 0.897053 0.957000 3.339372 3.768705 4.177696 2.680413	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329 -3.766697 -4.483149 -4.354052 -3.202667 -3.840727 -4.657273 -3.350321 -4.302771	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112 2.486729 3.068471 1.847111 3.202346 0.760715 1.376458 0.230561 -0.002167	H H H H H N C C C H C H C H C H C H C H	1.565106 0.458676 0.40275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291 -3.971107 -4.678956 -3.982537 -4.694742 -4.269168 -4.273260 -3.349446 -5.434321	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233 4.233247 4.592638 2.883281 2.184780 0.181803 -1.209661 -1.682231 -1.963296	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935 1.744368 2.507192 1.365476 1.830251 -0.138137 0.102714 0.462453 -0.099580
E (GFN2-E (GFN-I) COORDIN CO N C C C C C C C H C C C C H C C C C C C	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056 4.018328 1.579016 2.194663 0.897053 0.957000 3.339372 3.768705 4.177696 2.680413 3.489727	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329 -3.766697 -4.483149 -4.354052 -3.202667 -3.840727 -4.657273 -3.350321 -4.302771 -2.186937	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112 2.486729 3.068471 1.847111 3.202346 0.760715 1.376458 0.230561 -0.002167 2.678096	Н Н С Н Н Н С С С Н С Н С Н С Н С Н С Н	1.565106 0.458676 0.40275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291 -3.971107 -4.678956 -3.982537 -4.694742 -4.269168 -4.273260 -3.349446 -5.434321 -5.422650	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233 4.233247 4.592638 2.883281 2.184780 0.181803 -1.209661 -1.682231 -1.963296 -3.044497	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935 1.744368 2.507192 1.365476 1.830251 -0.138137 0.102714 0.462453 -0.099580 0.109482
E(GFN2-E(GFN-ICO) COORDINATE COORDINATE CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056 4.018328 1.579016 2.194663 0.897053 0.957000 3.339372 3.768705 4.177696 2.680413	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329 -3.766697 -4.483149 -4.354052 -3.202667 -3.840727 -4.657273 -3.350321 -4.302771	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112 2.486729 3.068471 1.847111 3.202346 0.760715 1.376458 0.230561 -0.002167	H H H H H N C C C H C H C H C H C H C H	1.565106 0.458676 0.40275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291 -3.971107 -4.678956 -3.982537 -4.694742 -4.269168 -4.273260 -3.349446 -5.434321	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233 4.233247 4.592638 2.883281 2.184780 0.181803 -1.209661 -1.682231 -1.963296	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935 1.744368 2.507192 1.365476 1.830251 -0.138137 0.102714 0.462453 -0.099580
E (GFN2-E (GFN-I) Coordin Co N C C C C H C C H C C H H C C H H H H H	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518  nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056 4.018328 1.579016 2.194663 0.897053 0.957000 3.339372 3.768705 4.177696 2.680413 3.489727 3.987086	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329 -3.766697 -4.483149 -4.354052 -3.202667 -3.840727 -4.657273 -3.350321 -4.302771 -2.186937 -2.948844	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112 2.486729 3.068471 1.847111 3.202346 0.760715 1.376458 0.230561 -0.002167 2.678096 3.313441	Н Н С Н Н Н Н С С С С Н С Н С Н С Н С Н	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291 -3.971107 -4.678956 -3.982537 -4.694742 -4.269168 -4.273260 -3.349446 -5.432321 -5.422650 -6.610122	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233 4.233247 4.592638 2.883281 2.184780 0.181803 -1.209661 -1.682231 -1.963296 -3.044497 -1.342518	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935 1.744368 2.507192 1.365476 1.830251 -0.138137 0.102714 0.462453 -0.099580 0.109482 -0.557540
E (GFN2-E (GFN-I) COORDIN CO N C C C C H C C C H H C C C H H H C H H H H H H	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518  nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056 4.018328 1.579016 2.194663 0.897053 0.957000 3.339372 3.768705 4.177696 2.680413 3.489727 3.987086 2.926655	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329 -3.766697 -4.483149 -4.354052 -3.202667 -3.840727 -4.657273 -3.350321 -4.302771 -2.186937 -2.948844 -1.502226	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112 2.486729 3.068471 1.847111 3.202346 0.760715 1.376458 0.230561 -0.002167 2.678096 3.313441 3.343865	Н Н Н Н Н С С С Н С Н С Н С Н С Н С Н С	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291 -3.971107 -4.678956 -3.982537 -4.694742 -4.269168 -4.273260 -3.349446 -5.434321 -5.422650 -6.610122 -7.523914	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233 4.233247 4.592638 2.883281 2.184780 0.181803 -1.209661 -1.682231 -1.963296 -3.044497 -1.342518 -1.935217	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935 1.744368 2.507192 1.365476 1.830251 -0.138137 0.102714 0.462453 -0.099580 0.109482 -0.557540 -0.717817
E (GFN2-E (GFN-E) COORDIN CO N C C C C H C C C H H C C C H H H H H H	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056 4.018328 1.579016 2.194663 0.897053 0.957000 3.339372 3.768705 4.177696 2.680413 3.489727 3.987086 2.926655 4.276494	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329 -3.766697 -4.483149 -4.354052 -3.202667 -3.840727 -4.657273 -3.350321 -4.302771 -2.186937 -2.948844 -1.502226 -1.592905	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112 2.486729 3.068471 1.847111 3.202346 0.760715 1.376458 0.230561 -0.002167 2.678096 3.313441 3.343865 2.174752	Н Н С Н Н Н И С С С Н С Н С Н С Н С С Н С Н	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291 -3.971107 -4.678956 -3.982537 -4.694742 -4.269168 -4.273260 -3.349446 -5.434321 -5.422650 -6.610122 -7.523914 -6.614569	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233 4.233247 4.592638 2.883281 2.184780 0.181803 -1.209661 -1.682231 -1.963296 -3.044497 -1.342518 -1.995217 0.039623	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935 1.744368 2.507192 1.365476 1.830251 -0.138137 0.102714 0.462453 -0.099580 0.109482 -0.557540 -0.717817 -0.806285
E (GFN2-E (GFN-I) COORDIN CO N C C C C C C C C H C C C H H C H H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C H C C H C C C C C C C C C C C C C C C C C C C C	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056 4.018328 1.579016 2.194663 0.897053 0.957000 3.339372 3.768705 4.177696 2.680413 3.489727 3.987086 2.926655 4.276494 3.913203	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329 -3.766697 -4.483149 -4.354052 -3.202667 -3.840727 -4.657273 -3.350321 -4.302771 -2.186937 -2.948844 -1.502226 -1.592905 1.698521	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112 2.486729 3.068471 1.847111 3.202346 0.760715 1.376458 0.230561 -0.002167 2.678096 3.313441 3.343865 2.174752 -2.541515	Н Н С Н Н Н И С С С Н С Н С Н С Н С Н С	1.565106 0.458676 0.40275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291 -3.971107 -4.678956 -3.982537 -4.694742 -4.269168 -4.273260 -3.349446 -5.434321 -5.422650 -6.610122 -7.523914 -6.614569 -7.529740	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233 4.233247 4.592638 2.883281 2.184780 0.181803 -1.209661 -1.682231 -1.963296 -3.044497 -1.342518 -1.935217 0.039623 0.530986	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935 1.744368 2.507192 1.365476 1.830251 -0.138137 0.102714 0.462453 -0.099580 0.109482 -0.557540 -0.717817 -0.806285 -1.171216
E (GFN2-E (GFN-E) COORDIN CO N C C C C H C C C H H C C C H H H H H H	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518 nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056 4.018328 1.579016 2.194663 0.897053 0.957000 3.339372 3.768705 4.177696 2.680413 3.489727 3.987086 2.926655 4.276494	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329 -3.766697 -4.483149 -4.354052 -3.202667 -3.840727 -4.657273 -3.350321 -4.302771 -2.186937 -2.948844 -1.502226 -1.592905	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112 2.486729 3.068471 1.847111 3.202346 0.760715 1.376458 0.230561 -0.002167 2.678096 3.313441 3.343865 2.174752	Н Н С Н Н Н И С С С Н С Н С Н С Н С С Н С Н	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291 -3.971107 -4.678956 -3.982537 -4.694742 -4.269168 -4.273260 -3.349446 -5.434321 -5.422650 -6.610122 -7.523914 -6.614569	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233 4.233247 4.592638 2.883281 2.184780 0.181803 -1.209661 -1.682231 -1.963296 -3.044497 -1.342518 -1.995217 0.039623	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935 1.744368 2.507192 1.365476 1.830251 -0.138137 0.102714 0.462453 -0.099580 0.109482 -0.557540 -0.717817 -0.806285
E (GFN2-E (GFN-I) COORDIN CO N C C C C C H C C C H H H H H H H C H H H H H H H H H H H H H H H H H H H H	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518  nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056 4.018328 1.579016 2.194663 0.897053 0.957000 3.339372 3.768705 4.177696 2.680413 3.469727 3.987086 2.926655 4.276494 3.913203 4.869939	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329 -3.766697 -4.483149 -4.354052 -3.202667 -3.840727 -4.657273 -3.350321 -4.302771 -2.186937 -2.948844 -1.502226 -1.592905 1.698521 1.807966	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112 2.486729 3.068471 1.847111 3.202346 0.760715 1.376458 0.230561 -0.002167 2.678096 3.313441 3.343865 2.174752 -2.541515 -3.091743	Н Н С Н Н Н И С С С Н С Н С Н С Н С Н С	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291 -3.971107 -4.678956 -3.982537 -4.694742 -4.269168 -4.273260 -3.349446 -5.434321 -5.422650 -6.610122 -7.523914 -6.614569 -7.529740 -5.454829	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233 4.233247 4.592638 2.883281 2.184780 0.181803 -1.209661 -1.682231 -1.963296 -3.044497 -1.342518 -1.935217 0.039623 0.530986 0.799839	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935 1.744368 2.507192 1.365476 1.830251 -0.138137 0.102714 0.462453 -0.099580 0.109482 -0.557540 -0.717817 -0.806285 -1.171216 -0.593411
E (GFN2-E (GFN-I) COORDIN CO N C C C C H C C C H H C C H H C H H H C H H H H H H H H C H H H H H H H H H H H H H H H H H H H H	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518  nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056 4.018328 1.579016 2.194663 0.897053 0.957000 3.3339372 3.768705 4.177696 2.680413 3.489727 3.987086 2.926655 4.276494 3.913203 4.869939 3.748863	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329 -3.766697 -4.483149 -4.354052 -3.202667 -3.840727 -4.657273 -3.350321 -4.302771 -2.186937 -2.948844 -1.502226 -1.592905 1.698521 1.807966 2.630319	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112 2.486729 3.068471 1.847111 3.202346 0.760715 1.376458 0.230561 -0.002167 2.678096 3.313441 3.343865 2.174752 -2.541515 -3.091743 -1.971223	Н Н С Н Н Н И С С С Н С Н С Н С Н С Н С	1.565106 0.458676 0.40275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291 -3.971107 -4.678956 -3.982537 -4.694742 -4.269168 -4.273260 -3.349446 -5.434321 -5.422650 -6.610122 -7.523914 -6.614569 -7.529740	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233 4.233247 4.592638 2.883281 2.184780 0.181803 -1.209661 -1.682231 -1.963296 -3.044497 -1.342518 -1.935217 0.039623 0.530986	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935 1.744368 2.507192 1.365476 1.830251 -0.138137 0.102714 0.462453 -0.099580 0.109482 -0.557540 -0.717817 -0.806285 -1.171216
E (GFN2-E (GFN-E) (GFN	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518  nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056 4.018328 1.579016 2.194663 0.897053 0.957000 3.339372 3.768705 4.177696 2.680413 3.489727 3.987086 2.926655 4.276494 3.913203 4.869939 3.748863 3.105093	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329 -3.766697 -4.483149 -4.354052 -3.202667 -3.840727 -4.657273 -3.350321 -4.302771 -2.186937 -2.948844 -1.502226 -1.592905 1.698521 1.807966 2.630319 1.620360	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112 2.486729 3.068471 1.847111 3.202346 0.760715 1.376458 0.230561 -0.002167 2.678096 3.313441 3.343865 2.174752 -2.541515 -3.091743 -1.971223 -3.291069	Н Н С Н Н Н И С С С Н С Н С Н С Н С Н С Н	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291 -3.971107 -4.678956 -3.982537 -4.694742 -4.269168 -4.273260 -3.349446 -5.434321 -5.422650 -6.610122 -7.523914 -6.614569 -7.529740 -5.454829 -5.460469	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233 4.233247 4.592638 2.883281 2.184780 0.181803 -1.209661 -1.682231 -1.963296 -3.044497 -1.342518 -1.935217 0.039623 0.530986 0.799839	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935 1.744368 2.507192 1.365476 1.830251 -0.138137 0.102714 0.462453 -0.099580 0.109482 -0.557540 -0.717817 -0.806285 -1.171216 -0.593411
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E (GFN2-E (GFN-E) (GFN	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518  nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056 4.018328 1.579016 2.194663 0.897053 0.957000 3.339372 3.768705 4.177696 2.680413 3.489727 3.987086 2.926655 4.276494 3.913203 4.869939 3.748863 3.105093 4.381760 5.303968 3.567736 4.554814	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329 -3.766697 -4.483149 -4.354052 -3.202667 -3.840727 -4.657273 -3.350321 -4.302771 -2.186937 -2.948844 -1.502226 -1.592905 1.698521 1.807966 2.630319 1.620360 -0.743355 -0.518687 -0.947956 -1.670294	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112 2.486729 3.068471 1.847111 3.202346 0.760715 1.376458 0.230561 -0.002167 2.678096 3.313441 3.343865 2.174752 -2.541515 -3.091743 -1.971223 -3.291069 -2.545150 -3.120183 -3.270035 -1.965698	H H H H H N C C C H C H C H C H C H C H	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291 -3.971107 -4.678956 -3.982537 -4.694742 -4.269168 -4.273260 -3.349446 -5.434321 -5.422650 -6.610122 -7.523914 -6.614569 -7.529740 -5.454829 -5.460469  mation 20. licity: 4: 0 3c) = -3413.53710	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233 4.233247 4.592638 2.883281 2.184780 0.181803 -1.209661 -1.682231 -1.963296 -3.044497 -1.342518 -1.935217 0.039623 0.799839 1.881413	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935 1.744368 2.507192 1.365476 1.830251 -0.138137 0.102714 0.462453 -0.099580 0.109482 -0.557540 -0.717817 -0.806285 -1.171216 -0.593411 -0.795476
E (GFN2-E (GFN-I) COORDING CO N CC CC CC CC H CC CC H H H CC H H H CC H H H CC H H CC H CC H CC H CC CC	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518  nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056 4.018328 1.579016 2.194663 0.897053 0.957000 3.339372 3.768705 4.177696 2.680413 3.489727 3.987086 2.926655 4.276494 3.913203 4.869939 3.748863 3.105093 4.381760 5.303968 3.567736 4.554814 5.168732	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329 -3.766697 -4.483149 -4.354052 -3.202667 -3.840727 -4.657273 -3.350321 -4.302771 -2.186937 -2.948844 -1.502226 -1.592905 1.698521 1.807966 2.630319 1.620360 -0.743355 -0.518687 -0.947956 -1.670294 0.720678	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112 2.486729 3.068471 1.847111 3.202346 0.760715 1.376458 0.230561 -0.002167 2.678096 3.313441 3.343865 2.174752 -2.541515 -3.091743 -1.971223 -3.291069 -2.545150 -3.120183 -3.270035 -1.965698 -0.635820	H H C H H N C C C H C H C H C H C H C H	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291 -3.971107 -4.678956 -3.982537 -4.694742 -4.269168 -4.273260 -3.349446 -5.434321 -5.422650 -6.610122 -7.523914 -6.614569 -7.529740 -5.454829 -5.460469  mation 20. licity: 4::0 3c) = -3413.53710 def2-TZVP) = -341	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233 4.233247 4.592638 2.883281 2.184780 0.181803 -1.209661 -1.682231 -1.963296 -3.044497 -1.342518 -1.935217 0.039623 0.530986 0.799839 1.881413	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935 1.744368 2.507192 1.365476 1.830251 -0.138137 0.102714 0.462453 -0.099580 0.109482 -0.557540 -0.717817 -0.806285 -1.171216 -0.593411 -0.795476
E (GFN2-E (GFN-I) COORDIN CO N CC CC CC H CC CC H H H H H H H H H H H H H H H H H H H H	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518  nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056 4.018328 1.579016 2.194663 0.897053 0.957000 3.339372 3.768705 4.177696 2.680413 3.489727 3.987086 2.926655 4.276494 3.913203 4.869939 3.748863 3.105093 4.381760 5.303968 3.567736 4.554814	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329 -3.766697 -4.483149 -4.354052 -3.202667 -3.840727 -4.657273 -3.350321 -4.302771 -2.186937 -2.948844 -1.502226 -1.592905 1.698521 1.807966 2.630319 1.620360 -0.743355 -0.518687 -0.947956 -1.670294 0.720678 1.003897	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112 2.486729 3.068471 1.847111 3.202346 0.760715 1.376458 0.230561 -0.002167 2.678096 3.313441 3.343865 2.174752 -2.541515 -3.091743 -1.971223 -3.291069 -2.545150 -3.120183 -3.270035 -1.965698 -0.635820 -1.188082	H H H H H C C C H C H C H C H C H C H C	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291 -3.971107 -4.678956 -3.982537 -4.694742 -4.269168 -4.273260 -3.349446 -5.434321 -5.422650 -6.610122 -7.523914 -6.614569 -7.529740 -5.454829 -5.460469  mation 20. licity: 4 : 0 3c) = -3413.53710 def2-TZVP) = -341 - D3(BJ)/def2-TZV	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233 4.233247 4.592638 2.883281 2.184780 0.181803 -1.209661 -1.682231 -1.963296 -3.044497 -1.342518 -1.935217 0.039623 0.530986 0.799839 1.881413	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935 1.744368 2.507192 1.365476 1.830251 -0.138137 0.102714 0.462453 -0.099580 0.109482 -0.557540 -0.717817 -0.806285 -1.171216 -0.593411 -0.795476
E (GFN2-E (GFN-I) COORDING CO N CC CC CC CC H CC CC H H H CC H H H CC H H H CC H H CC H CC H CC H CC CC	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518  nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056 4.018328 1.579016 2.194663 0.897053 0.957000 3.339372 3.768705 4.177696 2.680413 3.489727 3.987086 2.926655 4.276494 3.913203 4.869939 3.748863 3.105093 4.381760 5.303968 3.567736 4.554814 5.168732	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329 -3.766697 -4.483149 -4.354052 -3.202667 -3.840727 -4.657273 -3.350321 -4.302771 -2.186937 -2.948844 -1.502226 -1.592905 1.698521 1.807966 2.630319 1.620360 -0.743355 -0.518687 -0.947956 -1.670294 0.720678	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112 2.486729 3.068471 1.847111 3.202346 0.760715 1.376458 0.230561 -0.002167 2.678096 3.313441 3.343865 2.174752 -2.541515 -3.091743 -1.971223 -3.291069 -2.545150 -3.120183 -3.270035 -1.965698 -0.635820	H H H H H C C C H C H C H C H C H C H C	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291 -3.971107 -4.678956 -3.982537 -4.694742 -4.269168 -4.273260 -3.349446 -5.434321 -5.422650 -6.610122 -7.523914 -6.614569 -7.529740 -5.454829 -5.460469  mation 20. licity: 4 : 0 3c) = -3413.53710 def2-TZVP) = -341 - D3(BJ)/def2-TZV	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233 4.233247 4.592638 2.883281 2.184780 0.181803 -1.209661 -1.682231 -1.963296 -3.044497 -1.342518 -1.935217 0.039623 0.530986 0.799839 1.881413	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935 1.744368 2.507192 1.365476 1.830251 -0.138137 0.102714 0.462453 -0.099580 0.109482 -0.557540 -0.717817 -0.806285 -1.171216 -0.593411 -0.795476
E (GFN2-E (GFN-I) COORDIN CO N CC CC CC H CC CC H H H H H H H H H CC H H H H H H CC H H H H H CC H H H H H H H CC H H H H H H H CC H H H H H H H H H H H H H H H H H H H H	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518  nates: -0.135033	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329 -3.766697 -4.483149 -4.354052 -3.202667 -3.840727 -4.657273 -3.350321 -4.302771 -2.186937 -2.948844 -1.502226 -1.592905 1.698521 1.807966 2.630319 1.620360 -0.743355 -0.518687 -0.947956 -1.670294 0.720678 1.003897 -0.163591	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112 2.486729 3.068471 1.847111 3.202346 0.760715 1.376458 0.230561 -0.002167 2.678096 3.313441 3.343865 2.174752 -2.541515 -3.091743 -1.971223 -3.291069 -2.545150 -3.120183 -3.270035 -1.965698 -0.635820 -1.188082 -0.016077	H H H H H C C C C H C H C H C H C H C H	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291 -3.971107 -4.678956 -3.982537 -4.694742 -4.269168 -4.273260 -3.349446 -5.434321 -5.422650 -6.610122 -7.523914 -6.614569 -7.529740 -5.454829 -5.460469  mation 20. licity: 4 : 0 3c) = -3413.53710 def2-TZVP) = -341 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233 4.233247 4.592638 2.883281 2.184780 0.181803 -1.209661 -1.682231 -1.963296 -3.044497 -1.342518 -1.935217 0.039623 0.530986 0.799839 1.881413	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935 1.744368 2.507192 1.365476 1.830251 -0.138137 0.102714 0.462453 -0.099580 0.109482 -0.557540 -0.717817 -0.806285 -1.171216 -0.593411 -0.795476
E (GFN2-E (GFN-I) E (GFN-I) COORDIN CO N C C C C H H H C H H H C H H H C H H H H H H H H H H H H H H H H H H H H	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518  nates: -0.135033 0.588906 1.528759 2.536625 1.893502 2.845146 3.861765 2.719056 4.018328 1.579016 2.194663 0.897053 0.957000 3.339372 3.768705 4.177696 2.680413 3.489727 3.987086 2.926655 4.276494 3.913203 4.869939 3.748863 3.105093 4.381760 5.303968 3.567736 4.554814 5.168732 6.088108 5.411148	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329 -3.766697 -4.483149 -4.354052 -3.202667 -3.840727 -4.657273 -3.350321 -4.302771 -2.186937 -2.948844 -1.502226 -1.592905 1.698521 1.807966 2.630319 1.620360 -0.743355 -0.518687 -0.947956 -1.670294 0.720678 1.003897 -0.163591 1.555098	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112 2.486729 3.068471 1.847111 3.202346 0.760715 1.376458 0.230561 -0.002167 2.678096 3.313441 3.343865 2.174752 -2.541515 -3.091743 -1.971223 -3.291069 -2.545150 -3.120183 -3.270035 -1.965698 -0.635820 -1.188082 -0.016077 0.048410	H H H H H H C C C C H C H C H C H C H C	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291 -3.971107 -4.678956 -3.982537 -4.694742 -4.269168 -4.273260 -3.349446 -5.434321 -5.422650 -6.610122 -7.523914 -6.614569 -7.529740 -5.454829 -5.454829 -5.460469  mation 20. licity: 4 : 0 3c) = -3413.53710 def2-TZVP) = -341 - D3(BJ)/def2-TZ - D3(BJ)/def2-TZ - D3(BJ)/def2-TZ-3c) = -3408.8718	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233 4.233247 4.592638 2.883281 2.184780 0.181803 -1.209661 -1.682231 -1.963296 -3.044497 -1.342518 -1.935217 0.039623 0.530986 0.799839 1.881413	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935 1.744368 2.507192 1.365476 1.830251 -0.138137 0.102714 0.462453 -0.099580 0.109482 -0.557540 -0.717817 -0.806285 -1.171216 -0.593411 -0.795476
E (GFN2-E (GFN-I)  COORDIN  CO  N  CC  CC  CC  H  H  H  H  H  H  CC  H  H	-xTB) = -148.5414 -xTB) = -147.3205 FF) = -20.5044518  nates: -0.135033	-3415.59789474214 13151347 Hartree 08912646 Hartree 94755 Hartree  0.030378 -1.427145 0.658613 -2.876839 -1.747278 -1.044804 -1.438206 0.067523 0.457329 -3.766697 -4.483149 -4.354052 -3.202667 -3.840727 -4.657273 -3.350321 -4.302771 -2.186937 -2.948844 -1.502226 -1.592905 1.698521 1.807966 2.630319 1.620360 -0.743355 -0.518687 -0.947956 -1.670294 0.720678 1.003897 -0.163591	-0.336980 0.766997 -1.025825 1.670887 0.789058 0.002896 0.074038 -0.861254 -1.636112 2.486729 3.068471 1.847111 3.202346 0.760715 1.376458 0.230561 -0.002167 2.678096 3.313441 3.343865 2.174752 -2.541515 -3.091743 -1.971223 -3.291069 -2.545150 -3.120183 -3.270035 -1.965698 -0.635820 -1.188082 -0.016077	H H H H H H C C C C H C H C H C H C H C	1.565106 0.458676 0.400275 2.987664 3.736366 3.531408 2.363195 -1.865150 -2.996932 -3.065739 -2.148878 -1.435010 -2.152949 -1.439089 -3.059695 -3.058291 -3.971107 -4.678956 -3.982537 -4.694742 -4.269168 -4.273260 -3.349446 -5.434321 -5.422650 -6.610122 -7.523914 -6.614569 -7.529740 -5.454829 -5.460469  mation 20. licity: 4 : 0 3c) = -3413.53710 def2-TZVP) = -341 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV	2.755085 2.015674 3.772277 4.369369 4.546598 4.256473 5.282232 0.354268 0.945529 2.401774 3.302895 2.931818 4.655305 5.344225 5.124722 6.186233 4.233247 4.592638 2.883281 2.184780 0.181803 -1.209661 -1.682231 -1.963296 -3.044497 -1.342518 -1.935217 0.039623 0.530986 0.799839 1.881413	1.242523 1.528369 0.637582 -0.161547 1.597171 0.726908 -0.066474 0.053072 0.404656 -0.176154 -0.925655 0.189303 -0.287166 1.154322 1.445935 1.744368 2.507192 1.365476 1.830251 -0.138137 0.102714 0.462453 -0.099580 0.109482 -0.557540 -0.717817 -0.806285 -1.171216 -0.593411 -0.795476

E (PM7)	= 113.04935 Kcal	/mol		Н	-2.408803	1.281427	-3.059369
		-3415.593775659198	Uartroo	Н	-0.987159	0.819017	-2.066742
			пагстее				
	,	63096653 Hartree		H	-0.738643	1.587286	-3.656174
E (GFN2-	xTB) = -147.3148	73545114 Hartree		C	-1.943771	4.047712	-3.036963
E (GFN-F	F) = -20.5021256	05986 Hartree		H	-1.939030	5.054227	-2.570722
,	•			Н	-2.986998	3.809115	-3.326314
0						4.104081	
Coordin				H	-1.354129		-3.975206
Co	0.253011	0.121641	0.146248	N	1.529363	-0.817697	-0.671093
N	-1.268137	-0.929560	0.802848	C	2.475184	-1.164911	-1.464857
N	-0.498980	1.854874	0.427515	С	2.583257	-0.585400	-2.842748
C	-3.580710	-1.203577	1.877144	Ċ	2.236210	0.764810	-3.062297
С	-2.366018	-0.360834	1.350113	H	1.952055	1.388954	-2.204047
C	-2.474818	1.043648	1.496874	C	2.264731	1.306785	-4.353233
H	-3.371210	1.377552	2.017197	H	2.006958	2.367002	-4.499172
С	-1.622590	2.107823	1.104780	С	2.624286	0.504466	-5.449234
		3.522817					-6.464803
С	-2.063337		1.599858	H	2.641606	0.928916	
С	-4.766794	-0.320806	2.324850	C	2.966120	-0.842263	-5.242528
H	-5.602621	-0.982563	2.628080	H	3.241988	-1.478673	-6.097487
H	-5.136365	0.331473	1.509114	С	2.956188	-1.382049	-3.948365
H	-4.521986	0.311832	3.200949	Н	3.219660	-2.438418	-3.788559
С	-4.121367	-2.134451	0.772672	С	3.477651	-2.184664	-1.022440
H	-5.038527	-2.640640	1.136870	C	3.075253	-3.190029	-0.116639
H	-3.394222	-2.918557	0.503331	H	2.023801	-3.222183	0.200180
Н	-4.386082	-1.567175	-0.141477	С	3.997010	-4.129971	0.357760
С	-3.171022	-2.055156	3.098888	H	3.661947	-4.916145	1.052412
H	-4.067939	-2.560799	3.512258	C	5.339822	-4.074849	-0.055482
H	-2.734703	-1.427423	3.901217	H	6.066100	-4.812427	0.319276
H	-2.441672	-2.838401	2.827969	С	5.750661	-3.075814	-0.953071
C				Н			
	-2.017505	3.491765	3.149010		6.801931	-3.023525	-1.275985
H	-2.314922	4.480260	3.556042	С	4.825973	-2.139906	-1.440242
H	-0.992490	3.267469	3.507378	H	5.151640	-1.355200	-2.139754
H	-2.695762	2.726463	3.572272				
C	-3.506987	3.823750	1.134201	Confor	mation 21.		
H	-3.812565	4.829400	1.488753		licity: 4		
H	-4.243628	3.094802	1.522520	Charge	: 0		
H	-3.578778	3.820162	0.027690	E(B97-	3c) = -3413.53579	4721675 Hartree	
С	-1.177651	4.696278	1.142152	E (M06/	def2-TZVP) = -341	3.221368215538 На	rt.ree
Н	-1.544620	5.620658	1.632912		- D3(BJ)/def2-TZV		
						•	
H	-1.214220	4.861131	0.050599		- D3(BJ)/def2-TZ		8426199 Hartree
H	-0.116899	4.568100	1.423894	E (PBEh	-3c) = -3408.8714	39088500 Hartree	
C	-0.950632	-2.317055	0.731702	E(PM6)	= 99.56668 Kcal/	mol	
C	-1.185574	-3.047514	-0.471992		= 107.19404 Kcal		
							0 11
С	-0.765572	-4.388774	-0.535241		X-V/def2-TZVP) =	-3415.5921084//20	U Hartree
H	-0.945214	-4.960755	-1.458204	E(GFN1	-xTB) = $-148.5339$	34476783 Hartree	
С	-0.945214 -0.124636		-1.458204 0.543639		-xTB) = $-148.5339-xTB$ ) = $-147.3113$		
C	-0.124636	-4.960755 -5.009059	0.543639	E(GFN2	-xTB) = $-147.3113$	44835929 Hartree	
C H	-0.124636 0.187082	-4.960755 -5.009059 -6.061969	0.543639 0.473195	E(GFN2		44835929 Hartree	
C H C	-0.124636 0.187082 0.141613	-4.960755 -5.009059 -6.061969 -4.269531	0.543639 0.473195 1.703114	E (GFN2 E (GFN-	-xTB) = $-147.3113FF) = -20.4934755$	44835929 Hartree	
C H C H	-0.124636 0.187082	-4.960755 -5.009059 -6.061969	0.543639 0.473195	E(GFN2	-xTB) = $-147.3113FF) = -20.4934755nates:$	44835929 Hartree 06248 Hartree	
C H C	-0.124636 0.187082 0.141613	-4.960755 -5.009059 -6.061969 -4.269531	0.543639 0.473195 1.703114	E (GFN2 E (GFN-	-xTB) = $-147.3113FF) = -20.4934755$	44835929 Hartree	0.430065
C H C H C	-0.124636 0.187082 0.141613 0.677571 -0.238230	-4.960755 -5.009059 -6.061969 -4.269531 -4.745887 -2.919985	0.543639 0.473195 1.703114 2.537846 1.814734	E (GFN2 E (GFN- Coordi Co	-xTB) = -147.3113 FF) = -20.4934755 nates: -0.063504	44835929 Hartree 06248 Hartree -0.442176	
C H C H C	-0.124636 0.187082 0.141613 0.677571 -0.238230 -1.835962	-4.960755 -5.009059 -6.061969 -4.269531 -4.745887 -2.919985 -2.404319	0.543639 0.473195 1.703114 2.537846 1.814734 -1.696029	E (GFN2 E (GFN- Coordi Co N	-xTB) = -147.3113 FF) = -20.4934755 nates: -0.063504 0.872075	44835929 Hartree 06248 Hartree -0.442176 -0.398027	-1.320972
C H C H C C	-0.124636 0.187082 0.141613 0.677571 -0.238230 -1.835962 -2.286389	-4.960755 -5.009059 -6.061969 -4.269531 -4.745887 -2.919985 -2.404319 -1.447318	0.543639 0.473195 1.703114 2.537846 1.814734 -1.696029 -1.361885	E (GFN2 E (GFN- Coordi Co N	-xTB) = -147.3113 FF) = -20.4934755 nates: -0.063504 0.872075 -1.825498	44835929 Hartree 06248 Hartree -0.442176 -0.398027 -0.841831	-1.320972 -0.236113
C H C H C C H	-0.124636 0.187082 0.141613 0.677571 -0.238230 -1.835962 -2.286389 -0.785134	-4.960755 -5.009059 -6.061969 -4.269531 -4.745887 -2.919985 -2.404319 -1.447318 -2.062087	0.543639 0.473195 1.703114 2.537846 1.814734 -1.696029 -1.361885 -2.767004	E (GFN2 E (GFN- Coordi Co N N C	-xTB) = -147.3113 FF) = -20.4934755 nates: -0.063504 0.872075 -1.825498 0.925921	44835929 Hartree 06248 Hartree -0.442176 -0.398027 -0.841831 -0.779436	-1.320972 -0.236113 -3.892851
C H C H C C	-0.124636 0.187082 0.141613 0.677571 -0.238230 -1.835962 -2.286389	-4.960755 -5.009059 -6.061969 -4.269531 -4.745887 -2.919985 -2.404319 -1.447318	0.543639 0.473195 1.703114 2.537846 1.814734 -1.696029 -1.361885	E (GFN2 E (GFN- Coordi Co N	-xTB) = -147.3113 FF) = -20.4934755 nates: -0.063504 0.872075 -1.825498	44835929 Hartree 06248 Hartree -0.442176 -0.398027 -0.841831 -0.779436 -0.707443	-1.320972 -0.236113
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С Н С Н С С Н С Н Н Н Н Н Н Н Н Н Н Н Н	-0.124636 0.187082 0.141613 0.677571 -0.238230 -1.835962 -2.286389 -0.785134 -0.027595 -1.266368 -0.253372	-4.960755 -5.009059 -6.061969 -4.269531 -4.745887 -2.919985 -2.404319 -1.447318 -2.062087 -1.360431 -1.597100 -2.974663	0.543639 0.473195 1.703114 2.537846 1.814734 -1.696029 -1.361885 -2.767004 -2.374972 -3.651940 -3.108149	E(GFN2 E(GFN- Coordi Co N N C C C C	-xTB) = -147.3113 FF) = -20.4934755 nates: -0.063504 0.872075 -1.825498 0.925921 0.251307 -1.127114 -1.488826	44835929 Hartree 06248 Hartree -0.442176 -0.398027 -0.841831 -0.779436 -0.707443 -1.052104 -1.310049	-1.320972 -0.236113 -3.892851 -2.471938 -2.510432 -3.507905
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СНСНССНННСННСНСНННСССС	-0.124636 0.187082 0.141613 0.677571 -0.238230 -1.835962 -2.286389 -0.785134 -0.027595 -1.266368 -0.253372 -2.946847 -3.700444 -2.532749 -3.470872 0.195856 -0.456164 1.641377 1.765997 2.360874 1.922201 0.061236 -0.958341 0.289775 0.774446 0.382821 1.726335 2.615123	-4.960755 -5.009059 -6.061969 -4.269531 -4.745887 -2.919985 -2.404319 -1.447318 -2.062087 -1.360431 -1.597100 -2.974663 -3.271729 -3.586456 -4.189197 -2.711336 -2.103829 -1.208641 -1.600230 -1.078180 -2.444825 -0.904253 -2.856035 -3.261678 -2.177911 -3.703537 2.711731 2.847690 3.641838	0.543639 0.473195 1.703114 2.537846 1.814734 -1.696029 -1.361885 -2.767004 -2.374972 -3.651940 -3.108149 -2.312213 -1.565009 -2.779019 -3.113333 3.032011 3.080084 2.849837 1.879567 2.853767 3.667825 4.363651 4.514771 5.211087 4.430162 -0.270783 0.193365 -0.553014	E(GFN2 E(GFN- Coordi Co N C C C C C C H H C C C H H H C H H H H	-xTB) = -147.3113 FF) = -20.4934755  nates:	44835929 Hartree 06248 Hartree 06248 Hartree  -0.442176 -0.398027 -0.841831 -0.7779436 -0.707443 -1.052104 -1.310049 -1.088898 -1.456684 -2.252828 -2.349205 -2.625137 -2.918624 0.126511 0.092348 1.180175 -0.178490 -0.355297 -0.445030 -0.993359 0.689560 -2.830293 -3.100319 -3.629158	-1.320972 -0.236113 -3.892851 -2.471938 -2.510432 -3.507905 -1.518809 -2.054362 -4.367878 -5.368935 -4.442445 -3.670815 -4.871290 -5.873766 -4.527264 -4.991638 -4.014322 -5.082008 -3.430471 -3.707011 -2.768292 -3.158956 -2.068823
СНСНССНСНННСНННСНННСН	-0.124636 0.187082 0.141613 0.677571 -0.238230 -1.835962 -2.286389 -0.785134 -0.027595 -1.266368 -0.253372 -2.946847 -3.700444 -2.532749 -3.470872 0.195856 -0.456164 1.641377 1.765997 2.360874 1.922201 0.061236 -0.958341 0.289775 0.774446 0.382821 1.726335	-4.960755 -5.009059 -6.061969 -4.269531 -4.745887 -2.919985 -2.404319 -1.447318 -2.062087 -1.360431 -1.597100 -2.97463 -3.271729 -3.586456 -4.189197 -2.711336 -2.103829 -1.208641 -1.600230 -1.078180 -2.444825 -0.904253 -2.856035 -3.261678 -2.177911 -3.703537 2.711731 2.847690	0.543639 0.473195 1.703114 2.537846 1.814734 -1.696029 -1.361885 -2.767004 -2.374972 -3.651940 -3.108149 -2.312213 -1.565009 -2.779019 -3.113333 3.032011 3.080084 2.849837 1.879567 2.853767 3.667825 4.363651 4.514771 5.211087 4.430162 -0.270783 0.193365	E(GFN2 E(GFN- Coordi Co N C C C C C C C H C C C H H C C H H H H	-xTB) = -147.3113 FF) = -20.4934755  nates:	44835929 Hartree 06248 Hartree  -0.442176 -0.398027 -0.841831 -0.779436 -0.707443 -1.052104 -1.310049 -1.088898 -1.456684 -2.252828 -2.349205 -2.625137 -2.918624 0.126511 0.092348 1.180175 -0.178490 -0.355297 -0.445030 -0.993359 0.689560 -2.830293 -3.100319	-1.320972 -0.236113 -3.892851 -2.471938 -2.510432 -3.507905 -1.518809 -2.054362 -4.367878 -5.368935 -4.442445 -3.670815 -4.871290 -5.873766 -4.527264 -4.991638 -4.014322 -5.082008 -3.430471 -3.707011 -2.768292 -3.158956
СНСНССНННСНННСНСНННСНННСС	-0.124636 0.187082 0.141613 0.677571 -0.238230 -1.835962 -2.286389 -0.785134 -0.027595 -1.266368 -0.253372 -2.946847 -3.700444 -2.532749 -3.470872 0.195856 -0.456164 1.641377 1.765997 2.360874 1.922201 0.061236 -0.958341 0.289775 0.774446 0.382821 1.726335 2.615123 3.649863	-4.960755 -5.009059 -6.061969 -4.269531 -4.745887 -2.919985 -2.404319 -1.447318 -2.062087 -1.360431 -1.597100 -2.974663 -3.271729 -3.586456 -4.189197 -2.711336 -2.103829 -1.208641 -1.600230 -1.078180 -2.444825 -0.904253 -2.856035 -3.261678 -2.177911 -3.703537 -2.711731 -2.847690 -3.641838 -3.766075	0.543639 0.473195 1.703114 2.537846 1.814734 -1.696029 -1.361885 -2.767004 -2.374972 -3.651940 -3.108149 -2.312213 -1.565009 -2.779019 -3.113333 3.032011 3.080084 2.849837 1.879567 2.853767 3.667825 4.363651 4.514771 5.211087 4.430162 -0.270783 0.193365 -0.553014 -0.200072	E(GFN2 E(GFN- Coordi Co N C C C C H C C C H H H C H H H C H H H H C H H H H H H H H H H H H H H H H H H H H	-xTB) = -147.3113 FF) = -20.4934755  nates:	44835929 Hartree 06248 Hartree 06248 Hartree  -0.442176 -0.398027 -0.841831 -0.779436 -0.707443 -1.052104 -1.310049 -1.088898 -1.456684 -2.252828 -2.349205 -2.625137 -2.918624 0.126511 0.092348 1.180175 -0.178490 -0.355297 -0.445030 -0.993359 0.689560 -2.830293 -3.100319 -3.629158 -2.832257	-1.320972 -0.236113 -3.892851 -2.471938 -2.510432 -3.507905 -1.518809 -2.054362 -4.367878 -5.368935 -4.442445 -3.670815 -4.871290 -5.873766 -4.527264 -4.991638 -4.014322 -5.082008 -3.430471 -3.707011 -2.768292 -3.158956 -2.068823 -3.622299
СНСНССННННСНННСНННСНННСССНС	-0.124636 0.187082 0.141613 0.677571 -0.238230 -1.835962 -2.286389 -0.785134 -0.027595 -1.266368 -0.253372 -2.946847 -3.700444 -2.532749 -3.470872 0.195856 -0.456164 1.641377 1.765997 2.360874 1.922201 0.061236 -0.958341 0.289775 0.774446 0.382821 1.726335 2.615123 3.649863 2.208638	-4.960755 -5.009059 -6.061969 -4.269531 -4.745887 -2.919985 -2.404319 -1.447318 -2.062087 -1.360431 -1.597100 -2.974663 -3.271729 -3.586456 -4.189197 -2.711336 -2.103829 -1.208641 -1.600230 -1.078180 -2.444825 -0.904253 -2.856035 -3.261678 -2.177911 -3.703537 -2.711731 -3.847690 -3.641838 -3.766075 -4.271730	0.543639 0.473195 1.703114 2.537846 1.814734 -1.696029 -1.361885 -2.767004 -2.374972 -3.651940 -3.108149 -2.312213 -1.565009 -2.779019 -3.113333 3.032011 3.080084 2.849837 1.879567 2.853767 2.853767 3.667825 4.363651 4.514771 5.211087 4.430162 -0.270783 0.193365 -0.553014 -0.200072 -1.735187	E(GFN2 E(GFN- Coordi CO N CC CC H CC H H CC H H H C H H H C H H H C H H H C H H H C H H H C H H H H H H H H H H H H H H H H H H H H	-xTB) = -147.3113 FF) = -20.4934755  nates:	44835929 Hartree 06248 Hartree 06248 Hartree  -0.442176 -0.398027 -0.841831 -0.779436 -0.707443 -1.052104 -1.310049 -1.088898 -1.456684 -2.252828 -2.349205 -2.625137 -2.918624 0.126511 0.092348 1.180175 -0.178490 -0.355297 -0.445030 -0.993359 0.689560 -2.830293 -3.100319 -3.629158 -2.832257 -0.386553	-1.320972 -0.236113 -3.892851 -2.471938 -2.510432 -3.507905 -1.518809 -2.054362 -4.367878 -5.368935 -4.442445 -3.670815 -4.871290 -5.873766 -4.527264 -4.991638 -4.014322 -5.082008 -3.430471 -3.707011 -2.768292 -3.158956 -2.068823 -3.622299 -3.080369
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СНСНССННННСНННСНННСНННССН	-0.124636 0.187082 0.141613 0.677571 -0.238230 -1.835962 -2.286389 -0.785134 -0.027595 -1.266368 -0.253372 -2.946847 -3.700444 -2.532749 -3.470872 0.195856 -0.456164 1.641377 1.765997 2.360874 1.922201 0.061236 -0.958341 0.289775 0.774446 0.382821 1.726335 2.615123 3.649863 2.208638 2.916601 0.902741	-4.960755 -5.009059 -6.061969 -4.269531 -4.745887 -2.919985 -2.404319 -1.447318 -2.062087 -1.360431 -1.597100 -2.974663 -3.271729 -3.586456 -4.189197 -2.711336 -2.103829 -1.208641 -1.600230 -1.078180 -2.444825 -0.904253 -2.856035 -3.261678 -2.177911 -3.703537 -7.11731 -3.847690 -3.641838 -7.66075 -4.271730 -4.895640 -4.895640 -4.079475	0.543639 0.473195 1.703114 2.537846 1.814734 -1.696029 -1.361885 -2.767004 -2.374972 -3.651940 -3.108149 -2.312213 -1.565009 -2.779019 -3.113333 3.032011 3.080084 2.849837 1.879567 2.853767 3.667825 4.363651 4.514771 5.211087 4.430162 -0.270783 0.193365 -0.553014 -0.200072 -1.735187 -2.300737 -2.213089	E(GFN2 E(GFN- Coordi Co N CC CC H CC CC H H CC H H H H H H H H	-xTB) = -147.3113 FF) = -20.4934755  nates:	44835929 Hartree 06248 Hartree 06248 Hartree  -0.442176 -0.398027 -0.841831 -0.779436 -0.707443 -1.052104 -1.310049 -1.088898 -1.456684 -2.252828 -2.349205 -2.625137 -2.918624 0.126511 0.092348 1.180175 -0.178490 -0.355297 -0.445030 -0.993359 0.689560 -2.830293 -3.100319 -3.629158 -2.832257 -0.386553 -0.642350 -0.312277	-1.320972 -0.236113 -3.892851 -2.471938 -2.510432 -3.507905 -1.518809 -2.054362 -4.367878 -5.368935 -4.442445 -3.670815 -4.871290 -5.873766 -4.527264 -4.991638 -4.014322 -5.082008 -3.430471 -3.707011 -2.768292 -3.158956 -2.068823 -3.622299 -3.080369 -3.474212 -3.940362
СНСНССНННСНННСНННСНННССССНСНСН	-0.124636 0.187082 0.141613 0.677571 -0.238230 -1.835962 -2.286389 -0.785134 -0.027595 -1.266368 -0.253372 -2.946847 -3.700444 -2.532749 -3.470872 0.195856 -0.456164 1.641377 1.765997 2.360874 1.922201 0.061236 -0.958341 0.289775 0.774446 0.382821 1.726335 2.615123 3.649863 2.208638 2.916601 0.902741 0.601735	-4.960755 -5.009059 -6.061969 -4.269531 -4.745887 -2.919985 -2.404319 -1.447318 -2.062087 -1.360431 -1.597100 -2.974663 -3.271729 -3.586456 -4.189197 -2.711336 -2.103829 -1.208641 -1.600230 -1.078180 -2.444825 -0.904253 -2.856035 -3.261678 -2.177911 -3.703537 -2.711731 -2.847690 3.641838 3.766075 4.271730 4.895640 4.079475 4.548562	0.543639 0.473195 1.703114 2.537846 1.814734 -1.696029 -1.361885 -2.767004 -2.374972 -3.651940 -3.108149 -2.312213 -1.565009 -2.779019 -3.113333 3.032011 3.080084 2.849837 1.879567 2.853767 3.667825 4.363651 4.514771 5.211087 4.430162 -0.270783 0.193365 -0.553014 -0.200072 -1.735187 -2.300737 -2.213089 -3.161000	E(GFN2 E(GFN- Coordi Co N C C C C C C H H C C H H H C H H H C H H H H C H H H H H H H H H H H H H H H H H H H H	-xTB) = -147.3113 FF) = -20.4934755  nates:	44835929 Hartree 06248 Hartree 06248 Hartree  -0.442176 -0.398027 -0.841831 -0.779436 -0.707443 -1.052104 -1.310049 -1.088898 -1.456684 -2.252828 -2.349205 -2.625137 -2.918624 0.126511 0.092348 1.180175 -0.178490 -0.355297 -0.445030 -0.993359 0.689560 -2.830293 -3.100319 -3.629158 -2.832257 -0.386553 -0.642350 -0.312277 0.616010	-1.320972 -0.236113 -3.892851 -2.471938 -2.510432 -3.507905 -1.518809 -2.054362 -4.367878 -5.368935 -4.442445 -3.670815 -4.871290 -5.873766 -4.527264 -4.991638 -4.014322 -5.082008 -3.430471 -3.707011 -2.768292 -3.158956 -2.068823 -3.622299 -3.080369 -3.474212 -3.940362 -2.613666
СНСНССННННСНННСНННСНННССН	-0.124636 0.187082 0.141613 0.677571 -0.238230 -1.835962 -2.286389 -0.785134 -0.027595 -1.266368 -0.253372 -2.946847 -3.700444 -2.532749 -3.470872 0.195856 -0.456164 1.641377 1.765997 2.360874 1.922201 0.061236 -0.958341 0.289775 0.774446 0.382821 1.726335 2.615123 3.649863 2.208638 2.916601 0.902741	-4.960755 -5.009059 -6.061969 -4.269531 -4.745887 -2.919985 -2.404319 -1.447318 -2.062087 -1.360431 -1.597100 -2.974663 -3.271729 -3.586456 -4.189197 -2.711336 -2.103829 -1.208641 -1.600230 -1.078180 -2.444825 -0.904253 -2.856035 -3.261678 -2.177911 -3.703537 -7.11731 -3.847690 -3.641838 -7.66075 -4.271730 -4.895640 -4.895640 -4.079475	0.543639 0.473195 1.703114 2.537846 1.814734 -1.696029 -1.361885 -2.767004 -2.374972 -3.651940 -3.108149 -2.312213 -1.565009 -2.779019 -3.113333 3.032011 3.080084 2.849837 1.879567 2.853767 3.667825 4.363651 4.514771 5.211087 4.430162 -0.270783 0.193365 -0.553014 -0.200072 -1.735187 -2.300737 -2.213089	E(GFN2 E(GFN- Coordi Co N CC CC H CC CC H H CC H H H H H H H H	-xTB) = -147.3113 FF) = -20.4934755  nates:	44835929 Hartree 06248 Hartree 06248 Hartree  -0.442176 -0.398027 -0.841831 -0.779436 -0.707443 -1.052104 -1.310049 -1.088898 -1.456684 -2.252828 -2.349205 -2.625137 -2.918624 0.126511 0.092348 1.180175 -0.178490 -0.355297 -0.445030 -0.993359 0.689560 -2.830293 -3.100319 -3.629158 -2.832257 -0.386553 -0.642350 -0.312277	-1.320972 -0.236113 -3.892851 -2.471938 -2.510432 -3.507905 -1.518809 -2.054362 -4.367878 -5.368935 -4.442445 -3.670815 -4.871290 -5.873766 -4.527264 -4.991638 -4.014322 -5.082008 -3.430471 -3.707011 -2.768292 -3.158956 -2.068823 -3.622299 -3.080369 -3.474212 -3.940362
СНСНССНКННСИННСИННСИНННССССИСНСИС	-0.124636 0.187082 0.141613 0.677571 -0.238230 -1.835962 -2.286389 -0.785134 -0.027595 -1.266368 -0.253372 -2.946847 -3.700444 -2.532749 -3.470872 0.195856 -0.456164 1.641377 1.765997 2.360874 1.922201 0.061236 -0.958341 0.289775 0.774446 0.382821 1.726335 2.615123 3.649863 2.208638 2.916601 0.902741 0.601735 -0.023232	-4.960755 -5.009059 -6.061969 -4.269531 -4.745887 -2.919985 -2.404319 -1.447318 -2.062087 -1.360431 -1.597100 -2.974663 -3.271729 -3.586456 -4.189197 -2.711336 -2.103829 -1.208641 -1.600230 -1.078180 -2.444825 -0.904253 -2.856035 -3.261678 -2.177911 -3.703537 -2.711731 -3.703537 -2.711731 -3.847690 -3.641838 -3.766075 -4.271730 -4.895640 -4.079475 -4.548562 -3.289236	0.543639 0.473195 1.703114 2.537846 1.814734 -1.696029 -1.361885 -2.767004 -2.374972 -3.651940 -3.108149 -2.312213 -1.565009 -2.779019 -3.113333 3.032011 3.080084 2.849837 1.879567 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.853767 2.85377 2.853777 2.853777 2.853777 2.853777 2.853777 2.85377	E(GFN2 E(GFN- Coordi CO N CC CC H CC H H CC H H H CH H H H C H H H C H H H C H H H C H H H C H H H H C H H H H H H H H H H H H H H H H H H H H	-xTB) = -147.3113 FF) = -20.4934755  nates:	44835929 Hartree 06248 Hartree 06248 Hartree  -0.442176 -0.398027 -0.841831 -0.779436 -0.707443 -1.052104 -1.310049 -1.088898 -1.456684 -2.252828 -2.349205 -2.625137 -2.918624 -0.126511 -0.092348 -1.180175 -0.178490 -0.355297 -0.445030 -0.993359 0.689560 -2.830293 -3.100319 -3.629158 -2.832257 -0.386553 -0.642350 -0.312277 -0.616010 -1.569129	-1.320972 -0.236113 -3.892851 -2.471938 -2.510432 -3.507905 -1.518809 -2.054362 -4.367878 -5.368935 -4.442445 -3.670815 -4.871290 -5.873766 -4.527264 -4.991638 -4.014322 -5.082008 -3.430471 -3.707011 -2.768292 -3.158956 -2.068823 -3.622299 -3.080369 -3.474212 -3.940362 -2.613666 -0.989358
СНСНССНСНННСНННСНСНННССННССС	-0.124636 0.187082 0.141613 0.677571 -0.238230 -1.835962 -2.286389 -0.785134 -0.027595 -1.266368 -0.253372 -2.946847 -3.700444 -2.532749 -3.470872 0.195856 -0.456164 1.641377 1.765997 2.360874 1.922201 0.061236 -0.958341 0.289775 0.774446 0.382821 1.726335 2.615123 3.649863 2.208638 2.916601 0.902741 0.601735 -0.023232 2.190886	-4.960755 -5.009059 -6.061969 -4.269531 -4.745887 -2.919985 -2.404319 -1.447318 -2.062087 -1.360431 -1.597100 -2.974663 -3.271729 -3.586456 -4.189197 -2.711336 -2.103829 -1.208641 -1.600230 -1.078180 -2.444825 -0.904253 -2.856035 -3.261678 -2.177911 -3.703537 2.711731 2.847690 3.641838 3.766075 4.271730 4.895640 4.079475 4.548562 3.289236 2.159916	0.543639 0.473195 1.703114 2.537846 1.814734 -1.696029 -1.361885 -2.767004 -2.374972 -3.651940 -3.108149 -2.312213 -1.565009 -2.779019 -3.113333 3.032011 3.080084 2.849837 1.879567 2.853767 3.667825 4.363651 4.514771 5.211087 4.430162 -0.270783 0.193365 -0.270783 0.193365 -0.553014 -0.200072 -1.735187 -2.300737 -2.213089 -3.161000 -1.514672 1.473472	E(GFN2 E(GFN- Coordi Co N CC CC H CC H H CC H H H C H H H H C H H H C H H H C H H H H H H H H H H H H H H H H H H H H	-xTB) = -147.3113 FF) = -20.4934755  nates:	44835929 Hartree 06248 Hartree 06248 Hartree  -0.442176 -0.398027 -0.841831 -0.779436 -0.707443 -1.052104 -1.310049 -1.088898 -1.456684 -2.252828 -2.349205 -2.625137 -2.918624 0.126511 0.092348 1.180175 -0.178490 -0.355297 -0.445030 -0.993359 0.689560 -2.830293 -3.100319 -3.629158 -2.832257 -0.386553 -0.642350 -0.312277 0.616010 -1.569129 -1.925608	-1.320972 -0.236113 -3.892851 -2.471938 -2.510432 -3.507905 -1.518809 -2.054362 -4.367878 -5.368935 -4.442445 -3.670815 -4.871290 -5.873766 -4.527264 -4.991638 -4.014322 -5.082008 -3.430471 -3.707011 -2.768292 -3.158956 -2.068823 -3.622299 -3.080369 -3.474212 -3.940362 -2.613666 -0.989358 -1.486087
СНСНССНСНННСНННСНСНННССНССНСНССС	-0.124636 0.187082 0.141613 0.677571 -0.238230 -1.835962 -2.286389 -0.785134 -0.027595 -1.266368 -0.253372 -2.946847 -3.700444 -2.532749 -3.470872 0.195856 -0.456164 1.641377 1.765997 2.360874 1.922201 0.061236 -0.958341 0.289775 0.774446 0.382821 1.726335 2.615123 3.649863 2.208638 2.916601 0.902741 0.601735 -0.023232 2.190886 1.425341	-4.960755 -5.009059 -6.061969 -4.269531 -4.745887 -2.919985 -2.404319 -1.447318 -2.062087 -1.360431 -1.597100 -2.97463 -3.271729 -3.586456 -4.189197 -2.711336 -2.103829 -1.208641 -1.600230 -1.078180 -2.444825 -0.904253 -2.856035 -3.261678 -2.177911 -3.703537 -2.71731 -3.847690 -3.641838 -3.766075 -4.271730 -4.895640 -4.079475 -4.548562 -3.289236 -2.159916 -1.382437	0.543639 0.473195 1.703114 2.537846 1.814734 -1.696029 -1.361885 -2.767004 -2.374972 -3.651940 -3.108149 -2.312213 -1.565009 -2.779019 -3.113333 3.032011 3.080084 2.849837 1.879567 2.853767 3.667825 4.363651 4.514771 5.211087 4.430162 -0.270783 0.193365 -0.553014 -0.20072 -1.735187 -2.300737 -2.213089 -3.161000 -1.514672 1.473472 1.473472 1.473472 1.473472 1.771776	E(GFN2 E(GFN- Coordi Co N CC CC H CC CC H H H H H H H H H H H H	-xTB) = -147.3113 FF) = -20.4934755  nates:	44835929 Hartree 06248 Hartree 0.398027 0.841831 0.7779436 0.707443 1.052104 1.310049 1.088898 1.456684 2.252828 2.349205 2.625137 2.918624 0.126511 0.092348 1.180175 0.178490 0.355297 0.445030 0.993359 0.689560 2.830293 3.100319 -3.629158 -2.832257 0.386553 0.642350 -0.312277 0.616010 -1.569129 -1.925608 -0.603432	-1.320972 -0.236113 -3.892851 -2.471938 -2.510432 -3.507905 -1.518809 -2.054362 -4.367878 -5.368935 -4.442445 -3.670815 -4.871290 -5.873766 -4.527264 -4.991638 -4.014322 -5.082008 -3.430471 -3.707011 -2.768292 -3.158956 -2.068823 -3.622299 -3.080369 -3.474212 -3.940362 -2.613666 -0.989358 -1.486087 -0.507335
СНСНССНСНННСНННСННННССССНСНСНССНС	-0.124636 0.187082 0.141613 0.677571 -0.238230 -1.835962 -2.286389 -0.785134 -0.027595 -1.266368 -0.253372 -2.946847 -3.700444 -2.532749 -3.470872 0.195856 -0.456164 1.641377 1.765997 2.360874 1.922201 0.061236 -0.958341 0.289775 0.774446 0.382821 1.726335 2.615123 3.649863 2.208638 2.916601 0.902741 0.601735 -0.023232 2.190886 1.425341 3.533220	-4.960755 -5.009059 -6.061969 -4.269531 -4.745887 -2.919985 -2.404319 -1.447318 -2.062087 -1.360431 -1.597100 -2.974663 -3.271729 -3.586456 -4.189197 -2.711336 -2.103829 -1.208641 -1.600230 -1.078180 -2.444825 -0.904253 -2.856035 -3.261678 -2.177911 -3.703537 2.711731 2.847690 3.641838 3.766075 4.271730 4.895640 4.079475 4.548562 3.289236 2.159916 1.382437 1.435289	0.543639 0.473195 1.703114 2.537846 1.814734 -1.696029 -1.361885 -2.767004 -2.374972 -3.651940 -3.108149 -2.312213 -1.5655009 -2.779019 -3.113333 3.032011 3.080084 2.849837 1.879567 2.853767 3.667825 4.363651 4.514771 5.211087 4.430162 -0.2707387 -0.2707387 -1.735187 -2.300737 -2.300737 -2.213089 -3.161000 -1.514672 1.473472 1.473472 1.471776 1.305170	E(GFN2 E(GFN- Coordi Co N CC CC H CC CC H H H CC H H H C H H H C H H H C H H H H C H H H H H H H H H H H H H H H H H H H H	-xTB) = -147.3113 FF) = -20.4934755  nates:	44835929 Hartree 06248 Hartree 06248 Hartree 06248 Hartree  -0.442176 -0.398027 -0.841831 -0.7779436 -0.707443 -1.052104 -1.310049 -1.088898 -1.456684 -2.252828 -2.349205 -2.625137 -2.918624 0.126511 0.092348 1.180175 -0.178490 -0.355297 -0.445030 -0.993359 0.689560 -2.830293 -3.100319 -3.629158 -2.832257 -0.386553 -0.642350 -0.312277 0.616010 -1.569129 -1.925608 -0.603432 -2.289286	-1.320972 -0.236113 -3.892851 -2.471938 -2.510432 -3.507905 -1.518809 -2.054362 -4.367878 -5.368935 -4.442445 -3.670815 -4.871290 -5.873766 -4.527264 -4.991638 -4.014322 -5.082008 -3.430471 -3.707011 -2.768292 -3.158956 -2.068823 -3.622299 -3.080369 -3.474212 -3.940362 -2.613666 -0.989358 -1.486087 -0.507335 -0.190849
СНСНССНСНННСНННСНСНННССНССНСНССС	-0.124636 0.187082 0.141613 0.677571 -0.238230 -1.835962 -2.286389 -0.785134 -0.027595 -1.266368 -0.253372 -2.946847 -3.700444 -2.532749 -3.470872 0.195856 -0.456164 1.641377 1.765997 2.360874 1.922201 0.061236 -0.958341 0.289775 0.774446 0.382821 1.726335 2.615123 3.649863 2.208638 2.916601 0.902741 0.601735 -0.023232 2.190886 1.425341	-4.960755 -5.009059 -6.061969 -4.269531 -4.745887 -2.919985 -2.404319 -1.447318 -2.062087 -1.360431 -1.597100 -2.97463 -3.271729 -3.586456 -4.189197 -2.711336 -2.103829 -1.208641 -1.600230 -1.078180 -2.444825 -0.904253 -2.856035 -3.261678 -2.177911 -3.703537 -2.71731 -3.847690 -3.641838 -3.766075 -4.271730 -4.895640 -4.079475 -4.548562 -3.289236 -2.159916 -1.382437	0.543639 0.473195 1.703114 2.537846 1.814734 -1.696029 -1.361885 -2.767004 -2.374972 -3.651940 -3.108149 -2.312213 -1.565009 -2.779019 -3.113333 3.032011 3.080084 2.849837 1.879567 2.853767 3.667825 4.363651 4.514771 5.211087 4.430162 -0.270783 0.193365 -0.553014 -0.20072 -1.735187 -2.300737 -2.213089 -3.161000 -1.514672 1.473472 1.473472 1.473472 1.473472 1.771776	E(GFN2 E(GFN- Coordi Co N CC CC H CC CC H H H H H H H H H H H H	-xTB) = -147.3113 FF) = -20.4934755  nates:	44835929 Hartree 06248 Hartree 0.398027 0.841831 0.7779436 0.707443 1.052104 1.310049 1.088898 1.456684 2.252828 2.349205 2.625137 2.918624 0.126511 0.092348 1.180175 0.178490 0.355297 0.445030 0.993359 0.689560 2.830293 3.100319 -3.629158 -2.832257 0.386553 0.642350 -0.312277 0.616010 -1.569129 -1.925608 -0.603432	-1.320972 -0.236113 -3.892851 -2.471938 -2.510432 -3.507905 -1.518809 -2.054362 -4.367878 -5.368935 -4.442445 -3.670815 -4.871290 -5.873766 -4.527264 -4.991638 -4.014322 -5.082008 -3.430471 -3.707011 -2.768292 -3.158956 -2.068823 -3.622299 -3.080369 -3.474212 -3.940362 -2.613666 -0.989358 -1.486087 -0.507335
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СНСНССНСНННСНННСНСНННСССНСНСНСНСННН	-0.124636 0.187082 0.141613 0.677571 -0.238230 -1.835962 -2.286389 -0.785134 -0.027595 -1.266368 -0.253372 -2.946847 -3.700444 -2.532749 -3.470872 0.195856 -0.456164 1.641377 1.765997 2.360874 1.922201 0.061236 -0.958341 0.289775 0.774446 0.382821 1.726335 2.615123 3.649863 2.208638 2.916601 0.902741 0.601735 -0.023232 2.190886 1.425341 3.533220 3.491583 3.787060 4.363221 2.219897 1.230182 2.948597	-4.960755 -5.009059 -6.061969 -4.269531 -4.745887 -2.919985 -2.404319 -1.447318 -2.062087 -1.360431 -1.597100 -2.974663 -3.271729 -3.586456 -4.189197 -2.711336 -2.103829 -1.208641 -1.600230 -1.078180 -2.444825 -0.904253 -2.856035 -3.261678 -2.177911 -3.703537 2.711731 2.847690 3.641838 3.766075 4.271730 4.895640 4.079475 4.548562 3.289236 2.159916 1.382437 1.435289 0.707795 0.877529 2.144395 3.132545 3.599034 3.950594	0.543639 0.473195 1.703114 2.537846 1.814734 -1.696029 -1.361885 -2.767004 -2.374972 -3.651940 -3.108149 -2.312213 -1.565009 -2.779019 -3.113333 3.032011 3.080084 2.849837 1.879567 2.853767 3.667825 4.363651 4.514771 5.211087 4.430162 -0.270783 0.193365 -0.553014 -0.270783 0.193365 -0.553014 -0.200772 -1.735187 -2.300737 -2.213089 -3.161000 -1.514672 1.473472 1.717176 1.305170 0.471337 2.229057 1.108847 2.664265 2.837668 2.837668	E(GFN2 E(GFN-Coordi Coordi COONNCCCHCCCHHCCHHHCCHHHCCHHHHCCHHHHCCHHHHCCHHHH	-xTB) = -147.3113 FF) = -20.4934755  nates:	44835929 Hartree 06248 Hartree 06248 Hartree  -0.442176 -0.398027 -0.841831 -0.779436 -0.707443 -1.052104 -1.310049 -1.088898 -1.456684 -2.252828 -2.349205 -2.625137 -2.918624 0.126511 0.092348 1.180175 -0.178490 -0.355297 -0.445030 -0.993359 0.689560 -2.830293 -3.100319 -3.629158 -2.832257 -0.386553 -0.642350 -0.312277 0.616010 -1.569129 -1.925608 -0.603432 -2.289286 0.002874 1.387077 1.754828 2.821738 0.795751 1.105568	-1.320972 -0.236113 -3.892851 -2.471938 -2.510432 -3.507905 -1.518809 -2.054362 -4.367878 -5.368935 -4.44245 -3.670815 -4.871290 -5.873766 -4.527264 -4.991638 -4.014322 -5.082008 -3.430471 -3.707011 -2.768292 -3.158956 -2.068823 -3.622299 -3.080369 -3.474212 -3.940362 -2.613666 -0.989358 -1.486087 -0.507335 -0.190849 -1.196519 -1.224579 -1.113976 -1.151757 -0.988177 -0.9885873
СНСНССНСНННСНННСННННССНСНСНСНСНСНСНСН	-0.124636 0.187082 0.141613 0.677571 -0.238230 -1.835962 -2.286389 -0.785134 -0.027595 -1.266368 -0.253372 -2.946847 -3.700444 -2.532749 -3.470872 0.195856 -0.456164 1.641377 1.765997 2.360874 1.922201 0.061236 -0.958341 0.289775 0.774446 0.382821 1.726335 2.615123 3.649863 2.208638 2.916601 0.902741 0.601735 -0.023232 2.190886 1.425341 3.533220 3.491583 3.787060 4.363221 2.219887 1.230182 2.948597 2.518638	-4.960755 -5.009059 -6.061969 -4.269531 -4.745887 -2.919985 -2.404319 -1.447318 -2.062087 -1.360431 -1.597100 -2.974663 -3.271729 -3.586456 -4.189197 -2.711336 -2.103829 -1.208641 -1.600230 -1.078180 -2.444825 -0.904253 -2.856035 -3.261678 -2.177911 -3.703537 2.711731 2.847690 3.641838 3.766075 4.271730 4.895640 4.079475 4.548562 3.289236 2.159916 1.382437 1.435289 0.707795 0.877529 2.144395 3.132545 3.599034 3.950594 2.607487	0.543639 0.473195 1.703114 2.537846 1.814734 -1.696029 -1.361885 -2.767004 -2.374972 -3.651940 -3.108149 -2.312213 -1.565009 -2.779019 -3.113333 3.032011 3.080084 2.849837 1.879567 2.853767 3.667825 4.363651 4.514771 5.211087 4.430162 -0.270783 0.193365 -0.553014 -0.270783 0.193365 -0.553014 -0.270783 0.193365 -0.553014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 0.193365 -0.573014 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.270783 -0.2707	E(GFN2 E(GFN-di COONNCCCHCCHHHCHHHCHHHCHHHCCHHHCCHCHCHCCHCC	-xTB) = -147.3113 FF) = -20.4934755  nates:	44835929 Hartree 06248 Hartree 06248 Hartree  -0.442176 -0.398027 -0.841831 -0.779436 -0.707443 -1.052104 -1.310049 -1.088898 -1.456684 -2.252828 -2.349205 -2.625137 -2.918624 0.126511 0.092348 1.180175 -0.178490 -0.355297 -0.445030 -0.993359 0.689560 -2.830293 -3.100319 -3.629158 -2.832257 -0.386553 -0.642350 -0.312277 0.616010 -1.569129 -1.925608 -0.603432 -2.289286 0.002874 1.387077 1.754828 2.821738 0.795751 1.105568 -0.557582	-1.320972 -0.236113 -3.892851 -2.471938 -2.510432 -3.507905 -1.518809 -2.054362 -4.367878 -5.368935 -4.442445 -3.670815 -4.871290 -5.873766 -4.527264 -4.991638 -4.014322 -5.082008 -3.430471 -3.707011 -2.768292 -3.158956 -2.068823 -3.622299 -3.080369 -3.474212 -3.940362 -2.613666 -0.989358 -1.486087 -0.507335 -0.190849 -1.196519 -1.224579 -1.113976 -1.151757 -0.958177 -0.985873 -0.856161
СНСНССНСНННСНННСНСННННССССНСНССНСНННС	-0.124636 0.187082 0.141613 0.677571 -0.238230 -1.835962 -2.286389 -0.785134 -0.027595 -1.266368 -0.253372 -2.946847 -3.700444 -2.532749 -3.470872 0.195856 -0.456164 1.641377 1.765997 2.360874 1.922201 0.061236 -0.958341 0.289775 0.774446 0.382821 1.726335 2.615123 3.649863 2.208638 2.916601 0.902741 0.601735 -0.023232 2.190886 1.425341 3.533220 3.491583 3.787060 4.363221 2.219897 1.230182 2.948597 2.518638 -1.401735	-4.960755 -5.009059 -6.061969 -4.269531 -4.745887 -2.919985 -2.404319 -1.447318 -2.062087 -1.360431 -1.597100 -2.974663 -3.271729 -3.586456 -4.189197 -2.711336 -2.103829 -1.208641 -1.600230 -1.078180 -2.444825 -0.904253 -2.856035 -3.261678 -2.177911 -3.703537 2.711731 2.847690 3.641838 3.766075 4.271730 4.895640 4.079475 4.548562 3.289236 2.159916 1.382437 1.435289 0.707795 0.877529 2.144395 3.132545 3.599034 3.950594 2.607487 2.976037	0.543639 0.473195 1.703114 2.537846 1.814734 -1.696029 -1.361885 -2.767004 -2.374972 -3.651940 -3.108149 -2.312213 -1.565009 -2.779019 -3.113333 3.032011 3.080084 2.849837 1.879567 2.853767 3.667825 4.363651 4.514771 5.211087 4.430162 -0.270783 0.193365 -0.553014 -0.20072 -1.735187 -2.300737 -2.213089 -3.161000 -1.514672 1.473472 1.473472 1.473472 1.717176 1.305170 0.471337 2.229057 1.108847 2.664265 2.837668 2.485343 3.594724 -2.085651	E(GFN2 E(GFN-COON CCCHCCCHHHHCHHHCHHHCHHHCCHHHCCHHHCC	-xTB) = -147.3113 FF) = -20.4934755  nates:	44835929 Hartree 06248 Hartree 06248 Hartree  -0.442176 -0.398027 -0.841831 -0.7779436 -0.707443 -1.052104 -1.310049 -1.088898 -1.456684 -2.252828 -2.349205 -2.625137 -2.918624 0.126511 0.092348 1.180175 -0.178490 -0.355297 -0.445030 -0.993359 0.689560 -2.830293 -3.100319 -3.629158 -2.832257 -0.386553 -0.642350 -0.312277 0.616010 -1.569129 -1.925608 -0.603432 -2.289286 0.002874 1.387077 1.754828 2.821738 0.795751 1.105568 -0.557582 -1.309703	-1.320972 -0.236113 -3.892851 -2.471938 -2.510432 -3.507905 -1.518809 -2.054362 -4.367878 -5.368935 -4.442445 -3.670815 -4.871290 -5.873766 -4.527264 -4.991638 -4.014322 -5.082008 -3.430471 -3.707011 -2.768292 -3.158956 -2.068823 -3.622299 -3.080369 -3.474212 -3.940362 -2.613666 -0.989358 -1.486087 -0.507335 -0.190849 -1.196519 -1.224579 -1.113976 -1.151757 -0.958177 -0.885873 -0.856161 -0.687964
СНСНССНСНННСНННСНКННССССНСНСНСНСНННС	-0.124636 0.187082 0.141613 0.677571 -0.238230 -1.835962 -2.286389 -0.785134 -0.027595 -1.266368 -0.253372 -2.946847 -3.700444 -2.532749 -3.470872 0.195856 -0.456164 1.641377 1.765997 2.360874 1.922201 0.061236 -0.958341 0.289775 0.774446 0.382821 1.726335 2.615123 3.649863 2.208638 2.916601 0.902741 0.601735 -0.023232 2.190886 1.425341 3.533220 3.491583 3.787060 4.363221 2.219897 1.230182 2.948597 2.518638 -1.401735 -2.107175	-4.960755 -5.009059 -6.061969 -4.269531 -4.745887 -2.919985 -2.404319 -1.447318 -2.062087 -1.360431 -1.597100 -2.974663 -3.271729 -3.586456 -4.189197 -2.711336 -2.103829 -1.208641 -1.600230 -1.078180 -2.444825 -0.904253 -2.856035 -3.261678 -2.177911 -3.703537 -2.171731 -2.847690 -3.641838 -3.766075 -4.271730 -4.895640 -4.079475 -4.548562 -3.289236 -2.159916 -3.382437 -4.435289 -0.707795 -0.877529 -2.144395 -3.132545 -3.599034 -3.908513	0.543639 0.473195 1.703114 2.537846 1.814734 -1.696029 -1.361885 -2.767004 -2.374972 -3.651940 -3.108149 -2.312213 -1.565009 -2.779019 -3.113333 3.032011 3.080084 2.849837 1.879567 2.853767 2.853767 2.853767 2.6647825 4.363651 4.514771 5.211087 4.430162 -0.270783 0.193365 -0.553014 -0.200072 -1.735187 -2.300737 -2.213089 -3.161000 -1.514672 1.473472 1.717176 1.305170 0.471337 2.229057 1.108847 2.664265 2.837668 2.485343 3.594724 -2.085651 -1.232474	E(GFN2GFN-GFN-GFN-GFN-GFN-GFN-GFN-GFN-GFN-GFN-	-xTB) = -147.3113 FF) = -20.4934755  nates:	44835929 Hartree 06248 Hartree  -0.442176 -0.398027 -0.841831 -0.779436 -0.707443 -1.052104 -1.310049 -1.088898 -1.456684 -2.252828 -2.349205 -2.625137 -2.918624 -0.126511 -0.992348 -1.180175 -0.178490 -0.355297 -0.445030 -0.993359 0.689560 -2.830293 -3.100319 -3.629158 -2.832257 -0.386553 -0.642350 -0.312277 0.616010 -1.569129 -1.925608 -0.603432 -2.289286 0.002874 1.387077 1.754828 2.821738 0.795751 1.105568 -0.557582 -1.309703 -0.974991	-1.320972 -0.236113 -3.892851 -2.471938 -2.510432 -3.507905 -1.518809 -2.054362 -4.367878 -5.368935 -4.442445 -3.670815 -4.871290 -5.873766 -4.527264 -4.991638 -4.014322 -5.082008 -3.430471 -3.707011 -2.768292 -3.158956 -2.068823 -3.622299 -3.080369 -3.474212 -3.940362 -2.613666 -0.989358 -1.486087 -0.507335 -0.190849 -1.196519 -1.224579 -1.113976 -1.151757 -0.958177 -0.885873 -0.856161 -0.687964 -0.953100
СНСНССНСНННСНННСНСННННССССНСНССНСНННС	-0.124636 0.187082 0.141613 0.677571 -0.238230 -1.835962 -2.286389 -0.785134 -0.027595 -1.266368 -0.253372 -2.946847 -3.700444 -2.532749 -3.470872 0.195856 -0.456164 1.641377 1.765997 2.360874 1.922201 0.061236 -0.958341 0.289775 0.774446 0.382821 1.726335 2.615123 3.649863 2.208638 2.916601 0.902741 0.601735 -0.023232 2.190886 1.425341 3.533220 3.491583 3.787060 4.363221 2.219897 1.230182 2.948597 2.518638 -1.401735	-4.960755 -5.009059 -6.061969 -4.269531 -4.745887 -2.919985 -2.404319 -1.447318 -2.062087 -1.360431 -1.597100 -2.974663 -3.271729 -3.586456 -4.189197 -2.711336 -2.103829 -1.208641 -1.600230 -1.078180 -2.444825 -0.904253 -2.856035 -3.261678 -2.177911 -3.703537 2.711731 2.847690 3.641838 3.766075 4.271730 4.895640 4.079475 4.548562 3.289236 2.159916 1.382437 1.435289 0.707795 0.877529 2.144395 3.132545 3.599034 3.950594 2.607487 2.976037	0.543639 0.473195 1.703114 2.537846 1.814734 -1.696029 -1.361885 -2.767004 -2.374972 -3.651940 -3.108149 -2.312213 -1.565009 -2.779019 -3.113333 3.032011 3.080084 2.849837 1.879567 2.853767 3.667825 4.363651 4.514771 5.211087 4.430162 -0.270783 0.193365 -0.553014 -0.20072 -1.735187 -2.300737 -2.213089 -3.161000 -1.514672 1.473472 1.473472 1.473472 1.717176 1.305170 0.471337 2.229057 1.108847 2.664265 2.837668 2.485343 3.594724 -2.085651	E(GFN2 E(GFN-COON CCCHCCCHHHHCHHHCHHHCHHHCCHHHCCHHHCC	-xTB) = -147.3113 FF) = -20.4934755  nates:	44835929 Hartree 06248 Hartree 06248 Hartree  -0.442176 -0.398027 -0.841831 -0.7779436 -0.707443 -1.052104 -1.310049 -1.088898 -1.456684 -2.252828 -2.349205 -2.625137 -2.918624 0.126511 0.092348 1.180175 -0.178490 -0.355297 -0.445030 -0.993359 0.689560 -2.830293 -3.100319 -3.629158 -2.832257 -0.386553 -0.642350 -0.312277 0.616010 -1.569129 -1.925608 -0.603432 -2.289286 0.002874 1.387077 1.754828 2.821738 0.795751 1.105568 -0.557582 -1.309703	-1.320972 -0.236113 -3.892851 -2.471938 -2.510432 -3.507905 -1.518809 -2.054362 -4.367878 -5.368935 -4.442445 -3.670815 -4.871290 -5.873766 -4.527264 -4.991638 -4.014322 -5.082008 -3.430471 -3.707011 -2.768292 -3.158956 -2.068823 -3.622299 -3.080369 -3.474212 -3.940362 -2.613666 -0.989358 -1.486087 -0.507335 -0.190849 -1.196519 -1.224579 -1.113976 -1.151757 -0.958177 -0.885873 -0.856161 -0.687964

7.7	0.510693	1.951461	-1.389307	NT	1.588373	-0.130306	-0.977502
H				N			
С	1.491377	3.413728	-0.157450	С	-1.340369	-3.660095	-1.175660
H	1.329572	2.856563	0.783237	C	-0.629804	-2.258548	-1.098287
H	0.683932	4.168350	-0.250631	C	0.700031	-2.271449	-1.606204
H	2.452450	3.961894	-0.070471	H	0.970918	-3.202185	-2.107764
С	1.635820	3.260325	-2.677852	С	1.741778	-1.316941	-1.592437
Н	1.597568	2.603241	-3.568905	C	2.994293	-1.708320	-2.441373
H	2.599217	3.810739	-2.711085	С	-2.855688	-3.667729	-0.898945
H	0.821245	4.007837	-2.771725	H	-3.221392	-4.709991	-0.999778
C	2.877229	-2.441587	-0.747007	H	-3.416661	-3.040999	-1.615182
H	1.811012	-2.559182	-1.031511	H	-3.111439	-3.320703	0.114571
С	3.009019	-2.800029	0.745079	С	-1.150317	-4.329366	-2.560380
Н	2.428847	-2.094373	1.371206	Н	-1.689212	-5.298374	-2.564365
H	4.067567	-2.738583	1.072507	Н	-0.093443	-4.551844	-2.800837
H	2.651221	-3.832262	0.941091	H	-1.567085	-3.711434	-3.378262
C	3.699674	-3.398970	-1.623008	C	-0.645475	-4.552942	-0.116212
H	3.616040	-3.147504	-2.699457	H	-1.119705	-5.556277	-0.095332
H	3.353439	-4.444286	-1.488343	H	-0.727683	-4.114501	0.896810
Н	4.776534	-3.373962	-1.356675	Н	0.431969	-4.682149	-0.337802
	-2.667336	-0.649497	0.884605		2.517105	-1.784229	-3.915079
C				C			
С	-3.374942	0.585591	1.030532	H	3.367190	-2.054698	-4.575355
C	-4.179825	0.770718	2.164491	H	2.124616	-0.801905	-4.248888
H	-4.741908	1.709630	2.275490	H	1.715260	-2.533738	-4.058217
C	-4.267188	-0.208228	3.164285	С	3.541171	-3.085883	-2.003426
Н	-4.905717	-0.047503	4.045909	H	4.440991	-3.339981	-2.600609
C	-3.514527	-1.383151	3.044446	Н	2.808621	-3.903185	-2.146852
Н							
	-3.555570	-2.142920	3.841369	Н	3.833435	-3.077381	-0.935603
С	-2.701588	-1.630837	1.922071	С	4.163734	-0.708170	-2.407992
C	-3.195866	1.698269	0.004683	H	4.942375	-1.060705	-3.114769
H	-2.912894	1.220199	-0.953676	H	4.630705	-0.619022	-1.411820
С	-4.466095	2.518520	-0.250010	H	3.860310	0.305673	-2.724922
Н	-5.326850	1.872360	-0.518215	С	-2.507503	-0.898884	-0.214623
Н	-4.301128	3.231545	-1.083077	C	-3.351022	-0.343620	-1.231321
H	-4.757107	3.119848	0.635905	С	-4.701500	-0.094210	-0.929416
С	-2.015465	2.600921	0.408166	H	-5.351835	0.309024	-1.722468
H	-1.103161	1.999361	0.598692	C	-5.218469	-0.308832	0.353697
H	-2.231970	3.159436	1.341501	H	-6.274655	-0.096462	0.575765
H	-1.785241	3.331404	-0.394202	С	-4.351340	-0.732095	1.362418
C	-1.910808	-2.938968	1.883723	Н	-4.730021	-0.831710	2.392383
Н	-2.092612	-3.408790	2.874534	C	-2.992741	-1.026011	1.120686
C	-0.389079	-2.755174	1.781732	С	-2.870729	0.070987	-2.626576
H	0.139928	-3.708381	1.987858	H	-3.738427	0.616832	-3.055920
H	-0.001533	-2.003041	2.496205	C	-1.715174	1.084395	-2.606173
H	-0.069976	-2.487707	0.740530	H	-1.883308	1.884546	-1.860174
С	-2.405669	-3.934592	0.822304	H	-1.587949	1.558538	-3.601403
Н	-3.493880	-4.121552	0.913328	H	-0.744341	0.578012	-2.391149
Н	-1.882862	-4.906918	0.932519	C	-2.566281	-1.079003	-3.598451
H	-2.200752	-3.559094	-0.198734	Н	-3.392908	-1.816149	-3.631744
N	0.963398	0.318806	1.684879	H	-1.634026	-1.607370	-3.321602
C	1.299950	1.015162	2.707392	H	-2.426288	-0.681519	-4.625179
C	2.683802	0.921285	3.271110	С	-2.206069	-1.467667	2.365141
С	3.740403	0.504254	2.433004	H	-2.544933	-0.753498	3.149427
Н	3.520155	0.293007	1.378838	C	-0.678489	-1.361991	2.353825
C	5.040210	0.376356	2.933585	Н	-0.344409	-0.351518	2.049042
						-2.099554	
H	5.851486	0.064130	2.257522	H	-0.195251		1.685321
С	5.308400	0.654658	4.285477	H	-0.296769	-1.542326	3.379197
H	6.331033	0.554512	4.680708	C	-2.641978	-2.867552	2.846859
С	4.263875	1.066251	5.129431	H	-3.742888	-2.948506	2.941240
H	4.464443	1.281275	6.190454	H	-2.194924	-3.091172	3.837305
С	2.961288	1.204362	4.627064	H	-2.309777	-3.658525	2.146067
Н	2.146233	1.523788	5.293656	C	2.579195	0.780785	-0.523922
				_		0.700703	
C C		1 060000		C		0 447005	
(;	0.332226	1.962802	3.357386	С	3.401628	0.447805	0.597720
	0.711760	3.293065	3.644309	С	3.401628 4.301162	1.413905	0.597720 1.080545
H	0.711760 1.740060	3.293065 3.619087	3.644309 3.425659	C H	3.401628 4.301162 4.942712	1.413905 1.160514	0.597720 1.080545 1.938892
H C	0.711760 1.740060 -0.212444	3.293065 3.619087 4.196799	3.644309 3.425659 4.186614	C H C	3.401628 4.301162 4.942712 4.388479	1.413905 1.160514 2.690337	0.597720 1.080545 1.938892 0.510545
H C H	0.711760 1.740060 -0.212444 0.092068	3.293065 3.619087 4.196799 5.235448	3.644309 3.425659 4.186614 4.388131	C H C H	3.401628 4.301162 4.942712 4.388479 5.096225	1.413905 1.160514 2.690337 3.431428	0.597720 1.080545 1.938892 0.510545 0.911410
H C	0.711760 1.740060 -0.212444 0.092068 -1.520715	3.293065 3.619087 4.196799	3.644309 3.425659 4.186614	C H C	3.401628 4.301162 4.942712 4.388479	1.413905 1.160514 2.690337	0.597720 1.080545 1.938892 0.510545 0.911410
H C H	0.711760 1.740060 -0.212444 0.092068	3.293065 3.619087 4.196799 5.235448	3.644309 3.425659 4.186614 4.388131	C H C H	3.401628 4.301162 4.942712 4.388479 5.096225	1.413905 1.160514 2.690337 3.431428	0.597720 1.080545 1.938892 0.510545 0.911410
H C H C H	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595	C H C H C	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454
Н С Н С Н	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448 -1.901575	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192 2.452112	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595 4.208659	C H C H C H	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745 2.656704	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857 2.082016	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454 -1.107045
H C H C H C	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448 -1.901575 -2.921569	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192 2.452112 2.109498	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595 4.208659 4.435812	C H C H C H C	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745 2.656704 3.301768	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857 2.082016 -0.895303	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454 -1.107045 1.314405
H C H C H C H	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448 -1.901575 -2.921569 -0.987854	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192 2.452112 2.109498 1.555282	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595 4.208659 4.435812 3.637385	C H C H C H C H	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745 2.656704 3.301768 2.595041	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857 2.082016 -0.895303 -1.531088	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454 -1.107045 1.314405 0.744274
H C H C H C	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448 -1.901575 -2.921569	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192 2.452112 2.109498	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595 4.208659 4.435812	С Н С Н С Н С Н С Н	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745 2.656704 3.301768 2.595041 4.652060	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857 2.082016 -0.895303 -1.531088 -1.630006	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454 -1.107045 1.314405 0.744274 1.379385
H C H C H C H C	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448 -1.901575 -2.921569 -0.987854 -1.297769	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192 2.452112 2.109498 1.555282	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595 4.208659 4.435812 3.637385	С Н С Н С Н С Н С Н	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745 2.656704 3.301768 2.595041 4.652060 5.110603	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857 2.082016 -0.895303 -1.531088 -1.630006 -1.751187	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454 -1.107045 1.314405 0.744274 1.379385 0.378354
H C H C H C H C	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448 -1.901575 -2.921569 -0.987854	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192 2.452112 2.109498 1.555282	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595 4.208659 4.435812 3.637385	С Н С Н С Н С Н С Н	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745 2.656704 3.301768 2.595041 4.652060	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857 2.082016 -0.895303 -1.531088 -1.630006	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454 -1.107045 1.314405 0.744274 1.379385
H C H C H C H C H C H C H C	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448 -1.901575 -2.921569 -0.987854 -1.297769	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192 2.452112 2.109498 1.555282	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595 4.208659 4.435812 3.637385	С Н С Н С Н С Н С Н	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745 2.656704 3.301768 2.595041 4.652060 5.110603	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857 2.082016 -0.895303 -1.531088 -1.630006 -1.751187	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454 -1.107045 1.314405 0.744274 1.379385 0.378354
H C H C H C H C H C H C M H C M H C H M H C H H C H H C H H C H H H C H H H H	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448 -1.901575 -2.921569 -0.987854 -1.297769 mation 24.	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192 2.452112 2.109498 1.555282	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595 4.208659 4.435812 3.637385	С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745 2.656704 3.301768 2.595041 4.652060 5.110603 4.524913 5.379369	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857 2.082016 -0.895303 -1.531088 -1.630006 -1.751187 -2.639361 -1.082541	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454 -1.107045 1.314405 0.744274 1.379385 0.378354 1.821770 2.013918
H C H C H C H C H C H C H C H C H Conform	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448 -1.901575 -2.921569 -0.987854 -1.297769 mation 24. Licity: 4	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192 2.452112 2.109498 1.555282 0.524995	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595 4.208659 4.435812 3.637385	С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745 2.656704 3.301768 2.595041 4.652060 5.110603 4.524913 5.379369 2.723112	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857 2.082016 -0.895303 -1.531088 -1.630006 -1.751187 -2.639361 -1.082541 -0.716587	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454 -1.107045 1.314405 0.744274 1.379385 0.378354 1.821770 2.013918 2.728993
H C H C H C H Conform Multipl Charge: E(B97-3	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448 -1.901575 -2.921569 -0.987854 -1.297769 mation 24. Licity: 4 : 0 3c) = -3413.52221	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192 2.452112 2.109498 1.555282 0.524995	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595 4.208659 4.435812 3.637385 3.405889	С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н Н С Н Н Н Н Н Н Н Н Н Н Н Н Н	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745 2.656704 3.301768 2.595041 4.652060 5.110603 4.524913 5.379369 2.723112 1.775690	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857 2.082016 -0.895303 -1.531088 -1.630006 -1.751187 -2.639361 -1.082541 -0.716587 -0.148139	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454 -1.107045 1.314405 0.744274 1.379385 0.378354 1.821770 2.013918 2.728993 2.712223
H C H C H C H Conform Multipl Charge: E (B97-6	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448 -1.901575 -2.921569 -0.987854 -1.297769 mation 24. licity: 4 : 0 3c) = -3413.52221 def2-TZVP) = -341	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192 2.452112 2.109498 1.555282 0.524995	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595 4.208659 4.435812 3.637385 3.405889	С Н С Н С С Н С Н С Н С Н С Н С Н Н С Н Н С Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745 2.656704 3.301768 2.595041 4.652060 5.110603 4.524913 5.379369 2.723112 1.775690 3.425899	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857 2.082016 -0.895303 -1.531088 -1.630006 -1.751187 -2.639361 -1.082541 -0.716587 -0.148139 -0.158458	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454 -1.107045 1.314405 0.744274 1.379385 0.378354 1.821770 2.013918 2.728993 2.712223 3.381490
H C H C H C H Conform Multipl Charge: E (B97-3 E (M06/6 E (PBE -	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448 -1.901575 -2.921569 -0.987854 -1.297769 mation 24. licity: 4 : 0 3c) = -3413.52221 def2-TZVP) = -341 -D3(BU)/def2-TZV	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192 2.452112 2.109498 1.555282 0.524995 3598330 Hartree 3.209283793482 Hai	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595 4.208659 4.435812 3.637385 3.405889	С Н С Н С С Н С Н Н Н Н Н Н Н Н Н Н Н Н Н	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745 2.656704 3.301768 2.595041 4.652060 5.110603 4.524913 5.379369 2.723112 1.775690 3.425899 2.530962	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857 2.082016 -0.895303 -1.531088 -1.630006 -1.751187 -2.639361 -1.082541 -0.716587 -0.148139 -0.158458 -1.701847	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454 -1.107045 0.744274 1.379385 0.378354 1.821770 2.013918 2.728993 2.712223 3.381490 3.201181
H C H C H C H Conform Multipl Charge: E (B97-3 E (M06/c E (PBE - E (PBE0	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448 -1.901575 -2.921569 -0.987854 -1.297769 mation 24. licity: 4 : 0 3c) = -3413.52221 def2-TZVP) = -341 - D3(BJ)/def2-TZV	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192 2.452112 2.109498 1.555282 0.524995 33598330 Hartree 3.209283793482 Ham P) = -3412.0846063 VP) = -3412.298503	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595 4.208659 4.435812 3.637385 3.405889	С Н С Н С Н С Н Н С Н Н С Н Н С Н С Н С	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745 2.656704 3.301768 2.595041 4.652060 5.110603 4.524913 5.379369 2.723112 1.775690 3.425899 2.530962 1.786209	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857 2.082016 -0.895303 -1.531088 -1.630006 -1.751187 -2.639361 -1.082541 -0.716587 -0.148139 -0.158458 -1.701847 2.474450	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454 -1.107045 1.314405 0.744274 1.379385 0.378354 1.821770 2.013918 2.728993 2.712223 3.381490 3.201181 -2.294344
H C H C H C H Conform Multipl Charge: E (B97-3 E (M06/c E (PBE - E (PBE0	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448 -1.901575 -2.921569 -0.987854 -1.297769 mation 24. licity: 4 : 0 3c) = -3413.52221 def2-TZVP) = -341 -D3(BU)/def2-TZV	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192 2.452112 2.109498 1.555282 0.524995 33598330 Hartree 3.209283793482 Ham P) = -3412.0846063 VP) = -3412.298503	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595 4.208659 4.435812 3.637385 3.405889	С Н С Н С С Н С Н Н Н С Н Н Н Н Н Н Н Н Н Н Н Н Н	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745 2.656704 3.301768 2.595041 4.652060 5.110603 4.524913 5.379369 2.723112 1.775690 3.425899 2.530962	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857 2.082016 -0.895303 -1.531088 -1.630006 -1.751187 -2.639361 -1.082541 -0.716587 -0.148139 -0.158458 -1.701847	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454 -1.107045 0.744274 1.379385 0.378354 1.821770 2.013918 2.728993 2.712223 3.381490 3.201181
H C H C H C H Conform Multipl Charge: E(B97-3 E(M06/6 E(PBE-0 E(PBE0) E(PBE0-0 E(PBE0-0)	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448 -1.901575 -2.921569 -0.987854 -1.297769 mation 24. Licity: 4 : 0 3c) = -3413.52221 def2-TZVP) = -341 - D3(BJ)/def2-TZ - D3(BJ)/def2-TZ	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192 2.452112 2.109498 1.555282 0.524995 3598330 Hartree 3.209283793482 Hai P) = -3412.0846063 VP) = -3412.2986063	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595 4.208659 4.435812 3.637385 3.405889	СНСНССННННСН	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745 2.656704 3.301768 2.595041 4.652060 5.110603 4.524913 5.379369 2.723112 1.775690 3.425899 2.530962 1.786209 1.227581	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857 2.082016 -0.895303 -1.531088 -1.630006 -1.751187 -2.639361 -1.082541 -0.716587 -0.148139 -0.158458 -1.701847 2.474450 1.565673	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454 -1.107045 1.314405 0.744274 1.379385 0.378354 1.821770 2.013918 2.728993 2.712223 3.381490 3.201181 -2.294384 -2.599729
H C H C H C H Conform Multipl Conform E (B97-3 E (M06/6 E (PBE - E (PBE0- E (PBE0- E (PM6)	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448 -1.901575 -2.921569 -0.987854 -1.297769 mation 24. Licity: 4 : 0 3c) = -3413.52221 def2-TZVP) = -341 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192 2.452112 2.109498 1.555282 0.524995 3598330 Hartree 3.209283793482 Har P) = -3412.0846063 WP) = -3412.298501 80718656 Hartree	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595 4.208659 4.435812 3.637385 3.405889	СНСНССНСННС	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745 2.656704 3.301768 2.595041 4.652060 5.110603 4.524913 5.379369 2.723112 1.775690 3.425899 2.530962 1.786209 1.227581 2.620507	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857 2.082016 -0.895303 -1.531088 -1.630006 -1.751187 -2.639361 -1.082541 -0.716587 -0.148139 -0.158458 -1.701847 2.474450 1.565673 2.922995	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454 -1.107045 1.314405 0.744274 1.379385 0.378354 1.821770 2.013918 2.728993 2.712223 3.381490 3.201181 -2.294344 -2.599729 -3.505675
H C H C H C H Conform Multipl Charge: E (B97-3 E (M06/d E (PBE - E (PBED- E (PBED- E (PM6) E (PM7)	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448 -1.901575 -2.921569 -0.987854 -1.297769 mation 24. licity: 4 : 0 3c) = -3413.52221 def2-TZVP) = -341 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZO - D3(BJ)/de	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192 2.452112 2.109498 1.555282 0.524995 3598330 Hartree 3.209283793482 Har P) = -3412.0846063 VP) = -3412.298501 80718656 Hartree /mol	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595 4.208659 4.435812 3.637385 3.405889	СНСНССНННСНННСН	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745 2.656704 3.301768 2.595041 4.652060 5.110603 4.524913 5.379369 2.723112 1.775690 3.425899 2.530962 1.786209 1.227581 2.620507 1.963022	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857 2.082016 -0.895303 -1.531088 -1.630006 -1.751187 -2.639361 -1.082541 -0.716587 -0.148139 -0.158458 -1.701847 2.474450 1.565673 2.922995 3.139144	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454 -1.107045 1.314405 0.744274 1.379385 0.378354 1.821770 2.013918 2.728993 2.712223 3.381490 3.201181 -2.2943344 -2.599729 -3.505675 -4.372656
H C H C H C H C H C H C H C H C H C H C	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448 -1.901575 -2.921569 -0.987854 -1.297769 mation 24. licity: 4 : 0 3c) = -3413.52221 def2-TZVP) = -341 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192 2.452112 2.109498 1.555282 0.524995 33598330 Hartree 3.209283793482 Har P) = -3412.0846063 VP) = -3412.0846063 VP) = -3412.0845063 VP) = -3412.0845063	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595 4.208659 4.435812 3.637385 3.405889	С Н С Н С С Н С Н Н Н С Н С Н Н Н Н С Н С Н Н	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745 2.656704 3.301768 2.595041 4.652060 5.110603 4.524913 5.379369 2.723112 1.775690 3.425899 2.530962 1.786209 1.227581 2.665077 1.963022 3.344919	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857 2.082016 -0.895303 -1.531088 -1.630006 -1.751187 -2.639361 -1.082541 -0.716587 -0.148139 -0.158458 -1.701847 2.474450 1.565673 2.922995 3.139144 2.142197	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454 -1.107045 1.314405 0.744274 1.379385 0.378354 1.821770 2.013918 2.728993 2.712223 3.381490 3.201181 -2.294344 -2.599729 -3.505675 -4.372656 -3.813182
H C H C H C H Conform Multipl Charge: E(B97-3 E(M06/c E(PBE)- E(PBE)- E(PBE)- E(PM6) E(PM7) E(M97) E(GFN1-	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448 -1.901575 -2.921569 -0.987854 -1.297769 mation 24. licity: 4 : 0 3c) = -3413.52221 lef2-TZVP) = -341 -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -105.36936 Kcal =118.40729 Kcal -118.40729 Kcal -118.40729 Kcal -118.40729 Kcal	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192 2.452112 2.109498 1.555282 0.524995 3598330 Hartree 3.209283793482 Hai P) = -3412.0846063 VP) = -3412.298501 80718656 Hartree /mol /mol -3415.576821403597 28018604 Hartree	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595 4.208659 4.435812 3.637385 3.405889	СНСНССНКСНННСНКН	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745 2.656704 3.301768 2.595041 4.652060 5.110603 4.524913 5.379369 2.723112 1.775690 3.425899 2.530962 1.786209 1.227581 2.620507 1.963022 3.344919 3.195936	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857 2.082016 -0.895303 -1.531088 -1.630006 -1.751187 -2.639361 -1.082541 -0.716587 -0.148139 -0.158458 -1.701847 2.474450 1.565673 2.922995 3.139144 2.142197 3.846325	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454 -1.107045 1.314405 0.744274 1.379385 0.378354 1.821770 2.013918 2.728993 2.712223 3.381490 3.201181 -2.294344 -2.599729 -3.505675 -4.372656 -3.813182 -3.287332
H C H C H C H C H C H C H C H C H C H C	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448 -1.901575 -2.921569 -0.987854 -1.297769 mation 24. Licity: 4 : 0 3c) = -3413.52221 def2-TZVP) = -341 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - 3c) = -3408.8566 = 105.36936 Kcal = 118.40729 Kcal (-V/def2-TZVP) = -xTB) = -148.2248 -xTB) = -147.2998	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192 2.452112 2.109498 1.555282 0.524995 3598330 Hartree 3.209283793482 Hai P = -3412.0846063 VP) = -3412.298501 80718656 Hartree /mol /mol /mol 28018604 Hartree 72495061 Hartree	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595 4.208659 4.435812 3.637385 3.405889	СНСНССНННСНННСН	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745 2.656704 3.301768 2.595041 4.652060 5.110603 4.5224913 5.379369 2.723112 1.775690 3.425899 2.530962 1.786209 1.227581 2.620507 1.963022 3.344919 3.195936 0.759419	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857 2.082016 -0.895303 -1.531088 -1.630006 -1.751187 -2.639361 -1.082541 -0.716587 -0.148139 -0.158458 -1.701847 2.474450 1.565673 2.922995 3.139144 2.142197 3.846325 3.549495	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454 -1.107045 1.314405 0.744274 1.379385 0.378354 1.821770 2.013918 2.728993 2.712223 3.381490 3.201181 -2.294344 -2.599729 -3.505675 -4.372656 -3.813182 -3.287332 -1.896455
H C H C H C H C H C H C H C H C H C H C	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448 -1.901575 -2.921569 -0.987854 -1.297769 mation 24. licity: 4 : 0 3c) = -3413.52221 lef2-TZVP) = -341 -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -D3(BJ)/def2-TZV -105.36936 Kcal =118.40729 Kcal -118.40729 Kcal -118.40729 Kcal -118.40729 Kcal	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192 2.452112 2.109498 1.555282 0.524995 3598330 Hartree 3.209283793482 Hai P = -3412.0846063 VP) = -3412.298501 80718656 Hartree /mol /mol /mol 28018604 Hartree 72495061 Hartree	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595 4.208659 4.435812 3.637385 3.405889	СНСНССНСНННСННСН	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745 2.656704 3.301768 2.595041 4.652060 5.110603 4.524913 5.379369 2.723112 1.775690 3.425899 2.530962 1.786209 1.227581 2.620507 1.963022 3.344919 3.195936 0.759419 0.134785	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857 2.082016 -0.895303 -1.531088 -1.630006 -1.751187 -2.639361 -1.082541 -0.716587 -0.148139 -0.158458 -1.701847 2.474450 1.565673 2.922995 3.139144 2.142197 3.846325 3.549495 3.213011	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454 -1.107045 1.314405 0.744274 1.379385 0.378354 1.821770 2.013918 2.728993 2.712223 3.381490 3.201181 -2.294344 -2.599729 -3.505675 -4.372656 -3.813182 -3.287332 -1.896455 -1.043477
H C H C H C H C H C H C H C H C H C H C	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448 -1.901575 -2.921569 -0.987854 -1.297769 mation 24. licity: 4 : 0 3c) = -3413.52221 def2-TZVP) = -341 - D3(BJ)/def2-TZV - D3(BJ)/de	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192 2.452112 2.109498 1.555282 0.524995 3598330 Hartree 3.209283793482 Hai P = -3412.0846063 VP) = -3412.298501 80718656 Hartree /mol /mol /mol 28018604 Hartree 72495061 Hartree	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595 4.208659 4.435812 3.637385 3.405889	С Н С Н С С Н С Н Н Н С Н С Н Н Н С Н Н Н С Н Н	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745 2.656704 3.301768 2.595041 4.652060 5.110603 4.524913 5.379369 2.723112 1.775690 3.425899 2.530962 1.786209 1.227581 2.620507 1.963022 3.344919 3.195936 0.759419 0.134785 0.083791	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857 2.082016 -0.895303 -1.531088 -1.630006 -1.751187 -2.639361 -1.082541 -0.716587 -0.148139 -0.158458 -1.701847 2.474450 1.565673 2.922995 3.139144 2.142197 3.846325 3.549495 3.213011 3.787468	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454 -1.107045 1.314405 0.744274 1.379385 0.378354 1.821770 2.013918 2.728993 2.712223 3.381490 3.201181 -2.294344 -2.599729 -3.505675 -4.372656 -3.813182 -3.287332 -1.896455 -1.043477 -2.743450
H C H C H C H C H C H C H C H C H C H C	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448 -1.901575 -2.921569 -0.987854 -1.297769 mation 24. licity: 4 : 0 3c) = -3413.52221 def2-TZVP) = -341 - D3(BJ)/def2-TZV - D3(BJ)/de	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192 2.452112 2.109498 1.555282 0.524995 3598330 Hartree 3.209283793482 Hai P = -3412.0846063 VP) = -3412.298501 80718656 Hartree /mol /mol /mol 28018604 Hartree 72495061 Hartree	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595 4.208659 4.435812 3.637385 3.405889	СНСНССНСНННСННСН	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745 2.656704 3.301768 2.595041 4.652060 5.110603 4.524913 5.379369 2.723112 1.775690 3.425899 2.530962 1.786209 1.227581 2.620507 1.963022 3.344919 3.195936 0.759419 0.134785	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857 2.082016 -0.895303 -1.531088 -1.630006 -1.751187 -2.639361 -1.082541 -0.716587 -0.148139 -0.158458 -1.701847 2.474450 1.565673 2.922995 3.139144 2.142197 3.846325 3.549495 3.213011	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454 -1.107045 1.314405 0.744274 1.379385 0.378354 1.821770 2.013918 2.728993 2.712223 3.381490 3.201181 -2.294344 -2.599729 -3.505675 -4.372656 -3.813182 -3.287332 -1.896455 -1.043477
H C H C H C H C H C H C H C H C H C H C	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448 -1.901575 -2.921569 -0.987854 -1.297769 mation 24. licity: 4 : 0 3c) = -3413.52221 def2-TZVP) = -341 - D3(BJ)/def2-TZV - D3(BJ)/de	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192 2.452112 2.109498 1.555282 0.524995 3598330 Hartree 3.209283793482 Hai P = -3412.0846063 VP) = -3412.298501 80718656 Hartree /mol /mol /mol 28018604 Hartree 72495061 Hartree	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595 4.208659 4.435812 3.637385 3.405889	С Н С Н С С Н С Н Н Н С Н С Н Н Н С Н Н Н С Н Н	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745 2.656704 3.301768 2.595041 4.652060 5.110603 4.524913 5.379369 2.723112 1.775690 3.425899 2.530962 1.786209 1.227581 2.620507 1.963022 3.344919 3.195936 0.759419 0.134785 0.083791	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857 2.082016 -0.895303 -1.531088 -1.630006 -1.751187 -2.639361 -1.082541 -0.716587 -0.148139 -0.158458 -1.701847 2.474450 1.565673 2.922995 3.139144 2.142197 3.846325 3.549495 3.213011 3.787468	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454 -1.107045 1.314405 0.744274 1.379385 0.378354 1.821770 2.013918 2.728993 2.712223 3.381490 3.201181 -2.294344 -2.599729 -3.505675 -4.372656 -3.813182 -3.287332 -1.896455 -1.043477 -2.743450
H C H C H C H C H C H C H C H C H C H C	0.711760 1.740060 -0.212444 0.092068 -1.520715 -2.242448 -1.901575 -2.921569 -0.987854 -1.297769 mation 24. licity: 4 : 0 3c) = -3413.52221 def2-TZVP) = -341 - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - T3(BJ)/def2-TZV - T4(BJ)/def2-TZV - T4(BJ)/def2-TZV - T5(BJ)/def2-TZV - T5(BJ)/de	3.293065 3.619087 4.196799 5.235448 3.776364 4.481192 2.452112 2.109498 1.555282 0.524995 33598330 Hartree 3.209283793482 Han P) = -3412.0846063 VP) = -3412.298501 80718656 Hartree /mol /mol -3415.576821403597 28018604 Hartree 72495061 Hartree 03666 Hartree	3.644309 3.425659 4.186614 4.388131 4.478979 4.919595 4.208659 4.435812 3.637385 3.405889	С Н С Н С С Н С Н Н Н С Н С Н Н Н С Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н	3.401628 4.301162 4.942712 4.388479 5.096225 3.559356 3.620745 2.656704 3.301768 2.595041 4.652060 5.110603 4.524913 5.379369 2.723112 1.775690 3.425899 2.530962 1.786209 1.227581 2.620507 1.963022 3.344919 3.195936 0.759419 0.134785 0.083791 1.263269	1.413905 1.160514 2.690337 3.431428 3.016002 4.019857 2.082016 -0.895303 -1.531088 -1.630006 -1.751187 -2.639361 -1.082541 -0.716587 -0.148139 -0.158458 -1.701847 2.474450 1.565673 2.922995 3.139144 2.142197 3.846325 3.549495 3.213011 3.787468 4.489796	0.597720 1.080545 1.938892 0.510545 0.911410 -0.570117 -1.018454 -1.107045 1.314405 0.744274 1.379385 0.378354 1.821770 2.013918 2.728993 2.712223 3.381490 3.201181 -2.294344 -2.599729 -3.505675 -4.372656 -3.813182 -3.287332 -1.896455 -1.043477 -2.743450 -1.590601

~	0 400555	2 150001	1 050451	~	0 760001	2 120102	1 055060
C	-2.488557	3.152291	1.870471	C	0.762221	3.130183	1.255960
C	-3.574556	2.793098	1.040231	H	-0.198368	2.589222	1.130966
H	-3.458808	1.926680	0.374399	C	1.235472	3.551294	-0.146338
C	-4.771895	3.514096	1.080873	H	1.353903	2.673495	-0.805734
H	-5.611278	3.207243	0.437581	H	2.212754	4.075211	-0.098628
С	-4.906338	4.615754	1.944873	Н	0.504936	4.240488	-0.617463
Н	-5.849028	5.183375	1.977716	C	0.505359	4.370883	2.128986
C	-3.830592	4.987559	2.766979	H	0.183038	4.103862	3.154648
H	-3.925019	5.853837	3.439890	H	-0.284558	5.005502	1.677296
C	-2.630662	4.261240	2.734128	H	1.417518	4.996380	2.218746
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C	-0.226177	2.443533	2.904665	C	-2.537503	-0.217749	-2.261344
С	1.140574	2.651760	2.622366	С	-2.789287	-0.366164	-3.634618
H	1.460247	2.798492	1.579737	H	-3.329069	0.428682	-4.169731
C	2.083168	2.678679	3.659367	С	-2.340941	-1.490939	-4.342592
H	3.141808	2.857355	3.419395	H	-2.547233	-1.586039	-5.419367
С	1.680085	2.467596	4.987800	С	-1.606200	-2.478510	-3.676592
Н	2.422551	2.480057	5.800381	Н	-1.224623	-3.343088	-4.240752
С	0.324432	2.237347	5.275911	С	-1.347751	-2.394326	-2.295801
H	0.003505	2.059174	6.313920	С	-2.880778	1.082488	-1.538663
C	-0.625052	2.238207	4.243882	H	-3.057408	0.839750	-0.472562
H	-1.688856	2.066022	4.468850	С	-1.674241	2.037878	-1.581936
				H	-0.742692	1.540991	-1.235780
Conform	mation 25.			Н	-1.845778	2.923370	-0.936694
	licity: 4			H		2.387262	-2.615358
					-1.475935		
Charge:				С	-4.139534	1.779410	-2.068563
E(B97-3	3c) = -3413.53412	0938863 Hartree		H	-5.016223	1.101335	-2.076207
E(M06/c	def2-TZVP) = -341	3.218951084109 Ha:	rtree	H	-3.996454	2.162721	-3.099948
E (PBE -	- D3(BJ)/def2-TZV	$^{\prime}P) = -3412.0955809$	918157 Hartree	H	-4.388519	2.653808	-1.433796
		VP) = -3412.309826		С	-0.490891	-3.457137	-1.616727
	-3c) = -3408.8663		JOI US TO HAICICC	Н	-0.600249		-0.522140
						-3.309360	
	= 101.74523 Kcal			С	0.993083	-3.251305	-1.975075
E(PM7)	= 113.44669 Kcal	/mol		H	1.635902	-3.986385	-1.448560
E (ωB97)	X-V/def2-TZVP) =	-3415.587721198738	B Hartree	H	1.341617	-2.235121	-1.699714
E (GFN1-	-xTB) = $-148.5319$	34483411 Hartree		H	1.155902	-3.372205	-3.066066
	-xTB) = $-147.3100$			C	-0.933220	-4.892329	-1.940805
	FF) = -20.4958240			Н	-2.002661	-5.056782	-1.704123
E (GEN-I	er) = =20.4936240	33230 Haitiee					
				H	-0.336251	-5.620390	-1.354531
Coordin	nates:			H	-0.782301	-5.136722	-3.012534
Co	0.217598	-0.409987	-0.096342	N	1.657645	0.166187	-0.981753
N	0.128325	0.292893	1.748532	С	2.429732	0.556065	-1.928886
N	-1.562905	-1.110090	-0.192172	C	3.912601	0.407434	-1.793974
C	-1.163725	0.845506	3.920626	C	4.481359	0.344634	-0.502261
C	-0.960562	0.166169	2.518386	H	3.820491	0.452837	0.368439
C	-2.101575	-0.568137	2.079826	C	5.858787	0.162949	-0.338421
H	-2.879533	-0.657650	2.835042	H	6.283633	0.130611	0.677056
C	-2.421254	-1.173799	0.848536	С	6.694018	0.031664	-1.461960
C	-3.767831	-1.964179	0.758084	Н	7.778002	-0.111707	-1.333928
C	-2.115902	2.044260	3.676920	C	6.138019	0.087521	-2.750400
H	-2.305259	2.579150	4.630908	H	6.784710	-0.021407	-3.634783
H	-3.089496	1.712375	3.265852	C	4.758373	0.278461	-2.918046
H	-1.676098	2.767110	2.963291	H	4.326950	0.313401	-3.929537
C	-1.838259	-0.120667	4.928434	С	1.871371	1.178391	-3.173541
H	-1.884485	0.370806	5.920911	С	0.716271	0.636489	-3.775505
Н	-1.260476	-1.058253	5.042337	Н	0.259384	-0.268887	-3.349079
H	-2.877280	-0.388442	4.658176	C	0.156419	1.242145	-4.908515
C	0.102445	1.372558	4.624275	H	-0.735148	0.795593	-5.372944
H	-0.199990	1.801248	5.601620	C	0.726025	2.409749	-5.442357
H	0.618635	2.164995	4.060019	H	0.281408	2.887294	-6.328997
H	0.840581	0.574411	4.822507	C	1.867431	2.965189	-4.840723
С	-3.503850	-3.358946	0.152230	H	2.313968	3.885631	-5.247590
Н	-4.433855	-3.962323	0.185287	C	2.443341	2.348446	-3.721280
H	-2.722985	-3.904065	0.719776	H	3.337873	2.783464	-3.250346
H	-3.188035	-3.295340	-0.903853				
С	-4.819783	-1.228251	-0.102174		mation 26.		
H	-5.775483	-1.791605	-0.072954		licity: 4		
H	-4.514038	-1.146643	-1.160657	Charge	e: 0		
		-0.209968	0.288106		3c) = -3413.527433	3727270 Hartree	
H	-5.016740					3.214203684880 На	rtree
Н	-5.016740 -4.401452		2 148018			7.21 120000 1000 Ha	
С	-4.401452	-2.189812	2.148018		,	2412 000400	201210 11
C H	-4.401452 -5.295420	-2.189812 -2.834469	2.030865		- D3(BJ)/def2-TZVE		
C H H	-4.401452 -5.295420 -4.743648	-2.189812 -2.834469 -1.246221	2.030865 2.617564	E(PBEC	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZV	7P) = -3412.30414	
C H H H	-4.401452 -5.295420 -4.743648 -3.706838	-2.189812 -2.834469 -1.246221 -2.697055	2.030865 2.617564 2.846266	E(PBEC E(PBEh	- D3(BJ)/def2-TZVE - D3(BJ)/def2-TZV (-3c) = -3408.86484	7P) = -3412.30414 11198544 Hartree	
С Н Н С	-4.401452 -5.295420 -4.743648	-2.189812 -2.834469 -1.246221	2.030865 2.617564	E(PBEC E(PBEh	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZV	7P) = -3412.30414 11198544 Hartree	
C H H H	-4.401452 -5.295420 -4.743648 -3.706838	-2.189812 -2.834469 -1.246221 -2.697055	2.030865 2.617564 2.846266	E(PBEC E(PBEh E(PM6)	- D3(BJ)/def2-TZVE - D3(BJ)/def2-TZV (-3c) = -3408.86484	7P) = -3412.30414 11198544 Hartree 'mol	
C H H C C	-4.401452 -5.295420 -4.743648 -3.706838 1.401433 2.378174	-2.189812 -2.834469 -1.246221 -2.697055 0.792191 -0.122331	2.030865 2.617564 2.846266 2.133857 2.629154	E (PBEC E (PBEh E (PM6) E (PM7)	- D3(BJ)/def2-TZVE - D3(BJ)/def2-TZVE - D3(BJ)/def2-TZVE - 3c) = -3408.86484 = 101.41495 Kcal/ = 116.72492 Kcal/	7P) = -3412.30414 H1198544 Hartree (mol (mol	6377179 Hartree
C H H C C	-4.401452 -5.295420 -4.743648 -3.706838 1.401433 2.378174 3.635451	-2.189812 -2.834469 -1.246221 -2.697055 0.792191 -0.122331 0.387952	2.030865 2.617564 2.846266 2.133857 2.629154 3.005269	E (PBE 0 E (PBE h E (PM6) E (PM7) E (ωB97	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF -3c) = -3408.86484 = 101.41495 Kcal/ = 116.72492 Kcal/ X-V/def2-TZVP) = -	7P) = -3412.30414 11198544 Hartree (mol (mol -3415.58704461996	6377179 Hartree
C H H C C C	-4.401452 -5.295420 -4.743648 -3.706838 1.401433 2.378174 3.635451 4.384658	-2.189812 -2.834469 -1.246221 -2.697055 0.792191 -0.122331 0.387952 -0.311486	2.030865 2.617564 2.846266 2.133857 2.629154 3.005269 3.410241	E (PBEC E (PBEh E (PM6) E (PM7) E (ωB97 E (GFN1	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - 3408.86484 = 101.41495 Kcal/ = 116.72492 Kcal/ (X-V/def2-TZVF) = - -xTB) = -148.52744	7P) = -3412.30414 11198544 Hartree /mol /mol -3415.58704461996 11701144 Hartree	6377179 Hartree
C H H C C C H	-4.401452 -5.295420 -4.743648 -3.706838 1.401433 2.378174 3.635451 4.384658 3.960849	-2.189812 -2.834469 -1.246221 -2.697055 0.792191 -0.122331 0.387952 -0.311486 1.741279	2.030865 2.617564 2.846266 2.133857 2.629154 3.005269 3.410241 2.848459	E (PBEC E (PBEh E (PM6) E (PM7) E (ωB97 E (GFN1 E (GFN2	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - 3c) = -3408.86484 = 101.41495 Kcal/ = 116.72492 Kcal/ X-V/def2-TZVP) = - -xTB) = -148.52744 -xTB) = -147.30522	<pre>TP) = -3412.30414 11198544 Hartree fmol fmol 3415.58704461996 11701144 Hartree 21332721 Hartree</pre>	6377179 Hartree
C H H C C C H C	-4.401452 -5.295420 -4.743648 -3.706838 1.401433 2.378174 3.635451 4.384658 3.960849 4.952712	-2.189812 -2.834469 -1.24621 -2.697055 0.792191 -0.122331 0.387952 -0.311486 1.741279 2.113148	2.030865 2.617564 2.846266 2.133857 2.629154 3.005269 3.410241 2.848459 3.145585	E (PBEC E (PBEh E (PM6) E (PM7) E (ωB97 E (GFN1 E (GFN2	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - 3408.86484 = 101.41495 Kcal/ = 116.72492 Kcal/ (X-V/def2-TZVF) = - -xTB) = -148.52744	<pre>TP) = -3412.30414 11198544 Hartree fmol fmol 3415.58704461996 11701144 Hartree 21332721 Hartree</pre>	6377179 Hartree
С Н Н С С С Н С Н	-4.401452 -5.295420 -4.743648 -3.706838 1.401433 2.378174 3.635451 4.384658 3.960849 4.952712 3.023511	-2.189812 -2.834469 -1.246221 -2.697055 0.792191 -0.122331 0.387952 -0.311486 1.741279 2.113148 2.604258	2.030865 2.617564 2.846266 2.133857 2.629154 3.005269 3.410241 2.848459 3.145585 2.268804	E (PBEC E (PBEh E (PM6) E (PM7) E (WB97 E (GFN1 E (GFN2 E (GFN-	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF -3c) = -3408.86484 = 101.41495 Kcal/ = 116.72492 Kcal/ X-V/def2-TZVP) = - -XTB) = -148.52744 -XTB) = -147.30522 FFF) = -20.49233791	<pre>TP) = -3412.30414 11198544 Hartree fmol fmol 3415.58704461996 11701144 Hartree 21332721 Hartree</pre>	6377179 Hartree
C H H C C C H C	-4.401452 -5.295420 -4.743648 -3.706838 1.401433 2.378174 3.635451 4.384658 3.960849 4.952712	-2.189812 -2.834469 -1.24621 -2.697055 0.792191 -0.122331 0.387952 -0.311486 1.741279 2.113148	2.030865 2.617564 2.846266 2.133857 2.629154 3.005269 3.410241 2.848459 3.145585	E (PBEC E (PBEh E (PM6) E (PM7) E (WB97 E (GFN1 E (GFN2 E (GFN-	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - 3c) = -3408.86484 = 101.41495 Kcal/ = 116.72492 Kcal/ X-V/def2-TZVP) = - -xTB) = -148.52744 -xTB) = -147.30522	<pre>TP) = -3412.30414 11198544 Hartree fmol fmol 3415.58704461996 11701144 Hartree 21332721 Hartree</pre>	6377179 Hartree
С Н Н С С С Н С Н	-4.401452 -5.295420 -4.743648 -3.706838 1.401433 2.378174 3.635451 4.384658 3.960849 4.952712 3.023511 3.290593	-2.189812 -2.834469 -1.246221 -2.697055 0.792191 -0.122331 0.387952 -0.311486 1.741279 2.113148 2.604258 3.659364	2.030865 2.617564 2.846266 2.133857 2.629154 3.005269 3.410241 2.848459 3.145585 2.268804 2.101724	E (PBEC E (PBEh E (PM6) E (PM7) E (WB97 E (GFN1 E (GFN2 E (GFN-	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - C3(BJ)/def2-TZVF - 3(B)/def2-TZVP) = - (C3(B)/def2-TZVP) = - (C3(B)/d	<pre>TP) = -3412.30414 11198544 Hartree fmol fmol 3415.58704461996 11701144 Hartree 21332721 Hartree</pre>	6377179 Hartree
C H H C C C H C H C H	-4.401452 -5.295420 -4.743648 -3.706838 1.401433 2.378174 3.635451 4.384658 3.960849 4.952712 3.023511 3.290593 1.743471	-2.189812 -2.834469 -1.246221 -2.697055 0.792191 -0.122331 0.387952 -0.311486 1.741279 2.113148 2.604258 3.659364 2.155581	2.030865 2.617564 2.846266 2.133857 2.629154 3.005269 3.410241 2.848459 3.145585 2.268804 2.101724 1.898555	E (PBEC E (PBEh E (PM6) E (PM7) E (WB97 E (GFN1 E (GFN2 Coordi Co	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - 101.41495 Kcal/ = 116.72492 Kcal/ (X-V/def2-TZVP) = - -xTB) = -148.52744 -xTB) = -147.30522 	PP) = -3412.30414 11198544 Hartree (mol (mol 13415.58704461996 11701144 Hartree 11332721 Hartree -9882 Hartree -0.336096	6377179 Hartree  2 Hartree  -0.050237
С Н Н С С С Н С Н С С Н С С С Н С С С С Н С С С С С С С С С С С С С	-4.401452 -5.295420 -4.743648 -3.706838 1.401433 2.378174 3.635451 4.384658 3.960849 4.952712 3.023511 3.290593 1.743471 2.173679	-2.189812 -2.834469 -1.246221 -2.697055 0.792191 -0.122331 0.387952 -0.311486 1.741279 2.113148 2.604258 3.659364 2.155581 -1.636523	2.030865 2.617564 2.846266 2.133857 2.629154 3.005269 3.410241 2.848459 3.145585 2.268804 2.101724 1.898555 2.726200	E (PBEC E (PBEh E (PM6)) E (PM7) E (GFN1 E (GFN2 E (GFN- Coordi Co	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - 3408.86484 = 101.41495 Kcal/ = 116.72492 Kcal/ (X-V/def2-TZVP) = - -xTB) = -148.52744 (-xTB) = -147.30522 (-FF) = -20.49233791 (-xTB) = -1675722	<pre>TP) = -3412.30414 11198544 Hartree fmol fmol 3415.58704461996 11701144 Hartree 21332721 Hartree 9882 Hartree -0.336096 -1.037815</pre>	6377179 Hartree  2 Hartree  -0.050237 0.075784
С Н Н Н С С С Н С Н С Н С Н С Н С Н С Н	-4.401452 -5.295420 -4.743648 -3.706838 1.401433 2.378174 3.635451 4.384658 3.960849 4.952712 3.023511 3.290593 1.743471 2.173679 3.168811	-2.189812 -2.834469 -1.246221 -2.697055 0.792191 -0.122331 0.387952 -0.311486 1.741279 2.113148 2.604258 3.659364 2.155581 -1.636523 -2.025495	2.030865 2.617564 2.846266 2.133857 2.629154 3.005269 3.410241 2.848459 3.145585 2.268804 2.101724 1.898555 2.726200 3.033394	E (PBEC E (PBEh E (PM6) E (PM7) E (GB97 E (GFN1 E (GFN2 Coordi Co N	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF -3c) = -3408.86484 = 101.41495 Kcal/ = 116.72492 Kcal/ (X-V/def2-TZVP) = - -xTB) = -148.52744 (-xTB) = -147.30522 -FF) = -20.49233791 .nates: 0.099354 -1.675722 -0.106581	<pre>TP) = -3412.30414 11198544 Hartree (mol (mol) -3415.58704461996 11701144 Hartree 21332721 Hartree -9882 Hartree -0.336096 -1.037815 1.168039</pre>	6377179 Hartree  2 Hartree  -0.050237 0.075784 1.217054
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С Н Н С С С Н С Н С С Н С С Н С С Н С С С Н С С С Н С С С С С С С С С С С С С	-4.401452 -5.295420 -4.743648 -3.706838 1.401433 2.378174 3.635451 4.384658 3.960849 4.952712 3.023511 3.290593 1.743471 2.173679 3.168811 1.178451	-2.189812 -2.834469 -1.246221 -2.697055 0.792191 -0.122331 0.387952 -0.311486 1.741279 2.113148 2.604258 3.659364 2.155581 -1.636523 -2.025495 -2.103589	2.030865 2.617564 2.846266 2.133857 2.629154 3.005269 3.410241 2.848459 3.145585 2.268804 2.101724 1.898555 2.726200 3.033394 3.800164	E (PBEC E (PBEh E (PM6) E (PM7) E (GB91 E (GFN1 E (GFN- Coordi Co N	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - 30) = -3408.86484 = 101.41495 Kcal/ = 116.72492 Kcal/ (X-V/def2-TZVP) = - -XTB) = -148.52744 -XTB) = -147.30522 -FF) = -20.49233791 .nates: 0.099354 -1.675722 -0.106581 -3.981119	PP) = -3412.30414 11198544 Hartree (mol (mol -3415.58704461996 11701144 Hartree 11332721 Hartree -0.336096 -1.037815 1.168039 -1.348982	6377179 Hartree  2 Hartree  -0.050237 0.075784 1.217054 1.124036
С Н Н С С С Н С Н С Н С Н С Н Н Н Н Н Н Н Н Н Н Н Н Н	-4.401452 -5.295420 -4.743648 -3.706838 1.401433 2.378174 3.635451 4.384658 3.960849 4.952712 3.023511 3.290593 1.743471 2.173679 3.168811 1.178451 1.399875 1.233946	-2.189812 -2.834469 -1.246221 -2.697055 0.792191 -0.122331 0.387952 -0.311486 1.741279 2.113148 2.604258 3.659364 2.155581 -1.636523 -2.025495 -2.103589 -1.651154 -3.205980	2.030865 2.617564 2.846266 2.133857 2.629154 3.005269 3.410241 2.848459 3.145585 2.268804 2.101724 1.898555 2.726200 3.033394 3.800164 4.787379 3.915428	E (PBEC E (PBEC E (PMG) E (PM7) E (GFN1 E (GFN2 C (GFN- COORDI CO N N C C C	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - 101.41495 Kcal/ = 116.72492 Kcal/ (X-V/def2-TZVP) = - -xTB) = -148.52744 -xTB) = -147.30522 -FF) = -20.49233791 	PP) = -3412.30414 11198544 Hartree (mol (mol 13415.58704461996 11701144 Hartree 1332721 Hartree -0.336096 -1.037815 1.168039 -1.348982 -0.612522 0.528152	-0.050237 0.075784 1.217054 1.124036 0.943738 1.740116
С Н Н Н С С С Н С Н С Н С Н С Н Н Н Н Н Н Н Н Н Н Н Н Н	-4.401452 -5.295420 -4.743648 -3.706838 1.401433 2.378174 3.635451 4.384658 3.960849 4.952712 3.023511 3.290593 1.743471 2.173679 3.168811 1.178451 1.399875 1.233946 0.135136	-2.189812 -2.834469 -1.246221 -2.6697055 0.792191 -0.122331 0.387952 -0.311486 1.741279 2.113148 2.604258 3.659364 2.155581 -1.636523 -2.025495 -2.103589 -1.651154 -3.205980 -1.853859	2.030865 2.617564 2.846266 2.133857 2.629154 3.005269 3.410241 2.848459 3.145585 2.268804 2.101724 1.898555 2.726200 3.033394 3.800164 4.787379 3.915428 3.526300	E (PBEC E (PBEC E (PMT)) E (BMT) E (GFN1 E (GFN2 Coordi CO N N C C C C	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - 30) = -3408.86484 = 101.41495 Kcal/ = 116.72492 Kcal/ (X-V/def2-TZVP) = -4 -xTB) = -148.5274 -xTB) = -20.49233791 - xTB) = -20.49233791 - 20.106581 - 3.981119 - 2.613951 - 2.378130 - 3.216457	TP) = -3412.30414 11198544 Hartree (mol (mol -3415.58704461996 11701144 Hartree 21332721 Hartree -0.336096 -1.037815 1.168039 -1.348982 -0.612522 0.528152 0.810051	6377179 Hartree  2 Hartree  -0.050237 0.075784 1.217054 1.124036 0.943738 1.740116 2.374760
С Н Н Н С С С Н С Н С С Н С Н Н Н С	-4.401452 -5.295420 -4.743648 -3.706838 1.401433 2.378174 3.635451 4.384658 3.960849 4.952712 3.023511 3.290593 1.743471 2.173679 3.168811 1.178451 1.399875 1.233946 0.135136 1.873076	-2.189812 -2.834469 -1.246221 -2.697055 0.792191 -0.122331 0.387952 -0.311486 1.741279 2.113148 2.604258 3.659364 2.155581 -1.636523 -2.025495 -2.103589 -1.651154 -3.205980 -1.853859 -2.304640	2.030865 2.617564 2.846266 2.133857 2.629154 3.005269 3.410241 2.848459 3.145585 2.268804 2.101724 1.898555 2.726200 3.033394 3.800164 4.787379 3.915428 3.526300 1.373497	E (PBEC E (PPEH E (PMG)) E (PMT) E (GFN1 E (GFN2 E (GFN- Coordi CO N N C C C C C	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - 101.41495 Kcal/ = 116.72492 Kcal/ (X-V/def2-TZVP) = - -XTB) = -148.52744 -XTB) = -147.30522 -FF) = -20.49233791 .nates: 0.099354 -1.675722 -0.106581 -3.981119 -2.613951 -2.378130 -3.216457 -1.251610	PP) = -3412.30414 11198544 Hartree mol mol -3415.58704461996 11701144 Hartree 11332721 Hartree -0.336096 -1.037815 1.168039 -1.348982 -0.612522 0.528152 0.810051 1.391199	-0.050237 0.075784 1.217054 1.124036 0.943738 1.740116 2.374760 1.876049
СНННСССНСНССНСНН	-4.401452 -5.295420 -4.743648 -3.706838 1.401433 2.378174 3.635451 4.384658 3.960849 4.952712 3.023511 3.290593 1.743471 2.173679 3.168811 1.178451 1.399875 1.233946 0.135136 1.873076 2.551614	-2.189812 -2.834469 -1.246221 -2.697055 0.792191 -0.122331 0.387952 -0.311486 1.741279 2.113148 2.604258 3.659364 2.155581 -1.636523 -2.025495 -2.103589 -1.651154 -3.205980 -1.853859 -2.304640 -1.944995	2.030865 2.617564 2.846266 2.133857 2.629154 3.005269 3.410241 2.848459 3.145585 2.268804 2.101724 1.898555 2.726200 3.033394 3.800164 4.787379 3.915428 3.526300 1.373497 0.577346	E (PBEC E (PPEH E (PMG)) E (PMT) E (GFN1 E (GFN2 Coordi Co N C C C C C C	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - 3c) = -3408.86484 = 101.41495 Kcal/ = 116.72492 Kcal/ (X-V/def2-TZVP) = - -XTB) = -148.52744 -XTB) = -147.30522 -FF) = -20.49233791 nates: 0.099354 -1.675722 -0.106581 -3.981119 -2.613951 -2.378130 -3.216457 -1.251610 -1.524847	PP) = -3412.30414 11198544 Hartree (mol (mol -3415.58704461996 11701144 Hartree 11332721 Hartree -0.336096 -1.037815 1.168039 -1.348982 -0.612522 0.528152 0.810051 1.391199 2.592288	-0.050237 0.075784 1.217054 1.124036 0.943738 1.740116 2.374760 1.876049 2.853450
С н н н с с с н с н с с н с н н н с н н н н н	-4.401452 -5.295420 -4.743648 -3.706838 1.401433 2.378174 3.635451 4.384658 3.960849 4.952712 3.023511 3.290593 1.743471 2.173679 3.168811 1.178451 1.399875 1.233946 0.135136 1.873076 2.551614 0.814107	-2.189812 -2.834469 -1.246221 -2.697055 0.792191 -0.122331 0.387952 -0.311486 1.741279 2.113148 2.604258 3.659364 2.155581 -1.636523 -2.025495 -2.103589 -1.651154 -3.205980 -1.853859 -2.304640 -1.944995 -2.132366	2.030865 2.617564 2.846266 2.133857 2.629154 3.005269 3.410241 2.848459 3.145585 2.268804 2.101724 1.898555 2.726200 3.033394 3.800164 4.787379 3.915428 3.526300 1.373497 0.577346 1.057992	E (PBEC E (PBEC E (PMG)) E (PMG)) E (GFN1 E (GFN2 Coordi Co N N C C C C C C C	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - 101.41495 Kcal/ = 101.41495 Kcal/ (X-V/def2-TZVP) = - -xTB) = -148.52744 -xTB) = -147.30522 -FF) = -20.49233791 .nates: 0.099354 -1.675722 -0.106581 -3.981119 -2.613951 -2.378130 -3.216457 -1.251610 -1.524847 -4.860923	PP) = -3412.30414 11198544 Hartree (mol (mol (3415.58704461996 11701144 Hartree 11332721 Hartree -0.336096 -1.037815 1.168039 -1.348982 -0.612522 0.528152 0.810051 1.391199 2.592288 -0.705079	-0.050237 0.075784 1.217054 1.124036 0.943738 1.740116 2.374760 1.876049 2.853450 2.216482
СНННСССНСНССНСНН	-4.401452 -5.295420 -4.743648 -3.706838 1.401433 2.378174 3.635451 4.384658 3.960849 4.952712 3.023511 3.290593 1.743471 2.173679 3.168811 1.178451 1.399875 1.233946 0.135136 1.873076 2.551614	-2.189812 -2.834469 -1.246221 -2.697055 0.792191 -0.122331 0.387952 -0.311486 1.741279 2.113148 2.604258 3.659364 2.155581 -1.636523 -2.025495 -2.103589 -1.651154 -3.205980 -1.853859 -2.304640 -1.944995	2.030865 2.617564 2.846266 2.133857 2.629154 3.005269 3.410241 2.848459 3.145585 2.268804 2.101724 1.898555 2.726200 3.033394 3.800164 4.787379 3.915428 3.526300 1.373497 0.577346	E (PBEC E (PPEH E (PMG)) E (PMT) E (GFN1 E (GFN2 Coordi Co N C C C C C C	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - 3c) = -3408.86484 = 101.41495 Kcal/ = 116.72492 Kcal/ (X-V/def2-TZVP) = - -XTB) = -148.52744 -XTB) = -147.30522 -FF) = -20.49233791 nates: 0.099354 -1.675722 -0.106581 -3.981119 -2.613951 -2.378130 -3.216457 -1.251610 -1.524847	PP) = -3412.30414 11198544 Hartree (mol (mol -3415.58704461996 11701144 Hartree 11332721 Hartree -0.336096 -1.037815 1.168039 -1.348982 -0.612522 0.528152 0.810051 1.391199 2.592288	-0.050237 0.075784 1.217054 1.124036 0.943738 1.740116 2.374760 1.876049 2.853450

Н	-5.141739	0.338993	1.973891	С	4.453454	0.183741	-0.273820
Н	-4.370936	-0.716070	3.210101	Н	3.730801	0.780163	0.299155
С	-4.794379	-1.322083	-0.185701	C	2.190175	-0.478081	-3.260607
H	-5.779428	-1.806335	-0.024482	C	1.049766	-1.206368	-3.659609
H	-4.286180	-1.861645	-1.004025	H	0.478756	-1.763939	-2.902491
Н	-4.979742	-0.279540	-0.512930	С	0.658948	-1.234410	-5.005160
C	-3.743569	-2.814955	1.547295	Н	-0.219513	-1.827601	-5.303000
H	-4.715864	-3.292778	1.784733	C	1.388260	-0.517767	-5.969040
H	-3.106614	-2.875706	2.452394	H	1.076385	-0.533067	-7.024447
H	-3.271885	-3.408754	0.744378	С	2.522277	0.214472	-5.580470
C	-1.947816	2.029868	4.234091	Н	3.097508	0.780467	-6.329620
H	-2.109786	2.868970	4.941165	C	2.927986	0.225822	-4.238298
H	-1.154483	1.380314	4.656000	H	3.818065	0.797175	-3.933911
H	-2.883696	1.441018	4.198161				
С	-2.678910	3.428809	2.246161	Confo	rmation 27.		
Н	-2.904308	4.293207	2.904088		plicity: 4		
H	-3.608393	2.841564	2.122468	Charg			
H	-2.393200	3.823037	1.249991	E(B97	(-3c) = -3413.527900	)609814 Hartree	
C	-0.365962	3.570864	3.125898	E (M06	f/def2-TZVP) = -3413	3.218268966413 Ha	rtree
Н	-0.749163	4.366066	3.797583		- D3(BJ)/def2-TZVF		
H							
	0.014246	4.059903	2.213806		0 - D3(BJ)/def2-TZV		38U363U Hartree
H	0.493781	3.095453	3.628930	E(PBE	h-3c) = -3408.86198	35515107 Hartree	
С	-1.729035	-2.070544	-0.898051	E(PM6	i) = 104.83845 Kcal/	mol	
С	-1.208636	-3.362363	-0.543477	E(PM7	) = 111.70127 Kcal/	mol	
Č	-1.219392	-4.391609	-1.495370		7X-V/def2-TZVP) = -		0 Hartree
							U naitiee
H	-0.831200	-5.383441	-1.220448		11-xTB) = $-148.52708$		
C	-1.703376	-4.171365	-2.791243	E (GFN	(2-xTB) = -147.30301	.8689219 Hartree	
H	-1.714409	-4.989226	-3.526802	E (GFN	I-FF) = -20.49292598	31894 Hartree	
С	-2.124275	-2.889840	-3.153806		,		
				~			
H	-2.442637	-2.706601	-4.192494		linates:		
C	-2.125774	-1.804443	-2.250222	Co	0.315487	-0.117045	-0.137706
C	-0.534034	-3.588286	0.806992	N	-0.479683	1.076984	1.265000
Н	-0.892138	-2.798576	1.497690	N	-0.475661	0.709218	-1.690937
С	-0.846151	-4.947438	1.447047	C	-1.577513	3.331105	1.904620
H	-1.935610	-5.119624	1.550384	С	-1.203505	2.155317	0.922368
H	-0.392617	-5.005554	2.457183	С	-1.580603	2.414000	-0.424099
Н	-0.424937	-5.787540	0.857647	Н	-2.205619	3.298155	-0.537148
C	0.987347	-3.405771	0.648712	C	-1.288760	1.775593	-1.652881
H	1.238404	-2.422364	0.192432	С	-2.027229	2.383957	-2.894328
H	1.413450	-4.181301	-0.020818	C	-2.979384	3.918549	1.599386
Н	1.504788	-3.466381	1.626861	Н	-3.230074	4.669832	2.374663
С	-2.456553	-0.438309	-2.883957	H	-3.765158	3.138212	1.619335
H	-1.775202	-0.404889	-3.764235	H	-3.038377	4.440884	0.625471
C	-2.143733	0.833422	-2.088836	С	-1.571040	3.016691	3.415005
Н	-1.080121	0.863119	-1.774736	H	-1.888661	3.931603	3.955859
	-2.775074						
H		0.951712	-1.187832	H	-0.577906	2.734793	3.799255
H	-2.309139	1.716239	-2.739986	H	-2.273728	2.207859	3.682319
C	-3.885300	-0.368296	-3.461327	С	-0.518755	4.433343	1.644190
H	-4.136223	-1.261799	-4.065986	H	-0.713742	5.310535	2.295960
H	-3.982979	0.520220	-4.117699	H	-0.537337	4.770351	0.589109
H	-4.646070	-0.279764	-2.663351	H	0.502064	4.066589	1.866364
C	1.103315	1.904593	1.351502	С	-1.933771	3.930459	-2.892789
С	2.041949	1.525137	2.351407	Н	-2.429981	4.324885	-3.802555
C							-2.907235
	3.251972	2.236177	2.442503	H	-0.879704	4.270204	
H	3.978147	1.960272	3.222777	H	-2.433490	4.400628	-2.024964
С	3.554125	3.275511	1.553235	C	-3.515683	1.973663	-2.770972
H	4.508834	3.816011	1.635410	H	-4.096472	2.385839	-3.622345
C		3.603312				2.347637	-1.829513
	2.642039		0.541789	H	-3.963431		
H	2.887905	4.405858	-0.170708	H	-3.627104	0.871641	-2.784572
C	1.410296	2.936227	0.420599	C	-1.513917	1.925347	-4.273238
С	1.785442	0.338615	3.274414	H	-2.069599	2.482716	-5.054555
Н	0.733887	0.021420	3.121021	Н	-1.672863	0.850482	-4.458256
C	2.685695	-0.842205	2.867847	H	-0.437452	2.132672	-4.413125
H	2.549949	-1.087707	1.796626	С	-0.281077	0.593508	2.586459
H	2.455621	-1.744608	3.472010	С	0.918006	0.895602	3.294570
H	3.757829	-0.597409	3.018336	С	1.067591	0.428099	4.612021
C	1.952181	0.680815	4.762548	Н	1.984599	0.675187	5.168590
H	1.292703	1.517711	5.068048	С	0.079104	-0.350801	5.224089
H	2.995269	0.971707	5.003725	H	0.204141	-0.699826	6.260176
H	1.702995	-0.196896	5.393405	C	-1.052567	-0.716739	4.485466
C	0.431422	3.337282	-0.678830	Н	-1.811766	-1.373812	4.939448
H	-0.492358	2.744835	-0.519878	С	-1.253420	-0.278692	3.161843
C	0.969522	2.980344	-2.075299	C	2.043587	1.696277	2.653142
H	0.235099	3.257272	-2.859739	H	1.643926	2.116378	1.706876
Н	1.169952	1.896156	-2.159955	C	2.519785	2.870836	3.522909
H	1.916039	3.517840	-2.294085	H	1.683891	3.535072	3.820799
С	0.049199	4.825262	-0.604537	H	3.264439	3.483303	2.974047
H	-0.364517	5.096941	0.386927	H	3.011663	2.516054	4.451890
Н	-0.714228	5.068948	-1.371429	C	3.217417	0.766006	2.296109
H	0.924564	5.481367	-0.789642	H	2.877159	-0.061591	1.644757
N	1.663811	-0.268577	-0.903759	H	3.651917	0.311422	3.210122
С	2.561028	-0.407077	-1.809405	H	4.023042	1.326376	1.777690
C	4.007046	-0.484644	-1.434022	C	-2.500587	-0.796448	2.438892
С	4.929625	-1.249483	-2.181557	H	-2.900274	-1.580774	3.117882
H	4.587483	-1.783512	-3.080854	C	-2.211538	-1.500981	1.105768
C	6.267276	-1.346974	-1.770957	H	-1.394623	-2.241012	1.198313
Н	6.974023	-1.955895	-2.355782	Н	-1.938164	-0.774170	0.310454
С	6.704031	-0.672083	-0.619081	H	-3.118566	-2.030533	0.748703
H	7.756539	-0.742408	-0.304248	C	-3.626335	0.237734	2.269736
С	5.791525	0.095285	0.126282	H	-3.884178	0.728380	3.229397
Н	6.125184	0.636609	1.025424	Н	-4.542559	-0.258897	1.888162
11	0.123104	0.00000	1.023424	11	4.74777	0.230031	1.000102

H	-3.348218	1.020471	1.537665	H	1.360899	-3.720277	-2.962701
C	0.093348	0.037725	-2.802129	С	1.696691	2.951401	-3.600047
С	-0.585155	-1.067266	-3.400963	H	1.840722	3.880657	-4.189039
C	0.007402	-1.708661	-4.500362	H	1.902057	2.091018	-4.265227
Н	-0.517172	-2.551328	-4.975686	H	2.457448	2.938883	-2.793561
C	1.254336	-1.306599	-4.994497	C	0.076677	4.244361	-2.238121
Н	1.697888	-1.812940	-5.865097	Н	0.251244	5.075836	-2.951763
C	1.949128	-0.276657	-4.347273	Н	0.784241	4.369856	-1.401352
Н	2.950892	0.014690	-4.701782	Н	-0.941299	4.362658	-1.828149
C	1.403485	0.403070	-3.242750	C	-0.786575	2.918914	-4.137252
C	-1.906324	-1.579560	-2.842350	Н	-0.709610	3.861057	-4.717823
Н	-2.288664	-0.807103	-2.143879	H	-1.811964	2.861813	-3.719360
		-1.802825		Н	-0.666253	2.078706	-4.847314
C	-2.973963 -3.135675		-3.924315	н С			
H H		-0.894197	-4.538600	C	0.419166	-2.608659	-0.792242
	-3.942469	-2.078727	-3.459679		1.762406	-3.026629	-0.541663
H	-2.695112	-2.628341	-4.611012	С	1.967516	-4.250954	0.114010
C	-1.666368	-2.860020	-2.022994	H	2.996221	-4.594855	0.297585
H	-0.936015	-2.676567	-1.212255	С	0.889080	-5.033717	0.554010
H	-1.253988	-3.671742	-2.656575	H	1.072759	-5.988738	1.068172
H	-2.611139	-3.219164	-1.566408	С	-0.421970	-4.586610	0.347622
С	2.272129	1.456632	-2.555415	H	-1.265826	-5.192723	0.711358
H	3.242648	1.411191	-3.095146	С	-0.685212	-3.380256	-0.325158
С	2.590375	1.113426	-1.091833	С	2.931372	-2.118929	-0.905034
Н	3.412975	1.748078	-0.703357	Н	2.592071	-1.443244	-1.715886
H	2.895502	0.057355	-0.960304	С	3.289784	-1.223939	0.296988
H	1.727428	1.340789	-0.414390	H	2.398687	-0.684074	0.678663
C	1.770934	2.905167	-2.679098	H	4.056033	-0.472439	0.016345
H	1.542190	3.169463	-3.730525	H	3.685039	-1.828444	1.138653
H	2.549463	3.607988	-2.316880	С	4.159754	-2.876078	-1.424130
H	0.863239	3.075979	-2.068767	H	3.903595	-3.538687	-2.275982
N	1.123954	-1.546218	0.582389	H	4.623841	-3.504018	-0.635838
C	1.653619	-2.711635	0.655124	H	4.936164	-2.162004	-1.765639
C	1.602319	-3.684789	-0.487707	С	-2.121481	-2.918878	-0.549888
C	1.251592	-5.034912	-0.262407	H	-2.071898	-1.979242	-1.142005
H	1.045437	-5.371994	0.764909	С	-2.824631	-2.595804	0.780435
C	1.153302	-5.936587	-1.331643	H	-2.270723	-1.825239	1.353795
H	0.861742	-6.981227	-1.142027	H	-2.909608	-3.497791	1.420826
C	1.435801	-5.507240	-2.641570	H	-3.848820	-2.211312	0.598728
H	1.376707	-6.217407	-3.480601	С	-2.930157	-3.936103	-1.372517
С	1.795349	-4.169899	-2.872056	H	-2.449769	-4.150583	-2.348328
H	2.019245	-3.822718	-3.890883	H	-3.952496	-3.554319	-1.571104
C	1.861719	-3.260573	-1.807123	H	-3.032397	-4.900132	-0.833102
H	2.117979	-2.207549	-1.998166	С	-0.404328	2.576848	0.014640
С	2.346316	-3.143841	1.911632	С	-1.755828	3.007908	0.138583
C	1.941693	-2.593223	3.146587	С	-2.049700	4.041382	1.044714
H	1.097746	-1.890448	3.156316	H	-3.088611	4.391726	1.142864
С	2.600810	-2.941263	4.330932	С	-1.047926	4.621576	1.835116
H	2.263166	-2.505288	5.283676	H	-1.296069	5.430961	2.537362
С	3.681088	-3.840202	4.302009	С	0.267081	4.149397	1.739859
H	4.200657	-4.113034	5.233475	H	1.048758	4.589037	2.378658
С	4.093212	-4.392012	3.077837	С	0.614030	3.123925	0.842301
Н	4.942129	-5.092422	3.046407	C	-2.871830	2.323759	-0.643422
С	3.428129	-4.052155	1.890699	Н	-2.398786	1.755798	-1.470354
Н	3.757225	-4.482350	0.932852	С	-3.583949	1.298441	0.259111
				Н	-2.850863	0.605405	0.720154
Confor	mation 28.			H	-4.325047	0.703435	-0.314114
	olicity: 4			Н	-4.116751	1.803564	1.091234
Charge				C	-3.865057	3.310790	-1.272096
	-3c) = $-3413.540469$	9089547 Hartree		Н	-3.349091	4.052363	-1.915508
	def2-TZVP) = -3413		rt.ree	Н	-4.434102	3.872197	-0.502440
	- D3(BJ)/def2-TZVI			H	-4.605901	2.771452	-1.896849
	- D3(BJ)/def2-TZV				2.054718	2.629214	0.766518
	1-3c) = -3408.88149			Н	2.084599	1.838127	-0.011272
	= 94.93429 Kcal/r			С	2.499420	1.990579	2.092625
	= 109.90711 Kcal,			Н	3.535017	1.601658	2.011450
	X-V/def2-TZVP) = -		3 Hartree	H	1.837126	1.150662	2.373206
	-xTB) = $-148.54056$			Н	2.481640	2.729892	2.919965
	2-xTB) = $-147.31993$			С	3.025663	3.746192	0.344736
	-FF) = $-20.50468112$			Н	2.743794	4.194712	-0.628659
				Н	4.059361	3.354074	0.251730
Coordi	.nates:			H	3.047886	4.565225	1.093614
Co	-0.243746	-0.214629	0.088515	N	-0.427489	-0.047351	1.851404
N	0.182779	-1.344777	-1.387044	C	-0.403733	-0.283831	3.111920
N	-0.102051	1.501159	-0.863815	Č	0.667363	-1.132134	3.727495
C	0.443793	-1.917764	-3.879222	Č	1.158764	-2.253457	3.025794
Č	0.317346	-0.949778	-2.661128	Н	0.716260	-2.511173	2.052986
C	0.290029	0.425021	-2.985848	C	2.186682	-3.036331	3.566228
Н	0.420767	0.632785	-4.050013	Н	2.543478	-3.916236	3.009961
C	0.130700	1.585747	-2.183786	C	2.752565	-2.702045	4.808005
Č	0.267475	2.919210	-3.001755	Н	3.560915	-3.317314	5.232757
Č	-0.793753	-1.684454	-4.781708	C	2.278849	-1.580368	5.508834
Н	-0.751095	-2.359380	-5.661451	Н	2.724915	-1.306329	6.477404
Н	-0.856907	-0.643712	-5.152600	C	1.237112	-0.805834	4.978842
Н	-1.729445	-1.903195	-4.227890	Н	0.866635	0.071840	5.529870
C	1.733458	-1.597556	-4.668887	C	-1.465792	0.291448	3.996047
Н	1.813926	-2.275457	-5.543292	C	-1.942818	-0.398202	5.132383
Н	2.633206	-1.748924	-4.039003	Н	-1.497844	-1.367345	5.404109
Н	1.754359	-0.557590	-5.047191	C	-2.989465	0.135915	5.898486
C	0.471606	-3.420354	-3.544988	Н	-3.359451	-0.416388	6.775989
Н	0.490531	-3.983988	-4.500005	С	-3.563548	1.369409	5.549760
Н	-0.421459	-3.747524	-2.982988	Н	-4.379981	1.788959	6.157836

С	-3.084741	2.066518	4.426387	С	-1.122980	-0.491913	3.138431
H	-3.516243	3.042090	4.153346	С	2.665351	-1.039816	2.511625
С	-2.050330	1.529403	3.651676	H	2.420037	-1.510871	1.536983
H	-1.668780	2.063266	2.770903	С	3.448297	0.254821	2.228737
				Н	2.834905	0.970464	1.643999
Conform	mation 29.			Н	4.375557	0.047377	1.656536
	licity: 4			Н	3.739295	0.759159	3.173391
Charge:				C	3.511243	-2.046505	3.306530
		242741 !!		Н			
	3c) = -3413.522536				2.958986	-2.991788	3.481351
	def2-TZVP) = -3413			H	3.806273	-1.642131	4.296767
	- D3(BJ)/def2-TZVI			Н	4.443334	-2.293341	2.757891
	- D3(BJ)/def2-TZV		2016722 Hartree	C	-2.444515	-0.523193	2.379217
	-3c) = -3408.85896			H	-2.305682	-1.174881	1.493354
	= 109.03085 Kcal,			С	-2.771795	0.890530	1.863291
E(PM7)	= 117.05991 Kcal,	/mol		H	-3.692507	0.885696	1.245623
E (ωB97Σ	X-V/def2-TZVP) = -	-3415.577131082867	7 Hartree	H	-1.941554	1.287662	1.246273
E (GFN1-	-xTB) = $-148.5246$	78972839 Hartree		H	-2.917952	1.596676	2.706300
E (GFN2-	-xTB) = $-147.30103$	10405657 Hartree		C	-3.607210	-1.103058	3.197015
E (GFN-I	FF) = -20.4893090	74126 Hartree		H	-3.367239	-2.108008	3.599887
				H	-4.512823	-1.195945	2.563552
Coordin	nates:			H	-3.877076	-0.453356	4.055147
Co	0.468167	0.107570	0.035649	N	0.487904	1.896371	-0.048887
N	0.026595	-0.762849	-1.689490	C	0.417677	3.140020	0.251440
N	0.086625	-1.385977	1.185640	C	-0.291697	3.606056	1.491077
			-3.118885	C			
C	-0.636223	-2.846635			-0.038327	2.995316	2.736094
C	-0.333602	-2.051623	-1.785425	H	0.710190	2.191511	2.803306
C	-0.470167	-2.861009	-0.624192	C	-0.734107	3.406864	3.881368
H	-0.760389	-3.891447	-0.839979	Н	-0.511518	2.930075	4.846801
С	-0.301665	-2.600171	0.754200	С	-1.715517	4.407358	3.793395
С	-0.531859	-3.848046	1.672917	H	-2.267140	4.721871	4.692625
C	-0.431797	-2.087229	-4.443602	C	-1.990431	5.005696	2.552415
H	-0.651248	-2.786724	-5.276446	H	-2.765782	5.783342	2.473429
H	0.601474	-1.721702	-4.576691	C	-1.273149	4.618764	1.411781
H	-1.106611	-1.220233	-4.549121	H	-1.479470	5.093657	0.440432
С	0.273158	-4.103463	-3.179782	С	1.014085	4.171748	-0.656052
H	0.073699	-4.650203	-4.124102	С	1.238451	3.847008	-2.012498
Н	0.089801	-4.807803	-2.346591	Н	0.936119	2.854045	-2.371320
Н	1.344797	-3.834502	-3.167310	C	1.821917	4.775447	-2.881005
C	-2.105872	-3.340257	-3.109518	Н	1.975312	4.502977	-3.936720
Н	-2.263052	-4.035814	-3.959277	C	2.200023	6.044962	-2.409430
H		-2.502973		Н	2.658994		-3.092134
	-2.818275		-3.236351			6.776577	
H	-2.371630	-3.874399	-2.177233	C	1.986363	6.376533	-1.061550
C	0.488586	-4.934952	1.245888	H	2.285704	7.366278	-0.683371
H	0.365083	-5.834911	1.883016	C	1.394384	5.450033	-0.190196
H	1.527745	-4.567843	1.370981	H	1.234737	5.713327	0.866018
H H	1.527745 0.367074	-4.567843 -5.246846	0.191270			5.713327	0.866018
H H C	1.527745 0.367074 -1.971910	-4.567843 -5.246846 -4.375952	0.191270 1.470466		1.234737 nation 6.	5.713327	0.866018
H H	1.527745 0.367074	-4.567843 -5.246846	0.191270	Conform		5.713327	0.866018
H H C	1.527745 0.367074 -1.971910	-4.567843 -5.246846 -4.375952	0.191270 1.470466	Conform	nation 6. .icity: 4	5.713327	0.866018
H H C H	1.527745 0.367074 -1.971910 -2.137223	-4.567843 -5.246846 -4.375952 -5.269695	0.191270 1.470466 2.106732	Conform Multipl Charge:	nation 6. .icity: 4		0.866018
Н Н С Н Н	1.527745 0.367074 -1.971910 -2.137223 -2.175984	-4.567843 -5.246846 -4.375952 -5.269695 -4.666227	0.191270 1.470466 2.106732 0.421977	Conform Multipl Charge: E(B97-3	nation 6. icity: 4	5288374 Hartree	
Н Н С Н Н	1.527745 0.367074 -1.971910 -2.137223 -2.175984 -2.719142	-4.567843 -5.246846 -4.375952 -5.269695 -4.666227 -3.610591	0.191270 1.470466 2.106732 0.421977 1.760090	Conform Multipl Charge: E(B97-3	nation 6. icity: 4 0 8c) = -3413.532685	5288374 Hartree 3.222124048085 Ha	rtree
Н Н С Н Н С	1.527745 0.367074 -1.971910 -2.137223 -2.175984 -2.719142 -0.329576	-4.567843 -5.246846 -4.375952 -5.269695 -4.666227 -3.610591 -3.639053 -4.621291	0.191270 1.470466 2.106732 0.421977 1.760090 3.185700	Conform Multipl Charge: E(B97-3 E(M06/c	nation 6. .icity: 4 0 8c) = -3413.53268: lef2-TZVP) = -341: - D3(BJ)/def2-TZVP	5288374 Hartree 3.222124048085 Ha P) = -3412.094209	rtree 379966 Hartree
H H C H H C H	1.527745 0.367074 -1.971910 -2.137223 -2.175984 -2.719142 -0.329576 -0.451638 -1.061488	-4.567843 -5.246846 -4.375952 -5.269695 -4.666227 -3.610591 -3.639053 -4.621291 -2.942777	0.191270 1.470466 2.106732 0.421977 1.760090 3.185700 3.686402 3.630111	Conform Multipl Charge: E(B97-3 E(M06/d E(PBE - E(PBE0	nation 6. .icity: 4 0 8c) = -3413.532689 8cef2-TZVP) = -3413 - D3(BJ)/def2-TZVV	5288374 Hartree 3.222124048085 Ha P) = -3412.094209 PP) = -3412.30834	rtree 379966 Hartree
H H C H H C H H	1.527745 0.367074 -1.971910 -2.137223 -2.175984 -2.719142 -0.329576 -0.451638 -1.061488 0.679733	-4.567843 -5.246846 -4.375952 -5.269695 -4.666227 -3.610591 -3.639053 -4.621291 -2.942777 -3.263393	0.191270 1.470466 2.106732 0.421977 1.760090 3.185700 3.686402 3.630111 3.431721	Conform Multipl Charge: E(B97-3 E(M06/6 E(PBE - E(PBE0 E(PBEh-	mation 6. .icity: 4 0 8c) = -3413.532689 lef2-TZVP) = -341. - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV	5288374 Hartree 3.222124048085 Ha P) = -3412.094209 PP) = -3412.30834 57868448 Hartree	rtree 379966 Hartree
H C H H C H H C H	1.527745 0.367074 -1.971910 -2.137223 -2.175984 -2.719142 -0.329576 -0.451638 -1.061488 0.679733 0.188994	-4.567843 -5.246846 -4.375952 -5.269695 -4.666227 -3.610591 -3.639053 -4.621291 -2.942777 -3.263393 0.152333	0.191270 1.470466 2.106732 0.421977 1.760090 3.185700 3.686402 3.630111 3.431721 -2.759797	Conform Multipl Charge: E (B97-3 E (M06/d E (PBE - E (PBE0 E (PBEh- E (PM6)	mation 6. icity: 4 0 8c) = -3413.532689 def2-TZVP) = -3413 D3 (BJ) /def2-TZVI - D3 (BJ) /def2-TZVI - D3 (BJ) /def2-TZVI - B3 (BJ) /def2-TZVI - B4	5288374 Hartree 3.222124048085 Ha P) = -3412.094209 VP) = -3412.30834 57868448 Hartree mol	rtree 379966 Hartree
Н Н С Н Н С Н Н С С С С	1.527745 0.367074 -1.971910 -2.137223 -2.175984 -2.719142 -0.329576 -0.451638 -1.061488 0.679733 0.188994 1.502745	-4.567843 -5.246846 -4.375952 -5.269695 -4.666227 -3.610591 -3.639053 -4.621291 -2.942777 -3.263393 0.152333 0.368276	0.191270 1.470466 2.106732 0.421977 1.760090 3.185700 3.686402 3.630111 3.431721 -2.759797 -3.284171	Conform Multipl Charge: E (B97-3 E (M06/d E (PBE0- E (PBE0- E (PBE0- E (PM6)- E (PM7)	mation 6. icity: 4 0 8c) = -3413.53268! def2-TZVP) = -341: D3(BJ)/def2-TZV! - D3(BJ)/def2-TZV! - D4(BJ)/def2-TZV! - D4	5288374 Hartree 3.222124048085 Ha P) = -3412.094209 JP) = -3412.30834 57868448 Hartree mol /mol	rtree 379966 Hartree 2631976 Hartree
Н Н С Н Н С Н Н С С С С	1.527745 0.367074 -1.971910 -2.137223 -2.175984 -2.719142 -0.329576 -0.451638 -1.061488 0.679733 0.188994 1.502745 1.649833	-4.567843 -5.246846 -4.375952 -5.269695 -4.666227 -3.610591 -3.639053 -4.621291 -2.942777 -3.263393 0.152333 0.368276 1.198123	0.191270 1.470466 2.106732 0.421977 1.760090 3.185700 3.686402 3.630111 3.431721 -2.759797 -3.284171 -4.409433	Conform Multipl Charge: E(B97-3 E(M06/d E(PBE - E(PBE0- E(PBEh- E(PM6) E(PM7) E(WB97X	mation 6. .icity: 4 0 0c) = -3413.53268: def2-TZVP) = -341: D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - 3c) = -3408.8707! = 99.67616 Kcal/r = 114.02554 Kcal, (-V/def2-TZVP) = -	5288374 Hartree 3.222124048085 Ha P) = -3412.094209 JP) = -3412.30834 57868448 Hartree mol mol mol -3415.58905904635	rtree 379966 Hartree 2631976 Hartree
Н Н С Н Н С Н Н С С С С Н	1.527745 0.367074 -1.971910 -2.137223 -2.175984 -2.719142 -0.329576 -0.451638 -1.061488 0.679733 0.188994 1.502745 1.649833 2.657969	-4.567843 -5.246846 -4.375952 -5.269695 -4.666227 -3.610591 -3.639053 -4.621291 -2.942777 -3.263393 0.152333 0.368276 1.198123 1.341430	0.191270 1.470466 2.106732 0.421977 1.760090 3.185700 3.686402 3.630111 3.431721 -2.759797 -3.284171 -4.409433 -4.830228	Conform Multipl Charge: E (B97-3 E (M06/d E (PBE - E (PBE0 E (PBEh- E (PM6) E (PM7) E (GFN1-	mation 6. .icity: 4 0 8c) = -3413.532689 lef2-TZVP) = -341. - D3(BJ)/def2-TZV- - D3(BJ)/def2-TZV- - 3c) = -3408.87079 = 99.67616 Kcal/r = 114.02554 Kcal/r - V/def2-TZVP) = - - xTB) = -148.53509	5288374 Hartree 3.222124048085 Ha P) = -3412.094209 PF) = -3412.30834 57868448 Hartree nol /mol -3415.58905904635 57129350 Hartree	rtree 379966 Hartree 2631976 Hartree
Н Н С Н Н С Н Н С С С С Н С С С С С С С	1.527745 0.367074 -1.971910 -2.137223 -2.175984 -2.719142 -0.329576 -0.451638 -1.061488 0.679733 0.188994 1.502745 1.649833 2.657969 0.552253	-4.567843 -5.246846 -4.375952 -5.269695 -4.666227 -3.610591 -3.639053 -4.621291 -2.942777 -3.263393 0.152333 0.368276 1.198123 1.341430 1.846017	0.191270 1.470466 2.106732 0.421977 1.760090 3.185700 3.686402 3.630111 3.431721 -2.759797 -3.284171 -4.409433 -4.830228 -4.990401	Conform Multipl Charge: E (B97-3 E (M06/6 E (PBE - E (PBE0) E (PBEh- E (PM6)) E (PM7) E (GFN1- E (GFN1- E (GFN1-	mation 6. .icity: 4 0 8c) = -3413.532689 def2-TZVP) = -3413 - D3 (BJ) /def2-TZVI - D3 (BJ) /def2-TZVI 3c) = -3408.87079 = 99.67616 Kcal/r = 114.02554 Kcal/r = 114.02554 Kcal/r - C-V/def2-TZVP) = - .*xTB) = -148.53509 .*xTB) = -147.31314	5288374 Hartree 3.222124048085 Ha P) = -3412.094209 VP) = -3412.30834 57868448 Hartree mol /mol -3415.58905904635 57129350 Hartree 45160225 Hartree	rtree 379966 Hartree 2631976 Hartree
Н Н С Н Н С Н Н С С С Н С С Н Н С С Н Н С С Н Н С С С С С С С С С С С С С С С С С С С С	1.527745 0.367074 -1.971910 -2.137223 -2.175984 -2.719142 -0.329576 -0.451638 -1.061488 0.679733 0.188994 1.502745 1.649833 2.657969 0.552253 0.680785	-4.567843 -5.246846 -4.375952 -5.269695 -4.666227 -3.610591 -3.639053 -4.621291 -2.942777 -3.263393 0.152333 0.368276 1.198123 1.341430 1.846017 2.471147	0.191270 1.470466 2.106732 0.421977 1.760090 3.185700 3.686402 3.630111 3.431721 -2.759797 -3.284171 -4.409433 -4.830228 -4.990401 -5.886515	Conform Multipl Charge: E (B97-3 E (M06/6 E (PBE - E (PBE0) E (PBEh- E (PM6)) E (PM7) E (GFN1- E (GFN1- E (GFN1-	mation 6. .icity: 4 0 8c) = -3413.532689 lef2-TZVP) = -341. - D3(BJ)/def2-TZV- - D3(BJ)/def2-TZV- - 3c) = -3408.87079 = 99.67616 Kcal/r = 114.02554 Kcal/r - V/def2-TZVP) = - - xTB) = -148.53509	5288374 Hartree 3.222124048085 Ha P) = -3412.094209 VP) = -3412.30834 57868448 Hartree mol /mol -3415.58905904635 57129350 Hartree 45160225 Hartree	rtree 379966 Hartree 2631976 Hartree
Н Н С Н Н С Н Н С С С Н С С Н С С С Н С С С С С С С С С С С С С С С С С С С С	1.527745 0.367074 -1.971910 -2.137223 -2.175984 -2.719142 -0.329576 -0.451638 -1.061488 0.679733 0.188994 1.502745 1.649833 2.657969 0.552253 0.680785 -0.699025	-4.567843 -5.246846 -4.375952 -5.269695 -4.666227 -3.610591 -3.639053 -4.621291 -2.942777 -3.263393 0.152333 0.368276 1.198123 1.341430 1.846017 2.471147 1.728756	0.191270 1.470466 2.106732 0.421977 1.760090 3.185700 3.686402 3.630111 3.431721 -2.759797 -3.284171 -4.409433 -4.830228 -4.990401 -5.886515 -4.380242	Conform Multipl Charge: E (B97-3 E (M06/d E (PBE - E (PBE) E (PBE) E (PM6) E (PM7) E (GFN1- E (GFN2- E (GFN-F	mation 6. icity: 4 0 8c) = -3413.532688 8ef2-TZVP) = -3413 D3(BJ)/def2-TZVI D3(BJ)/def2-TZVI D3(BJ)/def2-TZVI D3(BJ)/def2-TZVI D3(BJ)/def2-TZVI B99.67616 Kcal/f = 114.02554 Kcal/f (-V/def2-TZVP) = -448.53508 EXTB) = -147.31314 FF) = -20.50069816	5288374 Hartree 3.222124048085 Ha P) = -3412.094209 VP) = -3412.30834 57868448 Hartree mol /mol -3415.58905904635 57129350 Hartree 45160225 Hartree	rtree 379966 Hartree 2631976 Hartree
Н Н С Н Н С Н Н С С С Н С Н С Н С Н С Н	1.527745 0.367074 -1.971910 -2.137223 -2.175984 -2.719142 -0.329576 -0.451638 -1.061488 0.679733 0.188994 1.502745 1.649833 2.657969 0.552253 0.680785 -0.699025 -1.555117	-4.567843 -5.246846 -4.375952 -5.269695 -4.666227 -3.610591 -3.639053 -4.621291 -2.942777 -3.263393 0.152333 0.368276 1.198123 1.341430 1.846017 2.471147 1.728756 2.289439	0.191270 1.470466 2.106732 0.421977 1.760090 3.185700 3.686402 3.630111 3.431721 -2.759797 -3.284171 -4.409433 -4.830228 -4.990401 -5.886515 -4.380242 -4.789033	Conform Multipl Charge: E (B97-3 E (M06/d E (PBE - E (PBE0- E (PBE0- E (PM6) E (PM7) E (GFN1- E (GFN1- E (GFN2- E (GFN-F	mation 6icity: 4 0 0c) = -3413.532688 def2-TZVP) = -3413.532688 def2-TZVP) = -3413.532688 def2-TZVP) = -3413.532688 def2-TZVP) = -3408.87078 = 99.67616 Kcal/r = 114.02554 Kcal/c-V/def2-TZVP) = -32788 = -148.53508 exTB) = -147.31314 exTB) = -147.31314 exTB) = -20.50069816	5288374 Hartree 3.222124048085 Ha 2) = -3412.094209 2P) = -3412.30834 57868448 Hartree mol /mol -3415.58905904635 57129350 Hartree 45160225 Hartree 17896 Hartree	rtree 379966 Hartree 2631976 Hartree 9 Hartree
Н Н С Н Н Н С С С С Н С Н С Н С С С С Н С Н С С С Н С С Н С С С Н С С С Н С С С Н С С С Н С С С Н С С С Н С С С Н С С С Н С С С С Н С С С С Н С С С С Н С С С С Н С С С С С С Н С С С С С Н С С С С С С С С С С С С С С С С С С С С	1.527745 0.367074 -1.971910 -2.137223 -2.175984 -2.719142 -0.329576 -0.451638 -1.061488 0.679733 0.188994 1.502745 1.649833 2.657969 0.552253 0.680785 -0.699025 -1.555117 -0.911465	-4.567843 -5.246846 -4.375952 -5.269695 -4.666227 -3.610591 -3.639053 -4.621291 -2.942777 -3.263393 0.152333 0.368276 1.198123 1.341430 1.846017 2.471147 1.728756 2.289439 0.922217	0.191270 1.470466 2.106732 0.421977 1.760090 3.185700 3.686402 3.630111 3.431721 -2.759797 -3.284171 -4.409433 -4.830228 -4.990401 -5.886515 -4.380242 -4.789033 -3.241669	Conform Multipl Charge: E (B97-3 E (M06/6 E (PBE) E (PBE) E (PM6) E (PM7) E (WB97X E (GFN1-E (GFN2-E (GFN-E) Coordin	mation 6. .icity: 4 0 0c) = -3413.532689 def2-TZVP) = -3411 - D3(BJ)/def2-TZV- -3c) = -3408.87079 = 99.67616 Kcal/r = 114.02554 Kcal/r = 114.02554 Kcal/r -147.02554 Kcal/r = 114.02554 Kcal/r = 115.0256 Kcal/r = 115.02	5288374 Hartree 3.22124048085 Ha 2) = -3412.094209 279 = -3412.30834 57868448 Hartree mol fmol -3415.58905904635 57129350 Hartree 45160225 Hartree 07896 Hartree 0.251105	rtree 379966 Hartree 2631976 Hartree 9 Hartree -0.055104
Н Н С Н Н Н С С С Н С Н С Н С С С С Н С С С С	1.527745 0.367074 -1.971910 -2.137223 -2.175984 -2.719142 -0.329576 -0.451638 -1.061488 0.679733 0.188994 1.502745 1.649833 2.657969 0.552253 0.680785 -0.699025 -1.555117 -0.911465 2.782859	-4.567843 -5.246846 -4.375952 -5.269695 -4.666227 -3.610591 -3.639053 -4.621291 -2.942777 -3.263393 0.152333 0.368276 1.198123 1.341430 1.846017 2.471147 1.728756 2.289439 0.922217 -0.213551	0.191270 1.470466 2.106732 0.421977 1.760090 3.185700 3.686402 3.630111 3.431721 -2.759797 -3.284171 -4.409433 -4.830228 -4.990401 -5.886515 -4.380242 -4.789033 -3.241669 -2.676614	Conform Multipl Charge: E (B97-3 E (M06/6 E (PBE - E (PBE0 - E (PBE0 - E (PM7) E (GFN1- E (GFN2- E (GFN-F	mation 6icity: 4 0 8c) = -3413.532689 8ef2-TZVP) = -3413 - D3 (BJ) /def2-TZVI - D3 (BJ) /def2-TZVI = 99.67616 Kcal/r = 114.02554 Kcal/r = 114.02554 Kcal/r = 174.02554 Kcal/r = 174.02554 Kcal/r = 174.02554 Kcal/r = 174.02554 Kcal/r = 174.03550	5288374 Hartree 3.222124048085 Ha 2) = -3412.094209 27) = -3412.30834 57868448 Hartree nol /mol -3415.58905904635 57129350 Hartree 15160225 Hartree 07896 Hartree 0.251105 -1.536927	rtree 379966 Hartree 2631976 Hartree 9 Hartree -0.055104 -0.711237
Н Н С Н Н Н С С С С Н С Н С Н С Н С Н С	1.527745 0.367074 -1.971910 -2.137223 -2.175984 -2.719142 -0.329576 -0.451638 -1.061488 0.679733 0.188994 1.502745 1.649833 2.657969 0.552253 0.680785 -0.699025 -1.555117 -0.911465 2.782859 3.599302	-4.567843 -5.246846 -4.375952 -5.269695 -4.666227 -3.610591 -3.639053 -4.621291 -2.942777 -3.263393 0.152333 0.368276 1.198123 1.341430 1.846017 2.471147 1.728756 2.289439 0.922217 -0.213551 0.286233	0.191270 1.470466 2.106732 0.421977 1.760090 3.185700 3.686402 3.630111 3.431721 -2.759797 -3.284171 -4.409433 -4.830228 -4.990401 -5.886515 -4.380242 -4.789033 -3.241669 -2.676614 -3.241539	Conform Multipl Charge: E (B97-3 E (M06/d E (PBE - E (PBE) - E (PBE) - E (PM7) E (GFN1- E (GFN1- E (GFN-F Coordin Co	mation 6icity: 4 0 8c) = -3413.532688 8ef2-TZVP) = -3413 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI = 99.67616 Kcal/r = 114.02554 Kcal/r = 114.02554 Kcal/r = 114.02554 Kcal/r = 114.03554	5288374 Hartree 3.222124048085 Ha 2) = -3412.094209 VP) = -3412.30834 57868448 Hartree mol /mol -3415.58905904635 57129350 Hartree 45160225 Hartree 0.251105 -1.536927 0.291787	rtree 379966 Hartree 2631976 Hartree 9 Hartree -0.055104 -0.711237 1.474187
Н Н С Н Н Н С С С Н С Н С С Н С Н С Н С	1.527745 0.367074 -1.971910 -2.137223 -2.175984 -2.719142 -0.329576 -0.451638 -1.061488 0.679733 0.188994 1.502745 1.649833 2.657969 0.552253 0.680785 -0.699025 -1.555117 -0.911465 2.782859 3.599302 3.009268	-4.567843 -5.246846 -4.375952 -5.269695 -4.666227 -3.610591 -3.639053 -4.621291 -2.942777 -3.263393 0.152333 0.368276 1.198123 1.341430 1.846017 2.471147 1.728756 2.289439 0.922217 -0.213551 0.286233 0.170489	0.191270 1.470466 2.106732 0.421977 1.760090 3.185700 3.686402 3.630111 3.431721 -2.759797 -3.284171 -4.409433 -4.830228 -4.990401 -5.886515 -4.380242 -4.789033 -3.241669 -2.676614 -3.241539 -1.207300	Conform Multipl Charge: E (B97-3 E (M06/d E (PBE - E (PBE0- E (PBE0- E (PM6) E (PM7) E (GFN1- E (GFN2- E (GFN-F Coordin Co N N C	mation 6icity: 4 0 8c) = -3413.532688 8ef2-TZVP) = -3413 D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI = 99.67616 Kcal/r = 114.02554 Kcal/r (-V/def2-TZVP) = -0.0000000000000000000000000000000000	5288374 Hartree 3.222124048085 Ha 2) = -3412.094209 VP) = -3412.30834 77868448 Hartree mol /mol -3415.58905904635 77129350 Hartree 45160225 Hartree 07896 Hartree  0.251105 -1.536927 0.291787 -3.607236	rtree 379966 Hartree 2631976 Hartree 9 Hartree -0.055104 -0.711237 1.474187 -0.718265
Н Н С Н Н С Н Н С С С Н С Н С С С Н С Н С Н	1.527745 0.367074 -1.971910 -2.137223 -2.175984 -2.719142 -0.329576 -0.451638 -1.061488 0.679733 0.188994 1.502745 1.649833 2.657969 0.552253 0.680785 -0.699025 -1.555117 -0.911465 2.782859 3.599302 3.009268 2.807746	-4.567843 -5.246846 -4.375952 -5.269695 -4.666227 -3.610591 -3.639053 -4.621291 -2.942777 -3.263393 0.152333 0.368276 1.198123 1.341430 1.846017 2.471147 1.728756 2.289439 0.922217 -0.213551 0.286233 0.170489 1.240545	0.191270 1.470466 2.106732 0.421977 1.760090 3.185700 3.686402 3.630111 3.431721 -2.759797 -3.284171 -4.409433 -4.830228 -4.990401 -5.886515 -4.380242 -4.789033 -3.241669 -2.676614 -3.241539 -1.207300 -1.017928	Conform Multipl Charge: E (B97-3 E (M06/6 E (PBE - E (PBE0) E (PM7) E (WB97X E (GFN1- E (GFN2- E (GFN-F Coordin Co	mation 6icity: 4 0 0c) = -3413.532689 def2-TZVP) = -3413 - D3(BJ)/def2-TZV3c) = -3408.87079 = 99.67616 Kcal/r = 114.02554 Kcal/r -174.02554 Kcal/r -174.02554 Kcal/r -175.0256 Kcal/r -175.	5288374 Hartree 3.22124048085 Ha 2) = -3412.094209 279 = -3412.30834 57868448 Hartree mol fmol -3415.58905904635 57129350 Hartree 45160225 Hartree 07896 Hartree  0.251105 -1.536927 0.291787 -3.607236 -2.236812	rtree 379966 Hartree 2631976 Hartree 9 Hartree -0.055104 -0.711237 1.474187 -0.718265 -0.179045
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Н Н С Н Н Н С С С Н С Н С Н С Н С Н Н Н С Н Н Н С Н Н Н С Н Н Н С	1.527745 0.367074 -1.971910 -2.137223 -2.175984 -2.719142 -0.329576 -0.451638 -1.061488 0.679733 0.188994 1.502745 1.649833 2.657969 0.552253 0.680785 -0.699025 -1.555117 -0.911465 2.782859 3.599302 3.009268 2.807746 4.051911 2.379282 2.983153 2.821437 2.295206 4.018326 -2.306428 -3.011684 -2.422033 -2.113270 -1.776081 -3.467728 -2.809613	-4.567843 -5.246846 -4.375952 -5.269695 -4.666227 -3.610591 -3.639053 -4.621291 -2.942777 -3.263393 0.152333 0.368276 1.198123 1.341430 1.846017 2.471147 1.728756 2.289439 0.922217 -0.213551 0.286233 0.170489 1.240545 -0.053544 -0.454983 -1.723795 -2.030876 -2.304053 -2.09863 1.054270 1.067761 2.432317 3.258857 2.467191 2.616892 -0.026737	0.191270 1.470466 2.106732 0.421977 1.760090 3.185700 3.686402 3.630111 3.431721 -2.759797 -3.284171 -4.409433 -4.830228 -4.990401 -5.886515 -4.380242 -4.789033 -3.241669 -2.676614 -3.241539 -1.207300 -1.017928 -0.901378 -0.521176 -2.869026 -3.921176 -2.224906 -2.589359 -2.608167 -3.470265 -1.919135 -2.588516 -1.021778 -1.597787 -1.645987	Conform Multipl Charge: E(B97-3 E(M06/6 E(PBE - E(PBE0 - E(PM6)) E(PM7) E(WB97X E(GFN1-E(GFN2-E(GFN-E)) COORDINATION CO N C C C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C C H C C C C H C C C C H C C C C C C C C C C C C C C C C C C C C	mation 6icity: 4 0 0c) = -3413.53268! def2-TZVP) = -341: - D3(BJ)/def2-TZV -3c) = -3408.8707! = 99.67616 Kcal/r = 114.02554 Kcal, -(-V/def2-TZVP) = -148.5350! extB) = -147.3131. extB) = -147.3131. extB) = -20.50069810  mates:  0.007013 0.505242 1.148615 2.079556 1.524447 2.239800 3.067312 2.118988 3.226605 1.309237 1.792597 1.326397 0.251761 3.530416 3.955323 4.194023 3.559861 2.099873	5288374 Hartree 3.222124048085 Ha 2) = -3412.094209 27) = -3412.30834 57868448 Hartree mol fmol -3415.58905904635 57129350 Hartree 07896 Hartree 0.251105 -1.536927 0.291787 -3.607236 -2.236812 -1.764932 -2.410069 -0.592049 -0.405489 -4.274197 -5.249953 -3.682998 -4.471800 -3.379141 -4.335613 -2.999984 -2.652343 -4.635825	rtree 379966 Hartree 2631976 Hartree 9 Hartree 9 Hartree -0.055104 -0.711237 1.474187 -0.718265 -0.179045 0.952926 1.256747 1.735336 2.821053 -1.875518 -2.087189 -2.807119 -1.627088 -1.210577 -1.579214 -0.409641 -2.045039 0.442524
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Н Н С Н Н Н С С С Н С Н С Н С Н С Н Н Н С Н Н Н С Н Н Н С Н Н Н С С Н С	1.527745 0.367074 -1.971910 -2.137223 -2.175984 -2.719142 -0.329576 -0.451638 -1.061488 0.679733 0.188994 1.502745 1.649833 2.657969 0.552253 0.680785 -0.699025 -1.555117 -0.911465 2.782859 3.599302 3.009268 2.807746 4.051911 2.379282 2.983153 2.821437 2.295206 4.018326 -2.306428 -3.011684 -2.422033 -2.113270 -1.776081 -3.467728 -2.809613 -2.828418 -3.467728 -2.809613 -2.828418 -3.845041 -2.190171 0.099619 1.342278 1.334192 2.289343 0.135257	-4.567843 -5.246846 -4.375952 -5.269695 -4.666227 -3.610591 -3.639053 -4.621291 -2.942777 -3.263393 0.152333 0.368276 1.198123 1.341430 1.846017 2.471147 1.728756 2.289439 0.922217 -0.213551 0.286233 0.170489 1.240545 -0.053544 -0.454983 -1.723795 -2.030876 -2.304053 -2.099863 1.054270 1.067761 2.432317 3.258857 2.467191 2.616892 -0.026737 -1.031718 0.220819 -0.088519 -0.088519 -0.088519 -0.088519 -0.088519 -0.088571 -0.068271 -0.135887	0.191270 1.470466 2.106732 0.421977 1.760090 3.185700 3.686402 3.630111 3.431721 -2.759797 -3.284171 -4.409433 -4.830228 -4.990401 -5.886515 -4.380242 -4.789033 -3.241669 -2.676614 -3.241539 -1.207300 -1.017928 -0.901378 -0.521176 -2.869026 -3.921176 -2.224906 -2.588516 -1.227300 -1.017928 -0.901378 -0.521176 -2.224906 -2.588516 -1.207300 -1.017928 -0.901378 -0.521176 -2.224906 -2.589359 -2.608167 -3.470265 -1.919135 -2.588516 -1.021778 -1.597787 -1.645987 -2.098773 -1.335299 -0.733379 2.518761 3.191840 4.501036 5.033183 5.142257	Conform Multipl Charge: E(B97-3 E(M06/6 E(PBE0-E(PM6)) E(PM7) E(GFN1-E(GFN2-E(GFN-F COORDING CO N N C C C C C H C C C H C C C C H C C C C	mation 6icity: 4 0 8c) = -3413.53268! def2-TZVP) = -341: - D3(BJ)/def2-TZV3c) = -3408.8707! = 99.67616 Kcal/r = 114.02554 Kcal/144.02554 Kcal/157 Kcal/r = 114.02554 Kcal/r = 114.0256 Kcal/	5288374 Hartree 3.22124048085 Ha 2) = -3412.094209 7P) = -3412.30834 57868448 Hartree nol fmol -3415.58905904635 57129350 Hartree 45160225 Hartree 07896 Hartree 0.251105 -1.536927 0.291787 -3.607236 -2.236812 -1.764932 -2.410069 -0.592049 -0.405489 -4.274197 -5.249953 -3.682998 -4.471800 -3.379141 -4.335613 -2.999984 -2.652343 -4.635825 -5.611194 -4.791730 -4.335004 -0.327961 -0.173310 0.521299 -1.248225 -1.617816	rtree 379966 Hartree 2631976 Hartree 2631976 Hartree  9 Hartree  -0.055104 -0.711237 1.474187 -0.718265 -0.179045 0.952926 1.256747 1.735336 2.821053 -1.875518 -2.821053 -1.875518 -2.807119 -1.627088 -1.210577 -1.579214 -0.409641 -2.045039 0.442524 0.063412 0.858400 1.277074 2.080833 2.811580 1.368017 1.507383 3.780913
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С	3.112723	0.862827	3.687164	Multip	licity: 5		
H	4.000929	0.909359	4.349620	Charge			
H H	2.216826 3.093442	0.863255 1.792277	4.333097 3.090028		3c) = -5596.386662 def2-TZVP) = -5596		rtree
C	-0.165167	-1.823712	-1.933732		- D3(BJ)/def2-TZVE		
С	0.430437	-1.365440	-3.149399		- D3(BJ)/def2-TZV		8439150 Hartree
C H	-0.222175 0.239005	-1.618923 -1.275952	-4.367571 -5.306190		-3c) = -5589.62401 = $-2.72851$ Kcal/m		
C	-1.448827	-2.293317	-4.404169		= 107.91092 Kcal/		
H	-1.946761	-2.495580	-5.364238		X-V/def2-TZVP) = -		4 Hartree
C H	-2.045017 -3.022168	-2.687732 -3.196771	-3.202115 -3.222591		-xTB) = $-152.46124$		
п С	-1.440551	-2.459028	-1.948853		-xTB) = $-152.11050FF) = -19.12483057$		
C	1.720999	-0.551122	-3.142352	, -	,		
H C	2.197725 2.731157	-0.685904 -1.005882	-2.150647 -4.206362	Coordi: Cr	nates: 0.291712	-0.318149	-0.695226
Н	2.731157	-2.093142	-4.141014	Al	-1.281855	4.319588	0.898640
H	3.691924	-0.465154	-4.084234	Cl	1.864300	-0.598462	-2.344844
H C	2.369887 1.401059	-0.796927 0.949056	-5.234363 -3.290636	Cl Cl	-1.083540 0.207347	4.500465 5.573835	3.083910 -0.059247
Н	0.660053	1.274317	-2.532238	N	-2.364441	-1.910997	-0.059247
H	0.961842	1.164507	-4.286862	H	-3.165912	-2.546264	-0.336617
H C	2.318600 -2.272358	1.564045 -2.858550	-3.178659 -0.724001	N N	-1.496735 -0.748368	0.192913 2.446158	0.235627 0.542139
Н	-2.272336	-3.665145	-1.095357	P	-1.052148	-2.118690	-1.468742
C	-3.181990	-1.692751	-0.292988	P	0.545103	2.015747	-0.522931
H	-3.769460	-1.298351	-1.145410	P	1.533467	-1.234139	1.320476
H H	-2.575774 -3.886293	-0.853878 -2.014756	0.098489 0.501416	C C	-2.498111 -3.600532	-0.733003 -0.529492	0.367642 1.212003
C	-1.538251	-3.439846	0.492045	Н	-4.383993	-1.294981	1.292187
H	-0.869825	-4.276483	0.211905	C	-3.634860	0.651449	1.969255
H H	-2.281589 -0.932177	-3.835002 -2.678929	1.214504 1.017443	H C	-4.451562 -2.652041	0.816661 1.625604	2.687915 1.812704
C	0.723738	1.446129	2.172981	Н	-2.656872	2.547420	2.409486
С	0.955264	2.729293	1.590717	С	-1.615251	1.428376	0.860846
C H	0.458567 0.640129	3.865367 4.861267	2.254737 1.822944	C C	-0.584736 -0.823394	-3.867759 -4.562137	-1.266398 -0.063397
C	-0.261978	3.752112	3.449933	Н	-1.384179	-4.080913	0.751466
H	-0.635310	4.653802	3.957892	C	-0.317553	-5.859983	0.104269
C H	-0.529010 -1.124021	2.481422 2.396231	3.982676 4.903932	H C	-0.508276 0.438403	-6.394227 -6.462462	1.046905 -0.913461
C	-0.066134	1.313661	3.356718	Н	0.838733	-7.478215	-0.775320
С	1.730686	2.879647	0.285226	C	0.688252	-5.765345	-2.107973
H C	1.825991 0.989838	1.858657 3.754470	-0.156294 -0.737208	H C	1.286529 0.181005	-6.231342 -4.472029	-2.905341 -2.287988
Н	-0.025889	3.360041	-0.936126	Н	0.389509	-3.920219	-3.217624
H	1.540004	3.774444	-1.699417	C	-1.760213	-2.005242	-3.154513
H C	0.893954 3.159883	4.802877 3.392207	-0.388043 0.532244	C H	-1.468553 -0.765369	-0.844624 -0.099099	-3.899986 -3.494275
Н	3.722607	2.726056	1.215808	C	-2.054885	-0.659809	-5.160942
H	3.140324	4.403010	0.990361	H	-1.821666	0.247594	-5.738488
H C	3.724491 -0.455647	3.461231 -0.068770	-0.420236 3.865886	C H	-2.927841 -3.387825	-1.629567 -1.483828	-5.678552 -6.667886
Н	0.346968	-0.771939	3.564634	C	-3.210796	-2.793171	-4.941201
C	-1.743197	-0.533729	3.160311	H	-3.888832	-3.555939	-5.353411
H H	-1.980612 -1.642606	-1.587091 -0.461159	3.413789 2.058795	C H	-2.626188 -2.835455	-2.986030 -3.904647	-3.681773 -3.110411
Н	-2.605880	0.100694	3.448165	C	2.138783	2.578138	0.155613
C	-0.592388	-0.155360	5.390300	C	2.253607	3.342143	1.331899
H H	0.320960 -0.770739	0.204799 -1.204713	5.906443 5.700683	H C	1.360298 3.526192	3.666798 3.677768	1.882358 1.814679
Н	-1.450150	0.441247	5.763658	Н	3.608693	4.274108	2.735169
N	-1.373514	0.992668	-0.903941	C	4.680879	3.259854	1.135667
C C	-2.450155 -3.415855	1.643992 1.982501	-1.150019 -0.054999	H C	5.675498 4.566132	3.533449 2.480710	1.520069 -0.026924
С	-2.930366	2.346612	1.218987	H	5.467693	2.136344	-0.556394
H	-1.845470	2.427663	1.375856	С	3.299532	2.128226	-0.514673
C H	-3.817865 -3.417024	2.613797 2.914188	2.269205 3.249151	H C	3.203820 0.229737	1.481235 2.887260	-1.401485 -2.100358
С	-5.204068	2.501860	2.070251	С	1.193807	3.663869	-2.766488
H	-5.901066	2.706837	2.897298	H	2.170448	3.847482	-2.296086
C H	-5.697385 -6.782024	2.130286 2.032656	0.808529 0.646958	C H	0.891979 1.645853	4.226375 4.840800	-4.014989 -4.529971
C	-4.811734	1.883145	-0.249990	C	-0.369059	4.025469	-4.598528
H	-5.200361	1.592488	-1.237685	H	-0.602782	4.476780	-5.574735
C C	-2.769244 -3.488974	2.053012 3.232726	-2.554081 -2.845991	C H	-1.335676 -2.330208	3.255309 3.102157	-3.930239 -4.376603
H	-3.855044	3.863305	-2.021760	С	-1.036153	2.679966	-2.687923
С	-3.721246	3.611529	-4.176583	Н	-1.791378	2.070205	-2.167091
H C	-4.273512 -3.250539	4.539415 2.813079	-4.391441 -5.231801	C H	-3.095137 -3.036711	4.652149 4.467243	0.187094 -0.910833
H	-3.440832	3.108673	-6.275051	H	-3.824933	3.908143	0.575501
С	-2.538918	1.634061	-4.948440	C	-3.593614	6.081255	0.454705
H C	-2.174268 -2.295068	0.995066 1.260161	-5.767860 -3.622280	H H	-4.591524 -2.889820	6.287302 6.836095	0.007757 0.044492
Н	-1.739261	0.341545	-3.390509	H	-3.676018	6.283993	1.543792
				C	2.006283	-0.000015	2.610672
ROB:	HUN			C H	3.328510 4.146712	0.159596 -0.442104	3.070931 2.651196
				С	3.617181	1.095785	4.076334
Conform	mation 10.			Н	4.655060	1.211416	4.424188

C H								
	2.597002	1.884375	4.628465	Н	-4.669184	1.202307	-3.347990	
	2.830289	2.622414	5.410780	C	-3.356632	0.148910	-1.987675	
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H	2.210294	-3.965839	2.477963	С	-2.016239	-5.591252	1.171020	
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Н								
	0.867203	-5.579147	3.794892	C	-1.218268	-4.664635	1.862550	
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С	-1.458249	-3.082439	3.482210	H	-0.477654	-2.623221	1.927870	
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С	-0.703801	-2.171622	2.730557	H	-3.389011	-0.805424	3.967420	
H	-1.155221	-1.212707	2.443645	H	-5.148954	-0.680962	3.866364	
С	3.116448	-2.076063	0.857735	С	-4.377314	-2.684916	3.451976	
Н	3.738233	-1.265957	0.421230	Н	-4.479652	-3.058172	4.495178	
H	3.630034	-2.426645	1.778220	H	-3.486092	-3.184260	3.016090	
C	2.926841	-3.199948	-0.165883	H	-5.250276	-3.058098	2.877950	
H	3.900848	-3.679984	-0.389681	С	-0.345715	2.155200	-2.888147	
H	2.522777	-2.789349	-1.110991	С	-0.299641	1.097543	-3.820203	
Н	2.234580	-3.989146	0.188292	Н	0.191126	0.150078	-3.545177	
11	2.234300	-3.909140	0.100292					
				С	-0.887899	1.253985	-5.083790	
Conform	mation 12.			H	-0.853024	0.422716	-5.803296	
Multip	licity: 5			С	-1.538943	2.450933	-5.418584	
Charge				Н	-2.011135	2.565046	-6.406358	
_		1005047						
	3c) = -5596.38874			C	-1.596850	3.500556	-4.487290	
E(M06/	def2-TZVP) = -559	6.637594551751 Has	rtree	H	-2.111449	4.439433	-4.743387	
E(PBE -	- D3(BJ)/def2-TZV	P) = -5594.6010500	21001 Hartree	C	-0.996727	3.359556	-3.227663	
E (PREO	- D3(BJ)/def2-T7	VP) = -5594.99789	7810705 Hartree	H	-1.041661	4.185528	-2.502070	
	-3c) = -5589.6280	,	OTO/OS HATCICC	C	-0.214163	3.147939	-0.156958	
	= -6.68397  Kcal/			С	0.563287	4.029920	0.623588	
E(PM7)	= 98.27049 Kcal/	mol		H	1.656995	4.056190	0.511733	
E (ωB97)	X-V/def2-TZVP) =	-5597.236224588247	Hartree	С	-0.053224	4.888683	1.547071	
	-xTB) = $-152.4666$			Н	0.565092	5.575069	2.145939	
	-xTB) = $-152.1175$			C	-1.447643	4.877889	1.703063	
E (GFN-1	FF) = -19.1251234	80387 Hartree		H	-1.928168	5.556537	2.424042	
				C	-2.227646	3.993874	0.940321	
Coordin	nates.			H	-3.317958	3.938767	1.074050	
Cr	0.656844	-0.379961	-0.274018	C	-1.615535	3.130393	0.023471	
Al	-4.161846	-0.434672	1.533698	H	-2.238089	2.430389	-0.552792	
Cl	1.473327	-1.631865	-2.018105	C	2.227326	2.625314	-1.665837	
Cl	-4.957010	1.599257	1.255293	H	2.108869	3.695717	-1.936639	
		-1.747188		Н				
Cl	-5.121756		0.091895		2.785595	2.577580	-0.709041	
N	2.217869	0.604282	2.237960	C	2.968037	1.840424	-2.747816	
H	2.839195	0.806981	3.025369	Н	4.014822	2.194317	-2.829976	
N	-0.020489	0.314123	1.563266	H	2.483831	1.963098	-3.736700	
N		-0.233928		Н	2.986025	0.755546	-2.521727	
	-2.271542		0.970368	н	2.986025	0./33346	-2.521/2/	
P	2.717882	-0.398610	0.919351					
P	-1.555925	-1.202514	-0.274614	Conform	nation 13.			
P	0.541348	1.924465	-1.295092	Multipl	licity: 5			
С	0.860636	0.832612	2.472878	Charge	4			
						000010 ***		
С	0.444902	1.568158	3.589012		3c) = -5596.381461			
H	1.184771	1.975574	4.291100	E(M06/c	def2-TZVP) = -5596	.630859369398 Ha	rtree	
С	-0.931520		0 0 40001	E (DDE	,			
Н		1.792032	3./4///1	E (PBE -			748065 Hartree	
	-1 293638	1.792032	3.747771 4 584625		- D3(BJ)/def2-TZVF	p) = -5594.594213		
~	-1.293638	2.407404	4.584625	E(PBE0	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZV	P(r) = -5594.594213 P(r) = -5594.99084		
C	-1.845276	2.407404 1.236667	4.584625 2.860118	E(PBE0 E(PBEh-	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZV -3c) = -5589.61881	P(r) = -5594.594213 P(r) = -5594.99084 P(r) = -8048475		
H	-1.845276 -2.920481	2.407404 1.236667 1.429788	4.584625 2.860118 2.961517	E(PBE0 E(PBEh- E(PM6)	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZV -3c) = -5589.61881 = 3.63514 Kcal/mo	P) = -5594.594213 PP) = -5594.99084 .8048475 Hartree		
H C	-1.845276 -2.920481 -1.384078	2.407404 1.236667 1.429788 0.436500	4.584625 2.860118 2.961517 1.781142	E (PBE0 E (PBEh- E (PM6) E (PM7)	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF -3c) = -5589.61881 = 3.63514 Kcal/mc = 116.33626 Kcal/	P) = -5594.594213 PP) = -5594.99084 .8048475 Hartree pl	1260730 Hartree	
H	-1.845276 -2.920481	2.407404 1.236667 1.429788	4.584625 2.860118 2.961517	E (PBE0 E (PBEh- E (PM6) E (PM7)	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZV -3c) = -5589.61881 = 3.63514 Kcal/mo	P) = -5594.594213 PP) = -5594.99084 .8048475 Hartree pl	1260730 Hartree	
H C	-1.845276 -2.920481 -1.384078	2.407404 1.236667 1.429788 0.436500	4.584625 2.860118 2.961517 1.781142	E (PBE0 E (PBEh- E (PM6) E (PM7) E (ωB97)	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF -3c) = -5589.61881 = 3.63514 Kcal/mc = 116.33626 Kcal/	P) = -5594.594213 PP) = -5594.99084 .8048475 Hartree pl (mol .5597.22901399056	1260730 Hartree	
H C C	-1.845276 -2.920481 -1.384078 4.283115 4.701681	2.407404 1.236667 1.429788 0.436500 0.368345 1.644539	4.584625 2.860118 2.961517 1.781142 0.377549 0.803723	E (PBE0 E (PBEh- E (PM6) E (PM7) E (ωB97) E (GFN1-	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZV -3c) = -5589.61881 = 3.63514 Kcal/mc = 116.33626 Kcal/ <-V/def2-TZVP) = - -xTB) = -152.46000	P) = -5594.594213 PP) = -5594.99084 8048475 Hartree ol 'mol -5597.22901399056 15404970 Hartree	1260730 Hartree	
H C C C H	-1.845276 -2.920481 -1.384078 4.283115 4.701681 4.097823	2.407404 1.236667 1.429788 0.436500 0.368345 1.644539 2.203652	4.584625 2.860118 2.961517 1.781142 0.377549 0.803723 1.534536	E (PBE0 E (PBEh- E (PM7) E (ωB97) E (GFN1- E (GFN2-	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZV - 3c) = -5589.61881 = 3.63514 Kcal/mc = 116.33626 Kcal/ <-V/def2-TZVP) = - -xTB) = -152.46000 -xTB) = -152.11134	P) = -5594.594213 PP) = -5594.99084 .8048475 Hartree Imol .5597.22901399056 .5404970 Hartree .2636979 Hartree	1260730 Hartree	
H C C C H C	-1.845276 -2.920481 -1.384078 4.283115 4.701681 4.097823 5.878472	2.407404 1.236667 1.429788 0.436500 0.368345 1.644539 2.203652 2.206362	4.584625 2.860118 2.961517 1.781142 0.377549 0.803723 1.534536 0.283625	E (PBE0 E (PBEh- E (PM7) E (ωB97) E (GFN1- E (GFN2-	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZV -3c) = -5589.61881 = 3.63514 Kcal/mc = 116.33626 Kcal/ <-V/def2-TZVP) = - -xTB) = -152.46000	P) = -5594.594213 PP) = -5594.99084 .8048475 Hartree Imol .5597.22901399056 .5404970 Hartree .2636979 Hartree	1260730 Hartree	
H C C C H C	-1.845276 -2.920481 -1.384078 4.283115 4.701681 4.097823 5.878472 6.204197	2.407404 1.236667 1.429788 0.436500 0.368345 1.644539 2.203652 2.206362 3.200920	4.584625 2.860118 2.961517 1.781142 0.377549 0.803723 1.534536 0.283625 0.624154	E (PBE0 E (PBEh- E (PM6) E (PM7) E (ωB97) E (GFN1- E (GFN-F	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF -3c) = -5589.61881 = 3.63514 Kcal/mc = 116.33626 Kcal/ (-V/def2-TZVP) = - -xTB) = -152.46000 -xTB) = -152.11134 FF) = -19.12619738	P) = -5594.594213 PP) = -5594.99084 .8048475 Hartree Imol .5597.22901399056 .5404970 Hartree .2636979 Hartree	1260730 Hartree	
H C C C H C H	-1.845276 -2.920481 -1.384078 4.283115 4.701681 4.097823 5.878472 6.204197 6.634226	2.407404 1.236667 1.429788 0.436500 0.368345 1.644539 2.203652 2.206362 3.200920 1.505113	4.584625 2.860118 2.961517 1.781142 0.377549 0.803723 1.534536 0.283625 0.624154 -0.668785	E (PBE0 E (PBEh- E (PM7) E (ωB97) E (GFN1- E (GFN2-	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF -3c) = -5589.61881 = 3.63514 Kcal/mc = 116.33626 Kcal/ <-V/def2-TZVP) = - -xTB) = -152.46000 -xTB) = -152.11134 FF) = -19.12619738	P) = -5594.594213 PP) = -5594.99084 8048475 Hartree Pl mol -5597.22901399056 15404970 Hartree 12636979 Hartree 16254 Hartree	1260730 Hartree	
H C C C H C	-1.845276 -2.920481 -1.384078 4.283115 4.701681 4.097823 5.878472 6.204197	2.407404 1.236667 1.429788 0.436500 0.368345 1.644539 2.203652 2.206362 3.200920	4.584625 2.860118 2.961517 1.781142 0.377549 0.803723 1.534536 0.283625 0.624154	E (PBE0 E (PBEh- E (PM6) E (PM7) E (ωB97) E (GFN1- E (GFN-F	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF -3c) = -5589.61881 = 3.63514 Kcal/mc = 116.33626 Kcal/ (-V/def2-TZVP) = - -xTB) = -152.46000 -xTB) = -152.11134 FF) = -19.12619738	P) = -5594.594213 PP) = -5594.99084 .8048475 Hartree Imol .5597.22901399056 .5404970 Hartree .2636979 Hartree	1260730 Hartree	
Н С С Н С Н С	-1.845276 -2.920481 -1.384078 4.283115 4.701681 4.097823 5.878472 6.204197 6.634226 7.554478	2.407404 1.236667 1.429788 0.436500 0.368345 1.644539 2.203652 2.206362 3.200920 1.505113 1.949305	4.584625 2.860118 2.961517 1.781142 0.377549 0.803723 1.534536 0.283625 0.624154 -0.668785 -1.077036	E (PBE0 E (PBEh- E (PM6) E (PM7) E (GB972- E (GFN1- E (GFN2- Coordin Cr	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF -3c) = -5589.61881 = 3.63514 Kcal/mc = 116.33626 Kcal/ K-V/def2-TZVP) = - -xTB) = -152.46000 -xTB) = -152.11134 FF) = -19.12619738 mates: 0.250465	P) = -5594.594213 PP) = -5594.99084 8048475 Hartree Ol mol 5597.22901399056 15404970 Hartree 16254 Hartree -0.792403	1260730 Hartree  1 Hartree  -0.175308	
H C C C H C H C H	-1.845276 -2.920481 -1.384078 4.283115 4.701681 4.097823 5.878472 6.204197 6.634226 7.554478 6.211034	2.407404 1.236667 1.429788 0.436500 0.368345 1.644539 2.203652 2.206362 3.200920 1.505113 1.949305 0.237676	4.584625 2.860118 2.961517 1.781142 0.377549 0.803723 1.534536 0.283625 0.624154 -0.668785 -1.077036 -1.104810	E (PBE0 E (PBEh- E (PM6) E (PM7) E (GB972- E (GFN-I Coordin Cr Al	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - 32() = -5589.61881 = 3.63514 Kcal/mc = 116.33626 Kcal/ (-V/def2-TZVP) = - -xTB) = -152.46000 -xTB) = -152.11134 FF) = -19.12619738 nates: 0.250465 -4.125790	P) = -5594.594213 P) = -5594.99084 8048475 Hartree 101 101 105597.22901399056 105404970 Hartree 12636979 Hartree 16254 Hartree -0.792403 0.766571	1260730 Hartree  1 Hartree  -0.175308 2.101154	
Н С С С Н С Н С Н С Н С	-1.845276 -2.920481 -1.384078 4.283115 4.701681 4.097823 5.878472 6.204197 6.634226 7.554478 6.211034 6.794802	2.407404 1.236667 1.429788 0.436500 0.368345 1.644539 2.203652 2.206362 3.200920 1.505113 1.949305 0.237676 -0.310232	4.584625 2.860118 2.961517 1.781142 0.377549 0.803723 1.534536 0.283625 0.624154 -0.668785 -1.077036 -1.104810 -1.859659	E (PBE0 E (PBEh- E (PM6) E (PM7) E (GFN1- E (GFN2- E (GFN-I Coordin Cr Al	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF -3c) = -5589.61881 = 3.63514 Kcal/mc = 116.33626 Kcal/ (-V/def2-TZVP) = - -xTB) = -152.46000 -xTB) = -152.11134 -15P) = -19.12619738 mates: 0.250465 -4.125790 0.493616	P) = -5594.594213 PP) = -5594.99084 .8048475 Hartree Imol .5597.22901399056 .5404970 Hartree .2636979 Hartree .6254 Hartree -0.792403 0.766571 -2.700074	1260730 Hartree  1 Hartree  -0.175308 2.101154 -1.421508	
Н С С С Н С Н С Н С Н С Н С Н С Н С Н С	-1.845276 -2.920481 -1.384078 4.283115 4.701681 4.097823 5.878472 6.204197 6.634226 7.554478 6.211034 6.794802 5.039893	2.407404 1.236667 1.429788 0.436500 0.368345 1.644539 2.203652 2.206362 3.200920 1.505113 1.949305 0.237676 -0.310232 -0.330897	4.584625 2.860118 2.961517 1.781142 0.377549 0.803723 1.534536 0.283625 0.624154 -0.668785 -1.077036 -1.104810 -1.859659 -0.588254	E (PBE0 E (PBEh- E (PM6) E (PM7) E (GB97) E (GFN1- E (GFN- Coordin Cr Al Cl	- D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF - D3(BJ)/def2-TZVF -3c) = -5589.61881 = 3.63514 Kcal/mc = 116.33626 Kcal/ (-V/def2-TZVP) = - -xTB) = -152.46000 -xTB) = -152.11134 FF) = -19.12619738 mates: 0.250465 -4.125790 0.493616 -5.360680	P) = -5594.594213 PP) = -5594.99084 .8048475 Hartree pl mol .5597.22901399056 .5404970 Hartree .2636979 Hartree .6254 Hartree -0.792403 0.766571 -2.700074 -0.980705	1260730 Hartree  1 Hartree  -0.175308 2.101154 -1.421508 1.721512	
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H	7.303089	-0.088180	-0.002979				
С	6.366015	-1.368798	-1.493524		inates:		
H C	7.300046 5.175980	-1.528122 -1.973806	-2.053719 -1.924567	Cr Al	-0.607837 4.408126	0.188841 1.392755	0.392782 0.460482
Н	5.171509	-2.608044	-2.824007	Cl	-2.283937	1.457888	1.318251
С	3.980905	-1.763248	-1.218672	Cl	5.175090	1.533398	-1.596487
H	3.032420	-2.214367	-1.557429	Cl	4.306360	3.393582	1.302840
С	2.708221	-1.750533	2.396819	N	-0.394205	-2.922169	0.282482
C H	2.269690 1.859444	-1.253785 -0.235195	3.642011 3.716915	H N	-0.462643 1.032814	-3.941699 -1.064697	0.336354 0.089690
C	2.349290	-2.061675	4.786559	N	2.536289	0.790138	0.215871
Н	2.007299	-1.666968	5.755223	P	-1.607128	-1.900671	0.979670
C	2.857235	-3.367659	4.695184	P	1.186570	1.659592	0.847923
H	2.915329	-4.000421	5.593588	P	-1.033162	0.626000	-2.038400
С	3.288217	-3.866218	3.453996	С	0.860815	-2.415280	-0.041582
H	3.684688	-4.890019	3.378255	C	1.879989	-3.266856	-0.488921
C H	3.213071 3.544706	-3.065132 -3.462537	2.306631 1.334637	H C	1.700606 3.097941	-4.347423 -2.683943	-0.570790 -0.868449
C	-3.141916	-1.449789	-0.833194	Н	3.899738	-3.310979	-1.286004
C	-3.064733	-2.683087	-1.517286	C	3.304807	-1.317720	-0.715645
Н	-2.377610	-3.467040	-1.166110	Н	4.242185	-0.841358	-1.030229
С	-3.840189	-2.894562	-2.665920	С	2.283069	-0.513135	-0.146950
H	-3.777534	-3.859269	-3.191748	С	-3.140036	-2.634534	0.313459
С	-4.680937	-1.879297	-3.150454	С	-3.142003	-3.342756	-0.905569
H	-5.284830	-2.047595	-4.055003	H	-2.197459	-3.499425	-1.447401
C H	-4.747728 -5.406947	-0.648709 0.151180	-2.478064 -2.847311	C H	-4.345347 -4.338459	-3.834020 -4.385067	-1.430112 -2.382260
C	-3.984238	-0.433055	-1.323221	C	-5.553797	-3.611003	-0.752013
Н	-4.051546	0.527458	-0.794752	Н	-6.497530	-3.995956	-1.166917
C	-2.131729	-2.535288	1.739490	C	-5.558634	-2.884242	0.450063
С	-1.065370	-2.660881	2.655174	H	-6.505208	-2.698369	0.979812
H	-0.221317	-1.954463	2.610370	С	-4.358674	-2.393171	0.982951
C H	-1.066741	-3.689581	3.604907	H	-4.364548	-1.822380	1.924367
C	-0.228119 -2.126792	-3.774085 -4.610824	4.312416 3.631943	C C	-1.668217 -2.088087	-2.277363 -3.527156	2.774832 3.276923
Н	-2.128642	-5.426173	4.371516	Н	-2.481077	-4.295067	2.591414
C	-3.183064	-4.495259	2.713664	C	-2.013995	-3.785315	4.652598
H	-4.016188	-5.213866	2.738561	H	-2.338108	-4.761094	5.045430
C	-3.194176	-3.457783	1.769767	C	-1.529561	-2.798545	5.530094
H	-4.034576	-3.348874	1.070985	H	-1.474555	-3.006167	6.609666
C H	-5.023967	2.352115 2.235949	1.299487	C H	-1.123985	-1.549712	5.034062
H H	-5.069743 -6.077495	2.235949	0.191175 1.623642	C C	-0.750873 -1.193144	-0.770386 -1.286430	5.715685 3.657744
C	-4.608021	3.782656	1.668784	Н	-0.890586	-0.304007	3.259180
Н	-5.339702	4.548640	1.328920	C	1.093714	3.265148	-0.004414
H	-3.629768	4.062984	1.223423	C	1.969758	3.606219	-1.055241
H	-4.505758	3.901369	2.768831	H	2.797015	2.936558	-1.333956
С	-0.492392	2.218381	-2.311518	С	1.777295	4.806084	-1.755446
C H	-1.687948	2.277959	-1.572818	H C	2.468414	5.069819 5.667888	-2.570082 -1.414118
C	-1.936889 -2.566837	1.470471 3.362002	-0.871950 -1.728366	Н	0.721695 0.579443	6.610020	-1.965069
Н	-3.494463	3.398629	-1.137788	C	-0.155879	5.322477	-0.373446
C	-2.253253	4.393686	-2.624939	Н	-0.994597	5.985643	-0.112952
H	-2.938647	5.246452	-2.745007	C	0.017917	4.118628	0.324937
С	-1.060514	4.340328	-3.367945	H	-0.703093	3.819465	1.101686
H	-0.812457	5.149165	-4.072236	С	1.528555	1.947500	2.624205
C H	-0.181777 0.757209	3.259635 3.227175	-3.212980 -3.787420	C H	1.513425 1.368336	3.212748 4.117101	3.238196 2.630587
C	2.277030	1.529945	-2.136994	C	1.721730	3.318235	4.620868
C	2.516839	2.644651	-1.301413	Н	1.716965	4.310854	5.095951
Н	1.686377	3.087352	-0.729492	С	1.958406	2.170111	5.393467
С	3.801191	3.194814	-1.202683	H	2.130896	2.260943	6.476654
H	3.970451	4.068334	-0.553824	С	1.985792	0.906462	4.780001
С	4.866868	2.640590	-1.932774	H	2.183360	0.002809	5.376712
H C	5.876358 4.635336	3.071521 1.538719	-1.853334 -2.769094	C H	1.762593 1.778063	0.792781 -0.199054	3.401050 2.921904
Н	5.462974	1.097239	-3.343870	C	5.364906	0.144353	1.656010
C	3.350150	0.984222	-2.870760	Н	4.793759	0.141146	2.613692
H	3.189285	0.112761	-3.521157	H	5.312052	-0.899106	1.275320
С	0.463127	-0.105166	-3.761541	С	6.825210	0.547165	1.915676
H	0.850956	0.571094	-4.552640	H	7.342290	-0.125361	2.635704
H	1.125176	-0.993219	-3.689796	H	6.891882	1.577342	2.325060
C H	-0.975748 -1.042725	-0.548591 -1.074827	-4.028026 -5.001145	H C	7.420780 0.343070	0.539747 -0.076947	0.977979 -3.021532
H	-1.673681	0.311795	-4.056808	C	0.401034	-1.466099	-3.272006
Н	-1.322347	-1.248536	-3.242667	Н	-0.441592	-2.110949	-2.977913
				С	1.526116	-2.028252	-3.889471
	rmation 14.			H	1.555061	-3.111440	-4.082721
	plicity: 5			C	2.622086	-1.220919	-4.234970
Charg		4000072 11		H	3.514198	-1.668274	-4.698405
	(-3c) = -5596.391804 (-3c) = -5596.391804		rtree	C H	2.585581 3.454924	0.154910 0.789887	-3.964815 -4.187957
	3/de12-TZVP) = -5590 1 - D3(BJ)/def2-TZV			н С	1.451061	0.725899	-3.370035
	10 - D3(BJ)/def2-TZV			Н	1.446465	1.803648	-3.154687
E (PBE	2h-3c) = -5589.63070	06915516 Hartree		С	-2.581171	-0.124688	-2.688667
	6) = -6.75326  Kcal/r			C	-3.709843	-0.094637	-1.839568
	() = 102.32169 Kcal		1	H	-3.607468	0.294967	-0.813041
	97X-V/def2-TZVP) = -107X-VP		ı Hartree	C H	-4.951613 -5.824924	-0.550921 -0.519612	-2.303845 -1.635863
	I2-xTB) = -152.46640 I2-xTB) = -152.11804			н С	-5.073234	-1.066661	-3.603595
	I-FF) = $-19.1239853$			Н	-6.045943	-1.437539	-3.961403
•							

C	-3.950652	-1.111736	-4.446544	H	2.119498	-3.206123	0.685277	
H	-4.042694	-1.511808	-5.468125	С	2.217915	-5.018282	-2.102469	
C	-2.710441	-0.632252	-3.997765	H	3.169192	-5.373346	-1.645572	
H	-1.838488	-0.651028	-4.669217	Н	1.486891	-4.985758	-1.261565	
C	-1.177867	2.387056	-2.632459	C	1.743823	-6.014866	-3.169758	
H	-0.266659	2.905367	-2.274383	H	1.600700	-7.042990	-2.769293	
H	-1.144388	2.367736	-3.742486	Н	2.464147	-6.089580	-4.010778	
С	-2.428472	3.090738	-2.107826	H	0.776599	-5.708090	-3.622430	
H	-2.403481	4.162092	-2.390446	С	-2.511310	1.767033	-1.347232	
H	-2.488872	3.027039	-1.003099	С	-3.387092	2.857538	-1.169843	
H	-3.354084	2.646601	-2.524987	H	-2.985454	3.840278	-0.882608	
				C	-4.769621	2.690833	-1.344831	
0	mation 19.			Н	-5.441893	3.550871	-1.201398	
Multip	licity: 5			C	-5.295869	1.438522	-1.701370	
Charge	. 0			Н	-6.380901	1.312034	-1.836053	
		7016550 *****						
	3c) = -5596.38747			C	-4.428210	0.350107	-1.892329	
E(M06/	def2-TZVP) = -559	6.635339660322 Har	tree	H	-4.824930	-0.636277	-2.177940	
F (DBF	- D3 (B.T) /def2-T7V	P) = -5594.5994771	23957 Hartree	С	-3.046934	0.511336	-1.712596	
E (PBEU	- D3(BJ)/def2-TZ	VP) = -5594.995563	611253 Hartree		-2.380299	-0.350555	-1.855445	
E (PBEh	-3c) = -5589.6226	42189024 Hartree		С	-0.433074	3.558439	-0.408313	
	= -0.77869 Kcal/			C	0.285444	4.574866	-1.068778	
E(PM7)	= 114.46982 Kcal	/mol		H	0.693591	4.408010	-2.075418	
E (wB97	X-V/def2-T7VP) =	-5597.232967487661	Hartree	C	0.496150	5.813062	-0.439770	
				Н				
	-xTB) = $-152.4577$				1.061719	6.598620	-0.963931	
E (GFN2	-xTB) = $-152.1102$	66014246 Hartree		C	-0.012428	6.050236	0.845888	
E (GEN-	FF) = -19.0974722	31007 Hartree		Н	0.153751	7.022296	1.334555	
T / GT II -	10.0014122	orgo, marcree						
				С	-0.724826	5.037957	1.510956	
Coordi	nates:			H	-1.117511	5.207614	2.525091	
Cr	0.200994	0.130735	0.478513	C	-0.921386	3.796035	0.896391	
Al	2.569220	-3.159814	-2.701227	H	-1.454726	3.000287	1.436763	
Cl	1.321595	1.431955	1.989730	С	-0.065781	2.014565	-2.863818	
Cl			-4.759525	Н		2.877496		
	1.955744	-2.716336			-0.583699		-3.333196	
Cl	4.604405	-2.481540	-2.381178	H	1.010179	2.269364	-2.780663	
N	-2.383548	-1.491453	1.085562	С	-0.242149	0.744195	-3.694170	
						0.879323		
H	-3.246383	-1.930378	1.416234	H	0.221993	0.8/9323	-4.691211	
N	-0.558688	-1.598024	-0.392419	H	-1.309649	0.496098	-3.855088	
N	1.459272	-1.908440	-1.639487	Н	0.254239	-0.131904	-3.234662	
				11	0.234239	-0.131904	-3.234002	
P	-1.462414	-0.397439	2.065064					
P	2.104997	-0.650091	-0.650570	Confor	emation 29.			
P	-0.683444	1.884797	-1.110424					
					olicity: 5			
C	-1.797372	-2.065107	-0.037940	Charge	e: 0			
С	-2.460604	-3.058337	-0.773935	E(B97-	-3c) = -5596.38966	9026221 Hartree		
							A Committee of the Comm	
H	-3.453470	-3.408466	-0.460870		def2-TZVP) = -559			
C	-1.825699	-3.556366	-1.922997	E(PBE	- D3(BJ)/def2-TZV	P) = -5594.601785	706922 Hartree	
H	-2 338298	-4 297781	-2 554066	E (PRE)	) = D3(B.T)/def2=T7		1417705 Hartree	
H	-2.338298	-4.297781	-2.554066		) - D3(BJ)/def2-TZ	VP) = -5594.99942	1417705 Hartree	
С	-2.338298 -0.543776	-4.297781 -3.134372	-2.554066 -2.265534		0 - D3(BJ)/def2-TZ 1-3c) = -5589.6282	VP) = -5594.99942	1417705 Hartree	
С	-0.543776	-3.134372	-2.265534	E (PBEh	n-3c) = -5589.6282	VP) = -5594.99942 70586791 Hartree	1417705 Hartree	
C H	-0.543776 -0.041437	-3.134372 -3.503947	-2.265534 -3.169098	E(PBEh E(PM6)	(n-3c) = -5589.6282 (n-3c) = -3.43148 Kcal/n	VP) = -5594.99942 70586791 Hartree mol	1417705 Hartree	
C H C	-0.543776 -0.041437 0.129802	-3.134372 -3.503947 -2.200073	-2.265534 -3.169098 -1.434959	E (PBEh E (PM6) E (PM7)	n-3c) = -5589.6282 0 = -3.43148 Kcal/n 1 = 116.09397 Kcal	VP) = -5594.99942 70586791 Hartree mol /mol		
C H C	-0.543776 -0.041437 0.129802 -2.675253	-3.134372 -3.503947	-2.265534 -3.169098 -1.434959 2.630168	E (PBEh E (PM6) E (PM7) E (ωB97	n-3c) = -5589.6282 = -3.43148 Kcal/n = 116.09397 Kcal TX-V/def2-TZVP) =	<pre>VP) = -5594.99942 70586791 Hartree mo1 /mo1 -5597.23730639242</pre>		
C H C	-0.543776 -0.041437 0.129802	-3.134372 -3.503947 -2.200073 0.834649	-2.265534 -3.169098 -1.434959 2.630168	E (PBEh E (PM6) E (PM7) E (ωB97	n-3c) = -5589.6282 0 = -3.43148 Kcal/n 1 = 116.09397 Kcal	<pre>VP) = -5594.99942 70586791 Hartree mo1 /mo1 -5597.23730639242</pre>		
C H C C	-0.543776 -0.041437 0.129802 -2.675253 -3.834322	-3.134372 -3.503947 -2.200073 0.834649 1.128347	-2.265534 -3.169098 -1.434959 2.630168 1.883145	E (PBE) E (PM6) E (PM7) E (ωB97) E (GFN1)	n-3c) = -5589.6282 = -3.43148 Kcal/n = 116.09397 Kcal 7X-V/def2-TZVP) = L-xTB) = -152.4661	<pre>VP) = -5594.99942 70586791 Hartree mo1 /mo1 -5597.23730639242 53330815 Hartree</pre>		
C H C C H	-0.543776 -0.041437 0.129802 -2.675253 -3.834322 -4.084816	-3.134372 -3.503947 -2.200073 0.834649 1.128347 0.530613	-2.265534 -3.169098 -1.434959 2.630168 1.883145 0.993944	E (PBE) E (PM6) E (PM7) E (ωB97) E (GFN1)	n-3c) = -5589.6282' n = -3.43148 Kcal/1 n = 116.09397 Kcal TX-V/def2-TZVP) = -152.4661 n-xTB) = -152.4661 n-xTB) = -152.1143	VP) = -5594.99942 70586791 Hartree mol /mol -5597.23730639242 53330815 Hartree 35810143 Hartree		
C H C C C H C	-0.543776 -0.041437 0.129802 -2.675253 -3.834322	-3.134372 -3.503947 -2.200073 0.834649 1.128347	-2.265534 -3.169098 -1.434959 2.630168 1.883145	E (PBE) E (PM6) E (PM7) E (ωB97) E (GFN1)	n-3c) = -5589.6282 = -3.43148 Kcal/n = 116.09397 Kcal 7X-V/def2-TZVP) = L-xTB) = -152.4661	VP) = -5594.99942 70586791 Hartree mol /mol -5597.23730639242 53330815 Hartree 35810143 Hartree		
C H C C C H C	-0.543776 -0.041437 0.129802 -2.675253 -3.834322 -4.084816 -4.648499	-3.134372 -3.503947 -2.200073 0.834649 1.128347 0.530613 2.207718	-2.265534 -3.169098 -1.434959 2.630168 1.883145 0.993944 2.256786	E (PBE) E (PM6) E (PM7) E (ωB97) E (GFN1)	n-3c) = -5589.6282' n = -3.43148 Kcal/1 n = 116.09397 Kcal TX-V/def2-TZVP) = -152.4661 n-xTB) = -152.4661 n-xTB) = -152.1143	VP) = -5594.99942 70586791 Hartree mol /mol -5597.23730639242 53330815 Hartree 35810143 Hartree		
C H C C H C	-0.543776 -0.041437 0.129802 -2.675253 -3.834322 -4.084816 -4.648499 -5.549807	-3.134372 -3.503947 -2.200073 0.834649 1.128347 0.530613 2.207718 2.430922	-2.265534 -3.169098 -1.434959 2.630168 1.883145 0.993944 2.256786 1.666843	E (PBE) E (PM6) E (PM7) E (ωB9) E (GFN2 E (GFN2	n-3c) = -5589.6282 = -3.43148 Kcal/n = 116.09397 Kcal /X-V/def2-TZVP) = -xTB) = -152.4661 2-xTB) = -152.1143 -FF) = -19.1310151	VP) = -5594.99942 70586791 Hartree mol /mol -5597.23730639242 53330815 Hartree 35810143 Hartree		
С Н С С С Н С Н	-0.543776 -0.041437 0.129802 -2.675253 -3.834322 -4.084816 -4.648499 -5.549807 -4.305305	-3.134372 -3.503947 -2.200073 0.834649 1.128347 0.530613 2.207718 2.430922 3.006814	-2.265534 -3.169098 -1.434959 2.630168 1.883145 0.993944 2.256786 1.666843 3.358613	E(PBEr E(PM6) E(PM7) E(\omega B97 E(GFN1) E(GFN2 E(GFN-	n-3c) = -5589.6282' = -3.43148 Kcal/i = 116.09397 Kcal /X-V/def2-TZVP) = -152.4661 2-xTB) = -152.1143 -FF) = -19.1310151	VP) = -5594.99942 70586791 Hartree mol /mol -5597.23730639242 53330815 Hartree 35810143 Hartree 48398 Hartree	6 Hartree	
C H C C H C H	-0.543776 -0.041437 0.129802 -2.675253 -3.834322 -4.084816 -4.648499 -5.549807	-3.134372 -3.503947 -2.200073 0.834649 1.128347 0.530613 2.207718 2.430922	-2.265534 -3.169098 -1.434959 2.630168 1.883145 0.993944 2.256786 1.666843	E (PBE) E (PM6) E (PM7) E (ωB9) E (GFN2 E (GFN2	n-3c) = -5589.6282 = -3.43148 Kcal/n = 116.09397 Kcal /X-V/def2-TZVP) = -xTB) = -152.4661 2-xTB) = -152.1143 -FF) = -19.1310151	VP) = -5594.99942 70586791 Hartree mol /mol -5597.23730639242 53330815 Hartree 35810143 Hartree		
С Н С С Н С Н С	-0.543776 -0.041437 0.129802 -2.675253 -3.834322 -4.084816 -4.648499 -5.549807 -4.305305 -4.942992	-3.134372 -3.503947 -2.200073 0.834649 1.128347 0.530613 2.207718 2.430922 3.006814 3.857594	-2.265534 -3.169098 -1.434959 2.630168 1.883145 0.993944 2.256786 1.666843 3.358613 3.642417	E(PBEr E(PM6) E(PM7) E(WB97) E(GFN1) E(GFN2) E(GFN-Coordi Cr	n-3c) = -5589.6282 n = -3.43148 Kcal// n = 116.09397 Kcal /X-V/def2-TZVP) = -1-xTB) = -152.4661 2-xTB) = -152.1143 -FF) = -19.1310151 inates: 0.137706	VP) = -5594.99942 70586791 Hartree mol /mol -5597.23730639242 53330815 Hartree 35810143 Hartree 48398 Hartree	0.213450	
С Н С С Н С Н С Н С Н	-0.543776 -0.041437 0.129802 -2.675253 -3.834322 -4.084816 -4.648499 -5.549807 -4.305305 -4.942992 -3.141833	-3.134372 -3.503947 -2.200073 0.834649 1.128347 0.530613 2.207718 2.430922 3.006814 3.857594 2.724058	-2.265534 -3.169098 -1.434959 2.630168 1.883145 0.993944 2.256786 1.666843 3.358613 3.642417 4.094890	E(PBER E(PM6) E(PM7) E(WB97) E(GFN1) E(GFN2) Coordi Cr A1	n-3c) = -5589.6282' 1 = -3.43148 Kcal/1   1 = 116.09397 Kcal 7X-V/def2-TZVP) = -1-xTB) = -152.4661.2-xTB) = -152.1143FF) = -19.1310151.  inates: 0.137706 -1.477923	VP) = -5594.99942 70586791 Hartree mol /mol -5597.23730639242 53330815 Hartree 35810143 Hartree 48398 Hartree -0.643828 2.050779	0.213450 -3.849012	
	-0.543776 -0.041437 0.129802 -2.675253 -3.834322 -4.084816 -4.648499 -5.549807 -4.305305 -4.942992 -3.141833 -2.865569	-3.134372 -3.503947 -2.200073 0.834649 1.128347 0.530613 2.207718 2.430922 3.006814 3.857594 2.724058 3.352465	-2.265534 -3.169098 -1.434959 2.630168 1.883145 0.993944 2.256786 1.666843 3.358613 3.642417 4.094890 4.955116	E (PBER E (PM6) E (PM7) E (WB97) E (GFN1) E (GFN2) Coordi Cr Al C1	n-3c) = -5589.6282' = -3.43148 Kcal/n = 116.09397 Kcal 7X-V/def2-TZVP) = -1-xTB) = -152.4661 2-xTB) = -152.1143 -FF) = -19.1310151 inates:	VP) = -5594.99942 70586791 Hartree mol /mol -5597.23730639242 53330815 Hartree 35810143 Hartree 48398 Hartree -0.643828 2.050779 -2.626509	0.213450 -3.849012 0.122526	
	-0.543776 -0.041437 0.129802 -2.675253 -3.834322 -4.084816 -4.648499 -5.549807 -4.305305 -4.942992 -3.141833 -2.865569 -2.325355	-3.134372 -3.503947 -2.200073 0.834649 1.128347 0.530613 2.207718 2.430922 3.006814 3.857594 2.724058 3.352465 1.643404	-2.265534 -3.169098 -1.434959 2.630168 1.883145 0.993944 2.256786 1.666843 3.358613 3.642417 4.094890 4.955116 3.735454	E (PBER E (PM6) E (PM7) E (WB97) E (GFN1) E (GFN2) E (GFN- Coordi Cr Al Cl	n-3c) = -5589.6282' = -3.43148 Kcal/n = 116.09397 Kcal 7X-V/def2-TZVP) = 1-xTB) = -152.4661 -xTB) = -152.1143 -FF) = -19.1310151 inates:	VP) = -5594.99942 70586791 Hartree mol /mol -5597.23730639242 53330815 Hartree 35810143 Hartree 48398 Hartree -0.643828 2.050779 -2.626509 2.374316	0.213450 -3.849012 0.122526 -3.544760	
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H	-5.710035	-4.565607	1.182985	P	0.547016	-2.061510	-0.550634
С	-4.144089	-3.321554	0.328843	С	0.936624	1.640612	-1.995074
Н	-4.461554	-3.478451	-0.713303	C	0.517820	2.202440	-3.207091
С	-3.026614	-2.519153	0.593871	Н	1.248584	2.417854	-3.998031
H	-2.466359	-2.056415	-0.235575	C	-0.846376	2.488924	-3.357576
C	1.384160	-0.247162	-3.077045	H	-1.214074	2.928983	-4.296435
С	1.854007	0.934293	-3.685905	С	-1.737337	2.254059	-2.316779
Н	1.261645	1.861661	-3.655091	Н	-2.786837	2.556049	-2.404178
C	3.093679	0.935843	-4.341045	C	-1.268454	1.696095	-1.097296
H	3.450059	1.864383	-4.811750	C	4.215403	-0.183027	-0.492760
C	3.868422	-0.233218	-4.400861	C	4.889032	-0.709680	0.631789
H	4.838576	-0.226664	-4.920556	H	4.597430	-0.390139	1.644334
С	3.408264	-1.407706	-3.784318	С	5.897052	-1.666632	0.456160
Н	4.020173	-2.322179	-3.807291	Н	6.413673	-2.079640	1.335585
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H	1.858895	-2.314914	-2.561014	H	7.028837	-2.862527	-0.966662
С	-1.369528	-1.374433	-2.984722	С	5.565539	-1.591298	-1.951963
С	-0.987979	-2.484959	-3.762911	H	5.826110	-1.938529	-2.963389
Н	0.074620	-2.682127	-3.963722	С	4.550980	-0.635526	-1.785012
С	-1.966259	-3.332768	-4.302536	H	3.997310	-0.260502	-2.658495
H	-1.658811	-4.191902	-4.917685	С	3.509400	2.404121	0.641244
С	-3.328575	-3.083812	-4.070709	С	4.841160	2.834343	0.471391
H	-4.092439	-3.747675	-4.502801	H	5.535318	2.249227	-0.152288
C	-3.711612	-1.970940	-3.304941	C	5.279798	4.002574	1.111621
H	-4.776630	-1.743948	-3.145738	H	6.319525	4.339958	0.982396
C	-2.740103	-1.120395	-2.757959	C	4.396743	4.738235	1.921322
H	-3.056392	-0.230862	-2.192995	H	4.748802	5.651440	2.425016
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C	-2.279250	0.316463	-6.145901	H	1.594454	2.782988	1.611251
H	-1.999738	-0.204473	-7.087947	С	-2.567093	-0.294362	2.089164
H	-3.042206	1.080106	-6.402114	C	-3.285112	-1.103799	1.185481
H	-2.788918			Н			
		-0.428905	-5.501970		-3.147669	-0.975335	0.102019
С	2.483920	2.328237	0.559810	C	-4.205578	-2.042256	1.664807
C	3.393146	3.164383	1.244136	H	-4.775559	-2.655220	0.951450
H	3.832114	2.835529	2.199272	С	-4.392229	-2.202487	3.046822
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Н	4.434940	5.066804	1.253362	C	-3.653341	-1.419383	3.947422
C	3.144111	4.856520	-0.488367	H	-3.801386	-1.536738	5.031696
H	3.398690	5.848477	-0.892098	C	-2.743308	-0.463208	3.474347
С	2.237080	4.033366	-1.170676	H	-2.199831	0.177062	4.183985
H	1.755417	4.360566	-2.105122	С	-1.119129	2.283349	2.571539
C	1.915029	2.770211	-0.647986	C	-0.327158	2.055079	3.720492
H	1.208422	2.129168	-1.189456	H	0.078103	1.050261	3.919633
C	1.755884	1.054497	2.998745	С	-0.007171	3.123073	4.570895
С	2.328944	0.299312	4.042764	H	0.606618	2.939559	5.465978
H	2.996855	-0.544388	3.818462	С	-0.450185	4.422397	4.270119
C	2.052388	0.617943	5.381056	Н	-0.194155	5.260367	4.936750
H	2.509817	0.022197	6.184807	C	-1.212211	4.651115	3.112785
С	1.192575	1.681705	5.693271	H	-1.557219	5.666685	2.866291
H	0.979189	1.929680	6.744185	С	-1.550233	3.589121	2.260520
С	0.606295	2.428786	4.657592	Н	-2.137387	3.786761	1.350507
Н	-0.066000	3.268620	4.892408	C	-4.932897	0.934737	-1.404373
C	0.885611	2.120022	3.320065	H	-4.154231	0.444687	-2.036141
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С	3.656141	-0.253147	1.206617	С	-5.981044	1.619757	-2.293581
H	4.362892	0.255557	1.895862	H	-6.457391	0.927428	-3.022966
Н	3.424374	-1.260739	1.610635	Н	-5.542881	2.460003	-2.872929
С	4.215297	-0.371114	-0.210067	Н	-6.798207	2.062400	-1.686278
H	5.164425	-0.943704	-0.205483	C	-0.738851	-3.196662	0.111777
H	4.417923	0.622884	-0.656694	C	-0.804069	-3.330960	1.516672
H	3.502630	-0.904532	-0.867520	H	-0.156784	-2.707116	2.154638
				C	-1.698487	-4.243231	2.091254
Conf-	rmation 3.			Н	-1.748295	-4.336077	3.186280
	plicity: 5			С	-2.549141	-5.009095	1.277778
Charg				H	-3.260587	-5.714542	1.733437
E(B97	-3c) = -5596.38828	5026355 Hartree		C	-2.502249	-4.860775	-0.117180
	/def2-TZVP) = -559		rtree	H	-3.170545	-5.454657	-0.759519
F (DBF	- D3(BJ)/def2-TZV	P) = -5594 600260	659020 Hartree	С	-1.595524	-3.963101	-0.702894
,	0 - D3(BJ)/def2-TZ	,		Н	-1.551745	-3.863281	-1.797774
			9040624 naitiee				
	h-3c) = -5589.6252			С	0.183298	-1.854489	-2.331640
E(PM6	) = -2.23795  Kcal/	mol		С	-1.068805	-1.305307	-2.692879
E(PM7	) = 106.40593  Kcal	/mol		H	-1.829674	-1.115500	-1.919563
	7X-V/def2-TZVP) =		7 Hartree	С	-1.347022	-0.978114	-4.025393
	1-xTB) = $-152.4618$			Н	-2.326700	-0.548199	-4.282674
	2-xTB) = $-152.1133$			С	-0.373057	-1.176373	-5.018277
E (GFN	-FF) = $-19.1246072$	//134 Hartree		H	-0.588834	-0.912561	-6.064581
				C	0.878585	-1.705754	-4.667815
Coord	inates:			H	1.647080	-1.862387	-5.440478
Cr	0.705972	0.132565	0.595169	C	1.158521	-2.042337	-3.333817
Al	-4.014180	2.106421	-0.092685	Н	2.147365		-3.076139
						-2.449675	
Cl	1.582480	-0.778067	2.518205	С	2.088074	-3.092535	-0.420949
Cl	-4.745132	2.057315	1.945252	H	2.885672	-2.533413	-0.951396
Cl		4.211337	-0.695184	H	2.349231	-3.020800	0.656134
CI	-3.916572		-1.761653	C	1.983027	-4.539923	-0.893573
N		1.391709					
N	2.289055	1.391709		H	2 957999	-5 056257	-0 776496
N H	2.289055 2.930406	1.842610	-2.419709	H	2.957989	-5.056257 -4.608362	-0.776496 -1.961084
N H N	2.289055 2.930406 0.064033	1.842610 1.327230	-2.419709 -0.986988	H	1.690770	-4.608362	-1.961084
N H N N	2.289055 2.930406 0.064033 -2.111295	1.842610 1.327230 1.526783	-2.419709 -0.986988 -0.023656				
N H N N	2.289055 2.930406 0.064033 -2.111295 2.805195	1.842610 1.327230 1.526783 0.924069	-2.419709 -0.986988 -0.023656 -0.176599	H H	1.690770 1.228506	-4.608362	-1.961084
N H N N	2.289055 2.930406 0.064033 -2.111295	1.842610 1.327230 1.526783	-2.419709 -0.986988 -0.023656	H H	1.690770	-4.608362	-1.961084

	licity: 5			C	3.667147	4.361418	-0.058699
Charge	: 0			H	3.946521	5.402306	-0.280360
E(B97-	3c) = -5596.38071	3574475 Hartree		С	4.397307	3.300598	-0.612231
E (M06/	def2-TZVP) = -559	6.629801015921 Ha	rtree	Н	5.257129	3.503805	-1.268848
	- D3(BJ)/def2-TZV			С	4.037442	1.971318	-0.336475
	- D3(BJ)/def2-TZ			Н	4.625839	1.156316	-0.780687
	(-3c) = -5589.6191		UJZ 1991 Hartice	C	2.370466	-0.075489	2.703600
	= -1.13712  Kcal/s			C	1.214400	0.349993	3.391299
,	= 122.68174 Kcal			Н	0.338193	0.703100	2.830244
			0 11				
	X-V/def2-TZVP) =		U Hartree	С	1.160806	0.312032	4.792776
	-xTB) = $-152.4590$			H	0.246869	0.646985	5.305948
	-xTB) = $-152.1076$			С	2.256787	-0.163314	5.527589
E (GFN-	FF) = -19.0859157	80954 Hartree		H	2.213412	-0.199065	6.626764
				С	3.412857	-0.590047	4.852851
Coordi	nates:			H	4.281262	-0.955362	5.422552
Cr	0.129793	-0.417705	-0.299332	C	3.473030	-0.543566	3.452214
Al	-3.785280	2.863836	0.270108	H	4.391648	-0.872794	2.946900
Cl	0.933795	-0.628176	-2.433145	C	3.825493	-1.098137	0.408356
Cl	-5.381433	1.452142	0.734459	Н	4.743702	-0.553889	0.717481
Cl	-3.525005	4.341928	1.874054	Н	3.743227	-1.986810	1.065479
N	-0.681760	-2.515237	1.858843	С	3.911036	-1.538834	-1.052716
Н	-0.852408	-3.305417	2.486562	Н	4.836938	-2.128456	-1.210743
N	-1.272409	-0.323860	1.253338	Н	3.909394	-0.685277	-1.757136
N	-2.154539	1.740641	0.434900	H	3.046608	-2.167944	-1.334324
P	0.050239	-2.750903	0.307031	11	3.040000	-2.10/944	-1.334324
	-1.143342			a c .			
P		1.457610	-0.923080		mation 4.		
P	2.367988	-0.024861	0.854439		olicity: 5		
С	-1.354178	-1.339171	2.168332	Charge			
С	-2.062479	-1.215831	3.371370		(3c) = -5596.393395		
H	-2.099340	-2.056833	4.077003		def2-TZVP) = -5596		
C	-2.683687	0.012293	3.644301	E(PBE	- D3(BJ)/def2-TZVE	P) = -5594.605472	482395 Hartree
H	-3.207532	0.161686	4.600272	E(PBEC	- D3(BJ)/def2-TZN	(7P) = -5595.00209	7578518 Hartree
C	-2.666753	1.037011	2.703179	E (PBEh	(-3c) = -5589.63142	20967067 Hartree	
H	-3.156575	2.002754	2.884772		= -8.32198  Kcal/m		
С	-2.020404	0.829707	1.457176		= 104.41180 Kcal/		
Č	1.455697	-3.832577	0.752123		X-V/def2-TZVP) = -		4 Hartree
C	2.042195	-3.750550	2.033464		-xTB) = $-152.46503$		1 Hartree
Н							
	1.611848	-3.082339	2.794261		(-xTB) = -152.11412		
С	3.188835	-4.502871	2.330303	E (GFN-	-FF) = -19.12790689	9//UI Hartree	
Н	3.637541	-4.431958	3.332801				
С	3.764305	-5.329577	1.352096		nates:		
H	4.665218	-5.916758	1.585509	Cr	0.851843	-0.149373	-0.042183
C	3.187831	-5.405326	0.072748	Al	-3.885964	-1.774537	1.024903
H	3.636931	-6.049866	-0.697847	Cl	2.164236	-0.764231	-1.829198
C	2.038888	-4.661306	-0.230036	Cl	-4.080215	-2.717974	2.999136
H	1.591533	-4.722528	-1.234203	Cl	-4.959790	0.140992	0.959741
С	-1.071553	-3.814460	-0.679321	N	1.860850	0.980238	2.673361
Č	-1.704277	-3.213000	-1.786817	Н	2.341399	1.266018	3.530539
Н	-1.445163	-2.180042	-2.072465	N	-0.115799	0.036732	1.795297
C	-2.648285	-3.938064	-2.530005	N	-2.007867	-1.157183	0.963230
Н	-3.140413	-3.459676	-3.390218	P	2.725289	0.339480	1.321347
C				P			
	-2.958500	-5.258870	-2.172178		-0.937174	-1.658414	-0.293193
H	-3.700714	-5.827060	-2.753468	P	0.222623	2.069408	-0.963426
С	-2.320010	-5.864125	-1.074323	С	0.501599	0.700581	2.821779
Н	-2.561267	-6.902545	-0.800340	С	-0.174235	1.085337	3.985224
С	-1.375054	-5.147045	-0.328029	Н	0.355450	1.634620	4.775190
H	-0.868863	-5.627354	0.524699	С	-1.528137	0.740354	4.098419
C	-0.331732	3.033875	-1.356030	H	-2.095532	1.031783	4.994738
С	0.716068	2.996921	-2.303507	C	-2.157537	0.007009	3.099648
H	1.038107	2.030546	-2.723733	Н	-3.199199	-0.310439	3.212984
C	1.357562	4.186273	-2.676424	C	-1.431623	-0.374869	1.942778
H	2.173178	4.154304	-3.414475	C	3.915021	1.654492	0.905656
С	0.975798	5.407216	-2.097276	C	3.852386	2.939148	1.482636
H	1.482404	6.338952	-2.392487	Н	3.113307	3.150376	2.269833
С	-0.032722	5.433899	-1.121660	С	4.706590	3.955245	1.026080
H	-0.321968	6.383447	-0.646231	Н	4.655916	4.955711	1.482051
С	-0.684030	4.251449	-0.740248	С	5.614564	3.699281	-0.013445
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C	-2.254327	0.975520	-2.299558	C	5.669857	2.421970	-0.597645
C		1.322813	-3.639736	Н	6.371452	2.221911	-1.421447
Н	2 001005		-3.039/30	C C		1.400608	-0.145016
н	-2.001985		2 005072				
	-1.185924	2.017348	-3.885873		4.824335		
C	-1.185924 -2.801176	2.017348 0.788616	-4.661168	H	4.842573	0.409871	-0.625320
C H	-1.185924 -2.801176 -2.603927	2.017348 0.788616 1.068575	-4.661168 -5.707064	H C	4.842573 3.735047	0.409871 -1.066958	-0.625320 1.918738
C H C	-1.185924 -2.801176 -2.603927 -3.848515	2.017348 0.788616 1.068575 -0.094944	-4.661168 -5.707064 -4.354324	H C C	4.842573 3.735047 3.169578	0.409871 -1.066958 -2.350054	-0.625320 1.918738 1.762197
C H C H	-1.185924 -2.801176 -2.603927 -3.848515 -4.475301	2.017348 0.788616 1.068575 -0.094944 -0.508371	-4.661168 -5.707064 -4.354324 -5.159064	H C C H	4.842573 3.735047 3.169578 2.194479	0.409871 -1.066958 -2.350054 -2.457054	-0.625320 1.918738 1.762197 1.257466
C H C H	-1.185924 -2.801176 -2.603927 -3.848515 -4.475301 -4.106204	2.017348 0.788616 1.068575 -0.094944 -0.508371 -0.434349	-4.661168 -5.707064 -4.354324 -5.159064 -3.015779	H C C H C	4.842573 3.735047 3.169578 2.194479 3.853924	0.409871 -1.066958 -2.350054 -2.457054 -3.478983	-0.625320 1.918738 1.762197 1.257466 2.232490
C H C H C	-1.185924 -2.801176 -2.603927 -3.848515 -4.475301 -4.106204 -4.942099	2.017348 0.788616 1.068575 -0.094944 -0.508371 -0.434349 -1.103491	-4.661168 -5.707064 -4.354324 -5.159064 -3.015779 -2.761826	H C C H C	4.842573 3.735047 3.169578 2.194479 3.853924 3.405862	0.409871 -1.066958 -2.350054 -2.457054 -3.478983 -4.475896	-0.625320 1.918738 1.762197 1.257466 2.232490 2.103173
C H C H C	-1.185924 -2.801176 -2.603927 -3.848515 -4.475301 -4.106204 -4.942099 -3.310777	2.017348 0.788616 1.068575 -0.094944 -0.508371 -0.434349 -1.103491 0.093136	-4.661168 -5.707064 -4.354324 -5.159064 -3.015779 -2.761826 -1.988719	H C C H C H	4.842573 3.735047 3.169578 2.194479 3.853924 3.405862 5.106209	0.409871 -1.066958 -2.350054 -2.457054 -3.478983 -4.475896 -3.330528	-0.625320 1.918738 1.762197 1.257466 2.232490 2.103173 2.851094
C H C H C H C	-1.185924 -2.801176 -2.603927 -3.848515 -4.475301 -4.106204 -4.942099	2.017348 0.788616 1.068575 -0.094944 -0.508371 -0.434349 -1.103491	-4.661168 -5.707064 -4.354324 -5.159064 -3.015779 -2.761826	H C C H C	4.842573 3.735047 3.169578 2.194479 3.853924 3.405862	0.409871 -1.066958 -2.350054 -2.457054 -3.478983 -4.475896	-0.625320 1.918738 1.762197 1.257466 2.232490 2.103173 2.851094 3.215641
C H C H C	-1.185924 -2.801176 -2.603927 -3.848515 -4.475301 -4.106204 -4.942099 -3.310777	2.017348 0.788616 1.068575 -0.094944 -0.508371 -0.434349 -1.103491 0.093136	-4.661168 -5.707064 -4.354324 -5.159064 -3.015779 -2.761826 -1.988719	H C C H C H	4.842573 3.735047 3.169578 2.194479 3.853924 3.405862 5.106209	0.409871 -1.066958 -2.350054 -2.457054 -3.478983 -4.475896 -3.330528	-0.625320 1.918738 1.762197 1.257466 2.232490 2.103173 2.851094
C H C H C H C	-1.185924 -2.801176 -2.603927 -3.848515 -4.475301 -4.106204 -4.942099 -3.310777 -3.535089	2.017348 0.788616 1.068575 -0.094944 -0.508371 -0.434349 -1.103491 0.093136 -0.160119	-4.661168 -5.707064 -4.354324 -5.159064 -3.015779 -2.761826 -1.988719 -0.941576	H C C H C H C	4.842573 3.735047 3.169578 2.194479 3.853924 3.405862 5.106209 5.647669	0.409871 -1.066958 -2.350054 -2.457054 -3.478983 -4.475896 -3.330528 -4.216837	-0.625320 1.918738 1.762197 1.257466 2.232490 2.103173 2.851094 3.215641
C H C H C H C	-1.185924 -2.801176 -2.603927 -3.848515 -4.475301 -4.106204 -4.942099 -3.310777 -3.535089 -3.978358	2.017348 0.788616 1.068575 -0.094944 -0.508371 -0.434349 -1.103491 0.093136 -0.160119 3.752862	-4.661168 -5.707064 -4.354324 -5.159064 -3.015779 -2.761826 -1.988719 -0.941576 -1.495381	H C C H C H C H C	4.842573 3.735047 3.169578 2.194479 3.853924 3.405862 5.106209 5.647669 5.677036	0.409871 -1.066958 -2.350054 -2.457054 -3.478983 -4.475896 -3.330528 -4.216837 -2.054197	-0.625320 1.918738 1.762197 1.257466 2.232490 2.103173 2.851094 3.215641 2.997800
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С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н	-1.185924 -2.801176 -2.603927 -3.848515 -4.475301 -4.106204 -4.942099 -3.310777 -3.535089 -3.978358 -4.128732 -3.026549 -5.133454 -5.271741	2.017348 0.788616 1.068575 -0.094944 -0.508371 -0.434349 -1.103491 0.093136 -0.160119 3.752862 4.825030 3.731971 3.261695 3.894228	-4.661168 -5.707064 -4.354324 -5.159064 -3.015779 -2.761826 -1.988719 -0.941576 -1.495381 -1.231117 -2.067795 -2.379842 -3.284305	Н С С Н С Н С Н С Н С Н С Н С С Н С С Н С С Н С С Н С С Н С С Н С С Н С С Н С С Н С С С Н С С С Н С С С Н С С С Н С С С С С Н С С С С С С С С С С С С С С С С С С С С	4.842573 3.735047 3.169578 2.194479 3.853924 3.405862 5.106209 5.647669 5.677036 6.662475 4.996232 5.448380 -1.927493	0.409871 -1.066958 -2.350054 -2.457054 -3.478983 -4.475896 -3.330528 -4.216837 -2.054197 -1.942990 -0.920234 0.079121 -1.646859	-0.625320 1.918738 1.762197 1.257466 2.232490 2.103173 2.851094 3.215641 2.997800 3.475389 2.531010 2.631680 -1.824788
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С Н С Н С Н С Н С Н С Н С Н С Н С Н С	-1.185924 -2.801176 -2.603927 -3.848515 -4.475301 -4.106204 -4.942099 -3.310777 -3.535089 -3.978358 -4.128732 -3.026549 -5.133454 -5.271741 -6.097822 -4.964546 2.938748	2.017348 0.788616 1.068575 -0.094944 -0.508371 -0.434349 -1.103491 0.093136 -0.160119 3.752862 4.825030 3.731971 3.261695 3.894228 3.253484 2.223701 1.691814	-4.661168 -5.707064 -4.354324 -5.159064 -3.015779 -2.761826 -1.988719 -0.941576 -1.495381 -1.231117 -2.067795 -2.379842 -3.284305 -1.831007 -2.731083 0.500435	H C C H C H C H C H C C H C	4.842573 3.735047 3.169578 2.194479 3.853924 3.405862 5.106209 5.647669 5.677036 6.662475 4.996232 5.448380 -1.927493 -2.877307 -3.075610 -3.623880	0.409871 -1.066958 -2.350054 -2.457054 -3.478983 -4.475896 -3.330528 -4.216837 -2.054197 -1.942990 -0.920234 0.079121 -1.646859 -0.622078 0.114492 -0.573765	-0.625320 1.918738 1.762197 1.257466 2.232490 2.103173 2.851094 3.215641 2.997800 3.475389 2.531010 2.631680 -1.824788 -2.017015 -1.225340 -3.200406
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С Н С Н С Н С Н С Н С Н С С Н С С Н С С С С С С С С С С С С С С С С С С С С	-1.185924 -2.801176 -2.603927 -3.848515 -4.475301 -4.106204 -4.942099 -3.310777 -3.535089 -3.978358 -4.128732 -3.026549 -5.133454 -5.271741 -6.097822 -4.964546 2.938748 2.194420	2.017348 0.788616 1.068575 -0.094944 -0.508371 -0.434349 -1.103491 0.093136 -0.160119 3.752862 4.825030 3.731971 3.261695 3.894228 3.253484 2.223701 1.691814 2.766557	-4.661168 -5.707064 -4.354324 -5.159064 -3.015779 -2.761826 -1.988719 -0.941576 -1.495381 -1.231117 -2.067795 -2.379842 -3.284305 -1.831007 -2.731083 0.500435 1.034192	H C C H C H C H C H C H C H	4.842573 3.735047 3.169578 2.194479 3.853924 3.405862 5.106209 5.647669 5.677036 6.662475 4.996232 5.448380 -1.927493 -2.877307 -3.075610 -3.623880 -4.378276	0.409871 -1.066958 -2.350054 -2.457054 -3.478983 -4.475896 -3.330528 -4.216837 -2.054197 -1.942990 -0.920234 0.079121 -1.646859 -0.622078 0.114492 -0.573765 0.215850	-0.625320 1.918738 1.762197 1.257466 2.232490 2.103173 2.851094 3.215641 2.997800 3.475389 2.531010 2.631680 -1.824788 -2.017015 -1.225340 -3.200406 -3.326719

H C	0 000104						
			4 01 7 0 5 4		0 004501	6 740010	
C	-2.277194	-3.280502	-4.817954	H	-0.284501	6.749312	0.617919
0	-1.707026	-2.595856	-2.841428	C	-2.420746	6.332378	0.653782
H	-0.974614	-3.403302	-2.695465	H	-2.703491	7.339414	0.311829
C	-0.444034	-3.389649	0.058823	С	-3.413199	5.372328	0.905498
C							
C	0.668593	-3.920845	-0.633533	H	-4.474942	5.623874	0.761679
H	1.192643	-3.305058	-1.383052	C	-3.055656	4.085053	1.336018
С	1.132743	-5.208042	-0.324981	H	-3.835531	3.327467	1.504317
H	1.997341	-5.618791	-0.868724	C	-0.504586	2.250409	3.699739
С	0.508058	-5.960706	0.684504	С	-0.986445	3.209863	4.612971
H	0.877141	-6.968743	0.928638	H	-1.740837	3.946192	4.293389
С	-0.580040	-5.420543	1.388938	С	-0.490514	3.229856	5.924772
H	-1.065651	-5.999574	2.189021	H	-0.864162	3.978533	6.639855
C	-1.059229	-4.137247	1.083809	C	0.487115	2.302173	6.324152
H	-1.899328	-3.718297	1.660732	H	0.876651	2.326394	7.353305
C	-4.376475	-3.111624	-0.352043	C	0.976444	1.353345	5.411353
H	-4.604370	-2.595893	-1.308771	H	1.752416	0.633650	5.713342
H	-3.493964	-3.753793	-0.572477	C	0.485712	1.328315	4.099101
C	-5.563813	-3.992574	0.070350	H	0.878121	0.599642	3.369269
Н	-5.814702	-4.761563	-0.693241	C	2.045361	-1.604276	-1.350956
H	-6.482067	-3.389334	0.234964	С	1.701389	-2.722554	-2.136700
H	-5.361642	-4.521362	1.024645	H	1.018901	-3.495179	-1.749540
C	-0.827882	2.041125	-2.472425	С	2.224268	-2.848395	-3.431947
С	-0.448574	1.147655	-3.498609	H	1.951606	-3.724721	-4.039238
H	0.389485	0.451036	-3.332442	C	3.088724	-1.869499	-3.946395
	-1.147348						
С		1.140423	-4.713011	H	3.492877	-1.970626	-4.965056
H	-0.850331	0.436629	-5.504826	C	3.424375	-0.751376	-3.166667
					4 070007		
С	-2.238601	2.002558	-4.906924	H	4.078907	0.032091	-3.575762
H	-2.794040	1.984526	-5.857021	C	2.895580	-0.606402	-1.876524
С	-2.631127	2.875353	-3.880032	Н	3.105517	0.300520	-1.286776
H	-3.490403	3.548183	-4.024319	C	2.604353	-1.629725	1.560474
С	-1.925719	2.902584	-2.666756	C	2.162093	-1.908921	2.872745
H	-2.228728	3.598082	-1.870029	H	1.089383	-2.049971	3.077173
C	-0.688830	3.054402	0.279541	C		-2.074679	3.904080
	-0.688830	3.054402		C	3.095556	-2.074679	3.904080
C	-0.095941	4.125885	0.980870	H	2.744483	-2.323639	4.917129
H	0.908303	4.482779	0.707310	C	4.470157	-1.948855	3.639917
C	-0.781852	4.743285	2.039057	H	5.202409	-2.083036	4.450418
H	-0.310932	5.581439	2.575751	C	4.908179	-1.665643	2.336823
C	-2.060337	4.298970	2.412145	H	5.984203	-1.578467	2.123044
H	-2.592648	4.784206	3.244280	C	3.980690	-1.503745	1.296347
C	-2.653466	3.226965	1.725209	H	4.331610	-1.298335	0.274385
H	-3.644236	2.842193	2.009876	C	2.497166	-4.905944	0.919731
C	-1.970446	2.605530	0.672607	H	2.972617	-4.400428	1.787983
Н							
	-2.445121	1.747272	0.172393	H	2.380643	-5.966156	1.251367
C	1.673233	3.091149	-1.517928	C	3.421012	-4.863424	-0.301196
Н	2.283412	3.281247	-0.611397	H	4.381291	-5.395621	-0.122645
H	2.269796	2.380705	-2.128452	H	3.682878	-3.824751	-0.588249
C	1.353274	4.374461	-2.279967	H	2.950509	-5.331028	-1.191507
H	2.288427	4.909599	-2.544476	С	0.110244	1.165780	-3.202847
H	0.725447	5.065632	-1.682093	C	1.182954	2.080875	-3.114966
H	0.806716	4.158980	-3.219161	H	1.384480		-2.160616
Н	0.806716	4.158980	-3.219161	H	1.384480	2.594410	-2.160616
Н	0.806716	4.158980	-3.219161	H C	1.384480 2.012302	2.594410 2.299621	-2.160616 -4.223631
		4.158980	-3.219161	С	2.012302	2.594410 2.299621	-4.223631
Confor	mation 8.	4.158980	-3.219161	C H	2.012302 2.843816	2.594410 2.299621 3.016901	-4.223631 -4.145799
Confor		4.158980	-3.219161	С	2.012302	2.594410 2.299621	-4.223631
Confor Multip	mation 8. licity: 5	4.158980	-3.219161	C H C	2.012302 2.843816 1.799504	2.594410 2.299621 3.016901 1.591740	-4.223631 -4.145799 -5.417759
Confor Multip Charge	mation 8. licity: 5 : 0		-3.219161	C H C H	2.012302 2.843816 1.799504 2.458750	2.594410 2.299621 3.016901 1.591740 1.756112	-4.223631 -4.145799 -5.417759 -6.283790
Confor Multip Charge E(B97-	mation 8. licity: 5 : 0 3c) = -5596.388164	1410458 Hartree		C H C	2.012302 2.843816 1.799504	2.594410 2.299621 3.016901 1.591740	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357
Confor Multip Charge E(B97-	mation 8. licity: 5 : 0 3c) = -5596.388164	1410458 Hartree		C H C H C	2.012302 2.843816 1.799504 2.458750 0.747341	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357
Confor Multip Charge E(B97- E(M06/	mation 8. licity: 5: 0 3c) = -5596.388164 def2-TZVP) = -5596	1410458 Hartree 5.635454850569 Har	tree	C H C H C	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358
Confor Multip Charge E(B97- E(M06/	mation 8. licity: 5 : 0 3c) = -5596.388164	1410458 Hartree 5.635454850569 Har	tree	C H C H C	2.012302 2.843816 1.799504 2.458750 0.747341	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357
Confor Multip Charge E(B97- E(M06/ E(PBE	mation 8.  clicity: 5 : 0 3c) = -5596.38816 def2-TZVP) = -5596 - D3(BJ)/def2-TZVI	1410458 Hartree 5.635454850569 Har P) = -5594.6002986	tree 70206 Hartree	C H C H C	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251 -0.102414	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642 0.459074	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358 -4.402829
Confor Multip Charge E (B97- E (M06/ E (PBE E (PBE0	mation 8. licity: 5 : 0 3c) = -5596.38816 def2-TZVP) = -5596 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI	1410458 Hartree 5.635454850569 Har 2) = -5594.6002986 VP) = -5594.997220	tree 70206 Hartree	C H C H C H C	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251 -0.102414 -0.935599	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642 0.459074 -0.254025	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358 -4.402829 -4.482813
Confor Multip Charge E (B97- E (M06/ E (PBE E (PBE0) E (PBEh	mation 8. licity: 5 : 0 3c) = -5596.388164 def2-TZVP) = -5596 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI	1410458 Hartree 5.635454850569 Har 2) = -5594.6002986 7P) = -5594.997220 18199500 Hartree	tree 70206 Hartree	C H C H C H C	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251 -0.102414 -0.935599 -2.148218	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642 0.459074 -0.254025 -0.337347	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358 -4.402829 -4.482813 -2.053274
Confor Multip Charge E (B97- E (M06/ E (PBE E (PBE0) E (PBEh	mation 8. licity: 5 : 0 3c) = -5596.38816 def2-TZVP) = -5596 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI	1410458 Hartree 5.635454850569 Har 2) = -5594.6002986 7P) = -5594.997220 18199500 Hartree	tree 70206 Hartree	C H C H C H C	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251 -0.102414 -0.935599	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642 0.459074 -0.254025	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358 -4.402829 -4.482813
Confor Multip Charge E (B97- E (M06/ E (PBE E (PBE0 E (PBEh E (PM6))	mation 8. licity: 5: 0 3c) = -5596.388164 def2-TZVP) = -5596 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - 3c) = -5589.62524 = -6.60257 Kcal/r	1410458 Hartree 5.635454850569 Har P) = -5594.6002986 VP) = -5594.997220 18199500 Hartree	tree 70206 Hartree	C H C H C H C H C	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251 -0.102414 -0.935599 -2.148218 -3.537136	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642 0.459074 -0.254025 -0.337347 -0.190543	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358 -4.402829 -4.482813 -2.053274 -1.852023
Confor Multip Charge E (B97- E (M06/ E (PBE E (PBE0 E (PBEh E (PM6) E (PM7)	mation 8. licity: 5 : 0 3c) = -5596.388164 def2-TZVP) = -5596 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - 3c) = -5589.6252 = -6.60257 Kcal/r = 97.36029 Kcal/r	1410458 Hartree 5.635454850569 Har P) = -5594.6002986 PP) = -5594.997220 18199500 Hartree nol	tree 70206 Hartree 541527 Hartree	C H C H C H C H C	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251 -0.102414 -0.935599 -2.148218 -3.537136 -3.962898	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642 0.459074 -0.254025 -0.337347 -0.190543 0.789998	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358 -4.402829 -4.482813 -2.053274 -1.852023 -1.593650
Confor Multip Charge E (B97- E (M06/ E (PBE E (PBE0 E (PBEh E (PM6) E (PM7)	mation 8. licity: 5: 0 3c) = -5596.388164 def2-TZVP) = -5596 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - 3c) = -5589.62524 = -6.60257 Kcal/r	1410458 Hartree 5.635454850569 Har P) = -5594.6002986 PP) = -5594.997220 18199500 Hartree nol	tree 70206 Hartree 541527 Hartree	C H C H C H C H C	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251 -0.102414 -0.935599 -2.148218 -3.537136	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642 0.459074 -0.254025 -0.337347 -0.190543	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358 -4.402829 -4.482813 -2.053274 -1.852023
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Confor Multip Charge E (B97- E (M06/ E (PBE E (PBE0 E (PBE0) E (PM6) E (PM7) E (\omega B97 E (GFN1	mation 8.  licity: 5 : 0 3c) = -5596.388164 def2-TZVP) = -5594 - D3(BJ)/def2-TZV1 - D3(BJ)/def2-TZV2-3c) = -5589.62524 = -6.60257 Kcal/r Z-V/def2-TZVP) = -xTB) = -152.46414	1410458 Hartree 5.635454850569 Har P) = -5594.6002986 PP) = -5594.997220 18199500 Hartree nol nol -5597.234767327922	tree 70206 Hartree 541527 Hartree	С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251 -0.102414 -0.935599 -2.148218 -3.537136 -3.962898 -4.390116 -5.471445	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642 0.459074 -0.254025 -0.337347 -0.190543 0.789998 -1.299247 -1.169279	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358 -4.402829 -4.482813 -2.053274 -1.852023 -1.593650 -1.966309 -1.806409
Confor Multip Charge E (B97- E (M06/ E (PBE E (PBE0 E (PBE0) E (PM6) E (PM7) E (\omega B97 E (GFN1	mation 8.  clicity: 5 : 0 3c) = -5596.388164 def2-TZVP) = -5596 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - 3c) = -5589.62524 = -6.60257 Kcal/r 297.36029 Kcal/r X-V/def2-TZVP) = -6.60257 Kcal/r	1410458 Hartree 5.635454850569 Har P) = -5594.6002986 PP) = -5594.997220 18199500 Hartree nol nol -5597.234767327922	tree 70206 Hartree 541527 Hartree	С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251 -0.102414 -0.935599 -2.148218 -3.537136 -3.962898 -4.390116	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642 0.459074 -0.254025 -0.337347 -0.190543 0.789998 -1.299247	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358 -4.402829 -4.482813 -2.053274 -1.852023 -1.593650 -1.966309
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Confor Multip Charge E (B97- E (M06/ E (PBE E (PBE0) E (PM6) E (PM7) E (GFN1 E (GFN1	mation 8.  licity: 5 : 0 3c) = -5596.388164 def2-TZVP) = -5594 - D3(BJ)/def2-TZV1 - D3(BJ)/def2-TZV2-3c) = -5589.62524 = -6.60257 Kcal/r Z-V/def2-TZVP) = -xTB) = -152.46414	1410458 Hartree 5.635454850569 Har 2) = -5594.6002986 7P) = -5594.997220 18199500 Hartree nol nol -5597.234767327922 11699474 Hartree 64681391 Hartree	tree 70206 Hartree 541527 Hartree	С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251 -0.102414 -0.935599 -2.148218 -3.537136 -3.962898 -4.390116 -5.471445 -3.870205 -4.540354	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642 0.459074 -0.254025 -0.337347 -0.190543 0.789998 -1.299247 -1.169279 -2.566435 -3.436062	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358 -4.402829 -4.482813 -2.053274 -1.852023 -1.593650 -1.966309 -1.806409 -2.270243 -2.344565
Confor Multip Charge E (B97- E (M06/ E (PBE E (PBE0 E (PBE0) E (PM7) E (GFN1 E (GFN1 E (GFN2	mation 8. licity: 5 : 0 3c) = -5596.388164 def2-TZVP) = -5596 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - 5589.6252 = -6.60257 Kcal/r = 97.36029 Kcal/r X-V/def2-TZVP) = -xTB) = -152.46414 -xTB) = -152.11345 FF) = -19.12687234	1410458 Hartree 5.635454850569 Har 2) = -5594.6002986 7P) = -5594.997220 18199500 Hartree nol nol -5597.234767327922 11699474 Hartree 64681391 Hartree	tree 70206 Hartree 541527 Hartree	C H C H C H C H C H C H C H C H C	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251 -0.102414 -0.935599 -2.148218 -3.537136 -3.962898 -4.390116 -5.471445 -3.870205 -4.540354 -2.487564	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642 0.459074 -0.254025 -0.337347 -0.190543 0.789998 -1.299247 -1.169279 -2.566435 -3.436062 -2.726149	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358 -4.402829 -4.482813 -2.053274 -1.852023 -1.593650 -1.966309 -1.806409 -2.270243 -2.344565 -2.454682
Confor Multip Charge E (B97- E (M06/ E (PBE E (PBE0) E (PM6) E (PM7) E (GFN1 E (GFN1	mation 8. licity: 5 : 0 3c) = -5596.388164 def2-TZVP) = -5596 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - 5589.6252 = -6.60257 Kcal/r = 97.36029 Kcal/r X-V/def2-TZVP) = -xTB) = -152.46414 -xTB) = -152.11345 FF) = -19.12687234	1410458 Hartree 5.635454850569 Har 2) = -5594.6002986 7P) = -5594.997220 18199500 Hartree nol nol -5597.234767327922 11699474 Hartree 64681391 Hartree	tree 70206 Hartree 541527 Hartree	С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251 -0.102414 -0.935599 -2.148218 -3.537136 -3.962898 -4.390116 -5.471445 -3.870205 -4.540354	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642 0.459074 -0.254025 -0.337347 -0.190543 0.789998 -1.299247 -1.169279 -2.566435 -3.436062	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358 -4.402829 -4.482813 -2.053274 -1.852023 -1.593650 -1.966309 -1.806409 -2.270243 -2.344565
Confor Multip Charge E (B97- E (M06/ E (PBE E (PBE0) E (PM7) E (WB97 E (GFN1 E (GFN2 E (GFN- Coordi	mation 8.  licity: 5 : 0 3c) = -5596.388164 def2-TZVP) = -5596 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - 3c) = -5589.62524 = -6.60257 Kcal/r = 97.36029 Kcal/r = 97.36029 Kcal/r X-V/def2-TZVP) = -xTB) = -152.46414 -xTB) = -152.11349 FF) = -19.12687234	1410458 Hartree 5.635454850569 Har P) = -5594.6002986 PP) = -5594.997220 18199500 Hartree and nol -5597.234767327922 11699474 Hartree 54681391 Hartree 13514 Hartree	etree 170206 Hartree 1541527 Hartree 18 Hartree	С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н С Н Н С Н Н Н Н Н Н Н Н Н Н Н Н Н	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251 -0.102414 -0.935599 -2.148218 -3.537136 -3.962898 -4.390116 -5.471445 -3.870205 -4.540354 -2.487564 -2.058513	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642 0.459074 -0.254025 -0.337347 -0.190543 0.789998 -1.299247 -1.169279 -2.566435 -3.436062 -2.726149 -3.722551	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358 -4.402829 -4.482813 -2.053274 -1.852023 -1.593650 -1.966309 -1.806409 -2.270243 -2.344565 -2.454682 -2.636493
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Confor Multip Charge E (B97-E (M06/E (PBE E (PBE) E (PBE) E (PBE) E (GFN1 E (GFN1 E (GFN1 C (GFN1 C)) GFN1 C (GFN1 C (GFN1 C (GFN1 C (GFN1 C (GFN1 C)) GFN1 C (GFN1 C)) GFN1 C (GFN1 C (GFN1 C)) GFN1 C (GFN1 C (GFN1 C)) GFN1 C (GFN1	mation 8. licity: 5: 0 3c) = -5596.388164 def2-TZVP) = -5596 - D3(BJ)/def2-TZV - 3c) = -5589.62524 = -6.60257 Kcal/r = 97.36029 Kcal/r = 97.36029 Kcal/r = 77.36029 Kcal/r = 77.36029 Kcal/r = 152.46414 -xTB) = -152.11345 FF) = -19.12687234  nates:  0.123190 0.588363 1.872643 -0.296884 -0.484770 -2.561846 -3.329178 -1.309315 0.100253	1410458 Hartree 5.635454850569 Har P) = -5594.6002986 18199500 Hartree 1001 1001 10597.234767327922 11699474 Hartree 13514 Hartree 13514 Hartree 13514 Hartree 135173 14.782115 15.444816 1.133173 1.365636 1.663051 1.2.500364	0.515218 0.869767 0.360448 2.826314 -0.747886 2.034900 2.671603 1.152324 0.560734	С H C H C H C H C H C H C H C H C H C H	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251 -0.102414 -0.935599 -2.148218 -3.537136 -3.962898 -4.390116 -5.471445 -3.870205 -4.540354 -2.487564 -2.058513 -1.634090 -0.550316 -1.963292 -2.710059 -1.250163 -2.598467 -3.156352	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642 0.459074 -0.254025 -0.337347 -0.190543 0.789998 -1.299247 -1.169279 -2.566435 -3.436062 -2.726149 -3.722551 -1.621146 -1.764304 2.598154 2.544717 3.389778 2.918549 3.876108	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358 -4.402829 -4.482813 -2.053274 -1.852023 -1.593650 -1.966309 -1.806409 -2.270243 -2.344565 -2.454682 -2.636493 -2.344565 -2.454682 -1.852083 -1.823988 -1.004560 -1.511290 -3.174667 -3.123129
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Confor Multip Charge E (B97- E (M06/ E (PBE) E (PBE0) E (PEM6) E (PM7) E (GB97 E (GFN12) E (GFN12) Coordi Cr Al Cl Cl Cl N H N N P P P	mation 8. licity: 5: 0 3c) = -5596.388164 def2-TZVP) = -5596 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - S1(BJ)/def2-TZVI - S1(BJ)/	1410458 Hartree 5.635454850569 Har 2) = -5594.6002986 7P) = -5594.997220 18199500 Hartree 18199500 Hartree 1801 1801 1802 1803 1804 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1805 1	0.515218 0.869767 0.360448 2.826314 -0.747886 2.034900 2.671603 1.152324 0.560734 1.982486 0.298436 -1.720486	С Н С Н С Н С Н С Н С Н С Н С Н Н Н Н Н	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251 -0.102414 -0.935599 -2.148218 -3.537136 -3.962898 -4.390116 -5.471445 -3.870205 -4.540354 -2.487564 -2.058513 -1.634090 -0.550316 -1.963292 -2.710059 -1.250163 -2.598467 -3.156352 -3.306067 -1.826980	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642 0.459074 -0.254025 -0.337347 -0.190543 0.789998 -1.299247 -1.169279 -2.566435 -3.436062 -2.726149 -3.722551 -1.621146 -1.764304 2.598154 2.544717 3.389778 2.918549 3.876108 2.128618	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358 -4.402829 -4.482813 -2.053274 -1.852023 -1.593650 -1.966309 -1.806409 -2.270243 -2.344565 -2.454682 -2.636493 -2.344342 -2.460853 -1.823988 -1.004560 -1.511290 -3.174667 -3.123129 -3.496055
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Confor Multip Charge E (B97-E (M06/E (PBE E (PBE0 E (PM6) E (PM7) E (GB97 E (GFN1 E (GFN2 E (GFN-C) Cordi Cr Al Cl Cl N H N N N P P P C C C C H C C C C C C C C C C C C	mation 8. licity: 5: 0 3c) = -5596.388164 def2-TZVP) = -5596 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - S1(BJ)/def2-TZVI - S1(BJ)/def2-TZVI = 97.36029 Kcal/r X-V/def2-TZVP) = -52.4641 -xTB) = -152.4641 -xTB) = -152.4641 -xTB) = -152.4641 -xTB) = -152.41345 FF) = -19.12687234  nates:	1410458 Hartree 5.635454850569 Har 2) = -5594.6002986 7P) = -5594.997220 18199500 Hartree 18199500 Hartree 18199500 Hartree 181699474 Hartree 184681391 Hartree 18514 Hartree 18514 Hartree 18514 Hartree 18515773 185773 185773 1865636 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 186305	0.515218 0.869767 0.360448 2.826314 -0.747886 2.034900 2.671603 1.152324 0.560734 1.982486 0.298436 -1.720486 1.675240 1.850922 2.267934 1.449493	CHCCHCCHCCHCCHCCCHCCCHCCCHCCCHCCCHCCCH	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251 -0.102414 -0.935599 -2.148218 -3.537136 -3.962898 -4.390116 -5.471445 -3.870205 -4.540354 -2.487564 -2.058513 -1.634090 -0.550316 -1.963292 -2.710059 -1.250163 -2.598467 -3.156352 -3.306067 -1.826980 YAA mation 14. slicity: 3	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642 0.459074 -0.254025 -0.337347 -0.190543 0.789998 -1.299247 -1.169279 -2.566435 -3.436062 -2.726149 -3.722551 -1.621146 -1.764304 2.598154 2.544717 3.389778 2.918549 3.876108 2.128618 3.015140	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358 -4.402829 -4.482813 -2.053274 -1.852023 -1.593650 -1.966309 -1.806409 -2.270243 -2.344565 -2.454682 -2.636493 -2.344342 -2.460853 -1.823988 -1.004560 -1.511290 -3.174667 -3.123129 -3.496055
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Confor Multip Charge E (B97-E (M06/E (PBE E (PBE0 E (PM6) E (PM7) E (GB97 E (GFN1 E (GFN2 E (GFN-C) Cordi Cr Al Cl Cl N H N N N P P P C C C C H C C C C C C C C C C C C	mation 8. licity: 5: 0 3c) = -5596.388164 def2-TZVP) = -5596 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - S1(BJ)/def2-TZVI - S1(BJ)/def2-TZVI = 97.36029 Kcal/r X-V/def2-TZVP) = -52.4641 -xTB) = -152.4641 -xTB) = -152.4641 -xTB) = -152.4641 -xTB) = -152.41345 FF) = -19.12687234  nates:	1410458 Hartree 5.635454850569 Har 2) = -5594.6002986 7P) = -5594.997220 18199500 Hartree 18199500 Hartree 18199500 Hartree 181699474 Hartree 184681391 Hartree 18514 Hartree 18514 Hartree 18514 Hartree 18515773 185773 185773 1865636 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 1863051 186305	0.515218 0.869767 0.360448 2.826314 -0.747886 2.034900 2.671603 1.152324 0.560734 1.982486 0.298436 -1.720486 1.675240 1.850922 2.267934 1.449493	CHCCHCCHCCCHCCCHCCCHCCCCHCCCHCCCCHCCCCHCCCC	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251 -0.102414 -0.935599 -2.148218 -3.537136 -3.962898 -4.390116 -5.471445 -3.870205 -4.540354 -2.487564 -2.058513 -1.634090 -0.550316 -1.963292 -2.710059 -1.250163 -2.598467 -3.156352 -3.306067 -1.826980 YAA mation 14. slicity: 3	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642 0.459074 -0.254025 -0.337347 -0.190543 0.789998 -1.299247 -1.169279 -2.566435 -3.436062 -2.726149 -3.722551 -1.621146 -1.764304 2.598154 2.544717 3.389778 2.918549 3.876108 2.128618 3.015140	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358 -4.402829 -4.482813 -2.053274 -1.852023 -1.593650 -1.966309 -1.806409 -2.270243 -2.344565 -2.454682 -2.636493 -2.344342 -2.460853 -1.823988 -1.004560 -1.511290 -3.174667 -3.123129 -3.496055 -3.963948
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Confor Multip Charge E (B97-E (M06/E (PBE E (PBE0 E (P	mation 8. licity: 5: 0 3c) = -5596.388164 def2-TZVP) = -5596 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - 3c) = -5589.62524 = -6.60257 Kcal/r = 97.36029 Kcal/r = 97.36029 Kcal/r = 97.36029 Kcal/r = 10.2020 Kcal/r	1410458 Hartree 5.635454850569 Har 2) = -5594.6002986 18199500 Hartree 18199500 Hartree 18199500 Hartree 18199500 Hartree 18199500 Hartree 18199500 Hartree 18199474 Hartree 183514 Hartree 18514 Hartree 18514 Hartree 18514 Hartree 18517 2.185773 185773 185773 1865636 1863051 1865636 1863051 1865636 1863051 1865635 1865635 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 18656777 1865677 1865677 1865677 1865677 1865677 1865677 1865677 1865677 1865677 1865677 1865677 1865677 1865677 1865677 1865677 1865677 1865677 1865677 1865677 1865677 1865677 1865677 1865677 1865677 1865677 1865677 1865	0.515218 0.869767 0.360448 2.826314 -0.747886 2.034900 2.671603 1.152324 0.560734 1.982486 0.298436 -1.720486 1.675240 1.850922 2.267934 1.449493 1.528337 0.966562 0.645429	CHCHHCCHHCCHHCCHHCCHHCCHHCCHHCCHHCCHHC	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251 -0.102414 -0.935599 -2.148218 -3.537136 -3.962898 -4.390116 -5.471445 -3.870205 -4.540354 -2.487564 -2.058513 -1.634090 -0.550316 -1.963292 -2.710059 -1.250163 -2.598467 -3.156352 -3.306067 -1.826980 YAA mation 14. clicity: 3 : 0 def2-TZVP) = -389 - 3893.56120 def2-TZVP) = -389 - D3 (BJ) / def2-TZVI	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642 0.459074 -0.254025 -0.337347 -0.190543 0.789998 -1.299247 -1.169279 -2.566435 -3.436062 -2.726149 -3.722551 -1.621146 -1.764304 2.598154 2.544717 3.389778 2.918549 3.876108 2.128618 3.015140	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358 -4.402829 -4.482813 -2.0553274 -1.852023 -1.593650 -1.966309 -1.806409 -2.270243 -2.344565 -2.454682 -2.636493 -2.344342 -2.460853 -1.823988 -1.004560 -1.511290 -3.174667 -3.123129 -3.496055 -3.963948
Confor Multip Charge E (B97-E (M06/E (PBE E (PBE0 E (PM6) E (PM7) E (GBN1 E (GFN1 C) Cordi Cr Al Cl Cl N H N N P P C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C C C C C C C C C C C C C C C C C C	mation 8. licity: 5: 0 3c) = -5596.388164 def2-TZVP) = -5596 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - 3c) = -5589.62524 = -6.60257 Kcal/r = 97.36029 Kcal/r = 1.52.46414 - xTB) = -152.11349 FF) = -19.12687234  nates: 0.123190 0.588363 1.872643 -0.296884 -0.48470 -2.561846 -3.329178 -1.309315 0.100253 -1.120322 1.319032 -0.969271 -2.493836 -3.599314 -4.534176 -3.476243 -4.339377 -2.267259	1410458 Hartree 5.635454850569 Har P) = -5594.002986 18199000 Hartree nol nol -5597.234767327922 11699474 Hartree 54681391 Hartree 13514 Hartree 0.706834 -4.396157 2.185773 -4.782115 -5.444816 1.133173 1.365636 -0.663051 -2.500364 2.091672 -1.315020 1.025835 -0.218117 -1.056777 -0.658322 -2.396458 -3.073743 -2.881104	0.515218 0.869767 0.360448 2.826314 -0.747886 2.034900 2.671603 1.152324 0.560734 1.982486 0.298436 -1.720486 1.675240 1.850922 2.267934 1.449493 1.528337 0.966562	CHCHHCCHHCCHHCCHHCCHHCCHHCCHHCCHHCCHHC	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251 -0.102414 -0.935599 -2.148218 -3.537136 -3.962898 -4.390116 -5.471445 -3.870205 -4.540354 -2.487564 -2.058513 -1.634090 -0.550316 -1.963292 -2.710059 -1.250163 -2.598467 -3.156352 -3.306067 -1.826980 YAA mation 14. dicity: 3 : 0 3c) = -3893.56120 def2-TZVP) = -3893	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642 0.459074 -0.254025 -0.337347 -0.190543 0.789998 -1.299247 -1.169279 -2.566435 -3.436062 -2.726149 -3.722551 -1.621146 -1.764304 2.598154 2.544717 3.389778 2.918549 3.876108 2.128618 3.015140	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358 -4.402829 -4.482813 -2.0553274 -1.852023 -1.593650 -1.966309 -1.806409 -2.270243 -2.344565 -2.454682 -2.636493 -2.344342 -2.460853 -1.823988 -1.004560 -1.511290 -3.174667 -3.123129 -3.496055 -3.963948
Confor Multip Charge E (B97-E (M06/E (PBE E (PBE0 E (PM6) E (PM7) E (GBN1 E (GFN1 C) Cordi Cr Al Cl Cl N H N N P P C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C C C C C C C C C C C C C C C C C C	mation 8. licity: 5: 0 3c) = -5596.388164 def2-TZVP) = -5596 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - S1(BJ)/def2-TZVI - S1(BJ)/def2-TZVI = 97.36029 Kcal/r X-V/def2-TZVP) = -2XTB) = -152.46414 -XTB) = -152.46414 -XTB) = -152.46414 -XTB) = -152.41344 FF) = -19.12687234  nates:	1410458 Hartree 5.635454850569 Har 2) = -5594.6002986 37P) = -5594.997220 18199500 Hartree 18199500 Hartree 18199500 Hartree 181699474 Hartree 184681391 Hartree 183514 Hartree 183514 Hartree 183514 Hartree 183516 Hartree 183517 2.185773 -4.782115 -5.444816 1.133173 1.365636 -0.663051 -2.500364 2.091672 -1.315020 1.025835 -0.218117 -1.056777 -0.658322 -2.396458 -3.073743 -2.881104 -3.923601 -2.012045	0.515218 0.869767 0.360448 2.826314 -0.747886 2.034900 2.671603 1.152324 0.560734 1.982486 0.298436 -1.720486 1.675240 1.850922 2.267934 1.449493 1.528337 0.966562 0.645429 0.876780	C H C H C H C C H C C H C C H C C H C C H C C H C C C H C C C C C C C C C C C C C C C C C C C C	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251 -0.102414 -0.935599 -2.148218 -3.537136 -3.962898 -4.390116 -5.471445 -3.870205 -4.540354 -2.487564 -2.058513 -1.634090 -0.550316 -1.963292 -2.710059 -1.250163 -2.598467 -3.156352 -3.306067 -1.826980 YAA mation 14. licity: 3 :: 0 3c) = -3893.561200 def2-TZVP) = -3893 -BBJ/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642 0.459074 -0.254025 -0.337347 -0.190543 0.789998 -1.299247 -1.169279 -2.566435 -3.436062 -2.726149 -3.722551 -1.621146 -1.764304 2.598154 2.544717 3.389778 2.918549 3.876108 2.128618 3.015140 4159994 Hartree 3.294578076202 Ha P) = -3891.975745 VP) = -3892.23733	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358 -4.402829 -4.482813 -2.0553274 -1.852023 -1.593650 -1.966309 -1.806409 -2.270243 -2.344565 -2.454682 -2.636493 -2.344342 -2.460853 -1.823988 -1.004560 -1.511290 -3.174667 -3.123129 -3.496055 -3.963948
Confor Multip Charge E (B97-E (M06/E (PBE E (PBE O E)))))))))))))))))))))	mation 8. licity: 5: 0 3c) = -5596.388164 def2-TZVP) = -5596 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - 3c) = -5589.62524 = -6.60257 Kcal/r = 97.36029 Kcal/r = 152.46414 -xTB) = -152.11345 FF) = -19.12687234  nates:  0.123190 0.588363 1.872643 -0.296884 -0.484770 -2.561846 -3.329178 -1.309315 0.100253 -1.120322 1.319032 -0.969271 -2.493836 -3.599314 -4.534176 -3.476243 -4.339377 -2.267259 -2.155508 -1.150562 -1.698563	1410458 Hartree 5.635454850569 Har 7P) = -5594.6002986 18199500 Hartree 18199500 Hartree 18199500 Hartree 18199500 Hartree 18199500 Hartree 18199474 Hartree 183514 Hartree 183514 Hartree 183514 Hartree 183514 Hartree 183516 Hartree 183517 2.185773 2.185773 4.782115 -5.444816 1.133173 1.365636 -0.663051 -2.500364 2.091672 -1.315020 1.025835 -0.218117 -1.056777 -0.658322 -2.396458 -3.073743 -2.881104 -3.923601 -2.012045 3.757594	0.515218 0.515218 0.869767 0.360448 2.826314 -0.747886 2.034900 2.671603 1.152324 0.560734 1.982486 0.298436 -1.720486 1.675240 1.850922 2.267934 1.449493 1.528337 0.966562 0.645429 0.876780 1.523453	CHCCHHCCHHCCHHCCHHCCHHCCHHCCHHCCHHCCHH	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251 -0.102414 -0.935599 -2.148218 -3.537136 -3.962898 -4.390116 -5.471445 -3.870205 -4.540354 -2.487564 -2.058513 -1.634090 -0.550316 -1.963292 -2.710059 -1.250163 -2.598467 -3.156352 -3.306067 -1.826980 YAA mation 14. clicity: 3 :: 0 3c) = -3893.5612000 def2-TZVP) = -38990 - D3 (BJ) / def2-TZVI - D3 (BJ) / def2-TZVI	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642 0.459074 -0.254025 -0.337347 -0.190543 0.789998 -1.299247 -1.169279 -2.566435 -3.436062 -2.726149 -3.722551 -1.621146 -1.764304 2.598154 2.544717 3.389778 2.918549 3.876108 2.128618 3.015140 4159994 Hartree 4159994 Hartree 43.294578076202 Ha P) = -3891.975745 VP) = -38992.23733 26142691 Hartree	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358 -4.402829 -4.482813 -2.0553274 -1.852023 -1.593650 -1.966309 -1.806409 -2.270243 -2.344565 -2.454682 -2.636493 -2.344342 -2.460853 -1.823988 -1.004560 -1.511290 -3.174667 -3.123129 -3.496055 -3.963948
Confor Multip Charge E (B97-E (M06/E (PBE E (PBE0 E (PM6) E (PM7) E (GBN1 E (GFN1 C) Cordi Cr Al Cl Cl N H N N P P C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C C C C C C C C C C C C C C C C C C	mation 8. licity: 5: 0 3c) = -5596.388164 def2-TZVP) = -5596 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - S1(BJ)/def2-TZVI - S1(BJ)/def2-TZVI = 97.36029 Kcal/r X-V/def2-TZVP) = -2XTB) = -152.46414 -XTB) = -152.46414 -XTB) = -152.41344 FF) = -19.12687234  nates:	1410458 Hartree 5.635454850569 Har 2) = -5594.6002986 37P) = -5594.997220 18199500 Hartree 18199500 Hartree 18199500 Hartree 181699474 Hartree 184681391 Hartree 183514 Hartree 183514 Hartree 183514 Hartree 183516 Hartree 183517 2.185773 -4.782115 -5.444816 1.133173 1.365636 -0.663051 -2.500364 2.091672 -1.315020 1.025835 -0.218117 -1.056777 -0.658322 -2.396458 -3.073743 -2.881104 -3.923601 -2.012045	0.515218 0.869767 0.360448 2.826314 -0.747886 2.034900 2.671603 1.152324 0.560734 1.982486 0.298436 -1.720486 1.675240 1.850922 2.267934 1.449493 1.528337 0.966562 0.645429 0.876780	CHCCHHCCHHCCHHCCHHCCHHCCHHCCHHCCHHCCHH	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251 -0.102414 -0.935599 -2.148218 -3.537136 -3.962898 -4.390116 -5.471445 -3.870205 -4.540354 -2.487564 -2.058513 -1.634090 -0.550316 -1.963292 -2.710059 -1.250163 -2.598467 -3.156352 -3.306067 -1.826980 YAA mation 14. licity: 3 :: 0 3c) = -3893.561200 def2-TZVP) = -3893 -BBJ/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642 0.459074 -0.254025 -0.337347 -0.190543 0.789998 -1.299247 -1.169279 -2.566435 -3.436062 -2.726149 -3.722551 -1.621146 -1.764304 2.598154 2.544717 3.389778 2.918549 3.876108 2.128618 3.015140 4159994 Hartree 4159994 Hartree 43.294578076202 Ha P) = -3891.975745 VP) = -38992.23733 26142691 Hartree	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358 -4.402829 -4.482813 -2.0553274 -1.852023 -1.593650 -1.966309 -1.806409 -2.270243 -2.344565 -2.454682 -2.636493 -2.344342 -2.460853 -1.823988 -1.004560 -1.511290 -3.174667 -3.123129 -3.496055 -3.963948
Confor Multip Charge E (B97-E (M06/E (PBE E E (PBE E (PBE E E (PBE E E (PBE E E (PBE E E E E E E E E E E E E E E E E E E	mation 8. licity: 5: 0 3c) = -5596.388164 def2-TZVP) = -5596 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - 3c) = -5589.62524 = -6.60257 Kcal/r = 97.36029 Kcal/r = 97.36029 Kcal/r = 97.36029 Kcal/r = 97.36029 Kcal/r = 78.36029 Kcal/r = 1.52.4641 - xTB) = -152.11345 FF) = -19.12687234  nates:  0.123190 0.588363 1.872643 -0.96884 -0.484770 -2.561846 -3.329178 -1.309315 0.100253 -1.120322 1.319032 -0.969271 -2.493836 -3.599314 -4.534176 -3.476243 -4.339377 -2.267259 -2.155508 -1.150562 -1.698563 -0.699507	1410458 Hartree 5.635454850569 Har 7P) = -5594.002986 18199500 Hartree 18199500 Hartree 18199500 Hartree 18199501 Hartree 18199501 Hartree 18199474 Hartree 183514 Hartree 183514 Hartree 183514 Hartree 183514 Hartree 183516 Hartree 183517 2.185773 -4.782115 -5.444816 1.133173 1.365636 -0.663051 -2.500364 2.091672 -1.315020 1.025835 -0.218117 -1.056777 -0.658322 -2.396458 -3.073743 -2.881104 -3.923601 -2.012045 3.757594 4.721022	0.515218 0.869767 0.360448 2.826314 -0.747886 2.034900 2.671603 1.152324 0.560734 1.982486 0.298436 -1.720486 1.675240 1.850922 2.267934 1.449493 1.528337 0.966562 0.645429 0.876780 1.523453 1.523453 1.523453	CHCCHHCCHHCCHHCCHHCCHHCCHHCCHHCCHHCCHH	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251 -0.102414 -0.935599 -2.148218 -3.537136 -3.962898 -4.390116 -5.471445 -3.870205 -4.540354 -2.487564 -2.058513 -1.634090 -0.550316 -1.963292 -2.710059 -1.250163 -2.598467 -3.156352 -3.306067 -1.826980 YAA mation 14. licity: 3 : 0 3c) = -3893.56120 def2-TZVP) = -389: -36 (BJ) / def2-TZVI -D3 (BJ) / def2-TZVI -D3 (BJ) / def2-TZVI -D3 (BJ) / def2-TZVI -D3 (BJ) / def2-TZVI -B3 (BJ) / def2-TZVI	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642 0.459074 -0.254025 -0.337347 -0.190543 0.789998 -1.299247 -1.169279 -2.566435 -3.436062 -2.726149 -3.722551 -1.621146 -1.764304 2.598154 2.544717 3.389778 2.918549 3.876108 2.128618 3.015140 4159994 Hartree 3.294578076202 Ha P) = -3891.23733 26142691 Hartree mol	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358 -4.402829 -4.482813 -2.0553274 -1.852023 -1.593650 -1.966309 -1.806409 -2.270243 -2.344565 -2.454682 -2.636493 -2.344342 -2.460853 -1.823988 -1.004560 -1.511290 -3.174667 -3.123129 -3.496055 -3.963948
Confor Multip Charge E (B97-E (M06/E (PBE E (PBE0 E (P	mation 8. licity: 5: 0 3c) = -5596.388164 def2-TZVP) = -5596 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - 3c) = -5589.6252 = -6.60257 Kcal/r = 97.36029 Kcal/r = 97.36029 Kcal/r = 97.36029 Kcal/r = 97.36029 Kcal/r = 1.0029 Kc	1410458 Hartree 5.635454850569 Har 7) = -5594.6002986 18199500 Hartree 18199500 Hartree 18199500 Hartree 18199501 Hartree 18199501 Hartree 18199474 Hartree 183514 Hartree 183514 Hartree 18514 Hartree 18516 Hartree 18517 2.185773 -4.782115 -5.444816 1.133173 1.365636 -0.663051 -2.500364 2.091672 -1.315020 1.025835 -0.218117 -1.056777 -0.658322 -2.396458 -3.073743 -2.881104 -3.923601 -2.012045 3.757594 4.721022 4.445443	0.515218 0.869767 0.360448 2.826314 -0.747886 2.034900 2.671603 1.152324 0.560734 1.982486 0.298436 -1.720486 1.675240 1.850922 2.267934 1.449493 1.528337 0.966562 0.645429 0.876780 1.523453 1.259306 1.356038	CHCHHCCHHCCHHCCHHCCHHCCHHCCHHCCHHCCHHC	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251 -0.102414 -0.935599 -2.148218 -3.537136 -3.962898 -4.390116 -5.471445 -3.870205 -4.540354 -2.487564 -2.058513 -1.634090 -0.550316 -1.963292 -2.710059 -1.250163 -2.598467 -3.156352 -3.306067 -1.826980  YAA  mation 14. licity: 3 : 0 def2-TZVP) = -389 - D3 (BJ) / def2-TZVI - D3 (BJ) / def2-TZVI - D3 (BJ) / def2-TZVI - 3c) = -3888.2919; -33c) = -3888.2919; -33c) = 88.99137 Kcal/i = 81.77057 Kcal/i	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642 0.459074 -0.254025 -0.337347 -0.190543 0.789998 -1.299247 -1.169279 -2.566435 -3.436062 -2.726149 -3.722551 -1.621146 -1.764304 2.598154 2.544717 3.389778 2.918549 3.876108 2.128618 3.015140 4159994 Hartree 3.294578076202 Ha P) = -3891.975745 VP) = -3892.23733 26142691 Hartree mol	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358 -4.402829 -4.482813 -2.055274 -1.852023 -1.593650 -1.966309 -1.806409 -2.270243 -2.344565 -2.454682 -2.636493 -2.344342 -2.460853 -1.823988 -1.004560 -1.511290 -3.174667 -3.123129 -3.496055 -3.963948
Confor Multip Charge E (B97-E (M06/E (PBE E E (PBE E (PBE E E (PBE E E (PBE E E (PBE E E E E E E E E E E E E E E E E E E	mation 8. licity: 5: 0 3c) = -5596.388164 def2-TZVP) = -5596 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - 3c) = -5589.62524 = -6.60257 Kcal/r = 97.36029 Kcal/r = 97.36029 Kcal/r = 97.36029 Kcal/r = 97.36029 Kcal/r = 78.36029 Kcal/r = 1.52.4641 - xTB) = -152.11345 FF) = -19.12687234  nates:  0.123190 0.588363 1.872643 -0.96884 -0.484770 -2.561846 -3.329178 -1.309315 0.100253 -1.120322 1.319032 -0.969271 -2.493836 -3.599314 -4.534176 -3.476243 -4.339377 -2.267259 -2.155508 -1.150562 -1.698563 -0.699507	1410458 Hartree 5.635454850569 Har 7P) = -5594.002986 18199500 Hartree 18199500 Hartree 18199500 Hartree 18199501 Hartree 18199501 Hartree 18199474 Hartree 183514 Hartree 183514 Hartree 183514 Hartree 183514 Hartree 183516 Hartree 183517 2.185773 -4.782115 -5.444816 1.133173 1.365636 -0.663051 -2.500364 2.091672 -1.315020 1.025835 -0.218117 -1.056777 -0.658322 -2.396458 -3.073743 -2.881104 -3.923601 -2.012045 3.757594 4.721022	0.515218 0.869767 0.360448 2.826314 -0.747886 2.034900 2.671603 1.152324 0.560734 1.982486 0.298436 -1.720486 1.675240 1.850922 2.267934 1.449493 1.528337 0.966562 0.645429 0.876780 1.523453 1.523453 1.523453	CHCHHCCHHCCHHCCHHCCHHCCHHCCHHCCHHCCHHC	2.012302 2.843816 1.799504 2.458750 0.747341 0.577251 -0.102414 -0.935599 -2.148218 -3.537136 -3.962898 -4.390116 -5.471445 -3.870205 -4.540354 -2.487564 -2.058513 -1.634090 -0.550316 -1.963292 -2.710059 -1.250163 -2.598467 -3.156352 -3.306067 -1.826980 YAA mation 14. licity: 3 : 0 3c) = -3893.56120 def2-TZVP) = -389: -36 (BJ) / def2-TZVI -D3 (BJ) / def2-TZVI -D3 (BJ) / def2-TZVI -D3 (BJ) / def2-TZVI -D3 (BJ) / def2-TZVI -B3 (BJ) / def2-TZVI	2.594410 2.299621 3.016901 1.591740 1.756112 0.666720 0.104642 0.459074 -0.254025 -0.337347 -0.190543 0.789998 -1.299247 -1.169279 -2.566435 -3.436062 -2.726149 -3.722551 -1.621146 -1.764304 2.598154 2.544717 3.389778 2.918549 3.876108 2.128618 3.015140 4159994 Hartree 3.294578076202 Ha P) = -3891.975745 VP) = -3892.23733 26142691 Hartree mol	-4.223631 -4.145799 -5.417759 -6.283790 -5.500357 -6.431358 -4.402829 -4.482813 -2.053274 -1.852023 -1.593650 -1.966309 -1.806409 -2.270243 -2.344565 -2.454682 -2.636493 -2.344342 -2.460853 -1.823988 -1.004560 -1.511290 -3.174667 -3.123129 -3.496055 -3.963948

	-xTB) = $-161.2712$			H C	0.185143	-1.129436 -3.221780	-3.294870
	-xTB) = $-160.1837$ ; FF) = $-22.3974067$ ;			Н	-0.969613 -1.725942	-3.827786	-1.867653 -1.331798
2 (021	22.037.1007	11170 110110100		H	-0.522305	-2.522959	-1.125472
Coordi				H	-0.164457	-3.890101	-2.236479
Co	-0.172086	-0.355137	-0.146222	P	-0.320275	-1.543158	1.769640
N N	1.456171 -1.116257	0.791283 0.306368	-0.325789 -1.709477	C C	0.928347 1.001858	-2.881029 -3.933327	2.127351 1.187153
C	3.008065	2.311970	-1.773283	Н	0.311895	-3.951087	0.331452
C	1.659692	1.578250	-1.395316	C	1.935903	-4.966107	1.336062
С	0.658924	1.768220	-2.381168	H	1.974861	-5.774196	0.589934
H C	0.950545 -0.648684	2.465317 1.261874	-3.166786 -2.536877	C H	2.817238 3.557192	-4.969073 -5.775518	2.430255 2.544208
C	-1.435931	1.934978	-3.721952	C	2.732604	-3.944576	3.384223
С	3.529501	1.635803	-3.068340	Н	3.401690	-3.946408	4.258448
H	4.478689	2.113246	-3.388851	С	1.792626	-2.910797	3.238433
H H	2.805356 3.732636	1.708164 0.559654	-3.901512 -2.896171	H C	1.733841 -1.853974	-2.129587 -2.587397	4.007128 1.921216
C	2.747324	3.812706	-2.056495	C	-2.946888	-2.397642	1.058984
Н	3.703940	4.307556	-2.321877	Н	-2.889367	-1.649480	0.257651
H	2.343030	4.324680	-1.159890	C	-4.119196	-3.156555	1.218374
H C	2.043950 4.171129	3.988571 2.275143	-2.891998 -0.761506	H C	-4.960042 -4.207065	-2.991349 -4.109934	0.529042 2.241999
Н	5.047609	2.759497	-1.239794	Н	-5.126096	-4.702315	2.369595
Н	4.472670	1.254091	-0.476320	C	-3.116813	-4.306359	3.107958
H	3.954404	2.829669	0.168250	H	-3.179140	-5.052765	3.914520
C	-0.577866	1.895495	-5.014534 -5.855480	C	-1.946942	-3.553149	2.948017
H H	-1.162781 -0.301085	2.320713 0.857109	-5.282098	H C	-1.095753 -0.437726	-3.711525 -0.584885	3.627589 3.347862
Н	0.355928	2.483684	-4.939513	C	-1.687450	-0.334924	3.955383
С	-2.798159	1.323355	-4.108763	H	-2.598479	-0.794661	3.546460
H	-3.183384	1.876833	-4.989614	C	-1.776473	0.499217	5.079974
H H	-3.556057 -2.721542	1.400715 0.257698	-3.311390 -4.391275	H C	-2.759855 -0.621010	0.688770 1.080622	5.537243 5.627177
C	-1.680168	3.414527	-3.334319	Н	-0.692652	1.729400	6.513423
H	-2.219043	3.939857	-4.150562	C	0.624345	0.834091	5.029944
H	-0.730033	3.950700	-3.145084	H	1.540338	1.289572	5.435309
H C	-2.295720 2.329780	3.491414 0.733371	-2.417065 0.785760	C H	0.713055 1.687599	0.022217	3.890265
C	3.182309	-0.387033	1.005607	п	1.00/399	-0.124273	3.411380
Ċ	3.999506	-0.382470	2.156430	Confor	mation 19.		
H	4.645038	-1.255786	2.343202		licity: 3		
C H	4.031331	0.700322	3.040993	Charge		2000102 ***	
н С	4.696379 3.196747	0.681996 1.803749	3.917343 2.806234		3c) = -3893.559999 def2-TZVP) = -3893		rtree
		1.000717	2.000231	D (1100)		J. 2 J 2 O 1 O 1 1 O O 7 O 11 a	LCICC
H	3.215304	2.651760	3.504811	E (PBE	- D3(BJ)/def2-TZVI	= -3891.974521	353261 Hartree
С	2.321054	1.831390	1.710609	E(PBE0	- D3(BJ)/def2-TZV	JP) = -3892.23586	
C C	2.321054 3.383554	1.831390 -1.579328	1.710609 0.058045	E (PBE0 E (PBEh	- D3(BJ)/def2-TZV -3c) = -3888.29228	JP) = -3892.23586 35114661 Hartree	
C C H	2.321054 3.383554 3.392207	1.831390 -1.579328 -2.469461	1.710609 0.058045 0.724277	E(PBE0 E(PBEh E(PM6)	- D3(BJ)/def2-TZV -3c) = -3888.29228 = 88.38083 Kcal/r	JP) = -3892.23586 35114661 Hartree nol	
C C	2.321054 3.383554	1.831390 -1.579328	1.710609 0.058045	E (PBE0 E (PBEh E (PM6) E (PM7)	- D3(BJ)/def2-TZV -3c) = -3888.29228	<pre>/P) = -3892.23586 35114661 Hartree mol mol</pre>	9461007 Hartree
C C H C H	2.321054 3.383554 3.392207 2.319985 1.304528 2.487907	1.831390 -1.579328 -2.469461 -1.848357 -1.874004 -2.845724	1.710609 0.058045 0.724277 -1.008978 -0.555576 -1.464396	E (PBE0 E (PBEh E (PM6) E (PM7) E (ωB97 E (GFN1	- D3(BJ)/def2-TZV -3c) = -3888.29222 = 88.38083 Kcal/r = 51.12475 Kcal/r X-V/def2-TZVP) = - -xTB) = -161.26948	<pre>7P) = -3892.23586 85114661 Hartree mol mol -3895.84969230863 86258523 Hartree</pre>	9461007 Hartree
C H C H H	2.321054 3.383554 3.392207 2.319985 1.304528 2.487907 2.320580	1.831390 -1.579328 -2.469461 -1.848357 -1.874004 -2.845724 -1.094320	1.710609 0.058045 0.724277 -1.008978 -0.555576 -1.464396 -1.817286	E (PBE0 E (PBEh E (PM6) E (PM7) E (ωB97 E (GFN1 E (GFN2	- D3(BJ)/def2-TZV -3c) = -3888.29228 = 88.38083 Kcal/r = 51.12475 Kcal/r X-V/def2-TZVP) = - -xTB) = -161.26948 -xTB) = -160.18294	<pre>VP) = -3892.23586 35114661 Hartree no1 no1 -3895.84969230863 36258523 Hartree 43194542 Hartree</pre>	9461007 Hartree
C H C H H C	2.321054 3.383554 3.392207 2.319985 1.304528 2.487907 2.320580 4.770392	1.831390 -1.579328 -2.469461 -1.848357 -1.874004 -2.845724 -1.094320 -1.520469	1.710609 0.058045 0.724277 -1.008978 -0.555576 -1.464396 -1.817286 -0.617138	E (PBE0 E (PBEh E (PM6) E (PM7) E (ωB97 E (GFN1 E (GFN2	- D3(BJ)/def2-TZV -3c) = -3888.29222 = 88.38083 Kcal/r = 51.12475 Kcal/r X-V/def2-TZVP) = - -xTB) = -161.26948	<pre>VP) = -3892.23586 35114661 Hartree no1 no1 -3895.84969230863 36258523 Hartree 43194542 Hartree</pre>	9461007 Hartree
C H C H H	2.321054 3.383554 3.392207 2.319985 1.304528 2.487907 2.320580	1.831390 -1.579328 -2.469461 -1.848357 -1.874004 -2.845724 -1.094320	1.710609 0.058045 0.724277 -1.008978 -0.555576 -1.464396 -1.817286 -0.617138 -1.177385	E (PBE0 E (PBEh E (PM6) E (PM7) E (ωB97 E (GFN1 E (GFN2	- D3(BJ)/def2-TZV -3c) = -3888.29221 = 88.38083 Kcal/r = 51.12475 Kcal/r X-V/def2-TZVP) = - -xTB) = -161.26941 -xTB) = -160.18294 FF) = -22.39590590	<pre>VP) = -3892.23586 35114661 Hartree no1 no1 -3895.84969230863 36258523 Hartree 43194542 Hartree</pre>	9461007 Hartree
С Н С Н Н С Н Н	2.321054 3.383554 3.392207 2.319985 1.304528 2.487907 2.320580 4.770392 4.967134 5.585328 4.824817	1.831390 -1.579328 -2.469461 -1.848357 -1.874004 -2.845724 -1.094320 -1.520469 -2.457704 -1.383478 -0.681408	1.710609 0.058045 0.724277 -1.008978 -0.555576 -1.464396 -1.817286 -0.617138 -1.177385 0.120339 -1.339620	E(PBE0 E(PBEh E(PM6) E(PM7) E(GFN1 E(GFN1 E(GFN2 E(GFN- Coordi	- D3(BJ)/def2-TZV -3c) = -3888.29221 = 88.38083 Kcal/r = 51.12475 Kcal/r X-V/def2-TZVP) = - -xTB) = -161.26940 -xTB) = -160.18294 FF) = -22.39590590 nates: 0.072310	VP) = -3892.23586 35114661 Hartree mol mol -3895.84969230863 36258523 Hartree 43194542 Hartree 07788 Hartree	9461007 Hartree  9 Hartree  0.235800
С С Н С Н Н С Н Н С Н С Н	2.321054 3.383554 3.392207 2.319985 1.304528 2.487907 2.320580 4.770392 4.967134 5.585328 4.824817 1.383818	1.831390 -1.579328 -2.469461 -1.848357 -1.874004 -2.845724 -1.094320 -1.520469 -2.457704 -1.383478 -0.681408 3.013068	1.710609 0.058045 0.724277 -1.008978 -0.555576 -1.464396 -1.817286 -0.617138 -1.177385 0.120339 -1.339620 1.476091	E(PBE0 E(PBEh E(PM6)) E(PM7) E(GB97 E(GFN1 E(GFN2 E(GFN- Coordi Co	- D3(BJ)/def2-TZV -3c) = -3888.2922( = 88.38083 Kcal/r = 51.12475 Kcal/r X-V/def2-TZVP) =xTB) = -161.2694( -xTB) = -160.18294 FF) = -22.39590590  nates:	<pre>VP) = -3892.23586 35114661 Hartree mol mol -3895.84969230863 36258523 Hartree 43194542 Hartree 07788 Hartree -0.206940 1.414448</pre>	9461007 Hartree 9 Hartree 0.235800 0.617536
С С Н С Н Н С Н Н С Н Н С Н	2.321054 3.383554 3.392207 2.319985 1.304528 2.487907 2.320580 4.770392 4.967134 5.585328 4.824817 1.383818 1.405824	1.831390 -1.579328 -2.469461 -1.848357 -1.874004 -2.845724 -1.094320 -1.520469 -2.457704 -1.383478 -0.681408 3.013068 3.232636	1.710609 0.058045 0.724277 -1.008978 -0.555576 -1.464396 -1.817286 -0.617138 -1.177385 0.120339 -1.339620 1.476091 0.388773	E(PBE0 E(PBEh E(PM6)) E(PM7)) E(WB97 E(GFN1 E(GFN2 COORDI CO	- D3(BJ)/def2-TZV -3c) = -3888.29221 = 88.38083 Kcal/r = 51.12475 Kcal/r X-V/def2-TZVP) = - -xTB) = -161.26941 -xTB) = -160.18294 FF) = -22.39590590 nates: 0.072310 -0.988378 1.791638	VP) = -3892.23586 35114661 Hartree mol mol -3895.84969230863 36258523 Hartree 43194542 Hartree 07788 Hartree -0.206940 1.414448 0.666641	9461007 Hartree  9 Hartree  0.235800 0.617536 0.001662
С С Н С Н Н С Н Н С Н С Н	2.321054 3.383554 3.392207 2.319985 1.304528 2.487907 2.320580 4.770392 4.967134 5.585328 4.824817 1.383818	1.831390 -1.579328 -2.469461 -1.848357 -1.874004 -2.845724 -1.094320 -1.520469 -2.457704 -1.383478 -0.681408 3.013068	1.710609 0.058045 0.724277 -1.008978 -0.555576 -1.464396 -1.817286 -0.617138 -1.177385 0.120339 -1.339620 1.476091	E(PBE0 E(PBEh E(PM6)) E(PM7) E(GB97 E(GFN1 E(GFN2 E(GFN- Coordi Co	- D3(BJ)/def2-TZV -3c) = -3888.2922( = 88.38083 Kcal/r = 51.12475 Kcal/r X-V/def2-TZVP) =xTB) = -161.2694( -xTB) = -160.18294 FF) = -22.39590590  nates:	<pre>VP) = -3892.23586 35114661 Hartree mol mol -3895.84969230863 36258523 Hartree 43194542 Hartree 07788 Hartree -0.206940 1.414448</pre>	9461007 Hartree 9 Hartree 0.235800 0.617536
C C H C H H C C H H C H C H C H H	2.321054 3.383554 3.392207 2.319985 1.304528 2.487907 2.320580 4.770392 4.967134 5.585328 4.824817 1.383818 1.405824 -0.071627 -0.357632 -0.357632	1.831390 -1.579328 -2.469461 -1.848357 -1.874004 -2.845724 -1.094320 -1.520469 -2.457704 -1.383478 -0.681408 3.013068 3.232636 2.644101 1.704679 3.442214	1.710609 0.058045 0.724277 -1.008978 -0.555576 -1.464396 -1.817286 -0.617138 -1.177385 0.120339 -1.339620 1.476091 0.388773 1.807343 1.293011 1.476091	E(PBE0 E(PBEh E(PMG)) E(PMT)) E(GB97 E(GFN1 E(GFN2 E(GFN- Coordi Co N N C C	- D3(BJ)/def2-TZV -3c) = -3888.29221 = 88.38083 Kcal/r = 51.12475 Kcal/r X-V/def2-TZVP) = -xTB) = -161.26948 -xTB) = -160.18294 FF) = -22.39590590  nates:  0.072310 -0.988378 1.791638 -1.223241 -0.437344 0.972101	VP) = -3892.23586 35114661 Hartree mol mol -3895.84969230863 36258523 Hartree 43194542 Hartree  -0.206940 1.414448 0.666641 4.002259 2.635647 2.802596	9461007 Hartree  9 Hartree  0.235800 0.617536 0.001662 0.800963 0.756076 0.752072
C C H C H H H C H C H H H H C H H H	2.321054 3.383554 3.392207 2.319985 1.304528 2.487907 2.320580 4.770392 4.967134 5.585328 4.824817 1.383818 1.405824 -0.071627 -0.357632 -0.766910 -0.212598	1.831390 -1.579328 -2.469461 -1.848357 -1.874004 -2.845724 -1.094320 -1.520469 -2.457704 -1.383478 -0.681408 3.013068 3.232636 2.644101 1.704679 3.442214 2.483261	1.710609 0.058045 0.724277 -1.008978 -0.555576 -1.464396 -1.817286 -0.617138 -1.177385 0.120339 -1.339620 1.476091 0.388773 1.807343 1.293011 1.476091 2.894493	E(PBE0 E(PBEh E(PMG)) E(PMT)) E(GB97 E(GFN1 E(GFN2 E(GFN- Coordi Co N N C C C C C	- D3(BJ)/def2-TZV -3c) = -3888.2922( = 88.38083 Kcal/r = 51.12475 Kcal/r X-V/def2-TZVP) =xTB) = -161.2694( -xTB) = -160.18294 FF) = -22.3959059(  nates:  0.072310 -0.988378 1.791638 -1.223241 -0.437344 0.972101 1.299783	VP) = -3892.23586 35114661 Hartree mol mol mol -3895.84969230863 36258523 Hartree 43194542 Hartree 07788 Hartree -0.206940 1.414448 0.666641 4.002259 2.635647 2.802596 3.809061	9461007 Hartree  9 Hartree  0.235800 0.617536 0.001662 0.800963 0.756076 0.752072 1.013280
C C H C H H H C H H H C H C H H H C C H C H H H C C H C C H C C C C C C C C C C C C C C C C C C C C	2.321054 3.383554 3.392207 2.319985 1.304528 2.487907 2.320580 4.770392 4.967134 5.585328 4.967134 5.585328 4.924817 1.383818 1.405824 -0.071627 -0.357632 -0.766910 -0.212598 1.799234	1.831390 -1.579328 -2.469461 -1.848357 -1.874004 -2.845724 -1.094320 -1.520469 -2.457704 -1.383478 -0.681408 3.013068 3.232636 2.644101 1.704679 3.442214 2.483261 4.296247	1.710609 0.058045 0.724277 -1.008978 -0.555576 -1.464396 -1.817286 -0.617138 -1.177385 0.120339 -1.339620 1.476091 0.388773 1.807343 1.293011 1.476091 2.894493 2.202392	E(PBE0 E(PBEh E(PMG)) E(PM7) E(GB97 E(GFN1 E(GFN2 E(GFN- Coordi Co N C C C C C	- D3(BJ)/def2-TZV -3c) = -3888.29221 = 88.38083 Kcal/r = 51.12475 Kcal/r X-V/def2-TZVP) = - -xTB) = -161.26941 -xTB) = -160.18294 FF) = -22.39590590 nates: 0.072310 -0.988378 1.791638 -1.223241 -0.437344 0.972101 1.299783 2.026508	VP) = -3892.23586 35114661 Hartree mol mol mol -3895.84969230863 36258523 Hartree 43194542 Hartree 07788 Hartree -0.206940 1.414448 0.666641 4.002259 2.635647 2.802596 3.809061 1.942003	9461007 Hartree  9 Hartree  0.235800 0.617536 0.001662 0.800963 0.756076 0.752072 1.013280 0.389678
C C H C H H H C H C H H H H C H H H	2.321054 3.383554 3.392207 2.319985 1.304528 2.487907 2.320580 4.770392 4.967134 5.585328 4.824817 1.383818 1.405824 -0.071627 -0.357632 -0.766910 -0.212598	1.831390 -1.579328 -2.469461 -1.848357 -1.874004 -2.845724 -1.094320 -1.520469 -2.457704 -1.383478 -0.681408 3.013068 3.232636 2.644101 1.704679 3.442214 2.483261	1.710609 0.058045 0.724277 -1.008978 -0.555576 -1.464396 -1.817286 -0.617138 -1.177385 0.120339 -1.339620 1.476091 0.388773 1.807343 1.293011 1.476091 2.894493	E(PBE0 E(PBEh E(PMG)) E(PMT)) E(GB97 E(GFN1 E(GFN2 E(GFN- Coordi Co N N C C C C C	- D3(BJ)/def2-TZV -3c) = -3888.2922( = 88.38083 Kcal/r = 51.12475 Kcal/r X-V/def2-TZVP) =xTB) = -161.2694( -xTB) = -160.18294 FF) = -22.3959059(  nates:  0.072310 -0.988378 1.791638 -1.223241 -0.437344 0.972101 1.299783	VP) = -3892.23586 35114661 Hartree mol mol mol -3895.84969230863 36258523 Hartree 43194542 Hartree 07788 Hartree -0.206940 1.414448 0.666641 4.002259 2.635647 2.802596 3.809061	9461007 Hartree  9 Hartree  0.235800 0.617536 0.001662 0.800963 0.756076 0.752072 1.013280
С С H C H H H C H H C H H H C H H H H C H H H	2.321054 3.383554 3.392207 2.319985 1.304528 2.487907 2.320580 4.770392 4.967134 5.585328 4.824817 1.383818 1.405824 -0.071627 -0.357632 -0.766910 -0.212598 1.799234 1.140766 2.845465 1.708230	1.831390 -1.579328 -2.469461 -1.848357 -1.874004 -2.845724 -1.094320 -1.520469 -2.457704 -1.383478 -0.681408 3.013068 3.232636 2.644101 1.704679 3.442214 2.483261 4.296247 5.135058 4.583912 4.195915	1.710609 0.058045 0.724277 -1.008978 -0.555576 -1.464396 -1.817286 -0.617138 -1.177385 0.120339 -1.339620 1.476091 0.388773 1.807343 1.293011 1.476091 2.894493 2.202392 1.898587 1.971535 3.304213	E (PBE0 E (PBEh E (PMG)) E (PMG)) E (GB97 E (GFN1 E (GFN2 E (GFN- Coordi Co N N C C C C C C H C C	- D3(BJ)/def2-TZV -3c) = -3888.29221 = 88.38083 Kcal/r = 51.12475 Kcal/r X-V/def2-TZVP) = -xTB) = -161.26948 -xTB) = -160.18294 FF) = -22.39590590  nates:  0.072310 -0.988378 1.791638 -1.223241 -0.437344 0.972101 1.299783 2.026508 3.455242 -0.562125 -1.203344	VP) = -3892.23586 35114661 Hartree mol mol -3895.84969230863 36258523 Hartree 43194542 Hartree  -0.206940 1.414448 0.666641 4.002259 2.635647 2.802596 3.809061 1.942003 2.581559 5.018420 5.920191	9461007 Hartree  9 Hartree  0.235800 0.617536 0.001662 0.800963 0.756076 0.752072 1.013280 0.389678 0.570517 1.769189 1.833875
С С H С H H H С H H H С H H H С H H H С	2.321054 3.383554 3.392207 2.319985 1.304528 2.487907 2.320580 4.770392 4.967134 5.585328 4.967134 5.585328 4.924817 1.383818 1.405824 -0.071627 -0.357632 -0.766910 -0.212598 1.799234 1.140766 2.845465 1.708230 -2.423759	1.831390 -1.579328 -2.469461 -1.848357 -1.874004 -2.845724 -1.094320 -1.520469 -2.457704 -1.383478 -0.681408 3.013068 3.232636 2.644101 1.704679 3.442214 2.483261 4.296247 5.135058 4.583912 4.195915 -0.248314	1.710609 0.058045 0.724277 -1.008978 -0.555576 -1.464396 -1.817286 -0.617138 -1.177385 0.120339 -1.339620 1.476091 0.388773 1.807343 1.293011 1.476091 2.894493 2.202392 1.898587 1.971535 3.304213 -1.750613	E(PBEO E(PBEA) E(PMGA) E(PMGA) E(GFN1 E(GFN2 E(GFN- COORDI CO N C C C C C C C C C C C H C C C C H H C C C C H H H	- D3(BJ)/def2-TZV -3c) = -3888.29221 = 88.38083 Kcal/r = 51.12475 Kcal/r X-V/def2-TZVP) =xTB) = -161.26941 -xTB) = -160.18294 FF) = -22.39590590 nates:	VP) = -3892.23586 35114661 Hartree mol mol mol -3895.84969230863 36258523 Hartree 43194542 Hartree 07788 Hartree -0.206940 1.414448 0.666641 4.002259 2.635647 2.802596 3.809061 1.942003 2.581559 5.018420 5.920191 5.365586	9461007 Hartree  9 Hartree  0.235800 0.617536 0.001662 0.800963 0.756076 0.752072 1.013280 0.389678 0.570517 1.769189 1.833875 1.433514
С С H С H H H С H H H С H H H C C	2.321054 3.383554 3.392207 2.319985 1.304528 2.487907 2.320580 4.770392 4.967134 5.585328 4.824817 1.383818 1.405824 -0.071627 -0.357632 -0.766910 -0.212598 1.799234 1.140766 2.845465 1.708230 -2.423759 -3.490978	1.831390 -1.579328 -2.469461 -1.848357 -1.874004 -2.845724 -1.094320 -1.520469 -2.457704 -1.383478 -0.681408 3.013068 3.232636 2.644101 1.704679 3.442214 2.483261 4.296247 5.135058 4.583912 4.195915 -0.248314 0.423753	1.710609 0.058045 0.724277 -1.008978 -0.555576 -1.464396 -1.817286 -0.617138 -1.177385 0.120339 -1.339620 1.476091 0.388773 1.807343 1.293011 1.476091 2.894493 2.202392 1.898587 1.971535 3.304213 -1.750613 -1.074408	E (PBE0 E (PBEh E (PMG)) E (PMG) E (GM97 E (GFN1 E (GFN2 E (GFN- Coordi Co N N C C C C C C C H H H H	- D3(BJ)/def2-TZV -3c) = -3888.29221 = 88.38083 Kcal/r = 51.12475 Kcal/r X-V/def2-TZVP) =xTB) = -161.2694( -xTB) = -160.1829( FF) = -22.39590590  nates:  0.072310 -0.988378 1.791638 -1.223241 -0.437344 0.972101 1.299783 2.026508 3.455242 -0.562125 -1.203344 0.433672 -0.457936	VP) = -3892.23586 35114661 Hartree mol mol mol -3895.84969230863 36258523 Hartree 33194542 Hartree -0.206940 1.414448 0.666641 4.002259 2.635647 2.802596 3.809061 1.942003 2.581559 5.018420 5.920191 5.365586 4.607175	9461007 Hartree  9 Hartree  0.235800 0.617536 0.001662 0.800963 0.756076 0.752072 1.013280 0.389678 0.570517 1.769189 1.833875 1.433514 2.791754
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ССНСНННСНННСНННССССНСНСССКНСНННСН	2.321054 3.383554 3.392207 2.319985 1.304528 2.487907 2.320580 4.770392 4.967134 5.585328 4.824817 1.383818 1.405824 -0.071627 -0.357632 -0.766910 -0.212598 1.799234 1.140766 2.845465 1.708230 -2.423759 -3.490978 -4.785132 -5.604989 -5.049467 -6.071361 -3.992710 -4.185388 -2.674686 -3.238094 -2.235947 -4.262279 -4.355346 -3.99846 -5.271842 -3.185725 -2.370043 -4.135582 -2.996059 -1.596805 -2.146261	1.831390 -1.579328 -2.469461 -1.848357 -1.874004 -2.845724 -1.094320 -1.520469 -2.457704 -1.383478 -0.681408 3.013068 3.232636 2.644101 1.704679 3.442214 2.483261 4.296247 5.135058 4.583912 4.195915 -0.248314 0.423753 -0.122078 0.398715 -1.310945 -1.717310 -1.986726 -2.939458 -1.491780 1.682342 2.064570 2.796408 3.023375 3.727799 2.526958 1.311588 0.585864 0.840646 2.198437 -2.399931 -3.112637	1.710609 0.058045 0.724277 -1.008978 -0.555576 -1.464396 -1.817286 -0.617138 -1.177385 0.120339 -1.339620 1.476091 0.388773 1.807343 1.293011 1.476091 2.894493 2.202392 1.898587 1.971535 3.304213 -1.750613 -1.750613 -1.750613 -1.16496 -0.598655 -1.807113 -1.849142 -2.428227 -2.947435 -2.410663 -0.253475 -0.534048 -0.515304 -1.596248 0.005608 -0.141934 1.237640 1.425560 1.565059 1.87458 -3.004499 -3.657550	E(PBEO E(PBEO E(PBEO E(PMEO)) E(DMEO) E(DMEO) E(GFN- COORDI CO N C C C C C C C C C C C C C C C C C	- D3(BJ)/def2-TZV -3c) = -3888.2922i = 88.38083 Kcal/r = 51.12475 Kcal/r X-V/def2-TZVP) = -xTB) = -161.2694i -xTB) = -160.18294 FFF) = -22.39590590  nates:	PP) = -3892.23586 35114661 Hartree mol mol mol -3895.84969230863 36258523 Hartree 43194542 Hartree -0.206940 1.414448 0.666641 4.002259 2.635647 2.802596 3.809061 1.942003 2.581559 5.018420 5.920191 5.365586 4.607175 4.594498 5.586859 3.942097 4.719508 3.947785 4.986951 3.500665 3.387046 2.826205 3.280711 1.873378 3.500570 1.733066 2.257266 1.598182 0.732324 3.939169 4.373724 4.682504	9461007 Hartree  9 Hartree  0.235800 0.617536 0.001662 0.800963 0.756076 0.752072 1.013280 0.389678 0.570517 1.769189 1.833875 1.433514 2.791754 -0.630191 -0.663194 -1.370708 -0.946250 1.205164 1.239547 2.203658 0.495278 2.093739 2.296755 2.656783 2.497204 0.112040 0.419265 -0.983518 0.573474 -0.163402 0.014887 0.179276

C	-4.052651	0.497484	2.532516	Confo	rmation 20.		
Н	-4.335280	0.252373	3.569383	Multi	plicity: 3		
C	-5.037171	0.543732	1.536610	Charo			
			1.786157			770442 !!	
H	-6.090152	0.343592			(-3c) = -3893.569504		
С	-4.661799	0.826281	0.216948		S/def2-TZVP) = -3893		
H	-5.428228	0.841967	-0.572396		: - D3(BJ)/def2-TZVP		
С	-3.326811	1.102416	-0.120003	E (PBE	0 - D3(BJ)/def2-TZV	P) = -3892.24517	1708628 Hartree
С	-1.711096	0.699771	3.422856	E(PBE	2h-3c) = -3888.30372	7951105 Hartree	
H	-2.277874	0.187423	4.231020	E(PM6	5) = 80.46644  Kcal/m	.01	
С	-0.473401	-0.170009	3.168296		r) = 36.81475 Kcal/m		
Н	-0.773426	-1.175459	2.828043		7X-V/def2-TZVP) = -		3 Hartree
Н	0.113701	-0.294931	4.102066		II-xTB) = -161.27561		3 Hareree
H	0.216194	0.286209	2.419129		I2-xTB) = $-160.19005$		
C	-1.303994	2.071020	3.987528	E (GFN	I-FF) = $-22.40634227$	6997 Hartree	
H	-0.752177	1.939153	4.941341				
H	-2.184377	2.712533	4.190405	Coord	linates:		
H	-0.631898	2.605704	3.289482	Co	-0.073153	-0.090218	-0.207773
С	-2.948549	1.449198	-1.555189	N	-0.032710	0.890436	1.500949
Н	-1.970486	1.967408	-1.502365	N	-1.710473	-1.076021	0.050916
C	-2.727622	0.185356	-2.398487	C	-1.011671	1.363790	3.881555
H	-1.927052	-0.432321	-1.949872	С	-1.009156	0.754402	2.422490
H	-2.425011	0.446838	-3.433216	С	-2.153635	-0.047294	2.174220
H	-3.643087	-0.438932	-2.445372	H	-2.895061	-0.005188	2.971909
C	-3.945996	2.398284	-2.235140	C	-2.522971	-0.899450	1.114239
H	-3.550909	2.730997	-3.216947	C	-3.967930	-1.505945	1.263680
H	-4.140908	3.301240	-1.621984	С	-2.405510	1.952481	4.232218
Н	-4.920854	1.905062	-2.428858	H	-2.351482	2.439974	5.226474
C	2.629897	-0.022689	-0.914115	Н	-3.207829	1.193333	4.295527
C	3.261841	-1.250040	-0.547923	Н	-2.718972	2.719947	3.497600
C	4.129259	-1.862478	-1.467633	C	-0.722858	0.191622	4.853128
H	4.639566	-2.794361	-1.188671	H	-0.743069	0.552977	5.902729
C	4.350670	-1.318803	-2.738404	H	0.275116	-0.249122	4.666120
H	5.040274	-1.813067	-3.439218	H	-1.473576	-0.616050	4.748995
С	3.662725	-0.161226	-3.122870	С	-0.008017	2.494865	4.190880
Н	3.813600	0.241474	-4.134636	Н	-0.195040	2.840295	5.228368
C	2.792356	0.499589	-2.238032	Н	-0.131884	3.365485	3.522207
С	2.963579	-1.901166	0.796799	Н	1.045276	2.177740	4.133953
H	1.855581	-1.789636	0.903283	С	-4.961029	-0.313481	1.243138
C	3.303658	-3.392837	0.846708	H	-6.001034	-0.685437	1.352807
H	2.866891	-3.946569	-0.006101	H	-4.898783	0.238497	0.284530
H	2.914682	-3.846225	1.780002	H	-4.764792	0.408930	2.058021
Н	4.401726	-3.556461	0.841324	С	-4.421828	-2.485696	0.164189
C	3.579364	-1.178129	2.005290	Н	-5.486333	-2.739831	0.346488
Н	3.243133	-0.127374	2.063312	Н	-3.847022	-3.428668	0.165762
H	4.687991	-1.191703	1.957616	H	-4.352164	-2.054013	-0.848911
H	3.279989	-1.681634	2.948724	С	-4.118773	-2.244735	2.615242
C	2.009384	1.730902	-2.689733	H	-5.150518	-2.642063	2.706333
H	2.003718	2.450758	-1.847369	H	-3.938845	-1.587721	3.487854
С	2.618560	2.458145	-3.892871	H	-3.423316	-3.104665	2.690641
H	3.685092	2.710497	-3.723405	C	1.088287	1.747820	1.650857
Н	2.070968	3.403312	-4.083455	С	1.030236	3.072722	1.115127
Н	2.556770	1.855681	-4.823086	Ċ	2.099078	3.949055	1.376373
C	0.536687	1.376704	-2.948935	Н	2.053499	4.980950	1.000233
H	0.065261	0.970751	-2.031116	C	3.226058	3.533817	2.100194
H	0.437243	0.623504	-3.757797	H	4.043817	4.241016	2.306186
H	-0.043480	2.275697	-3.242498	С	3.320101	2.201573	2.518948
P	-0.819367	-2.295139	0.026847	H	4.226981	1.860627	3.040201
С	-0.771255	-3.515786	1.437677	С	2.271579	1.290365	2.302121
С	-1.672987	-4.599593	1.514330	C	-0.147535	3.503994	0.247392
H	-2.447547	-4.720376	0.743448	H	-0.383640	2.602589	-0.365575
C	-1.590090	-5.526150	2.565105	C	-1.417361	3.851819	1.042125
Н	-2.302356	-6.364444	2.606654	Н	-1.767661	2.998598	1.649492
С	-0.606682	-5.387388	3.556910	H H	-2.239540	4.127918	0.349759
H	-0.545002	-6.113409	4.381824	H	-1.240172	4.715714	1.716488
С	0.293935	-4.313361	3.491608	С	0.197105	4.650697	-0.709900
H	1.066822	-4.189574	4.265691	H	-0.639502	4.823036	-1.415013
C	0.209256	-3.386190	2.442789	H	1.102167	4.435417	-1.311470
H	0.912629	-2.543884	2.410533	H	0.361796	5.603016	-0.163608
С	0.222019	-3.147810	-1.246983	С	2.408867	-0.155035	2.764218
C	0.665264	-2.377075	-2.340560	Н	1.384304	-0.574047	2.823080
Н	0.438079	-1.301862	-2.368871	C	3.175470	-0.980451	1.717291
C	1.398471	-2.967069	-3.378849	Н	2.642564	-0.972160	0.747719
H	1.744764	-2.346218	-4.217672	H	3.282848	-2.035509	2.042651
C	1.710723	-4.334394	-3.326662	H	4.187185	-0.562938	1.537768
H	2.297412	-4.798105	-4.134302	С	3.055122	-0.295170	4.150518
C	1.281059	-5.107626	-2.235954	H	3.001397	-1.348192	4.495123
H	1.527657	-6.179454	-2.188059	H	2.552681	0.339648	4.907859
С	0.535707	-4.520648	-1.201079	H	4.128337	-0.014603	4.134882
Н	0.199387	-5.132950	-0.351597	C	-1.737507	-2.202812	-0.809925
C	-2.516700	-2.650447	-0.623430	C	-1.397119	-3.491570	-0.287093
C	-2.745878	-3.274597	-1.865924	C	-1.475832	-4.606480	-1.139509
Н	-1.896520		-2.491570	Н		-5.605941	-0.746166
		-3.584275			-1.241794		
C	-4.057787	-3.500322	-2.311114	C	-1.859829	-4.470775	-2.480668
H	-4.224994	-3.985755	-3.284963	H	-1.935177	-5.358065	-3.127239
С	-5.150452	-3.115456	-1.518055	С	-2.104635	-3.195459	-3.003901
H	-6.178492	-3.295859	-1.867613	H	-2.348874	-3.090541	-4.070155
С	-4.924270	-2.495243	-0.278585	С	-2.025132	-2.046391	-2.200066
H	-5.770873	-2.177265	0.348015	C	-0.929457	-3.631680	1.159241
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Н	-3.450541	-1.750126	1.127610	C	-0.974629	-5.062308	1.703668
				Н	-1.980540	-5.515630	1.591836
				**	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	01000	

Н	-0.717117	-5.066987	2.781932	H	3.177992	4.174846	0.550559
Н	-0.245225	-5.724189	1.191998	С	4.537473	1.704269	-1.484346
C	0.471607	-3.024998	1.335302	Н	5.469549	2.295508	-1.596625
Н	0.467759	-1.953187	1.040006	H	4.336584	1.208666	-2.450944
Н	1.225719	-3.555335	0.718590	H	4.732352	0.914406	-0.738747
H	0.799235	-3.063973	2.393758	С	3.245053	3.705393	-2.186678
C	-2.182790	-0.654946	-2.796929	H	4.222191	4.191801	-2.384710
H	-1.384435	-0.062586	-2.284913	H	2.522547	4.504054	-1.931859
С	-1.917578	-0.597419	-4.303401	H	2.910270	3.234736	-3.132414
H	-0.970743	-1.102149	-4.573859	С	-2.108773	1.217564	0.817374
Н	-1.847588	0.457115	-4.638897	С	-2.216485	0.982520	2.217242
Н	-2.740953	-1.068781	-4.880263	C	-3.491398	0.688104	2.741042
C	-3.516476	0.026740	-2.456126	Н	-3.586736	0.492791	3.821528
Н	-3.658593	0.114875	-1.363568	C	-4.630607	0.632764	1.933698
H	-4.373275	-0.540022	-2.876391	H	-5.611178	0.402976	2.374907
Н	-3.547673	1.050271	-2.885357	С	-4.500989	0.827044	0.551765
P	1.486500	0.403082	-1.729798	H	-5.391850	0.754869	-0.091189
С	1.475730	-0.984483	-2.962297	С	-3.254972	1.102053	-0.028796
C	1.268472	-2.291580	-2.477267	С	-1.072843	1.060359	3.241184
H	1.053924	-2.447265	-1.409296	H	-1.248117	0.184327	3.908531
С	1.321745	-3.391564	-3.345348	C	0.380425	0.944011	2.757737
H	1.148810	-4.402189	-2.948275	H	0.543087	0.027567	2.132787
С	1.565338	-3.193790	-4.713101	H	1.051102	0.816463	3.633839
H	1.595341	-4.054276	-5.398815	H	0.734955	1.826980	2.195800
C	1.762810	-1.893321	-5.206216	С	-1.207845	2.313446	4.130764
Н	1.949489	-1.732467	-6.279156	Н	-0.480155	2.282397	4.968010
C	1.724430	-0.792925	-4.336256	Н	-2.224773	2.402166	4.560261
Н	1.883204	0.221949	-4.729547	Н	-1.008789	3.234977	3.547824
C	3.306292	0.510152	-1.386435	C	-3.128412	1.284824	-1.538654
C	4.194057	-0.537491	-1.707786	Н	-2.145756	1.762926	-1.724045
			-2.238123				
H	3.827180	-1.427944		C	-3.107346	-0.072980	-2.260810
С	5.549325	-0.452492	-1.353244	H	-2.299560	-0.721589	-1.868641
H	6.229624	-1.279442	-1.608856	H	-2.936173	0.056972	-3.348731
С	6.037669	0.681233	-0.685065	H	-4.073773	-0.603700	-2.130770
H	7.101619	0.747172	-0.410715	С	-4.212139	2.195232	-2.136476
С	5.158460	1.728872	-0.367102	H	-4.009987	2.383199	-3.211002
H	5.521455	2.620410	0.166157	H	-4.257571	3.175888	-1.622173
С	3.801508	1.641165	-0.705439	H	-5.220009	1.735406	-2.070773
H	3.120737	2.459349	-0.429408	C	2.520778	-0.351067	-1.286972
C	1.220801	1.878533	-2.825135	С	3.214891	-1.387309	-0.583773
С	-0.101948	2.299143	-3.071126	С	3.847576	-2.395381	-1.331863
Н	-0.934779	1.790773	-2.563535	Н	4.392493	-3.191923	-0.807926
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				C			
С	2.013865	3.637954	-4.322757		2.425169	-0.390552	-2.717644
H	2.850685	4.164546	-4.806807	C	3.213911	-1.427703	0.942895
C	2.278545	2.561514	-3.460878	H	2.136951	-1.329600	1.226745
H	3.317395	2.249461	-3.279617	С	3.723608	-2.747697	1.523949
				H	3.177640	-3.620754	1.118240
Confor	rmation 22.			H	3.589112	-2.754153	2.622613
Multip	olicity: 3			H	4.806468	-2.887988	1.322444
Charge	e: 0			C	3.945023	-0.248554	1.602523
E(B97-	-3c) = -3893.560355	371872 Hartree		H	3.517036	0.718639	1.286554
E(M06/	def2-TZVP) = -3893	3.289586107422 на	rtree	H	5.026003	-0.256569	1.350734
	- D3(BJ)/def2-TZVE			H	3.855886	-0.314933	2.706601
	) - D3(BJ)/def2-TZV				1.585532	0.643545	-3.461877
	1-3c) = -3888.28774			Н	1.780327	1.627629	-2.992181
	= 89.32346 Kcal/m			C	1.935326	0.785554	-4.946929
	= 46.70307 Kcal/n			Н	3.017422	0.975248	-5.099015
	7X-V/def2-TZVP) = -		3 Hartree	Н	1.374729	1.633697	-5.389275
	L-xTB) = $-161.27402$		3 Hareree	Н	1.664228	-0.119882	-5.528966
	2-xTB) = $-160.18398-FF) = -22.39561490$			C H	0.083942 -0.188321	0.379240 0.400821	-3.273817 -2.197519
E (GFN-	-FF) = -22.39361490	00441 Hartree					
C	nn+nn.			H	-0.212242	-0.605092	-3.688895
	inates:	0 151400	0 155004	H	-0.519538	1.164669	-3.773213
Co	0.231587	-0.151408	0.155394	P	-0.774077	-2.112437	0.663390
N	-0.845371	1.502766	0.250229	C	0.192724	-3.185877	1.847956
N	1.833264	0.658761	-0.574761	С	0.515708	-4.527643	1.561809
С	-1.094032	4.093513	0.238618	H	0.240706	-4.961350	0.590017
С	-0.335625	2.726165	0.050867	С	1.184017	-5.320332	2.508607
С	1.009140	2.903777	-0.378422	H	1.427007	-6.365952	2.264677
Н	1.308200	3.948929	-0.477163	C	1.540286	-4.788143	3.756518
С	2.030629	1.988090	-0.698480	H	2.061236	-5.412299	4.498203
С	3.407923	2.660817	-1.057056	С	1.237663	-3.448524	4.046835
С	-0.251219	5.031763	1.141437	H	1.521048	-3.014018	5.017766
Н	-0.815024	5.967866	1.331893	C	0.579992	-2.652863	3.097127
H	0.718826	5.318028	0.694083	Н	0.361607	-1.603338	3.337545
Н	-0.040489	4.556999	2.121016	C	-0.833107	-3.206241	-0.835007
C		4.733318	-1.163603	C	0.104270	-2.940553	-1.851777
-	-1.246340		-1.080548	Н	0.800685	-2.096016	-1.741464
H	-1.246340 -1.748247	5.720024		44		2.000010	
H H	-1.748247	5.720024		C	0 164792	-3 744527	
H	-1.748247 -1.864512	4.092949	-1.824013	C H	0.164792	-3.744527 -3.513769	-2.999564
H H	-1.748247 -1.864512 -0.269209	4.092949 4.884923	-1.824013 -1.661854	H	0.911233	-3.513769	-2.999564 -3.774170
H H C	-1.748247 -1.864512 -0.269209 -2.496450	4.092949 4.884923 4.049283	-1.824013 -1.661854 0.876377	H C	0.911233 -0.719925	-3.513769 -4.823348	-2.999564 -3.774170 -3.147279
H H C H	-1.748247 -1.864512 -0.269209 -2.496450 -2.862989	4.092949 4.884923 4.049283 5.092646	-1.824013 -1.661854 0.876377 0.967261	H C H	0.911233 -0.719925 -0.681992	-3.513769 -4.823348 -5.451553	-2.999564 -3.774170 -3.147279 -4.050462
Н Н С Н	-1.748247 -1.864512 -0.269209 -2.496450 -2.862989 -2.494362	4.092949 4.884923 4.049283 5.092646 3.605218	-1.824013 -1.661854 0.876377 0.967261 1.887234	H C H C	0.911233 -0.719925 -0.681992 -1.654360	-3.513769 -4.823348 -5.451553 -5.100981	-2.999564 -3.774170 -3.147279 -4.050462 -2.135107
H H C H H	-1.748247 -1.864512 -0.269209 -2.496450 -2.862989 -2.494362 -3.230403	4.092949 4.884923 4.049283 5.092646 3.605218 3.490264	-1.824013 -1.661854 0.876377 0.967261 1.887234 0.274375	H C H C	0.911233 -0.719925 -0.681992 -1.654360 -2.346779	-3.513769 -4.823348 -5.451553 -5.100981 -5.950293	-2.999564 -3.774170 -3.147279 -4.050462 -2.135107 -2.241782
Н Н С Н Н С	-1.748247 -1.864512 -0.269209 -2.496450 -2.862989 -2.494362 -3.230403 3.894139	4.092949 4.884923 4.049283 5.092646 3.605218 3.490264 3.398706	-1.824013 -1.661854 0.876377 0.967261 1.887234 0.274375 0.218849	H C H C H	0.911233 -0.719925 -0.681992 -1.654360 -2.346779 -1.709016	-3.513769 -4.823348 -5.451553 -5.100981 -5.950293 -4.303453	-2.999564 -3.774170 -3.147279 -4.050462 -2.135107 -2.241782 -0.982064
H C H H C H	-1.748247 -1.864512 -0.269209 -2.496450 -2.862989 -2.494362 -3.230403 3.894139 4.868621	4.092949 4.884923 4.049283 5.092646 3.605218 3.490264 3.398706 3.891810	-1.824013 -1.661854 0.876377 0.967261 1.887234 0.274375 0.218849 0.020313	H C H C H C	0.911233 -0.719925 -0.681992 -1.654360 -2.346779 -1.709016 -2.437233	-3.513769 -4.823348 -5.451553 -5.100981 -5.950293 -4.303453 -4.537308	-2.999564 -3.774170 -3.147279 -4.050462 -2.135107 -2.241782 -0.982064 -0.191824
Н Н С Н Н С	-1.748247 -1.864512 -0.269209 -2.496450 -2.862989 -2.494362 -3.230403 3.894139	4.092949 4.884923 4.049283 5.092646 3.605218 3.490264 3.398706	-1.824013 -1.661854 0.876377 0.967261 1.887234 0.274375 0.218849	H C H C H	0.911233 -0.719925 -0.681992 -1.654360 -2.346779 -1.709016	-3.513769 -4.823348 -5.451553 -5.100981 -5.950293 -4.303453	-2.999564 -3.774170 -3.147279 -4.050462 -2.135107 -2.241782 -0.982064

С	-3.597333	-2.298938	0.525716	С	1.732131	1.015086	-4.435297
H	-3.457328	-2.076965	-0.539506	H	1.256953	1.578472	-5.253453
C	-4.889292	-2.532501	1.016109	C	3.128438	0.999284	-4.328873
H	-5.746265	-2.479546	0.327192	H	3.745056	1.536851	-5.065257
С	-5.091092	-2.818467	2.374166	С	3.737385	0.311170	-3.267808
Н	-6.105889	-3.000694	2.759295	Н	4.833247	0.322186	-3.176108
C	-3.986070	-2.868762	3.236968	C	2.972689	-0.399119	-2.329362
Н	-4.127679	-3.092379	4.305586	C	-0.595251	0.400559	-3.623398
С	-2.690489	-2.652716	2.744305	H	-1.007061	-0.247897	-2.822711
H	-1.838557	-2.731191	3.433810	С	-1.073906	1.835575	-3.349687
				H	-0.761345	2.166770	-2.340024
Conforma	ation 23.			H	-2.178948	1.907123	-3.398834
Multipl:	icity: 3			Н	-0.650900	2.552444	-4.083333
Charge:				С	-1.119550	-0.122491	-4.969999
	c) = $-3893.56532$	8902517 Hartree		Н	-0.802898	-1.169053	-5.152051
	.,	3.296543162907 Hai	r+ r00	H	-0.753627	0.490626	-5.819750
•		P) = -3891.9798589		H	-2.228223	-0.093163	-4.994002
		VP) = -3892.24206	/120452 Hartree	С	3.619541	-1.116309	-1.152810
E(PBEh-	3c) = -3888.3001	30612013 Hartree		H	2.964935	-1.975859	-0.899187
E(PM6) =	= 82.56325 Kcal/	mol		C	5.018871	-1.668666	-1.444766
E(PM7) =	= 41.17791 Kcal/	mol		Н	5.020352	-2.320337	-2.342065
E (0B97X-	-V/def2-TZVP) =	-3895.861757008122	) Hartree	Н	5.381860	-2.268660	-0.586105
	xTB) = -161.2763		11010100	Н	5.761658	-0.861074	-1.609994
	xTB) = -160.1906			C	3.627343	-0.182863	0.068484
E (GFN-F)	F) = -22.4002221	0/330 Hartree		H	2.597422	0.190807	0.272736
				H	4.266671	0.705011	-0.117244
Coordina	ates:			H	3.988275	-0.698359	0.981351
Co	0.238553	0.074257	-0.119211	P	0.384851	2.210722	0.664842
N	-0.898731	-1.251626	0.853661	C	-1.174761	3.210920	0.642683
N	0.761726	-1.133172	-1.542082	С	-1.432455	4.134352	-0.394277
C	-1.857502	-3.660229	1.222990	Н	-0.667657	4.329368	-1.158819
C	-1.023874	-2.540483	0.479085	C	-2.657352	4.814978	-0.456074
C	-0.363194	-3.050223	-0.663371	H	-2.836949	5.532586	-1.271174
H	-0.531714	-4.114296	-0.837000	C	-3.642875	4.594725	0.519582
C	0.439522	-2.435116	-1.645641	H	-4.599679	5.136782	0.475674
C	0.865666	-3.410455	-2.803028	C	-3.399506	3.668995	1.545309
С	-2.862423	-4.293041	0.225907	H	-4.165400	3.463933	2.308906
Н	-3.448343	-5.083787	0.738157	С	-2.184215	2.971121	1.595494
H	-2.372141	-4.756181	-0.650730	Н	-2.044354	2.210472	2.372153
H	-3.577627	-3.534628	-0.151436	C	1.489841	3.354604	-0.306649
С	-0.861786	-4.748538	1.701668	С	1.719592	4.663006	0.178523
H	-1.414543	-5.572306	2.199361	H	1.251118	4.984364	1.120688
H	-0.142415	-4.333148	2.436483	C	2.536493	5.549205	-0.532326
H	-0.275437	-5.184821	0.870978	H	2.707253	6.565048	-0.144447
С	-2.689930	-3.261673	2.459698	С	3.138871	5.142148	-1.736844
Н	-3.175657	-4.181295	2.846837	Н	3.781646	5.839925	-2.295550
H	-3.489107	-2.536109	2.228410	C	2.917501	3.846749	-2.221257
H		-2.841540	3.279727	Н		3.509389	-3.159626
	-2.083403				3.381426		
C	-0.419175	-3.963504	-3.469691	С	2.095349	2.955669	-1.507426
H	-0.146668	-4.660652	-4.289086	H	1.926025	1.943434	-1.892880
H	-1.019726	-3.140195	-3.906433	C	1.143286	2.568397	2.333036
H	-1.067867	-4.511178	-2.760555	C	2.550014	2.453602	2.415705
С	1.734584	-2.845936	-3.945051	Н	3.132568	2,219824	1.512831
Н	1.908236	-3.666278	-4.671872	С	3.217208	2.643342	3.631778
H	2.723677	-2.494546	-3.603282	Н	4.313346	2.550658	3.670504
H	1.254822	-2.015042	-4.491262	C	2.491886	2.955360	4.793725
С	1.675299	-4.579423	-2.187484	H	3.013287	3.107704	5.750555
H	1.974384	-5.289866	-2.985964	С	1.097360	3.079018	4.720289
H	1.104905	-5.147824	-1.428128	H	0.516087	3.334055	5.619575
H	2.600453	-4.203482	-1.705026	C	0.426463	2.888798	3.500415
C	-1.656081	-0.660338	1.894057	H	-0.662965	3.007532	3.472853
C	-2.979563	-0.197389	1.622149				
C	-3.716151	0.385235	2.667386	Confor	rmation 3.		
Н	-4.743669	0.726892	2.476618		olicity: 3		
C	-3.158883	0.551863	3.943880	Charge			
Н	-3.743276	1.031142	4.744304		-3c) = -3893.562220°	761271 Hartron	
C	-1.867246	0.069280	4.205646		def2-TZVP) = -3893		
H	-1.457935	0.150502	5.223079		- D3(BJ)/def2-TZVP		
C	-1.113198	-0.578508	3.211062		) - D3(BJ)/def2-TZV		0477379 Hartree
С	-3.578780	-0.395058	0.233326	E (PBEh	n-3c) = -3888.29765	5951989 Hartree	
H	-3.204178	-1.372740	-0.136363	E(PM6)	= 81.61264  Kcal/m	01	
С	-5.109795	-0.460329	0.220196	E(PM7)	= 38.74997  Kcal/m	ol	
H	-5.496124	-1.220164	0.929762		7X-V/def2-TZVP) = -		8 Hartree
H	-5.472730	-0.722555	-0.794376		1-xTB) = $-161.27195$		
H	-5.565126	0.516635	0.484702		2-xTB) = $-160.18479$		
C	-3.074630	0.662208	-0.760860	r (GFN-	-FF) = -22.40377582	ous/ martree	
H	-3.362026	0.398108	-1.798450	_			
H	-1.966846	0.742412	-0.721572		inates:		
H	-3.478084	1.667125	-0.527035	Co	0.051448	-0.208423	0.187197
C	0.174239	-1.329716	3.544612	N	-1.017070	0.937339	-1.016851
Н	0.168336	-2.228536	2.892048	N	-1.040254	-0.025945	1.764722
C	1.445629	-0.551482	3.191046	C	-3.038280	2.546004	-1.452888
Н	1.391114	-0.170768	2.151954	C	-2.177724	1.507303	-0.627000
H	2.343067	-1.197741	3.279511	C	-2.722249	1.271390	0.659974
H	1.577198	0.318103	3.862347	H	-3.687531	1.750947	0.823237
С	0.232173	-1.818696	4.997791	С	-2.232547	0.597358	1.798263
H	1.106113	-2.486260	5.142657	C	-3.204093	0.659900	3.035353
H	-0.680223	-2.380962	5.284129	С	-4.549232	2.194113	-1.388202
H	0.349914	-0.974727	5.709084	H	-5.113638	2.921549	-2.006041
				H			
C	1.551111	-0.413399	-2.4/1909		-4.9//153	2.24249/	-0.369272
C C	1.551111 0.921976	-0.413399 0.325487	-2.471909 -3.515316	H	-4.977153 -4.749550	2.242492 1.183743	-0.369272 -1.794420

С	-2.835304	3.924545	-0.774261	С	3.557311	-3.165919	0.619972
H	-3.398331	4.707666	-1.324083	H	3.496891	-3.762201	-0.301888
H	-1.767928	4.215277	-0.765534	С	4.334286	-3.623091	1.694611
					4.876789	-4.576980	
H	-3.188889	3.915491	0.275223	H			1.605977
C	-2.727711	2.702056	-2.956201	C	4.422259	-2.870156	2.877059
H	-3.465280	3.410902	-3.385553	Н	5.032297	-3.232670	3.718579
H	-2.819236	1.749754	-3.508174	C	3.723950	-1.657812	2.983173
H	-1.723864	3.107004	-3.159265	H	3.772117	-1.063026	3.906728
С	-4.591916	0.127742	2.590920	С	2.934603	-1.207183	1.915147
H	-5.288080	0.136273	3.454905	H	2.365031	-0.273346	2.011970
H	-4.520452	-0.915336	2.222317	С	3.144616	-0.424475	-1.659683
H	-5.048346	0.733866	1.786161	C	4.378080	-0.048690	-1.087780
C	-2.808649	-0.163036	4.278300	H	4.601521	-0.308041	-0.042725
Н	-3.628012	-0.074774	5.021308	C		0.655389	
					5.325725		-1.846387
H	-1.882082	0.194265	4.760175	H	6.283337	0.943790	-1.386216
H	-2.683553	-1.237456	4.052517	С	5.060797	0.981178	-3.185918
C	-3.356804	2.130934	3.491190	H	5.807804	1.528719	-3.780713
H	-4.087022	2.195389	4.324536	C	3.835400	0.606782	-3.760114
Н	-3.714137	2.787737	2.674459	Н	3.606618	0.864164	-4.805379
H	-2.394413	2.539359	3.856750	C	2.878609	-0.080459	-3.001181
C	-0.467612	1.066270	-2.319459	H	1.916380	-0.351003	-3.459711
C	0.392600	2.154855	-2.649746				
C	0.835010	2.289996	-3.978023	Confo	rmation 30.		
H	1.483129	3.139703	-4.241575	Multi	plicity: 3		
C	0.461658	1.375602	-4.968737	Charge	e: 0		
H	0.795684	1.512251	-6.008452	E(B97	-3c) = -3893.563746	6418426 Hartree	
C		0.258089			,		
	-0.309301		-4.615607		/def2-TZVP) = -3893		
H	-0.559683	-0.485439	-5.385402	E (PBE	- D3(BJ)/def2-TZVI	P) = -3891.97833	5656992 Hartree
С	-0.768554	0.068015	-3.299978	F ( DBF)	0 - D3(BJ)/def2-TZV	7D1 = -3892 2387	82841677 Hartree
C	0.831614	3.179235	-1.609382	E (PBE	h-3c) = -3888.29779	91553374 Hartree	
H	0.211082	3.010496	-0.705347	E (PM6	) = 84.72964  Kcal/r	nol	
					) = 39.87404 Kcal/r		
С	2.301389	2.955684	-1.216142	•	,		
H	2.455552	1.944233	-0.799359	E (ωB9'	7X-V/def2-TZVP) = -	-3895.8551287309	57 Hartree
H	2.627592	3.698473	-0.459492	F (CFN	1-xTB) = $-161.27018$	20153085 Hartree	
H	2.967556	3.051294	-2.097703		2-xTB) = $-160.18224$		
С	0.621433	4.631457	-2.071499	E (GFN-	-FF) = $-22.39976222$	25851 Hartree	
Н	0.820474	5.335304	-1.237342		,		
H	-0.410580	4.811222	-2.431362	Coord	inates:		
H	1.314222	4.899886	-2.895623	Co	-0.313747	0.051608	-0.068013
C	-1.538120	-1.190266	-2.910220	N	1.147533	-0.859228	0.924850
H	-1.145266	-1.448691	-1.898566	N	-1.020207	1.135697	1.355752
С	-3.054164	-0.984405	-2.753279	С	2.307882	-1.407810	3.204964
H	-3.290976	-0.251612	-1.962510	C	1.369049	-0.586641	2.229665
H	-3.541040	-1.941537	-2.473187	C	0.654220	0.428840	2.916019
Н				Н			
	-3.511418	-0.639234	-3.704167		1.001424	0.587335	3.934772
С	-1.277371	-2.367921	-3.855521	С	-0.452074	1.234629	2.573956
H	-1.727294	-3.293291	-3.446670	С	-0.859322	2.268446	3.682579
H	-0.196380	-2.555811	-4.004640	C	3.080707	-0.475993	4.178336
H	-1.739381	-2.195123	-4.850138	H	3.774357	-1.088060	4.789201
					2.428364		
С	-0.301303	-0.413506	2.913043	H		0.061483	4.892016
С	0.386321	0.623298	3.630968	H	3.687170	0.276207	3.636873
С	1.103318	0.297168	4.790942	С	1.354560	-2.296222	4.045826
H	1.622761	1.089754	5.349018	H	1.937130	-2.933094	4.744386
С	1.148074	-1.023472	5.261510	H	0.754143	-2.963216	3.398547
H	1.691705	-1.267150	6.186705	H	0.648369	-1.681802	4.637947
C	0.497893	-2.027199	4.541473	C	3.382562	-2.321856	2.578855
Н	0.532181	-3.063133	4.914694	Н	3.972129	-2.770493	3.404558
C	-0.223567	-1.764191	3.357967	H	4.084352	-1.772260	1.927116
С	0.359948	2.056730	3.109448	Н	2.963875	-3.150678	1.987210
H	-0.619047	2.211997	2.614701	C	0.178076	3.416106	3.597217
C	0.492606	3.121486	4.204720	H	-0.055226	4.207642	4.340424
H	-0.249155	2.969977	5.014940	Н	0.176268	3.879850	2.592292
H	0.332105	4.131711	3.776910	H	1.203316	3.045132	3.793884
H	1.501466	3.122581	4.667099	C	-2.273684	2.871193	3.564287
C	1.428290	2.259450	2.025149	Н	-2.439796	3.545349	4.429508
H	1.312127	1.522835	1.197287	H	-3.062585	2.097379	3.583688
H	2.452331	2.133304	2.433897	H	-2.420826	3.466360	2.649269
				C	-0.785577		
H	1.355745	3.268976	1.574913			1.644597	5.100064
C	-0.864247	-2.995581	2.701005	H	-1.161101	2.379738	5.840354
H	-1.376982	-3.528260	3.535186	H	0.242284	1.378079	5.411774
С	-1.930086	-2.784817	1.616947	H	-1.412853	0.735344	5.175978
H	-2.787168	-2.185717	1.974785	C	1.953926	-1.750931	0.164839
Н	-2.315758	-3.771057	1.286290	C	1.614512	-3.130232	0.039714
H	-1.530819	-2.254199	0.729973	C	2.491733	-3.989713	-0.645279
С	0.244773	-3.938160	2.191097	Н	2.237109	-5.057770	-0.724644
H	0.959785	-4.207933	2.992300	C	3.681519	-3.519381	-1.209905
H	0.834286	-3.449029	1.394737	H	4.371474	-4.212409	-1.715403
H	-0.185650	-4.874338	1.779933	С	3.969089	-2.148427	-1.153719
P	1.823115	-1.266035	-0.671034	H	4.881459	-1.772266	-1.637412
С	1.537628	-2.813806	-1.659140	С	3.117467	-1.242349	-0.495358
C	0.421657	-3.603050	-1.318098	C	0.340443	-3.708447	
							0.641401
H	-0.279736	-3.241241	-0.554215	H	-0.081409	-2.934789	1.313489
С	0.196970	-4.837625	-1.941507	С	-0.692614	-3.989779	-0.462049
H	-0.677090	-5.442023	-1.654352	H	-0.946841	-3.067644	-1.015111
C	1.072416	-5.289264	-2.941403	H	-1.626347	-4.411693	-0.037076
Н	0.891962	-6.252508	-3.442291	Н	-0.297026	-4.715771	-1.201919
С	2.175214	-4.500420	-3.305100	C	0.584995	-4.973766	1.480213
H	2.864460	-4.844668	-4.091488	H	-0.346728	-5.272570	2.003635
C	2.413714	-3.274042	-2.663537	Н	1.371874	-4.822577	2.245316
H	3.291564	-2.674193	-2.944332	H	0.892123	-5.831850	0.847450
С	2.847795	-1.951783	0.722705	С	3.417409	0.253651	-0.513646
-		, , , , , , , , , , , , , , , , , , , ,		-			

Н	2.420365	0.739892	-0.600401	N	-0.839855	-1.804060	-0.282236
C C	4.059045	0.785009	0.778945	C	-1.869082	1.176890	-3.605762
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H	3.397921			C	-1.377925	0.418189	-2.309043
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Н	5.026163	0.279214	0.982769	H	-2.480720	-1.190465	-3.110811
C	4.272872	0.675909	-1.713661	С	-1.668221	-1.960302	-1.331094
H	4.330887	1.779945	-1.770583	С	-2.525565	-3.237008	-1.651318
H	3.857805	0.312294	-2.673469	С	-1.225184	0.462258	-4.821687
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C	-2.314182	1.586366	0.980224	H	-1.485424	-0.612354	-4.868668
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H	-3.937656	4.202714	-0.552968	H	-3.753228	1.636924	-4.615119
С	-4.920643	2.474905	0.301429	H	-3.903318	1.539954	-2.833742
H	-5.934438	2.830004	0.061926	H	-3.783490	0.044588	-3.808700
C	-4.730464	1.230188	0.915066	C	-1.532000	2.674763	-3.748868
H	-5.601551	0.595497	1.145715	H	-1.895427	3.008381	-4.742930
C	-3.449747	0.752479	1.247806	H	-0.451628	2.888256	-3.703825
С	-1.326578	3.709857	-0.122712	H	-2.027411	3.301800	-2.987370
H	-0.398762	3.184410	0.191715	C	-2.094127	-3.785097	-3.033869
С	-1.299181	3.898794	-1.649442	H	-2.702048	-4.676417	-3.294363
H	-1.316098	2.930031	-2.180967	Н	-1.029638	-4.095841	-3.015944
H	-0.394630	4.456215	-1.966796	H	-2.214856	-3.044506	-3.847141
H	-2.181778	4.477931	-1.991359	C	-2.445451	-4.423791	-0.670747
С	-1.354631	5.086055	0.566973	Н	-3.136060	-5.210943	-1.037462
Н	-1.380533	5.006579	1.669959	Н	-2.757540	-4.158628	0.354585
H	-2.245165	5.669654	0.254062	Н	-1.437812	-4.870287	-0.608496
H	-0.457379	5.677542	0.290699	C	-4.015854	-2.813174	-1.692700
C	-3.365640	-0.669221	1.806302	Н	-4.654430	-3.695124	-1.907249
Н	-4.415655	-1.034559	1.785472	H	-4.222984	-2.046283	-2.462736
C	-2.571417	-1.609988	0.891140	H	-4.328041	-2.396057	-0.713622
Н	-2.938824	-1.594480	-0.152538	C	-0.223366		-1.243377
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H	-2.639269	-2.656701	1.248423	C	1.056155	2.755210	
H	-1.479844	-1.363247	0.905704	C	1.336805	4.126857	-1.467924
C	-2.892017	-0.812301	3.262260	H	2.332758	4.499505	-1.756465
H	-3.429162	-0.119796	3.940358	С	0.388400	5.021877	-0.961764
H	-1.804606	-0.627189	3.359437	H	0.634111	6.089098	-0.854514
H	-3.086162	-1.845891	3.616975	С	-0.875520	4.542961	-0.582672
P	-0.237454	-0.152440	-2.285693	H	-1.621361	5.243842	-0.181222
С	1.031797	0.868325	-3.175744	С	-1.191696	3.180891	-0.686808
С	1.394761	2.096317	-2.588571	С	2.152638	1.944732	-2.358698
H	1.005073	2.348802	-1.590920	H	3.091974	2.242000	-1.844194
C	2.241912	2.987818	-3.260349	C	2.094211	0.414720	-2.296793
H	2.505801	3.948220	-2.792042	H	1.956435	0.062870	-1.253240
C	2.763565	2.648759	-4.519011	H	3.055569	-0.005982	-2.656353
H	3.435866	3.343403	-5.044728	H	1.277984	-0.012048	-2.909280
C	2.433552	1.413728	-5.098856	C	2.310694	2.389850	-3.828596
H	2.849019	1.135021	-6.079708	H	3.214247	1.925993	-4.275462
C	1.566027	0.529987	-4.436331	H	2.411037	3.489203	-3.920477
H	1.298716	-0.428762	-4.904574	H	1.440265	2.081466	-4.442346
С	-1.792226	0.541870	-3.047074	С	-2.543798	2.642419	-0.230122
С	-1.823680	1.076315	-4.352289	Н	-2.847338	1.867423	-0.963478
H	-0.901580	1.125361	-4.949884	С	-2.414048	1.926674	1.123813
С	-3.026459	1.554936	-4.891718	Н	-1.581078	1.193891	1.089795
Н	-3.036244	1.975250	-5.909324	Н	-3.343835	1.377728	1.376695
С	-4.212821	1.499278	-4.140823	H	-2.186055	2.639082	1.941290
Н	-5.154235	1.877391	-4.567218	C	-3.659894	3.690527	-0.192800
C	-4.189738	0.967958	-2.843436	Н	-4.631079	3.204577	0.031223
Н	-5.104096	0.930088	-2.234097	Н	-3.759605	4.222110	-1.161279
C	-2.984261	0.500185	-2.299833	Н	-3.490543	4.451607	0.597274
Н	-2.964435	0.117154	-1.271020	C	-0.576269	-2.779574	0.713389
C	-0.144594	-1.770292	-3.183775	C	0.462929	-3.738189	0.509018
C	-1.293264	-2.372575	-3.738846	C	0.711732	-4.689228	1.511897
Н	-2.257728	-1.844511	-3.711130	Н	1.503704	-5.438119	1.361909
C	-1.212755	-3.641698	-4.331721	C	-0.035609	-4.707724	2.699138
Н	-2.117878	-4.097999	-4.761226	Н	0.164807	-5.470756	3.466661
C	0.014618	-4.320911	-4.387902	C	-1.027511	-3.740942	2.907361
Н	0.014018	-5.313781	-4.858409	Н	-1.598096	-3.742776	3.849174
C	1.160730	-3.726163	-3.836468	C	-1.313279	-2.767716	1.933537
Н	2.129297	-4.248078	-3.860439	C	1.316130	-3.681703	-0.750348
п С	1.081489		-3.228567		0.709901		
		-2.466152		H		-3.179834	-1.532025
H	1.983972	-2.024504	-2.782065	C	2.537055	-2.783317	-0.488601
~ .				H	2.195818	-1.787133	-0.132938
Conformat				H	3.138970	-2.632697	-1.408279
Multiplio				H	3.189326	-3.212216	0.299908
Charge: (		05004120		C	1.730170	-5.056783	-1.287788
		85664138 Hartree		H	0.850858	-5.714326	-1.443821
		93.299025540857 Har		H	2.426738	-5.580443	-0.600861
		VP) = -3891.9816269		H	2.253805	-4.948747	-2.259258
		ZVP) = -3892.243500	924945 Hartree	С	-2.361288	-1.697427	2.205504
		583467721 Hartree		H	-2.482533	-1.120768	1.265711
	82.74895 Kcal			С	-3.732534	-2.277935	2.581341
	38.42901 Kcal			H	-4.112154	-2.968364	1.801422
		-3895.860393132127	Hartree	H	-4.475654	-1.463649	2.705691
		079756721 Hartree		H	-3.695478	-2.838940	3.538320
		653523218 Hartree		С	-1.846046	-0.723322	3.278269
E (GFN-FF)	= -22.404095	107430 Hartree		H	-0.900929	-0.249576	2.948010
				H	-1.643136	-1.244803	4.236612
Coordinat				H	-2.575798	0.087960	3.472868
Co	0.173462	-0.209516	0.122077	P	1.613228	0.811292	1.526097
N	-0.571785	0.912887	-1.354090	С	2.401526	-0.315754	2.778152

С	3.480070	0.150805	3.562878	С	1.630752	1.969387	-2.523902
Н					2.575720	2.358015	-2.086855
	3.859621	1.173342	3.415403	H			
С	4.066202	-0.679969	4.525749	С	1.710566	0.443484	-2.412222
H	4.905982	-0.305612	5.131205	H	1.657860	0.119786	-1.353582
C	3.585548	-1.988063	4.716128	H	2.682522	0.098283	-2.819682
H	4.049968	-2.641499	5.470692	H	0.902920	-0.078825	-2.958915
С	2.515930	-2.456061	3.940928	С	1.656709	2.373473	-4.014002
H	2.127559	-3.476185	4.074356	H	2.570206	1.973344	-4.500002
C	1.926378	-1.622244	2.974939	Н	1.652778	3.472634	-4.149623
Н	1.090087	-1.994987	2.369898	H	0.783611	1.964314	-4.560255
С	0.916593	2.106667	2.649224	С	-2.841208	2.453476	0.182651
C	0.610289	1.817498	3.996839	H	-2.817427	1.351362	0.060933
H	0.874497	0.838910	4.422081	C	-2.831776	2.769125	1.688575
C	-0.030681	2.772090	4.800651	H	-1.902727	2.426561	2.178477
H	-0.265445	2.528196	5.848188	H	-3.695638	2.287982	2.192854
С	-0.364657	4.032092	4.278520	H	-2.910179	3.861455	1.867128
Н	-0.862502	4.780648	4.913589	С	-4.150750	2.974385	-0.436615
C	-0.063658	4.325592	2.939479	Н	-5.026155	2.499818	0.052838
				H			
H	-0.328375	5.302564	2.506669		-4.217561	2.768120	-1.521541
С	0.558586	3.366316	2.128101	H	-4.249986	4.071263	-0.299278
H	0.747838	3.600636	1.074193	C	-0.309223	-2.844542	0.995720
C	3.185306	1.559846	0.864054	C	0.825913	-3.702208	0.851115
C	3.510136	2.928933	0.887351	C	1.186950	-4.541167	1.917331
H	2.834784	3.652030	1.362270	H	2.054899	-5.207776	1.807752
С	4.706759	3.386380	0.310076	С	0.460652	-4.546484	3.116330
Н	4.941118	4.461744	0.335184	Н	0.746896	-5.221563	3.936962
C	5.598109	2.485130	-0.290425	C	-0.621249	-3.669507	3.267395
Н	6.532262		-0.745375	Н		-3.644680	
		2.847840			-1.177079		4.218490
C	5.294734	1.112867	-0.293048	С	-1.020735	-2.802701	2.233017
H	5.993171	0.391236	-0.743663	С	1.650370	-3.661144	-0.428029
C	4.101263	0.656161	0.279501	H	0.965956	-3.350181	-1.242451
H	3.878536	-0.421412	0.282080	C	2.716882	-2.561804	-0.308823
				H	2.219494	-1.595279	-0.077135
Conform	nation 33.			Н	3.283014	-2.439190	-1.255273
	Licity: 3			Н	3.431453	-2.780097	0.511252
Charge:				C	2.265328	-5.008019	-0.824459
	3c) = -3893.560975			H	1.500354	-5.809681	-0.872863
	def2-TZVP) = -3893			H	3.052084	-5.334335	-0.113076
E(PBE -	- D3(BJ)/def2-TZVI	P) = -3891.975968	812902 Hartree	H	2.743816	-4.931922	-1.821922
E(PBE0	- D3(BJ)/def2-TZV	VP) = -3892.23706	3850715 Hartree	C	-2.144894	-1.811715	2.521527
E(PBEh-	-3c) = -3888.29029	90971566 Hartree		H	-2.466645	-2.043840	3.560178
E(PM6)	= 89.87465  Kcal/r	nol		С	-1.641589	-0.362181	2.548253
E (PM7)	= 44.26548 Kcal/r	mol 1		H	-0.724588	-0.243421	3.155070
	<pre>K-V/def2-TZVP) = -</pre>		9 Hartree	Н	-2.410234	0.311176	2.975460
	-xTB) = $-161.2714$		J Hartree	Н	-1.471168	0.038273	1.510883
	,						
	-xTB) = $-160.18298$			С	-3.394768	-1.929101	1.634314
E (GFN-F	FF) = -22.39230159	94608 Hartree		Н	-3.769759	-2.970873	1.590728
				H	-3.193059	-1.584814	0.601823
Coordin	nates:			H	-4.207973	-1.295935	2.045688
Co	0.087454	-0.233351	0.313362	P	1.625722	0.982187	1.434962
N	-0.866734	0.756632	-1.156659	С	3.069040	1.768798	0.558088
N	-0.682750	-1.977049	-0.057434	C	3.959690	0.883187	-0.088864
С	-2.252776	0.761238	-3.377266	Н	3.792851	-0.200668	-0.020574
C	-1.578541	0.116829	-2.100766	C	5.058638	1.366895	-0.809539
C	-1.801576	-1.283351	-2.051539	Н	5.736472	0.657104	-1.307921
H	-2.385390	-1.662690	-2.890785	C	5.293372	2.749438	-0.895238
С	-1.451663	-2.280815	-1.117617	H	6.152052	3.132629	-1.467126
C	-2.030905	-3.701684	-1.469226	C	4.431592	3.635476	-0.232323
C	-1.655203	0.090000	-4.641324	H	4.614597	4.720221	-0.274039
H	-2.117396	0.528706	-5.549799	C	3.330602	3.150692	0.493490
H	-1.825548	-1.002694	-4.671866	H	2.679413	3.864149	1.014134
H	-0.561958	0.259155	-4.704067	С	2.599835	-0.005683	2.676797
С	-3.774825	0.469196	-3.325280	С	2.172881	-1.286541	3.065949
H	-4.280033	0.952908	-4.186971	H	1.276157	-1.728068	2.610367
Н	-4.225864	0.870142	-2.396880	C	2.888800	-2.011930	4.034209
H	-4.007471	-0.611678	-3.364914	Н	2.537023	-3.014253	4.318850
C	-2.107473	2.281139	-3.595823	C	4.038726	-1.462512	4.617447
H	-2.627035	2.536178	-4.542573	H	4.602653	-2.032101	5.372128
H	-1.059176	2.606565	-3.694726	С	4.471864	-0.180993	4.233223
H	-2.564162	2.883525	-2.793834	H	5.374035	0.256842	4.687586
С	-1.336346	-4.197484	-2.761276	C	3.758064	0.543259	3.270049
H	-1.742504	-5.188217	-3.053901	H	4.100648	1.546314	2.973652
H	-0.244329	-4.312021	-2.611992	С	0.985239	2.322059	2.542742
Н	-1.488618	-3.501300	-3.608730	Č	0.539761	3.540788	1.990380
C	-1.869841	-4.804238	-0.403774	Н	0.602386	3.712260	0.909146
Н	-2.405048	-5.707732	-0.761461	C	-0.006418	4.539924	2.808129
п Н							
	-2.304577	-4.522543	0.572367	H	-0.337984	5.484322	2.349956
H	-0.819436	-5.092025	-0.228946	C	-0.155887	4.324328	4.186409
C	-3.554616	-3.591575	-1.737811	H	-0.595695	5.103791	4.827003
H	-3.961663	-4.597434	-1.968840	С	0.250844	3.099976	4.740741
H	-3.799483	-2.932969	-2.591969	H	0.131207	2.914886	5.819383
H	-4.089561	-3.203567	-0.849824	С	0.824711	2.109036	3.929839
С	-0.640931	2.156848	-1.150985	Н	1.159776	1.164554	4.382878
C	0.529249	2.717801	-1.750672				
C	0.697709	4.117579	-1.685901	Confo	rmation 7.		
Н	1.609619	4.554595	-2.123351		plicity: 3		
C	-0.256401	4.963062	-1.108778	Charg		110551 ***	
H	-0.101310	6.052443	-1.099726		-3c) = -3893.568404		
C	-1.399665	4.400374	-0.527003		/def2-TZVP) = -3893		
H	-2.149335	5.055949	-0.056788		- D3(BJ)/def2-TZVP		
C	-1.597885	3.010453	-0.508805	E (PBE	0 - D3(BJ)/def2-TZV	P) = -3892.24405	6380075 Hartree
C	1.007000						

E (PBEh	-3c) = -3888.3038	60858014 Hartree		Н	-1.181613	-0.533904	-2.320935
E(PM6)	= 81.92260 Kcal/	mol		C	-2.850919	-0.783253	-3.656606
E(PM7)	= 42.27180 Kcal/	mol		H	-3.606203	-0.995906	-2.874235
E(ωB97	X-V/def2-TZVP) =	-3895.86115901387	1 Hartree	H	-2.476222	-1.755543	-4.030745
E (GFN1	-xTB) = $-161.2776$	16075449 Hartree		H	-3.360689	-0.283213	-4.506588
	-xTB) = $-160.1912$			C	-0.650142	0.289787	-4.235351
E(GFN-	FF) = -22.4075442	64399 Hartree		H	0.260832	0.779210	-3.849222
				H	-1.072645	0.922544	-5.043804
Coordi				H	-0.346001	-0.677023	-4.686865
Co	-0.138952	-0.048740	-0.094793	P	-1.694636	-1.321365	0.853363
N	1.787715	-0.451862	0.080884	C	-2.687894	-2.417500	-0.276256
N	0.015544	1.476534	-1.245135	C	-4.069008	-2.635472	-0.081967
С	4.275924	-0.094617	-0.649100	H C	-4.591891	-2.122448 -3.503852	0.738502
C C	2.725024 2.388677	0.225306 1.306222	-0.619242 -1.468679	Н	-4.779200 -5.856839	-3.659259	-0.925051 -0.762395
Н	3.248381	1.754246	-1.969055	C	-4.119595	-4.177468	-1.965732
C	1.164292	1.948127	-1.762229	Н	-4.677334	-4.861357	-2.623432
C	1.316631	3.222924	-2.667072	C	-2.746821	-3.967638	-2.166057
C	4.658395	-0.417133	-2.119772	Н	-2.220740	-4.483892	-2.983599
Н	5.742373	-0.646357	-2.180722	C	-2.041224	-3.084962	-1.335207
Н	4.449986	0.419481	-2.812456	Н	-0.970746	-2.910176	-1.514271
Н	4.105605	-1.302635	-2.490346	С	-3.030972	-0.236376	1.555577
С	5.080793	1.148073	-0.194394	C	-3.252137	-0.107298	2.942086
H	6.167099	0.935247	-0.270884	H	-2.657215	-0.699493	3.652017
H	4.865596	1.406457	0.861115	С	-4.237328	0.768275	3.425755
H	4.870454	2.043379	-0.810638	H	-4.394891	0.858990	4.511537
C	4.786421	-1.282887	0.191985	C	-5.025334	1.511788	2.534184
H	5.863669	-1.419006	-0.036971	H	-5.802261	2.191844	2.915503
H	4.276157	-2.230511	-0.047919	C	-4.812894	1.383732	1.152069
H	4.695958	-1.117934	1.278989	H	-5.414627	1.965350	0.438228
C	2.178316	2.897847	-3.915003	С	-3.816811	0.527169	0.665190
H	2.262689	3.805957	-4.546133	H	-3.650808	0.459867	-0.420374
H	1.713268	2.102564	-4.529642	C	-1.389161	-2.457228	2.283834
H	3.207015	2.576442	-3.666117	C	-2.012326	-3.713770	2.425084
C H	0.013163 0.283591	3.845477 4.682157	-3.205524 -3.881812	H C	-2.697576 -1.758085	-4.080068 -4.505100	1.647208 3.556123
Н	-0.632896	4.255784	-2.412079	Н	-2.245711	-5.487506	3.651901
Н	-0.592001	3.126575	-3.786990	п С	-0.891027	-4.047481	4.561012
C	2.051954	4.297355	-1.828478	Н	-0.694443	-4.670546	5.446881
Н	2.174173	5.227449	-2.422326	C	-0.267446	-2.797705	4.424303
H	3.056925	3.954378	-1.514118	Н	0.432107	-2.436205	5.192115
Н	1.483383	4.550672	-0.913055	C	-0.504774	-2.014005	3.286800
C	2.110478	-1.268658	1.192667	Н	0.018146	-1.055934	3.164019
С	1.962612	-2.686445	1.130265				
С	2.386643	-3.455135	2.227194	T-TT TD	VOT		
Н	2.298544	-4.549727	2.182895	WUD	IOT		
С	2.913959	-2.857924	3.378896				
H	3.252443	-3.481821	4.219749	Confor	mation 0.		
C	2.968654	-1.460370	3.469627		licity: 2		
H	3.346382	-0.994341	4.391268	Charge			
С	2.565240	-0.646061	2.397459	•	3c) = -3367.159383		
С	1.328883	-3.330913	-0.093825		def2-TZVP) = -336		
H	0.504389	-2.625732	-0.352391	•	- D3(BJ)/def2-TZV	•	
C	2.244933	-3.388750	-1.327111	•	- D3(BJ)/def2-TZ	,	66/249/ Hartree
H H	2.589204	-2.382051 -3.825856	-1.624443		(-3c) = -3362.5770		
Н	1.699275 3.135297	-4.024154	-2.189786 -1.138105		= 65.51977 Kcal/r = 111.42633 Kcal		
C	0.723392	-4.710405	0.181968		- 111.42033 KCal, X-V/def2-TZVP) = -		6 Uartroo
Н	0.133165	-5.052859	-0.692144		-xTB) = $-130.5379$		o narciee
Н	0.051773	-4.697542	1.061668		(-xTB) = -127.3734		
Н	1.510390	-5.473506	0.357955		FF) = -15.7799681		
С	2.571956	0.875266	2.511979		,		
H	2.885866	1.283686	1.530380	Coordi	nates:		
C	1.147065	1.395716	2.748765	Co	0.341013	0.113855	-0.487642
H	0.453945	1.001026	1.972767	N	-0.075237	-1.560856	-1.426005
H	1.107811	2.502018	2.702701	0	-4.499134	-2.980696	1.497517
H	0.754976	1.077128	3.737108	0	-4.262037	-1.995241	3.533288
С	3.539802	1.426877	3.563208	C	-1.841110	0.832557	1.483856
H	3.568871	2.534249	3.514100	C	1.651714	-1.541399	-3.199741
H H	4.571164 3.233726	1.050073	3.407621	N C	0.734389	1.818529 -2.377129	0.398168
н С	-1.296961	1.156049 1.973433	4.595175 -1.454534	Н	-1.947420 -2.681466	-2.377129	-0.031781 0.129091
C	-1.806488	3.046219	-0.662456	C C	-2.055820	-1.239553	0.764479
C	-3.087222	3.549921	-0.947673	C	3.703608	-0.111425	-3.065595
Н	-3.476316	4.389504	-0.351473	Н	4.250731	-0.599106	-3.878587
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Н	-4.053229	1.428098	-3.436616	Н	2.623779	-4.085865	-3.476158
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С	-1.014790	3.632314	0.500453	H	2.803205	-1.473087	-7.741458
H	0.008684	3.206556	0.450122	C	2.253641	-1.460059	-5.642264
С	-0.900954	5.164477	0.439317	H	1.891459	-0.421098	-5.660861
H	-0.496002	5.513578	-0.530911	C	3.166838	-4.110141	-5.582848
	-0.231713	5.536048	1.242255	H	3.532881	-5.147746	-5.552004
H					4 000505	3.141545	-0.337265
H	-1.886917	5.652403	0.584167	C	4.223585		
H C	-1.886917 -1.638431	5.652403 3.190979	1.836499	С	3.221974	-3.379379	-6.780415
H C H	-1.886917 -1.638431 -1.669630	5.652403 3.190979 2.088458	1.836499 1.921906	C H	3.221974 3.624036	-3.379379 -3.843831	-6.780415 -7.693581
Н С Н Н	-1.886917 -1.638431 -1.669630 -2.681658	5.652403 3.190979 2.088458 3.555706	1.836499 1.921906 1.930366	C H C	3.221974 3.624036 4.650452	-3.379379 -3.843831 3.926134	-6.780415 -7.693581 -1.430494
Н С Н Н	-1.886917 -1.638431 -1.669630 -2.681658 -1.059514	5.652403 3.190979 2.088458 3.555706 3.589148	1.836499 1.921906 1.930366 2.694765	C H C H	3.221974 3.624036 4.650452 4.083884	-3.379379 -3.843831 3.926134 3.884868	-6.780415 -7.693581 -1.430494 -2.372880
Н С Н Н	-1.886917 -1.638431 -1.669630 -2.681658	5.652403 3.190979 2.088458 3.555706	1.836499 1.921906 1.930366	C H C	3.221974 3.624036 4.650452	-3.379379 -3.843831 3.926134	-6.780415 -7.693581 -1.430494

Н	7.362924	5.482203	-0.019288	С	-5.410338	5.681984	-2.230206
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Н	4.615301	2.612289	1.731061	C	-4.756923	3.457096	-1.494447
C	6.065112	4.054752	0.987280	H	-5.019409	2.416583	-1.250524
H	6.618569	4.099227	1.937656	C	-5.746261	4.353746	-1.923966
С	5.771338	4.761429	-1.316463	H	-6.788580	4.012388	-2.016494
H	6.086966	5.371197	-2.176779	C	-4.078327	6.107966	-2.106571
C	-3.105522	-1.036081	1.739198	H	-3.805256	7.145206	-2.353817
C C	-1.071571 3.030937	-2.472445 1.179525	-1.103797 -1.336226	C C	1.198298 1.537177	-3.440328 -0.855322	-0.469669 2.266759
C	0.496979	-2.052838	-2.589715	C	-1.688815	3.130830	0.292431
C	-1.139844	-3.529522	-2.085129	C	1.283380	1.271953	2.770148
H	-1.856481	-4.358306	-2.051026	С	2.288167	-0.625883	3.478783
C	2.372548	-0.477456	-2.634775	H	2.861570	-1.397335	4.005792
C	-0.121255	2.549725	1.212490	C	-0.205357	3.022076	1.921389
C H	4.124697 5.088510	0.895360 1.413633	-2.238691 -2.235397	C C	-1.078776 -1.892953	0.056150 4.297018	-2.618450 1.123157
C	0.486804	3.798779	1.607350	Н	-2.661852	5.057490	0.955793
Н	0.000063	4.550140	2.239942	C	-1.917352	0.610717	-3.655193
C	1.887620	2.580734	0.315671	H	-2.026386	0.181090	-4.657766
C	-0.190768	-3.249967	-3.031525	C	-2.033038	1.844730	-1.763527
H	0.045182	-3.804524	-3.945114	C	2.164654	0.705731	3.772081
C	-3.000553	0.285090	2.156746	H	2.611448	1.267341	4.598326
C H	1.745072 2.515787	3.811415 4.585077	1.067531 1.144008	C C	0.746133 -2.528550	-3.137837 1.712328	-1.749171 -3.118984
C	-1.345191	2.115999	1.700734	Н	-3.238520	2.399410	-3.590371
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C	3.024679	2.259446	-0.441487	H	-0.479074	-1.695714	-3.700524
N	-1.272067	-0.105557	0.640876	С	-2.367332	2.911565	-0.915220
C	-4.035362	-2.094656	2.200627	N	0.409199	-1.246849	-0.428003
C 0	-3.904282 -3.567182	1.063319 2.011896	3.034904 3.730208	C C	1.713350 0.804543	-4.725365 -3.960613	0.058738 -2.980743
0	-5.187722	0.633076	2.925563	0	-0.007831	-3.926996	-3.894336
C	-6.159390	1.314822	3.746010	0	1.912052	-4.739917	-3.001689
H	-7.112635	1.217988	3.190410	C	2.019351	-5.645575	-4.116426
H	-5.879889	2.385791	3.810960	H	1.983597	-5.063081	-5.061311
C	-5.176717	-2.951087	4.104967	H	1.129403	-6.311740	-4.121305
H H	-5.058026 -6.213166	-3.920906 -2.598950	3.580085 3.905589	C H	1.596703 1.460452	-7.080923 -7.213088	-0.159283 0.935134
C	-6.254541	0.698726	5.132620	H	2.691013	-7.122633	-0.349229
Н	-6.534060	-0.371557	5.078165	С	3.313870	-6.417510	-3.964223
H	-7.025427	1.227222	5.729101	H	4.184403	-5.732417	-3.949202
H	-5.287378	0.787410	5.664597	H	3.439561	-7.120727	-4.811122
C H	-4.888903	-3.051242	5.589343	H C	3.321997	-7.003255 -8.113988	-3.023241
н Н	-3.856717 -5.592806	-3.412567 -3.762648	5.767003 6.065237	Н	0.833490 -0.254894	-8.113988	-0.962649 -0.768365
H	-4.999192	-2.067808	6.087567	H	1.169813	-9.133638	-0.689271
				H	0.997929	-7.974901	-2.049957
	ation 16.			~ .			
Multipl: Charge:	icity: 2				mation 19.		
	c) = converged!)	Hartree		Charge			
		6.992755779787 на	rtree	_	3c) = -3367.158645	3434764 Hartree	
		$^{\prime}P) = -3365.969028$			def2-TZVP) = -3366		
		(VP) = -3366.03507	2868632 Hartree		- D3(BJ)/def2-TZVI		
		05776997 Hartree			- D3(BJ)/def2-TZV		9476244 Hartree
	= 66.49799 Kcal/ = 111.32898 Kcal				(-3c) = -3362.57679 = 64.33428 Kcal/n		
		-3368.99945860901	8 Hartree		= 110.92964 Kcal/		
		71835805 Hartree		Ε(ωΒ97	X-V/def2-TZVP) = -	-3368.99638844292	5 Hartree
		.31539602 Hartree			-xTB) = $-130.53991$		
E (GFN-F	F) = -15.7795200	185293 Hartree			(-xTB) = -127.37403 (-FF) = -15.78335048		
Coordin	ates:			E (GIN	11) - 13.70333040	JJ140 Haltiee	
Co	-0.118933	0.558760	0.187646	Coordi	nates:		
N	0.929731	0.314755	1.831395	Со	-0.155954	0.564459	0.005685
0	2.544749	-4.846189	0.947708	N	0.879508	0.764894	1.654840
0 C	1.109161 0.233181	-5.780035 -1.786510	-0.538752 -1.690206	0	3.336556 3.236691	-4.045908 -5.017685	1.690732 -0.357162
C	0.780993	2.580355	2.817137	C	0.069683	-2.246691	-1.087189
N	-1.137944	0.830647	-1.466642	C	-0.066657	2.876640	2.542636
C	1.519281	-2.076623	1.608507	N	-1.157831	0.397655	-1.672848
Н	2.031912	-2.934244	2.062618	С	2.252474	-1.287605	1.549980
C	1.021321	-2.239018	0.317827	H	3.045510	-1.876659	2.026768
C H	-0.949883 -0.786036	4.246616 4.951506	2.114400 2.935627	C C	1.543959 -1.605773	-1.888577 4.358232	0.510781 1.224029
C	1.232789	3.509237	3.894048	Н	-1.769836	5.113404	1.998953
N	-0.674315	2.333564	0.811366	C	-0.099353	3.817167	3.700480
С	1.945019	4.682805	3.565295	N	-0.868709	2.374609	0.244321
Н	2.171143	4.891689	2.508761	C	0.385605	5.137890	3.584475
C H	1.366761 1.129111	4.135925	6.253545	H C	0.794490	5.475291	2.620220
н С	0.945565	3.921320 3.249508	7.306651 5.251585	Н	-0.621596 -1.020711	4.256238 3.906068	6.048768 7.012932
Н	0.373151	2.347358	5.514760	C	-0.599460	3.386783	4.948536
С	2.367366	5.567814	4.567966	H	-0.978901	2.358396	5.045994
H	2.927851	6.474771	4.294453	C	0.364716	6.006181	4.685755
C C	-3.415557 2.080889	3.875670	-1.360580 5 915211	H	0.752646 -2.674273	7.030828 3.700308	4.579877 -2.838737
Н	2.080889	5.296397 5.991111	5.915211 6.701961	C C	-2.6/42/3	5.568785	5.920581

-1.675789

-1.590929

C

5.212440

5.540942

2.927851 -3.415557 2.080889 2.411994

-3.088711

-2.042003

C H

-0.156436 -1.996073

6.784266 -3.289864

6.250721

4.853413

H	-0.945532	5.003011	-2.998373	C	-1.459927	4.930310	-3.013446
C	-3.984230	5.597119	-4.477610	H	-1.811679	3.989537	-3.463234
H	-4.494041	6.334602	-5.115920	C	-1.304572	7.357779	-3.045686
C	-4.022247	3.516801	-3.216288	H	-1.532099	8.321824	-3.525397
H	-4.564688	2.631675	-2.851522	С	-0.273263	6.092130	-1.241805
C	-4.671100	4.457628	-4.029302	H	0.319035	6.061040	-0.314943
H	-5.724357	4.302520 5.792680	-4.308890 -4.104376	C H	-0.563298 -0.201468	7.320282 8.255151	-1.853872 -1.399207
C H	-2.645088 -2.099187	6.682763	-4.104376	н С	-1.751403	6.158857	-3.623820
C	1.738395	-3.257745	0.078128	Н	-2.334868	6.179707	-4.556933
C	1.902698	-0.063096	2.099165	C	1.475676	-3.494166	-0.831431
C	-1.608297	3.116463	-0.665572	C	-0.254135	-1.821378	2.092674
Č	0.795539	1.770691	2.602335	Č	-0.912458	3.266144	0.092619
C	2.489694	0.452388	3.314190	С	-0.840980	0.098235	2.992133
H	3.321959	-0.021131	3.847884	C	-0.656689	-2.108006	3.449342
C	-0.828973	3.150814	1.397945	H	-0.652709	-3.107978	3.898838
C	-1.340118	-0.757068	-2.421336	С	-1.220673	2.333446	2.066161
C	-2.060367	4.353168	-0.067469	C	1.663841	0.934073	-2.404282
H	-2.682290 -2.058657	5.097957 -0.471576	-0.574082 -3.641388	C H	-1.700921 -2.070122	4.192801 5.157710	0.874147 0.513069
C H	-2.058657	-1.222015	-4.399082	н С	1.949691	1.955185	-3.384809
C	-1.773390	1.400888	-2.406023	Н	2.639300	1.826782	-4.227219
C	1.787126	1.580866	3.642234	C	0.456413	2.686912	-1.852726
Н	1.926408	2.251235	4.496387	C	-0.986578	-0.909581	4.023217
C	0.774275	-3.498346	-0.897635	Н	-1.316371	-0.709819	5.047485
С	-2.293517	0.877215	-3.653731	C	2.080113	-2.787091	-1.863645
H	-2.788698	1.476954	-4.423800	C	1.184119	3.041107	-3.054959
C	-0.845130	-2.015769	-2.112987	H	1.116664	4.010896	-3.558229
H	-1.075983	-2.855415	-2.780422	С	2.138509	-0.364445	-2.507681
C	-1.974921	2.716444	-1.961666	H	2.824340	-0.623890	-3.324180
N C	0.525635 2.824180	-1.284133 -4.132646	-0.204083 0.581797	C	-0.403922 0.949955	3.566695 -1.238124	-1.178979 -0.535148
C	0.425839	-4.132646 -4.751491	-1.611120	N C	1.631084	-1.238124	-0.535148
0	-0.030838	-4.805774	-2.746012	C	2.862189	-3.306064	-3.009471
0	0.611571	-5.844458	-0.833746	0	3.680602	-2.662168	-3.653423
C	0.321264	-7.115880	-1.453920	0	2.539216	-4.592364	-3.278648
H	-0.636747	-7.032102	-2.007082	C	3.306031	-5.252324	-4.306368
H	0.188008	-7.809917	-0.601226	H	3.348507	-6.311914	-3.985574
C	4.268032	-5.939953	0.055299	Н	4.331179	-4.830874	-4.312750
H	5.049475	-5.377547	0.606493	С	0.517570	-6.894655	0.229770
H	4.694162	-6.314498	-0.895853	H	1.276414	-7.038253	1.028502
C H	1.435503 1.539893	-7.574244 -6.879073	-2.382665 -3.237124	H C	0.880034 2.647436	-7.460810 -5.098452	-0.654281 -5.667658
H	1.199427	-8.581053	-2.782741	Н	1.609567	-5.486400	-5.654059
				Н	3.218238	-5.662911	-6.432510
Н	2.405021	-7.631615	-1.850726				
H C	2.405021 3.720965	-7.631615 -7.072254	-1.850726 0.911358				
H C H	2.405021 3.720965 3.323979	-7.631615 -7.072254 -6.679695	-1.850726 0.911358 1.866578	H C	2.624366 -0.867704	-4.033859 -7.328137	-5.970929 0.662940
С	3.720965	-7.072254	0.911358	H	2.624366	-4.033859	-5.970929
C H	3.720965 3.323979	-7.072254 -6.679695	0.911358 1.866578	H C H H	2.624366 -0.867704 -1.205530 -0.864417	-4.033859 -7.328137 -6.760536 -8.405467	-5.970929 0.662940 1.553018 0.921984
C H H H	3.720965 3.323979 4.530949 2.910996	-7.072254 -6.679695 -7.792990	0.911358 1.866578 1.143629	H C H	2.624366 -0.867704 -1.205530	-4.033859 -7.328137 -6.760536	-5.970929 0.662940 1.553018
C H H H	3.720965 3.323979 4.530949 2.910996 ation 20.	-7.072254 -6.679695 -7.792990	0.911358 1.866578 1.143629	H C H H	2.624366 -0.867704 -1.205530 -0.864417 -1.605655	-4.033859 -7.328137 -6.760536 -8.405467	-5.970929 0.662940 1.553018 0.921984
C H H H Conform	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2	-7.072254 -6.679695 -7.792990	0.911358 1.866578 1.143629	H C H H Confor	2.624366 -0.867704 -1.205530 -0.864417 -1.605655 mation 21.	-4.033859 -7.328137 -6.760536 -8.405467	-5.970929 0.662940 1.553018 0.921984
C H H Conform Multipl Charge:	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2	-7.072254 -6.679695 -7.792990 -7.617236	0.911358 1.866578 1.143629	H C H H Confor	2.624366 -0.867704 -1.205530 -0.864417 -1.605655 mation 21. licity: 2	-4.033859 -7.328137 -6.760536 -8.405467	-5.970929 0.662940 1.553018 0.921984
C H H H Conform Multipl Charge: E(B97-3	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777	-7.072254 -6.679695 -7.792990 -7.617236	0.911358 1.866578 1.143629 0.388202	H C H H Confor Multip Charge	2.624366 -0.867704 -1.205530 -0.864417 -1.605655 mation 21. licity: 2	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832	-5.970929 0.662940 1.553018 0.921984
C H H H Conform Multipl Charge: E(B97-3) E(M06/d.	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336	-7.072254 -6.679695 -7.792990 -7.617236	0.911358 1.866578 1.143629 0.388202	H C H H Confor Multip Charge E(B97-	2.624366 -0.867704 -1.205530 -0.864417 -1.605655 mation 21. licity: 2 : 0 3c) = -3367.157794	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832	-5.970929 0.662940 1.553018 0.921984 -0.147790
C H H Conform Multipl Charge: E(B97-3 E(M06/d: E(PBE - E(PBE0	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV - D3(BJ)/def2-TZV	-7.072254 -6.679695 -7.792990 -7.617236 0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199	0.911358 1.866578 1.143629 0.388202	H C H H Confor Multip Charge E(B97- E(M06/ E(PBE	2.624366 -0.867704 -1.205530 -0.864417 -1.605655 mation 21. licity: 2: 0 3c) = -3367.157794 def2-TZVP) = -3364 - D3(BJ)/def2-TZVI	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832 4361162 Hartree 5.990631836714 Ha P) = -3365.966807	-5.970929 0.662940 1.553018 0.921984 -0.147790
C H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE - E(PBE0 E(PBEh-	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV - D3(BJ)/def2-TZV 5c) = -3362.5753	-7.072254 -6.679695 -7.792990 -7.617236 0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199 36082713 Hartree	0.911358 1.866578 1.143629 0.388202	H C H H Confor Multip Charge E(B97- E(M06/ E(PBE E(PBE)	2.624366 -0.867704 -1.205530 -0.864417 -1.605655 mation 21. licity: 2: 0 3c) = -3367.157794 def2-TZVP) = -3364 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832 4361162 Hartree 6.990631836714 Ha P) = -3365.966807 PP) = -3366.03244	-5.970929 0.662940 1.553018 0.921984 -0.147790
C H H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE - E(PBE0 - E(PBE0 - E(PM6) - E	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV - D3(BJ)/def2-TZV 3c) = -3362.5753 = 66.96457 Kcal/s	-7.072254 -6.679695 -7.792990 -7.617236 0368557 Hartree 6.989652078966 Ha P) = -3365.03199 36082713 Hartree mol	0.911358 1.866578 1.143629 0.388202	H C H H Confor Multip Charge E(B97- E(M06/ E(PBE E(PBE) E(PBE)	2.624366 -0.867704 -1.205530 -0.864417 -1.605655 mation 21. licity: 2 : 0 3c) = -3367.15779 def2-TZVP) = -3364 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZV-3c) = -3362.57528	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832 4361162 Hartree 5.990631836714 Ha 9) = -3365.966807 VP) = -3366.03244 35059553 Hartree	-5.970929 0.662940 1.553018 0.921984 -0.147790
C H H H Conform Multipl Charge: E (B97-3 E (M06/d E (PBE - E (PBE) E (PBE) E (PM6) E (PM7)	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' 3c) = -3362.5753 = 66.96457 Kcal/t = 112.31984 Kcal	-7.072254 -6.679695 -7.792990 -7.617236 0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199 36082713 Hartree mol /mol	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree	H C H H H Confor Multip Charge E(B97- E(M06/ E(PBE E(PBEC) E(PBEC) E(PBEC)	2.624366 -0.867704 -1.205530 -0.864417 -1.605655 mation 21. licity: 2 : 0 3c) = -3367.157794 def2-TZVP) = -3360 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - 3c) = -3362.57521 = 66.17919 Kcal/r	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832 4361162 Hartree 6.990631836714 Ha P) = -3365.966807 VP) = -3366.03244 35059553 Hartree mol	-5.970929 0.662940 1.553018 0.921984 -0.147790
C H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE - E(PBE0 E(PBEh - E(PBEh - E(PM6)) E(PM7) E(MB97X	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' 3c) = -3362.5753 = 66.96457 Kcal/i = 112.31984 Kcal -V/def2-TZVP) =	-7.072254 -6.679695 -7.792990 -7.617236 0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199 36082713 Hartree mol /mol -3368.99750545310	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree	H C H H H Confor Multip Charge E (B97- E (M06/ E (PBE E (PBEC E (PBE) E (PMF) E (PMF)	2.624366 -0.867704 -1.205530 -0.864417 -1.605655 mation 21. licity: 2: : 0 3c) = -3367.157799 def2-TZVP) = -3366 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - S362.57528 = 66.17919 Kcal/r = 111.82583 Kcal,	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832 4361162 Hartree 6.990631836714 Ha P) = -3365.966807 VP) = -3366.03244 85059553 Hartree mol	-5.970929 0.662940 1.553018 0.921984 -0.147790
C H H H H Conform Multipl Charge: E (B97-3 E (M06/d E (PBE - E (PBE0 - E (PM6) E (PM7) E (GFN1- E (GFN	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' 3c) = -3362.5753 = 66.96457 Kcal/s = 112.31984 Kcal - V/def2-TZVP) = xTB) = -130.5352	-7.072254 -6.679695 -7.792990 -7.617236 0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199 36082713 Hartree mol /mol -3368.99750545310 78876975 Hartree	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree	H C H H H Confor Multip Charge E(B97- E(M06/ E(PBE E(PBE) E(PBE) E(PMT) E(PMT)	2.624366 -0.867704 -1.205530 -0.864417 -1.605655 mation 21. licity: 2: 0 3c) = -3367.15779 def2-TZVP) = -3364 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - 3c) = -3362.57528 = 66.17919 Kcal/r = 111.82583 Kcal, X-V/def2-TZVP) = -	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832 4361162 Hartree 6.990631836714 Ha P) = -3366.03244 85059553 Hartree mol /mol -3368.99679956236	-5.970929 0.662940 1.553018 0.921984 -0.147790
C H H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE - E(PBE0 E(PM6) E(PM7) E(GFN1-E(GFN1-E(GFN1-E(GFN2-E(FN1-E(GFN2-E(FN1-E(GFN2-E(FN1-E(GFN2-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-E(FN1-	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' 3c) = -3362.5753 = 66.96457 Kcal/s = 112.31984 Kcal - V/def2-TZVP) = xTB) = -130.5352	-7.072254 -6.679695 -7.792990 -7.617236  0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199 36082713 Hartree mol /mol 7mol 78876975 Hartree 37819746 Hartree	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree	H C H H H Confor Multip Charge E(B97- E(M06/ E(PBE E(PBEC E(PBEC E(PBEC E(PM6) E(PM7) E(M97) E(GFN1)	2.624366 -0.867704 -1.205530 -0.864417 -1.605655 mation 21. licity: 2: 0: 3c) = -3367.157794 def2-TZVP) = -3364 - D3 (BJ) / def2-TZV- - D3 (BJ) / def2-TZV- -3c) = -3362.57524 = 66.17919 Kcal/r = 111.82583 Kcal, X-V/def2-TZVP) = - -xTB) = -130.53633 -xTB) = -127.37205	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832 4361162 Hartree 6.990631836714 Ha P) = -3365.966807 VP) = -3366.03244 35059553 Hartree mol /mol /mol 20680686 Hartree 68919929 Hartree	-5.970929 0.662940 1.553018 0.921984 -0.147790
C H H Conform Multipl Charge: E (B97-3 E (M06/d E (PBE - E (PBE0 - E (PBE0 - E (PM7)) E (\omega B97X E (GFN1 - E (GFN2 - E (GFN-F	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' 3c) = -3362.5753 = 66.96457 Kcal/: = 112.31984 Kcal -V/def2-TZVP) = xTB) = -130.5352 xTB) = -127.3708 F) = -15.7772397	-7.072254 -6.679695 -7.792990 -7.617236  0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199 36082713 Hartree mol /mol 7mol 78876975 Hartree 37819746 Hartree	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree	H C H H H Confor Multip Charge E(B97- E(M06/ E(PBE E(PBEC E(PBEC E(PBEC E(PM6) E(PM7) E(M97) E(GFN1)	2.624366 -0.867704 -1.205530 -0.864417 -1.605655 mation 21. licity: 2: : 0 3c) = -3367.15779: def2-TZVP) = -3366. D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - 3c) = -3362.57520: = 66.17919 Kcal/r = 111.82583 Kcal, X-V/def2-TZVP) = -xTB) = -130.53632	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832 4361162 Hartree 6.990631836714 Ha P) = -3365.966807 VP) = -3366.03244 35059553 Hartree mol /mol /mol 20680686 Hartree 68919929 Hartree	-5.970929 0.662940 1.553018 0.921984 -0.147790
C H H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE- E(PBE0- E(PBE0- E(PM6)- E(PM7)- E(GFN1- E(GFN2- E(GFN-F	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' 3c) = -3362.5753 = 66.96457 Kcal/i = 112.31984 Kcal -V/def2-TZVP) = xTB) = -130.5352 xTB) = -127.3708 F) = -15.7772397 ates:	-7.072254 -6.679695 -7.792990 -7.617236 0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199 36082713 Hartree mol /mol -3368.99750545310 78876975 Hartree 37819746 Hartree 15432 Hartree	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree	H C H H H H Confor Multip Charge E (B97- E (M06/ E (PBEC E (PBEC) E (PMF) E (PMF) E (GFN1 E (GFN2 E (GFN-	2.624366 -0.867704 -1.205530 -0.864417 -1.605655 mation 21. licity: 2: : 0 3c) = -3367.1577994 def2-TZVP) = -3366 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - S3c) = -3362.57528 = 66.17919 Kcal/r = 111.82583 Kcal, X-V/def2-TZVP) = -xTB) = -130.53633 -xTB) = -127.37209 FF) = -15.77829153	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832 4361162 Hartree 6.990631836714 Ha P) = -3365.966807 VP) = -3366.03244 35059553 Hartree mol /mol /mol 20680686 Hartree 68919929 Hartree	-5.970929 0.662940 1.553018 0.921984 -0.147790
C H H H H Conform Multipl Charge: E (B97-3 E (M06/d E (PBE) - E (PBE) E (PM7) E (GFN1-E (GFN2-E (GFN1-E (GFN2-E (GFN-F Coordin. Co	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV - D3(BJ)/def2-TZV 3c) = -3362.5753 = 66.96457 Kcal/: = 112.31984 Kcal -V/def2-TZVP) = xTB) = -130.5352 xTB) = -127.3708 F) = -15.7772397 ates: 0.176251	-7.072254 -6.679695 -7.792990 -7.617236  0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199 36082713 Hartree mol /mol 7mol 78876975 Hartree 37819746 Hartree 15432 Hartree	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree	H C H H H Confor Multip Charge E(B97- E(M66/ E(PBE) E(PM6) E(PM7) E(GFN1) E(GFN2) E(GFN- Coordi	2.624366 -0.867704 -1.205530 -0.864417 -1.605655 mation 21. licity: 2: : 0 3c) = -3367.15779 def2-TZVP) = -3366 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - 3c) = -3362.57520 = 66.17919 Kcal/r = 111.82583 Kcal, X-V/def2-TZVP) = - -xTB) = -130.53632 -xTB) = -127.37201 FF) = -15.77829153	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832 4361162 Hartree 5.990631836714 Ha 9) = -3365.966807 VP) = -3366.03244 35059553 Hartree mol (mol -3368.99679956236 20680686 Hartree 58919929 Hartree 12796 Hartree	-5.970929 0.662940 1.553018 0.921984 -0.147790 ertree 133785 Hartree 6827778 Hartree
C H H H H Conform Multipl Charge: E (B97-3 E (M06/d E (PBE - E (PBE) E (PM7) E (GFN1-E (GFN1-E (GFN2-E (GFN2-E (GFN-F Coording Co	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV - D3(BJ)/def2-TZV 3c) = -3362.5753 = 66.96457 Kcal/s = 112.31984 Kcal -V/def2-TZVP) = -130.5352 xTB) = -127.3708 F) = -15.7772397 ates: 0.176251 -0.355268	-7.072254 -6.679695 -7.792990 -7.617236  0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199 36082713 Hartree mol /mol -3368.99750545310 78876975 Hartree 37819746 Hartree 15432 Hartree  0.451465 -0.463877	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree 3 Hartree	H C H H H H Confor Multip Charge E(B97- E(M06/ E(PBE E(PBE) E(PM6) E(PM7) E(GFN1) E(GFN2 Coordi Co	2.624366 -0.867704 -1.205530 -0.864417 -1.605655 mation 21. licity: 2: 0: 3c) = -3367.157794 def2-TZVP) = -3364 - D3(BJ)/def2-TZV- - D3(BJ)/def2-TZV- 3c) = -3362.57528 = 66.17919 Kcal/r = 111.82583 Kcal/r = 111.	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832 4361162 Hartree 5.990631836714 Ha 9) = -3365.966807 7P) = -3366.03244 35059553 Hartree mol /mol -3368.99679956236 20680686 Hartree 58919929 Hartree 12796 Hartree	-5.970929 0.662940 1.553018 0.921984 -0.147790 artree 133785 Hartree 6827778 Hartree
C H H H H Conform Multipl Charge: E (B97-3 E (M06/d E (PBE - E (PBE) E (PM7) E (GFN1- E (GFN1- E (GFN2- E (GFN2- E (GFN2- Coording Coordin	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' 3c) = -3362.5753 3c) = -3362.5753 = 66.96457 Kcal/i = 112.31984 Kcal -V/def2-TZVP) = xTB) = -130.5352 xTB) = -127.3708 F) = -15.7772397 ates: 0.176251 -0.355268 2.671290	-7.072254 -6.679695 -7.792990 -7.617236 0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199 36082713 Hartree mol /mol -3368.99750545310 78819746 Hartree 15432 Hartree 0.451465 -0.463877 -5.568840	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree 3 Hartree 0.164384 1.820653 -0.608473	H C H H H H Confor Multip Charge E(B97- E(M06/ E(PBE E(PBEC E(PBEC E(PM6) E(PM7) E(GFN1) E(GFN2) E(GFN- Coordi Co	2.624366 -0.867704 -1.205530 -0.864417 -1.605655 mation 21. licity: 2: 0: 3c) = -3367.157794 def2-TZVP) = -3364 - D3 (BJ) / def2-TZV - D3 (BJ) / def2-TZV -3c) = -3362.57524 = 66.17919 Kcal/r = 111.82583 Kcal/r X-V/def2-TZVP) = -73760 -xTB) = -127.37205 FF) = -15.77829153 nates: -0.087975 1.590202	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832 4361162 Hartree 6.990631836714 Ha P) = -3365.966807 VP) = -3366.03244 35059553 Hartree mol /mol -3368.99679956236 20680686 Hartree 58919929 Hartree 12796 Hartree -0.505802 -1.403556	-5.970929 0.662940 1.553018 0.921984 -0.147790 Artree 133785 Hartree 6827778 Hartree 6827778 Hartree
C H H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE- E(PBE0- E(PBE0- E(PM7)) E(MB97X E(GFN1- E(GFN2- E(GFN2- COOrdin CO N O	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV - D3(BJ)/def2-TZ 50 = -3362.5753 = 66.96457 Kcal/i = 112.31984 Kcal -V/def2-TZVP) = xTB) = -130.5352 xTB) = -127.3708 F) = -15.7772397 ates: 0.176251 -0.355268 2.671290 0.457046	-7.072254 -6.679695 -7.792990 -7.617236 0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199 36082713 Hartree mol /mol -3368.99750545310 78876975 Hartree 37819746 Hartree 15432 Hartree 0.451465 -0.463877 -5.568840 -5.493827	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree 3 Hartree 0.164384 1.820653 -0.608473 -0.112872	H C H H H H Confor Multige E(B97- E(M06/ E(PBE E(PBEC E(PBEC) E(PM7) E(GFN1 E(GFN2) E(GFN1 COordi Co N O	2.624366 -0.867704 -1.205530 -0.864417 -1.605655 mation 21. licity: 2: 0: 3c) = -3367.157794 def2-TZVP) = -3366 - D3 (BJ)/def2-TZVI - D3 (BJ)/def2-TZVI - D3 (BJ)/def2-TZVI - S362.5752i = 66.17919 Kcal/r = 111.82583 Kcal, X-V/def2-TZVP) = - -xTB) = -130.53632 -xTB) = -137.37201 FF) = -15.778291531 nates: -0.087975 1.590202 5.036760	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832 4361162 Hartree 6.990631836714 Ha P) = -3365.966807 VP) = -3366.03244 35059553 Hartree mol -3368.99679956236 20680686 Hartree 20680686 Hartree -0.505802 -1.403556 2.641169	-5.970929 0.662940 1.553018 0.921984 -0.147790 Artree 133785 Hartree 6827778 Hartree 6827778 Hartree
C H H H H Conform Multipl Charge: E (B97-3 E (M06/d E (PBE - E (PBE) E (PM7) E (GFN1- E (GFN1- E (GFN2- E (GFN2- E (GFN2- Coording Coordin	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' 3c) = -3362.5753 3c) = -3362.5753 = 66.96457 Kcal/i = 112.31984 Kcal -V/def2-TZVP) = xTB) = -130.5352 xTB) = -127.3708 F) = -15.7772397 ates: 0.176251 -0.355268 2.671290	-7.072254 -6.679695 -7.792990 -7.617236 0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199 36082713 Hartree mol /mol -3368.99750545310 78819746 Hartree 15432 Hartree 0.451465 -0.463877 -5.568840	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree 3 Hartree 0.164384 1.820653 -0.608473	H C H H H H Confor Multip Charge E(B97- E(M06/ E(PBE E(PBEC E(PBEC E(PM6) E(PM7) E(GFN1) E(GFN2) E(GFN- Coordi Co	2.624366 -0.867704 -1.205530 -0.864417 -1.605655 mation 21. licity: 2: 0: 3c) = -3367.157794 def2-TZVP) = -3364 - D3 (BJ) / def2-TZV - D3 (BJ) / def2-TZV -3c) = -3362.57524 = 66.17919 Kcal/r = 111.82583 Kcal/r X-V/def2-TZVP) = -73760 -xTB) = -127.37205 FF) = -15.77829153 nates: -0.087975 1.590202	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832 4361162 Hartree 6.990631836714 Ha P) = -3365.966807 VP) = -3366.03244 35059553 Hartree mol /mol -3368.99679956236 20680686 Hartree 58919929 Hartree 12796 Hartree -0.505802 -1.403556	-5.970929 0.662940 1.553018 0.921984 -0.147790 Artree 133785 Hartree 6827778 Hartree 6827778 Hartree
C H H H H Conform Multipl Charge: E (B97-3 E (M06/d E (PBE - E (PM6) E (PM7) E (GFN1-E (GFN2-E (GFN1-Conform Conform C	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZ' 3c) = -3362.5753 = 66.96457 Kcal/; = 112.31984 Kcal -V/def2-TZVP) = xTB) = -130.5352 xTB) = -127.3708 F) = -15.7772397 ates: 0.176251 -0.355268 2.671290 0.457046 1.742223	-7.072254 -6.679695 -7.792990 -7.617236  0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199 36082713 Hartree mol /mol 78876975 Hartree 37819746 Hartree 15432 Hartree 15432 Hartree  0.451465 -0.463877 -5.568840 -5.493827 -1.394655	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree 3 Hartree 0.164384 1.820653 -0.608473 -0.112872 -1.658225	H C H H H H Confor Multip Charge E(B97- E(M06/ E(PBE) E(PM6) E(PM7) E(GFN1 E(GFN2 E(GFN- Coordi Co N O	2.624366 -0.867704 -1.205530 -0.864417 -1.605655  mation 21. licity: 2: 0 3c) = -3367.15779 def2-TZVP) = -3366 -0.864) / def2-TZVI -0.86 / D3 (BJ) / def2-TZVI -0.86 / D3 (BJ) / def2-TZVI -0.87919 Kcal/r =111.82583 Kcal, X-V/def2-TZVP) = -xTB) = -130.53632 -xTB) = -127.37201 FF) = -15.77829151  nates: -0.087975 1.590202 5.036760 4.018935	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832 4361162 Hartree 6.990631836714 Ha P) = -3365.966807 JP) = -3366.03244 35059553 Hartree mol /mol -3368.99679956236 20680686 Hartree 58919929 Hartree 12796 Hartree -0.505802 -1.403556 2.641169 4.208668	-5.970929 0.662940 1.553018 0.921984 -0.147790 Artree 133785 Hartree 6827778 Hartree 6827778 Hartree -0.248083 -0.721929 0.412672 1.700868 0.463700 -1.779348
C H H H H COnform Multipl Charge: E (B97-3 E (M06/d E (PBE - E (PBE) E (PM7)) E (WB97X E (GFN2-E (GFN2	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' 3c) = -3362.5753 = 66.96457 Kcal/i = 112.31984 Kcal -V/def2-TZVP) = xTB) = -130.5352 xTB) = -127.3708 F) = -15.7772397 ates: 0.176251 -0.355268 2.671290 0.457046 1.742223 -1.244887 0.769822 0.217402	-7.072254 -6.679695 -7.792990 -7.617236  0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199 36082713 Hartree mol /mol -3368.99750545310 7388.99750545310 73819746 Hartree 15432 Hartree  0.451465 -0.463877 -5.568840 -5.493827 -1.394655 1.432565 1.399734 -2.793868	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree 3 Hartree 0.164384 1.820653 -0.608473 -0.112872 -1.658225 3.141628 -1.448300 1.223514	H C H H H H Confor Multip Charge E(B87- E(M06/ E(PBE E(PBE) E(PM6) E(PM7) E(GFN1) E(GFN2) E(GFN- Coordi Co N O C C N	2.624366 -0.867704 -1.205530 -0.864417 -1.605655  mation 21. licity: 2: 0 3c) = -3367.157794 def2-TZVP) = -3366 - D3 (BJ) / def2-TZVI - D3 (BJ) / def2-TZVI = 66.17919 Kcal/r = 111.82583 Kcal, X-V/def2-TZVP) =xTB) = -130.5363; -xTB) = -127.3720; FF) = -15.7782915:  nates: -0.087975 1.590202 5.036760 4.018935 0.389861 0.728149 -1.773785	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832 4361162 Hartree 6.990631836714 Ha P) = -3365.966807 VP) = -3366.03244 35059553 Hartree mol -3368.99679956236 20680686 Hartree 20680686 Hartree -0.505802 -1.403556 2.641169 4.208668 2.402209 -3.473674 0.366226	-5.970929 0.662940 1.553018 0.921984 -0.147790 Artree 133785 Hartree 6827778 Hartree 6827778 Hartree -0.248083 -0.721929 0.412672 1.700868 0.463700 -1.779348 0.255004
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C H H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE) - E(PBE0) E(PBE0) E(PBE0) E(PBF0) E(GFN1-E(GFN2-E(GFN1-F Coordin CO N O C C C N C C H C	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV - D3(BJ)/def2-TZV 3c) = -3362.5753 = 66.96457 Kcal/s = 112.31984 Kcal -V/def2-TZVP) = xTB) = -130.5352 xTB) = -127.3708 F) = -15.7772397 ates: 0.176251 -0.355268 2.671290 0.457046 1.742223 -1.244887 0.769822 0.217402 0.182066 0.800580	-7.072254 -6.679695 -7.792990 -7.617236  0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199 36082713 Hartree mol /mol 78876975 Hartree 37819746 Hartree 15432 Hartree 15432 Hartree 15432 Hartree 15432 Hartree 15432 Hartree 15432 Hartree	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree 3 Hartree 0.164384 1.820653 -0.608473 -0.112872 -1.658225 3.141628 -1.448300 1.223514 1.547580 -0.009808	H C H H H H Confor Multip Charge E(B97- E(M06/ E(PBE) E(PM6) E(PM7) E(GFN1 E(GFN2 COORDI CO N O C C H	2.624366 -0.867704 -1.205530 -0.864417 -1.605655  mation 21. licity: 2: 0 3c) = -3367.15779 def2-TZVP) = -3361 - D3(BJ)/def2-TZV1 - D3(BJ)/def2-TZV2 = 66.17919 Kcal/r = 111.82583 Kcal, X-V/def2-TZVP) = -xTB) = -127.3720 FF) = -15.7782915  nates: -0.087975 1.590202 5.036760 4.018935 0.389861 0.728149 -1.773785 3.217156 4.277368	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832 4361162 Hartree 5.990631836714 Ha 9) = -3365.966807 7P) = -3366.03244 35059553 Hartree mol /mol -3368.99679956236 20680686 Hartree 58919929 Hartree 12796 Hartree -0.505802 -1.403556 2.641169 4.208668 2.402209 -3.473674 0.366226 0.281723 0.537481	-5.970929 0.662940 1.553018 0.921984 -0.147790 artree 133785 Hartree 16827778 Hartree 10 Hartree -0.248083 -0.721929 0.412672 1.700868 0.463700 -1.779348 0.255004 0.066193 0.187542
C H H H H Conform Multipl Charge: E (B97-3 E (M06/d E (PBE - E (PBE) E (PM7) E (GFN1- E (GFN2- E (GFN2- C (C ) N ) C C C C C C C C C C C C C C C C	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV = 112.31984 Kcal/ = 112.31984 Kcal/ = 112.31984 Kcal/ = 112.71990 Kcal/ - V/def2-TZVP) = -130.5352 xTB) = -127.3708 F) = -15.7772397 ates: 0.176251 -0.355268 2.671290 0.457046 1.742223 -1.244887 0.769822 0.217402 0.182066 0.800580 -1.866845	-7.072254 -6.679695 -7.792990 -7.617236  0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199 36082713 Hartree mol /mol -3368.99750545310 78876975 Hartree 37819746 Hartree 15432 Hartree  0.451465 -0.463877 -5.568840 -5.993827 -1.394655 1.432565 1.399734 -2.793868 -3.840468 -2.511683 3.626435	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree 34115 Hartree 0.164384 1.820653 -0.608473 -0.112872 -1.658225 3.141628 -1.448300 1.223514 1.547580 -0.009808 2.109352	H C H H H H Confor Multip Charge E(B97- E(M06/ E(PBE) E(PM6) E(PM7) E(GFN1) E(GFN2) Coordi Co N O C C C N C C H C	2.624366 -0.867704 -1.205530 -0.864417 -1.605655  mation 21. licity: 2: 0 3c) = -3367.157794 def2-TZVP) = -3364 - D3(BJ)/def2-TZV1 - D3(BJ)/def2-TZV3 = 66.17919 Kcal/f = 111.82583 Kcal/f = 111.82583 Kcal/f = 111.82583 Kcal/f = 111.82583 Kcal/f = 112.82583 Kcal/f = 112.82583 Kcal/f = 113.82583 Kcal	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832 4361162 Hartree 6.990631836714 Ha P) = -3365.966807 27) = -3366.03244 35059553 Hartree mol /mol -3368.99679956236 20680686 Hartree 58919929 Hartree 12796 Hartree -0.505802 -1.403556 2.641169 4.208668 2.402209 -3.473674 0.366226 0.281723 0.537481 1.289487	-5.970929 0.662940 1.553018 0.921984 -0.147790 Artree 133785 Hartree 16827778 Hartree 10 Hartree -0.248083 -0.721929 0.412672 1.700868 0.463700 -1.779348 0.255004 0.066193 0.187542 0.304178
C H H H H CONFORM Multipl: Charge: E (B97-3 E (M06/d E (PBE - E (PM6) E (PM7) E (GFN1-E (GFN1-E (GFN2-E (GFN2-E (GFN-F COORD N O C C C C C H C C H	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' 3c) = -3362.5753 = 66.96457 Kcal/i = 112.31984 Kcal -V/def2-TZVP) = xTB) = -130.5352 xTB) = -127.3708 F) = -15.7772397 ates: 0.176251 -0.355268 2.671290 0.457046 1.74223 -1.244887 0.769822 0.217402 0.182066 0.800580 -1.866845 -2.406283	-7.072254 -6.679695 -7.792990 -7.617236  0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199 36082713 Hartree mol /mol -3368.99750545310 78876975 Hartree 37817946 Hartree 15432 Hartree  0.451465 -0.463877 -5.568840 -5.493827 -1.394655 1.432565 1.399734 -2.793868 -3.840468 -2.511683 3.626435 4.023677	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree 3362115 Hartree 0.164384 1.820653 -0.608473 -0.112872 -1.65825 3.141628 -1.448300 1.223514 1.547580 -0.009808 2.109352 2.974984	H C H H H H Confor Multip Charge E(B97- E(M06/ E(PBE E(PBEC E(PBEC E(PBEC E(GFN1) E(GFN2) E(GFN2) COORD C C C N C C H C C C C C C C C C C C C C	2.624366 -0.867704 -1.205530 -0.864417 -1.605655  mation 21. licity: 2: 0 3c) = -3367.157794 def2-TZVP) = -3364 - D3 (BJ) / def2-TZV - 3c) = -3362.57524 = 66.17919 Kcal/r = 111.82583 Kcal/x - X-V/def2-TZVP) =xTB) = -127.37205 FF) = -15.77829155  nates: -0.087975 1.590202 5.036760 4.018935 0.389861 0.728149 -1.773785 3.217156 4.277368 2.285796 -1.687035	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832  4361162 Hartree 6.990631836714 Ha 2) = -3365.966807 //mol /mol /mol /mol 20680686 Hartree 68919929 Hartree 12796 Hartree 12796 Hartree 12796 Hartree 2402209 -3.473674 0.366226 0.281723 0.537481 1.289487 -4.150807	-5.970929 0.662940 1.553018 0.921984 -0.147790 Artree 133785 Hartree 133785 Hartree 16827778 Hartree 10 Hartree 10 Hartree 11 170868 0.463700 -1.779348 0.255004 0.066193 0.187542 0.304178 -1.723312
C H H H H Conform Multipl Charge: E (B97-3 E (M06/d E (PBE - E (PBE) E (PM7) E (GFN1- E (GFN2- E (GFN2- C (C ) N ) C C C C C C C C C C C C C C C C	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZ' 3c) = -3362.5753 = 66.96457 Kcal/; = 112.31984 Kcal -V/def2-TZVP) = xTB) = -130.5352 xTB) = -127.3708 F) = -15.7772397 ates: 0.176251 -0.355268 2.671290 0.457046 1.742223 -1.244887 0.769822 0.217402 0.182066 0.800580 -1.866845 -2.406283 -1.787950	-7.072254 -6.679695 -7.792990 -7.617236  0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199 36082713 Hartree mol /mol 78876975 Hartree 37819746 Hartree 15432 Hartree 15432 Hartree  0.451465 -0.463877 -5.568840 -5.493827 -1.394655 1.432565 1.399734 -2.793868 -3.840468 -2.511683 3.626435 4.023677 1.899328	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree 3 Hartree 0.164384 1.820653 -0.608473 -0.112872 -1.658225 3.141628 -1.448300 1.223514 1.547580 -0.009808 2.109352 2.974984 4.450757	H C H H H H Confor Multip Charge E(B97- E(M06/ E(PBE) E(PM6) E(PM7) E(GFN1) E(GFN2) Coordi Co N O C C C N C C H C	2.624366 -0.867704 -1.205530 -0.864417 -1.605655  mation 21. licity: 2: 0 3c) = -3367.15779 def2-TZVP) = -3366 -D3(BJ)/def2-TZVI -D3(BJ)/def2-TZVI -D3(BJ)/def2-TZVI -B111.82583 Kcal, X-V/def2-TZVP) =xTB) = -130.5363; -xTB) = -127.3720; FF) = -15.7782915; nates: -0.087975 1.590202 5.036760 4.018935 0.389861 0.728149 -1.773785 3.217156 4.277368 2.285796 -1.687035 -1.584682	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832 4361162 Hartree 6.990631836714 Ha 2) = -3365.966807 /P) = -3366.03244 35059553 Hartree mol /mol -3368.99679956236 20680686 Hartree 5891929 Hartree 12796 Hartree -0.505802 -1.403556 2.641169 4.208668 2.402209 -3.473674 0.366226 0.281723 0.537481 1.289487 -4.150807 -5.068311	-5.970929 0.662940 1.553018 0.921984 -0.147790 artree 133785 Hartree 16827778 Hartree 16827778 Hartree 170868 0.463700 -1.779348 0.255004 0.066193 0.187542 0.304178 -1.723312 -2.310830
C H H H H Conform Multipl Charge: E (B97-3 E (M06/d E (PBE) - E (PBE) E (PM6) E (GFN1-E (GFN2-E (GFN1-E (GFN2-E (GFN-F Coordin CO N C C C C C C C C C C C C C C C C C	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV - D3(BJ)/def2-TZ' 3c) = -3362.5753 = 66.96457 Kcal/i = 112.31984 Kcal -V/def2-TZVP) = xTB) = -130.5352 xTB) = -127.3708 F) = -15.7772397 ates: 0.176251 -0.355268 2.671290 0.457046 1.74223 -1.244887 0.769822 0.217402 0.182066 0.800580 -1.866845 -2.406283	-7.072254 -6.679695 -7.792990 -7.617236  0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199 36082713 Hartree mol /mol -3368.99750545310 78876975 Hartree 37817946 Hartree 15432 Hartree  0.451465 -0.463877 -5.568840 -5.493827 -1.394655 1.432565 1.399734 -2.793868 -3.840468 -2.511683 3.626435 4.023677	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree 3362115 Hartree 0.164384 1.820653 -0.608473 -0.112872 -1.65825 3.141628 -1.448300 1.223514 1.547580 -0.009808 2.109352 2.974984	H C H H H H  Confor Multip Charge E(B97- E(M06/ E(PBEC E(PBEC E(PBEC E(PFMG)) E(GFN1 E(GFN2 COORD C C C C H C H	2.624366 -0.867704 -1.205530 -0.864417 -1.605655  mation 21. licity: 2: 0 3c) = -3367.157794 def2-TZVP) = -3364 - D3 (BJ) / def2-TZV - 3c) = -3362.57524 = 66.17919 Kcal/r = 111.82583 Kcal/x - X-V/def2-TZVP) =xTB) = -127.37205 FF) = -15.77829155  nates: -0.087975 1.590202 5.036760 4.018935 0.389861 0.728149 -1.773785 3.217156 4.277368 2.285796 -1.687035	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832  4361162 Hartree 6.990631836714 Ha 2) = -3365.966807 //mol /mol /mol /mol 20680686 Hartree 68919929 Hartree 12796 Hartree 12796 Hartree 12796 Hartree 2402209 -3.473674 0.366226 0.281723 0.537481 1.289487 -4.150807	-5.970929 0.662940 1.553018 0.921984 -0.147790 Artree 133785 Hartree 133785 Hartree 16827778 Hartree 10 Hartree 10 Hartree 11 170868 0.463700 -1.779348 0.255004 0.066193 0.187542 0.304178 -1.723312
C H H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE) - E(PBE0) E(PBE0) E(PBF0) E(PBF0) E(GFN1-E(GFN2-E(GFN1-F Coordin CO N O C C C N C C H C C H C N	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV -D3(BJ)/def2-TZV 3c) = -3362.5753 = 66.96457 Kcal/s = 112.31984 Kcal -V/def2-TZVP) = xTB) = -130.5352 xTB) = -127.3708 F) = -15.7772397 ates: 0.176251 -0.355268 2.671290 0.457046 1.742223 -1.244887 0.769822 0.217402 0.182066 0.800580 -1.866845 -2.406283 -1.787950 -0.657517	-7.072254 -6.679695 -7.792990 -7.617236  0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199 36082713 Hartree mol /mol 78876975 Hartree 37819746 Hartree 15432 Hartree 15432 Hartree  0.451465 -0.463877 -5.568840 -5.493827 -1.394655 1.432565 1.399734 -2.793868 -3.840468 -2.511683 3.626435 4.023677 1.899328 2.106863	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree 3 Hartree 0.164384 1.820653 -0.608473 -0.112872 -1.658225 3.141628 -1.448300 1.223514 1.547580 -0.009808 2.109352 2.974984 4.450757 0.817524	H C H H H H Confor Multip Charge E(B97- E(M06/ E(PBE) E(PM6) E(PM7) E(GFN1 E(GFN2 COORDI CO N O C C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C C H C C C H C C C H C C C H C C C C H C C C C H C C C C C C C C C C C C C C C C C C C C	2.624366 -0.867704 -1.205530 -0.864417 -1.605655  mation 21. licity: 2: 0 3c) = -3367.157794 def2-TZVP) = -3367 -D3(BJ)/def2-TZVI -D3(BJ)/def2-TZVI -D3(BJ)/def2-TZVI -B11.82583 Kcal, X-V/def2-TZVP) = -xTB) = -130.53632 -xTB) = -127.37201 FF) = -15.77829151  nates: -0.087975 1.590202 5.036760 4.018935 0.389861 0.728149 -1.773785 3.217156 4.277368 2.285796 -1.687035 -1.584682 1.086368	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832 4361162 Hartree 5.990631836714 Ha 9) = -3365.966807 7P) = -3366.03244 35059553 Hartree mol 'Mol -3368.99679956236 20680686 Hartree 58919929 Hartree 12796 Hartree -0.505802 -1.403556 2.641169 4.208668 2.402209 -3.473674 0.366226 0.281723 0.537481 1.289487 -4.150807 -5.068311 -4.710284	-5.970929 0.662940 1.553018 0.921984 -0.147790 artree 133785 Hartree 16827778 Hartree 16827778 Hartree 1733785 Hartree 1733785 Hartree 1827778 Hartree 1827778 Hartree 1827778 Hartree 1827778 Hartree 1827778 Hartree 1827778 Hartree 182778 Hartree 182778 Hartree 182778 Hartree 182778 Hartree 182778 Hartree 182778 Hartree 182788 0.463700 -1.779348 0.255004 0.066193 0.187542 0.304178 -1.723312 -2.310830 -2.533947
C H H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE)- E(PM6): E(PPM7) E(GFN1- E(GFN2- E(GFN-F Coordin CO N O C C H C H C H C H C H C H C H C H C H	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV 3c) = -3362.5753 = 66.96457 Kcal/; = 112.31984 Kcal -V/def2-TZVP) = xTB) = -130.5352 xTB) = -127.3708 F) = -15.7772397 ates: 0.176251 -0.355268 2.671290 0.457046 1.742223 -1.244887 0.769822 0.217402 0.182066 0.800580 -1.866845 -2.406283 -1.787950 -0.657517 -2.991544 -3.537486 -1.615814	-7.072254 -6.679695 -7.792990 -7.617236  0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199 36082713 Hartree mol /mol -3368.99750545310 78876975 Hartree 37819746 Hartree 15432 Hartree  0.451465 -0.463877 -5.568840 -5.493827 -1.394655 1.432565 1.399734 -2.793868 -3.840468 -2.511683 3.626435 4.023677 1.899328 2.106863 1.376104 0.613420 3.349643	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree 3 Hartree 0.164384 1.820653 -0.608473 -0.112872 -1.658225 3.141628 -1.448300 1.223514 1.547580 -0.009808 2.109352 2.974984 4.450757 0.817524 4.971315 4.395770 6.412472	H C H H H H Confor Multip Charge E(B97- E(M06/ E(PBEC E(PBEC E(PFMC) E(GFN1) E(GFN2) E(GFN1) Coordi Co C C C H C H C H C H C H C H	2.624366 -0.867704 -1.205530 -0.864417 -1.605655  mation 21. licity: 2: 0 3c) = -3367.15779 def2-TZVP) = -3366 -D3(BJ)/def2-TZVI -D3(BJ)/def2-TZVI -D3(BJ)/def2-TZVI -B11.82583 Kcal, X-V/def2-TZVP) =xTB) = -130.5363; -xTB) = -127.3720; FF) = -15.7782915;  nates: -0.087975 1.590202 5.036760 4.018935 0.389861 0.728149 -1.773785 3.217156 4.277368 2.285796 -1.687035 -1.584682 1.086368 -1.080474 0.899345 0.483658	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832 4361162 Hartree 6.990631836714 Ha 2) = -3365.966807 (P) = -3366.03244 35059553 Hartree mol (Mol -3368.99679956236 20680686 Hartree 58919929 Hartree 12796 Hartree -0.505802 -1.403556 2.641169 4.208668 2.402209 -3.473674 0.366226 0.281723 0.537481 1.289487 -4.150807 -5.068311 -4.710284 -2.130939 -5.990362 -6.071182	-5.970929 0.662940 1.553018 0.921984 -0.147790 artree '133785 Hartree :6827778 Hartree :6827778 Hartree :0 Hartree -0.248083 -0.721929 0.412672 1.700868 0.463700 -1.779348 0.255004 0.066193 0.187542 0.304178 -1.723312 -2.310830 -2.533947 -0.727216 -1.968825 -0.953226
C H H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE) - E(PM6) E(PM7) E(GFN7-E(GFN1-E(GFN2-E(GFN-F COORDING C C C C C C H C C H C C H C H C H C H	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV 3c) = -3362.5753 = 66.96457 Kcal/s = 112.31984 Kcal -V/def2-TZVP) = xTB) = -130.5352 xTB) = -127.3708 F) = -15.7772397 ates: 0.176251 -0.355268 2.671290 0.457046 1.742223 -1.244887 0.769822 0.217402 0.182066 0.800580 -1.866845 -2.406283 -1.787950 -0.657517 -2.991544 -3.537486 -1.615814 -1.070240	-7.072254 -6.679695 -7.792990 -7.617236  0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199 36082713 Hartree mol /mol 78876975 Hartree 37819746 Hartree 15432 Hartree 15432 Hartree  0.451465 -0.463877 -5.568840 -5.493827 -1.394655 1.432565 1.399734 -2.793868 -3.840468 -2.511683 3.626435 4.023677 1.899328 2.106863 1.376104 0.613420 3.349643 4.122197	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree 3 Hartree 0.164384 1.820653 -0.608473 -0.112872 -1.658225 3.141628 -1.448300 1.223514 1.547580 -0.009808 2.109352 2.974984 4.450757 0.817524 4.971315 4.395770 6.412472 6.975578	H C H H H H Confor Multip Charge E(B97- E(M66/ E(PBEC E(PBEC E(PBEC E(PFM6)) E(GFN1) E(GFN2) E(GFN1- Coordi Co N C C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C R C C R C R	2.624366 -0.867704 -1.205530 -0.864417 -1.605655  mation 21. licity: 2: 0 3c) = -3367.157794 def2-TZVP) = -3366 -D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - 3c) = -3362.57524 = 66.17919 Kcal/r = 111.82583 Kcal, X-V/def2-TZVP) = -xTB) = -130.53632 -xTB) = -127.37201 FF) = -15.77829153  nates: -0.087975 1.590202 5.036760 4.018935 0.389861 0.728149 -1.773785 3.217156 4.277368 2.285796 -1.687035 -1.584682 1.086368 -1.080474 0.899345 0.483658 1.992920	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832 4361162 Hartree 5.990631836714 Ha 9) = -3365.966807 7P) = -3366.03244 35059553 Hartree nol (mol -3368.99679956236 20680686 Hartree 58919929 Hartree 12796 Hartree -0.505802 -1.403556 2.641169 4.208668 2.402209 -3.473674 0.366226 0.281723 0.537481 1.289487 -4.150807 -5.068311 -4.710284 -2.130939 -5.990362 -6.071182 -6.071182 -5.771527	-5.970929 0.662940 1.553018 0.921984 -0.147790 artree 133785 Hartree 16827778 Hartree 16827778 Hartree 17921929 0.412672 1.70868 0.463700 -1.779348 0.255004 0.066193 0.187542 0.304178 -1.723312 -2.310830 -2.533947 -0.727216 -1.968825 -0.953226 -4.541656
C H H H Conform Multipl Charge: E (B97-3 E (M06/d E (PBE - E (PBE0 - E (PBE0 - E (PM7)) E (GFN1- E (GFN2- E (GFN-F Coordin C C C N C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C R C R	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV - D3(BJ)/def2-TZV 3c) = -3362.5753 = 66.96457 Kcal/s = 112.31984 Kcal -V/def2-TZVP) = xTB) = -130.5352 xTB) = -127.3708 F) = -15.7772397 ates: 0.176251 -0.355268 2.671290 0.457046 1.742223 -1.244887 0.769822 0.217402 0.182066 0.800580 -1.866845 -2.406283 -1.787950 -0.657517 -2.991544 -3.537486 -1.615814 -1.070240 -1.109449	-7.072254 -6.679695 -7.792990 -7.617236  0368557 Hartree 6.989652078966 Ha P) = -3365.966264 WP) = -3366.03199 36082713 Hartree mol /mol -3368.99750545310 78876975 Hartree 37819746 Hartree 15432 Hartree 15432 Hartree 15432 Hartree 15432 Hartree 27819746 Hartree 15432 Hartree	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree 3 Hartree 0.164384 1.820653 -0.608473 -0.112872 -1.658225 3.141628 -1.448300 1.223514 1.547580 -0.009808 2.109352 2.974984 4.450757 0.817524 4.971315 4.395770 6.412472 6.975578 5.185985	H C H H H H Confor Multip Charge E(B97- E(M06/ E(PBE) E(PM6) E(PM7) E(GFN2) E(GFN1 CO C C C N C C C H C H C H C H	2.624366 -0.867704 -1.205530 -0.864417 -1.605655  mation 21. licity: 2: 0 3c) = -3367.157794 def2-TZVP) = -3364 - D3 (BJ) / def2-TZVP) - D3 (BJ) / def2-TZVP) = 66.17919 Kcal/r = 111.82583 Kcal, X-V/def2-TZVP) = -xTB) = -130.53632 -xTB) = -127.37203 FF) = -15.77829153  nates: -0.087975 1.590202 5.036760 4.018935 0.389861 0.728149 -1.773785 3.217156 4.277368 2.285796 -1.687035 -1.584682 1.086368 -1.080474 0.899345 0.483658 1.992920 2.419384	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832  4361162 Hartree 5.990631836714 Ha 9) = -3365.966807 7P) = -3366.03244 35059553 Hartree mol /mol -3368.99679956236 20680686 Hartree 58919929 Hartree 12796 Hartree 12796 Hartree 208668 2.402209 -3.473674 0.366226 0.281723 0.537481 1.289487 -4.150807 -5.068311 -4.710284 -2.130939 -5.990362 -6.071182 -5.771527 -5.680110	-5.970929 0.662940 1.553018 0.921984 -0.147790 Artree 133785 Hartree 6827778 Hartree 6827778 Hartree 10 Hartree 10 Hartree 10 Hartree 10 Hartree 11 Hartree 12 Hartree 13 Hartree 14 Hartree 15 Hartree 16 Hartree 17 Hartree 18 O. 463700 -1.779348 0.255004 0.066193 0.187542 0.304178 -1.723312 -2.310830 -2.533947 -0.727216 -1.968825 -0.953226 -4.541656 -5.552234
C H H H H Conform Multipl Charge: E (B97-3 E (M06/d E (PBE - E (PBE) E (PM7)) E (GFN1- E (GFN2- E (GFN2- C C C C C C C C C C C C C C C C C C C	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV - D3(BJ)/def2-TZV = 112.31984 Kcal/ = 12.31984 Kcal/ = 12.31984 Kcal/ = 12.31984 Kcal/ = 13.31984 Kcal/ = 13.91984 Kcal/ = 13.91984 Kcal/ = 13.91984 Kcal/ = 13.91984 Kcal/ = 13.91984 Kcal/ = 13.91984 Kcal/ = 13.91988 Kcal/	-7.072254 -6.679695 -7.792990 -7.617236  0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199 36082713 Hartree mol /mol -3368.99750545310 78876975 Hartree 37819746 Hartree 15432 Hartree  0.451465 -0.463877 -5.568840 -5.493827 -1.394655 1.432565 1.399734 -2.793868 -3.840468 -2.511683 3.626435 4.023677 1.899328 2.106863 1.376104 0.613420 3.349643 4.122197 2.895367 3.308485	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree 3362115 Hartree 3 Hartree 0.164384 1.820653 -0.608473 -0.112872 -1.658225 3.141628 -1.448300 1.223514 1.547580 -0.009808 2.109352 2.974984 4.450757 0.817524 4.971315 4.395770 6.412472 6.975578 5.185985 4.786074	H C H H H H Confor Multip Charge E(B97- E(M06/ E(PBE) E(PM6) E(PM7) E(GFN1) E(GFN2) COOrdi CO C C C N C C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C R C R	2.624366 -0.867704 -1.205530 -0.864417 -1.605655  mation 21. licity: 2: 0 3c) = -3367.157794 def2-TZVP) = -3364 - D3 (BJ) /def2-TZVP) - D3 (BJ) /def2-TZVP) = 66.17919 Kcal/r = 111.82583 Kcal/r X-V/def2-TZVP) = -3362.57528 = 66.17919 Kcal/r = 111.82583 Kcal/r X-V/def2-TZVP) = -37829153  nates: -0.087975 -1.590202 -5.036760 -4.018935 -0.389861 -0.728149 -1.773785 -3.217156 -4.277368 -2.285796 -1.687035 -1.584682 -1.086368 -1.080474 -0.899345 -0.483658 -1.992920 -2.419384 -642117	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832  4361162 Hartree 6.990631836714 Ha 20) = -3365.966807 470 = -3366.03244 35059553 Hartree and 436188.99679956236 43680686 Hartree 58919929 Hartree 12796 Hartree 12796 Hartree 4.208668 2.402209 -3.473674 0.366226 0.281723 0.537481 1.289487 -4.150807 -5.068311 -4.710284 -2.130939 -5.990362 -6.071182 -5.771527 -5.680110 -4.616157	-5.970929 0.662940 1.553018 0.921984 -0.147790 Artree 133785 Hartree 16827778 Hartree 16827778 Hartree 10 Hartree 10 Hartree 11 Hartree 12 Hartree 13 Hartree 14 Hartree 15 Hartree 16 Hartree 17 Hartree 18 Hartree 19 Hartree 10 Hartree 10 Hartree 10 Hartree 11 Hartree 12 Hartree 13 Hartree 14 Hartree 15 Hartree 16 Hartree 17 Hartree 17 Hartree 18 Hartree 18 Hartree 19 Hartree 10 Hartree 10 Hartree 10 Hartree 11 Hartree 12 Hartree 13 Hartree 14 Hartree 16 Hartree 17 Hartree 18
C H H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE)- E(PM6) E(PPM7) E(GFN1- E(GFN2- E(GFN-F Coordin CO N O C C H C H C H C H C H C H C H C H C H	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV 3c) = -3362.5753 = 66.96457 Kcal/; = 112.31984 Kcal -V/def2-TZVP) = xTB) = -130.5352 xTB) = -127.3708 F) = -15.7772397 ates: 0.176251 -0.355268 2.671290 0.457046 1.742223 -1.244887 0.769822 0.217402 0.182066 0.800580 -1.866845 -2.406283 -1.787950 -0.657517 -2.991544 -3.537486 -1.615814 -1.070240 -1.109449 -0.171079 -3.498369	-7.072254 -6.679695 -7.792990 -7.617236  0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199 36082713 Hartree mol /mol -3368.99750545310 78876975 Hartree 37819746 Hartree 15432 Hartree  0.451465 -0.463877 -5.568840 -5.493827 -1.394655 1.392565 1.399734 -2.793868 -3.840468 -2.511683 3.626435 4.023677 1.899328 2.106863 1.376104 0.613420 3.349643 4.122197 2.895367 3.308485 1.832277	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree 3 Hartree 3 Hartree 0.164384 1.820653 -0.608473 -0.112872 -1.658225 3.141628 -1.448300 1.223514 1.547580 -0.009808 2.109352 2.974984 4.450757 0.817524 4.971315 4.395770 6.412472 6.975578 5.185985 4.786074 6.196991	H C H H H H Confor Multip Charge E(B97- E(M06/ E(PBEC E(PBEC E(PFMC) E(GFN1) E(GFN2) E(GFN1) Coordi Co C C C H C C H C H C H C H C H C H C	2.624366 -0.867704 -1.205530 -0.864417 -1.605655  mation 21. licity: 2: 0 3c) = -3367.157794 def2-TZVP) = -3366 -D3(BJ)/def2-TZVI -D3(BJ)/def2-TZVI -D3(BJ)/def2-TZVI -B11.82583 Kcal, X-V/def2-TZVP) = -xTB) = -130.53632 -xTB) = -127.37203 FF) = -15.77829153  nates: -0.087975 1.590202 5.036760 4.018935 0.389861 0.728149 -1.773785 3.217156 4.277368 2.285796 -1.687035 -1.584682 1.086368 -1.080474 0.899345 0.483658 1.992920 2.419384 1.642117 1.791519	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832  4361162 Hartree 6.990631836714 Ha 2) = -3365.966807 /P) = -3366.03244 35059553 Hartree mol //mol -3368.99679956236 20680686 Hartree 58919929 Hartree 12796 Hartree 12796 Hartree 208668 2.402209 -3.473674 0.366226 0.281723 0.537481 1.289487 -4.150807 -5.068311 -4.710284 -2.130939 -5.990362 -6.071182 -5.771527 -5.680110 -4.616157 -3.621370	-5.970929 0.662940 1.553018 0.921984 -0.147790 artree 133785 Hartree 16827778 Hartree 16827778 Hartree 1733785 Hartree 1733785 Hartree 1721929 0.412672 1.700868 0.463700 -1.779348 0.255004 0.066193 0.187542 0.304178 -1.723312 -2.310830 -2.533947 -0.727216 -1.968825 -0.953226 -4.541656 -5.552234 -3.828145 -4.274331
C H H H H Conform Multipl Charge: E (B97-3 E (M06/d E (PBE - E (PBE) E (PM7)) E (GFN1- E (GFN2- E (GFN2- C C C C C C C C C C C C C C C C C C C	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV - D3(BJ)/def2-TZV = 112.31984 Kcal/ = 12.31984 Kcal/ = 12.31984 Kcal/ = 12.31984 Kcal/ = 13.31984 Kcal/ = 13.91984 Kcal/ = 13.91984 Kcal/ = 13.91984 Kcal/ = 13.91984 Kcal/ = 13.91984 Kcal/ = 13.91984 Kcal/ = 13.91988 Kcal/	-7.072254 -6.679695 -7.792990 -7.617236  0368557 Hartree 6.989652078966 Ha P) = -3365.966264 Wy) = -3366.03199 36082713 Hartree mol /mol 78876975 Hartree 37819746 Hartree 15432 Hartree 15432 Hartree  0.451465 -0.463877 -5.568840 -5.493827 -1.394655 1.432565 1.399734 -2.793868 -3.840468 -2.511683 3.626435 4.023677 1.899328 2.106863 1.376104 0.613420 3.349643 4.122197 2.895367 3.308485 1.832277 1.418311	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree 3362115 Hartree 3 Hartree 0.164384 1.820653 -0.608473 -0.112872 -1.658225 3.141628 -1.448300 1.223514 1.547580 -0.009808 2.109352 2.974984 4.450757 0.817524 4.971315 4.395770 6.412472 6.975578 5.185985 4.786074	H C H H H H Confor Multip Charge E(B97- E(M06/ E(PBE) E(PM6) E(PM7) E(GFN1) E(GFN2) COOrdi CO C C C N C C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C R C R	2.624366 -0.867704 -1.205530 -0.864417 -1.605655  mation 21. licity: 2: 0 3c) = -3367.15779 def2-TZVP) = -3367 -D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - 3c) = -3362.57528 = 66.17919 Kcal/r = 111.82583 Kcal, X-V/def2-TZVP) = -xTB) = -130.53632 -xTB) = -127.37201 FF) = -15.77829153  nates: -0.087975 1.590202 5.036760 4.018935 0.389861 0.728149 -1.773785 3.217156 4.277368 2.285796 -1.687035 -1.584682 1.086368 -1.080474 0.899345 0.483658 1.992920 2.419384 1.642117 1.791519 1.251865	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832  4361162 Hartree 6.990631836714 Ha 20) = -3365.966807 470 = -3366.03244 35059553 Hartree and 436188.99679956236 43680686 Hartree 58919929 Hartree 12796 Hartree 12796 Hartree 4.208668 2.402209 -3.473674 0.366226 0.281723 0.537481 1.289487 -4.150807 -5.068311 -4.710284 -2.130939 -5.990362 -6.071182 -5.771527 -5.680110 -4.616157	-5.970929 0.662940 1.553018 0.921984 -0.147790 artree 133785 Hartree 16827778 Hartree 16827778 Hartree 1733785 Hartree 1733785 Hartree 1733785 Hartree 1733785 Hartree 1733785 Hartree 1721929 0.412672 1.70868 0.463700 -1.779348 0.255004 0.066193 0.187542 0.304178 -1.723312 -2.310830 -2.533947 -0.727216 -1.968825 -0.953226 -4.541656 -5.552234 -3.828145 -4.274331 -2.682327
C H H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE0 - E(PM6) - E(PM7) E(GFN1-E(GFN1-E(GFN2-E(GFN-F COORDING CONCONCONCONCONCONCONCONCONCONCONCONCONC	3.720965 3.323979 4.530949 2.910996 ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZY 3c) = -3362.5753 = 66.96457 Kcal/s = 112.31984 Kcal/s = 112.31984 Kcal/s = 112.31984 Kcal/s = 17.3708 E 12.31984 Kcal/s = 17.3708 E 12.31984 Kcal/s = 17.3708 E 12.31984 Kcal/s = 17.3708 E 12.31988 E 12.31988 E 12.31988 E 12.31988 E 12.31988 E 12.31988 E 13.31988 E	-7.072254 -6.679695 -7.792990 -7.617236  0368557 Hartree 6.989652078966 Ha P) = -3365.966264 VP) = -3366.03199 36082713 Hartree mol /mol -3368.99750545310 78876975 Hartree 37819746 Hartree 15432 Hartree  0.451465 -0.463877 -5.568840 -5.493827 -1.394655 1.392565 1.399734 -2.793868 -3.840468 -2.511683 3.626435 4.023677 1.899328 2.106863 1.376104 0.613420 3.349643 4.122197 2.895367 3.308485 1.832277	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree 3 Hartree 0.164384 1.820653 -0.608473 -0.112872 -1.658225 3.141628 -1.448300 1.223514 1.547580 -0.009808 2.109352 2.974984 4.450757 0.817524 4.971315 4.395770 6.412472 6.975578 5.185985 4.786074 6.196991 6.585027	H C H H H H Confor Multip Charge E(B97- E(M66/ E(PBEC E(PBEC E(PBEC E(PFM6)) E(GFN1) E(GFN2) E(GFN1- Coordi Co N C C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C R C C R C R	2.624366 -0.867704 -1.205530 -0.864417 -1.605655  mation 21. licity: 2: 0 3c) = -3367.157794 def2-TZVP) = -3366 -D3(BJ)/def2-TZVI -D3(BJ)/def2-TZVI -D3(BJ)/def2-TZVI -B11.82583 Kcal, X-V/def2-TZVP) = -xTB) = -130.53632 -xTB) = -127.37203 FF) = -15.77829153  nates: -0.087975 1.590202 5.036760 4.018935 0.389861 0.728149 -1.773785 3.217156 4.277368 2.285796 -1.687035 -1.584682 1.086368 -1.080474 0.899345 0.483658 1.992920 2.419384 1.642117 1.791519	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832 4361162 Hartree 5.990631836714 Ha 9) = -3365.966807 7P) = -3366.03244 35059553 Hartree nol (mol -3368.99679956236 20680686 Hartree 58919929 Hartree 12796 Hartree -0.505802 -1.403556 2.641169 4.208668 2.402209 -3.473674 0.366226 0.281723 0.537481 1.289487 -4.150807 -5.068311 -4.710284 -2.130939 -5.990362 -6.071182 -5.771527 -5.680110 -4.616157 -3.621370 -7.145174	-5.970929 0.662940 1.553018 0.921984 -0.147790 artree 133785 Hartree 16827778 Hartree 16827778 Hartree 1733785 Hartree 1827778 Hartree 1827778 Hartree 1827778 Hartree 1827778 Hartree 1827778 Hartree 1827778 Hartree 1827778 Hartree 182778 Hartree 1827798 O.412672 1.70868 O.463700 -1.779348 O.255004 0.066193 O.187542 0.304178 -1.723312 -2.310830 -2.533947 -0.727216 -1.968825 -0.953226 -4.541656 -5.552234 -3.828145 -4.274331
C H H H Conform Multipl Charge: E(B97-3 E(M06/d E(PBE - E(PBE0 - E(PBE0 - E(PM7)) E(GFN1-E(GFN2-E(GFN1-C CON CC C N CC C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C	3.720965 3.323979 4.530949 2.910996  ation 20. icity: 2 0 c) = -3367.15777 ef2-TZVP) = -336 D3(BJ)/def2-TZV - D3(BJ)/def2-TZV 3c) = -3362.5753 = 66.96457 Kcal/s = 112.31984 Kcal -V/def2-TZVP) = xTB) = -130.5352 xTB) = -127.3708 F) = -15.7772397  ates: 0.176251 -0.355268 2.671290 0.457046 1.742223 -1.244887 0.769822 0.217402 0.182066 0.800580 -1.866845 -2.406283 -1.787950 -0.657517 -2.991544 -3.537486 -1.615814 -1.070240 -1.109449 -0.171079 -3.498369 -4.441613 -0.720107	-7.072254 -6.679695 -7.792990 -7.617236  0368557 Hartree 6.989652078966 Ha P) = -3365.966264 WP) = -3366.03199 36082713 Hartree mol /mol -3368.99750545310 78876975 Hartree 37819746 Hartree 15432 Hartree  0.451465 -0.463877 -5.568840 -5.493827 -1.394655 1.399734 -2.793868 -3.840468 -2.511683 3.626435 4.023677 1.899328 2.106863 1.376104 0.613420 3.349643 4.122197 2.895367 3.308485 1.832277 1.418311 4.880359	0.911358 1.866578 1.143629 0.388202 rtree 661020 Hartree 3362115 Hartree 3362115 Hartree 3 Hartree 0.164384 1.820653 -0.608473 -0.112872 -1.658225 3.141628 -1.448300 1.223514 1.547580 -0.009808 2.109352 2.974984 4.450757 0.817524 4.971315 4.395770 6.412472 6.975578 5.185985 4.786074 6.196991 6.585027 -1.811932	H C H H H H Confor Multip Charge E(B97- E(M06/ E(PBE) E(PM6) E(PM7) E(GFN2) E(GFN1- Coordi Co N C C C H C H C H C H C H C H C H C H C	2.624366 -0.867704 -1.205530 -0.864417 -1.605655  mation 21. licity: 2: 0 3c) = -3367.157794 def2-TZVP) = -3364 - D3(BJ)/def2-TZVP) - D3(BJ)/def2-TZVP) = 66.17919 Kcal/r = 111.82583 Kcal, X-V/def2-TZVP) = -xTB) = -130.53632 -xTB) = -127.37204 FF) = -15.77829153  nates: -0.087975 1.590202 5.036760 4.018935 0.389861 0.728149 -1.7773785 3.217156 4.277368 2.285796 -1.687035 -1.584682 1.086368 -1.080474 0.899345 0.483658 1.992920 2.419384 1.642117 1.791519 1.251865 1.105029	-4.033859 -7.328137 -6.760536 -8.405467 -7.167832  4361162 Hartree 5.990631836714 Ha 9) = -3365.966807 /P) = -3366.03244 35059553 Hartree mol /mol -3368.99679956236 20680686 Hartree 58919929 Hartree 12796 Hartree -0.505802 -1.403556 2.641169 4.208668 2.402209 -3.473674 0.366226 0.281723 0.537481 1.289487 -4.150807 -5.068311 -4.710284 -2.130939 -5.990362 -6.071182 -5.771527 -5.680110 -4.616157 -3.621370 -7.145174 -8.135372	-5.970929 0.662940 1.553018 0.921984 -0.147790 Artree 133785 Hartree 16827778 Hartree 16827778 Hartree 17929 0.412672 1.700868 0.463700 -1.779348 0.255004 0.066193 0.187542 0.304178 -1.723312 -2.310830 -2.533947 -0.727216 -1.968825 -0.953226 -4.541656 -5.552234 -3.828145 -4.274331 -2.682327 -2.682327 -2.224588

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H C	2.074315 -5.837810	-7.946016 -1.500347	-4.531044	C H	7.738456	1.429339	-0.562200
Н	-5.670927	-0.695702	-0.325733 -1.057484	н С	8.800591 0.618761	1.701280 -5.401715	-0.657691 -2.840162
С	-7.340861	-3.030751	0.822424	Н	0.118779	-4.728578	-3.552662
Н	-8.356605	-3.414668	1.001600	C	1.541440	-7.585608	-2.292743
C	-4.952522	-3.093046	1.279495	Н	1.750130	-8.629593	-2.571538
Н	-4.093739	-3.521193	1.818189	C	1.668180	-5.768370	-0.681084
C	-6.247085	-3.581439	1.508863	Н	1.971963	-5.385127	0.304714
Н	-6.402594	-4.396570	2.231993	С	1.932992	-7.099218	-1.035428
С	-7.131890	-1.990455	-0.097025	H	2.446585	-7.761963	-0.322356
H	-7.982927	-1.560804	-0.647235	C	0.885716	-6.732346	-3.194409
C	2.639574	2.653413	0.632303	H	0.585244	-7.103365	-4.186179
C	2.877826	-0.960840	-0.447825	C	-2.818874	2.424984	1.269609
C	-2.425507	-2.394376	-0.507197	С	0.959894	2.208512	1.423451
С	1.760332	-2.620864	-1.360255	С	1.836069	-2.622289	-1.030706
С	3.859119	-1.926086	-0.885267	С	2.720974	1.272756	0.495217
H	4.941848	-1.802974	-0.766355	C	2.102803	2.995865	1.822323
C	-0.610862	-3.226042	-1.444045	H	2.050102	3.884019	2.462815
C	-1.956869	1.706977	0.562879	C	3.096732	-0.850116	-0.665890
C	-2.805954	-3.651197	-1.112948	C	-2.323213	-1.694752	-0.915096
H C	-3.818430 -3.321979	-4.066967 1.963629	-1.099365 0.957300	C H	3.181319 3.473492	-2.977501 -3.949299	-1.424515 -1.834821
Н	-3.706119	2.946158	1.255516	н С	-2.822658	-2.977769	-1.834821
С	-3.018175	-0.216838	0.442964	Н	-3.878524	-3.197779	-1.546566
C	3.167099	-2.950992	-1.472427	C	-0.578830	-3.026234	-1.075723
Н	3.554466	-3.867490	-1.928864	C	3.197799	2.429254	1.226092
C	1.447153	3.364618	0.697273	Н	4.246089	2.739674	1.281911
C	-3.974718	0.760528	0.922278	C	-3.603373	1.563841	0.517455
Н	-5.015032	0.540229	1.180981	C	-1.744412	-3.819665	-1.410444
C	-0.969242	2.681276	0.586822	Н	-1.721614	-4.882111	-1.671979
Н	-1.259694	3.708544	0.834419	С	-3.149771	-0.614904	-0.638580
С	-3.346919	-1.541140	0.119257	H	-4.217051	-0.698994	-0.875700
N	0.913917	1.146222	0.202448	С	0.740922	-3.485942	-1.190300
C	4.018710	3.139063	0.873932	N	-1.410545	0.782231	0.399276
C	1.307074	4.838168	0.851742	С	-3.296527	3.685209	1.895448
0	2.007985	5.660563	0.290300	C	-5.083209	1.629980	0.404975
0	0.280199	5.164508	1.686232	0	-5.827303	1.946588	1.314626
C	0.069253	6.576576	1.915633	0	-5.510400	1.288193	-0.842593
H	-1.011757	6.666388	2.140948	С	-6.934781	1.405419	-1.068389
H	0.297310	7.128722	0.981745	H	-7.470204	1.055403	-0.162628
С	5.274185	4.894631	1.877121	H	-7.142508	0.714697	-1.908935
H	5.838888	4.857209	0.923015	C	-3.065851	5.162375	3.735527
H	5.877305	4.344071	2.631711	H	-4.162987	5.122690	3.900704
C	0.923782	7.075517	3.069053	H	-2.878216	6.025634	3.061746
H	0.728573	6.489486	3.988960	С	-7.314953	2.838146	-1.405465
H H	0.695546 1.999552	8.140041 6.995428	3.278774 2.820403	H H	-7.092867 -8.399614	3.507214 2.902624	-0.551580 -1.626020
С	4.966619	6.313431	2.820403	н Н	-6.756422	3.197494	-2.292314
Н	4.341367	6.819817	1.551956	C	-2.291281	5.262186	5.033277
H	5.906609	6.885864	2.442473	Н	-2.487868	4.384520	5.680180
H	4.420161	6.325777	3.277538	H	-2.592845	6.174323	5.585311
11	4.420101	0.323777	3.277330	H	-1.199696	5.317507	4.848450
Charge E (B97- E (M06/ E (PBE E (PBE0 E (PBE0) E (PM6) E (PM7) E (\omega B97 E (GFN1 E (GFN2	3c) = -3367.15620 def2-TZVP) = -336 - D3(BJ)/def2-TZV	6.987783231865 Ha P) = -3365.964460 VP) = -3366.02999 07430876 Hartree mol /mol -3368.99595168908 67801393 Hartree 16359100 Hartree	512888 Hartree 8563644 Hartree	Multip Charge E(B97- E(M06/ E(PBE E(PBE) E(PM6) E(PM7) E(WB97) E(GFN1	mation 32.  plicity: 2  e: 0  -3c) = -3367.153712  /def2-TZVP) = -3366  - D3(BJ)/def2-TZVP  n-3c) = -3362.57125  = 71.05000 Kcal/r  i = 116.59040 Kcal/r  7X-V/def2-TZVP) = -  1-xTB) = -130.52786  2-xTB) = -127.36499	6.984177544703 Ha P) = -3365.961902 PP) = -3366.02731 52763582 Hartree mol /mol -3368.99096690792 60062174 Hartree	2676208 Hartree 1552042 Hartree
Coordi	nates:				(2-x18) = -127.36491 -FF) = -15.76990151		
Co	0.194843	-0.280317	-0.073901	,	,		
N	1.349045	1.137849	0.630146	Coordi	inates:		
0	-4.152780	4.409292	1.421693	Co	-0.122564	-0.369242	0.189884
0	-2.657441	3.949513	3.067284	N	-1.877384	-0.032880	-0.630422
С	-2.717278	0.539068	0.010474	0	-1.788608	5.429839	-0.313928
С	3.564754	0.380850	-0.183752	0	0.338059	6.198859	-0.050214
N	-0.947487	-1.731738	-0.740020	С	1.467154	2.187713	0.459883
C	-0.348073	2.572008	1.710517	С	-2.598935	-2.343740	-1.149505
H	-0.521376	3.450836	2.342341	N	1.628222	-0.717769	1.013939
C	-1.461245	1.929738	1.173128	C	-1.946107	2.436805	-0.491640
C	3.957191	-1.866188	-1.229844	H	-2.538025	3.345224	-0.661635
H C	5.023409	-1.736013	-1.439166	C	-0.629733	2.604021	-0.072701
N C	5.009650 1.786909	0.729480 -1.309898	-0.317856 -0.582374	C H	-1.532105 -2.276170	-4.361851 -5.085261	-0.125772 -0.473950
N C	5.402717	1.827916	-1.112342	н С	-3.610841	-3.220994	-1.808354
Н	4.631615	2.408042	-1.641370	N	-0.495262	-2.296494	0.183507
C	7.358551	0.338668	0.236017	C	-4.944599	-3.271643	-1.348948
Н	8.121755	-0.243547	0.774595	Н	-5.238572	-2.655128	-0.486146

-5.238572 -4.177515 -3.872088

-3.238531

-2.199882 -5.882542

-2.655128 -4.872148 -5.496223

-4.035588

-4.001578 -4.109793

-0.486146 -3.520290 -4.373989

-2.899290

-3.261439

-1.969611

C H C H C

С

Н

С

8.121755 6.005172 5.705219

6.756522

7.046326

1.003365

-0.243547 -0.008810 -0.854588 2.173349

3.028847

-4.903074

0.774595 0.357847 0.994612

-1.235217

-1.864193 -1.576767

H C H

С

H	-6.917041	-4.142021	-1.594967	С	7.255461	0.709407	2.044659
С	2.049475	-4.305975	2.208220	H	7.858296	1.629669	2.079106
С	-5.502559	-4.910861	-3.058171	С	-0.635081	2.717026	4.080621
Н	-6.239154	-5.567951	-3.544898	С	7.826073	-0.520444	2.408982
С	2.199715	-4.323447	3.611463	H	8.876331	-0.568071	2.734445
H	1.831165	-3.469359	4.199478	С	0.096330	3.858648	4.474641
C	3.268360	-6.506007	3.499726	Н	0.943475	4.191383	3.856301
Н	3.742317	-7.362663	4.002471	C	-1.350275	4.156345	6.407629
C	2.524973	-5.405394	1.461443	Н	-1.628187	4.715794	7.313733
Н	2.426602	-5.390986	0.365551	C	-1.734586	2.312397	4.867965
C	3.129249	-6.496675	2.102715	Н	-2.309205	1.423207	4.567506
Н	3.499955	-7.343578	1.505286	C	-2.087501	3.025180	6.023307
C	2.802741	-5.415950	4.251925	Н	-2.943231	2.691503	6.629860
Н	2.906458	-5.416606	5.347708	C	-0.258616	4.571939	5.628737
C	0.034631	3.891022	0.031141	Н	0.318360	5.463481	5.918236
C	-2.490043	1.199256	-0.809012	C	-1.355089	-1.909088	-3.235864
C	0.201652	-3.295187	0.855880	C	2.013241	-1.947909	-1.536676
C	-2.750484	-0.951281	-1.195121	C	0.976259	1.327939	2.759405
C	-3.755687	1.052515	-1.488927	C	3.287216	-0.988462	-0.022209
Н	-4.418964	1.886649	-1.745714	C	3.347392	-2.461742	-1.736613
C	-1.556956	-2.947964	-0.428250	Н	3.621547	-3.189344	-2.509407
C	2.673671	0.183000	1.175431	С	2.792799	0.372112	1.953252
C	-0.459097	-4.571652	0.698022	C	-2.120536	1.583431	-0.179322
Н	-0.131134	-5.506421	1.162912	C	1.983288	1.403592	3.794339
С	3.815884	-0.454120	1.786291	Н	1.830018	1.845255	4.783773
Н	4.763518	0.051226	2.006351	С	-2.935988	2.568989	0.491324
			1.542700		-2.935988		
C C	2.100886	-1.907763 -0.280307	-1.766326	H C	-1.167939	3.005389 1.968919	0.072341 1.766260
Н	-3.901075			C			
С	-4.715004 1.363190	-0.782496	-2.298443 0.332972	Н	4.149434 5.228210	-1.839152 -1.947527	-0.818044
C		3.620885		С			-0.668865
	3.455230	-1.751642	2.033356		-2.296868	-0.904691	-3.046836
H C	4.047748 2.624307	-2.552668 1.537533	2.486757 0.880817	C H	-2.356514 -2.680360	2.795112 3.470508	1.711488 2.509814
					-2.493381	0.983157	
H	3.515280	2.145076	1.088438	C			-1.374738
C	1.417311	-3.133091	1.534986	H	-3.412713	1.320318	-1.865119
N	0.254010	1.574036	0.188803	C	-0.272811	1.961286	2.846044
C	-0.598542	5.212010	-0.130668	N	-0.610271	-0.586106	-1.465785
С	2.501659	4.555775	0.614538	С	-1.255946	-2.967524	-4.297549
0	2.904498	4.752895	1.743085	С	-3.506855	-0.788810	-3.881575
0	3.127608	5.130999	-0.438340	0	-3.831911	-1.633290	-4.707572
С	2.708035	4.851656	-1.789318	0	-4.227056	0.340948	-3.656723
H	1.699010	5.283452	-1.951807	С	-5.406807	0.521224	-4.474390
H	2.635453	3.752622	-1.939367	H	-6.055269	1.191933	-3.877444
C	-0.138044	7.560799	-0.086329	Н	-5.908306	-0.459953	-4.595687
H	-0.981403	7.623790	-0.803592	С	-2.984075	-4.287199	-3.159646
H	0.720339	8.143445	-0.473805	H	-3.122144	-3.358786	-2.570259
C	3.729515	5.468636	-2.724008	H	-2.565971	-5.060926	-2.479340
H	3.794424	6.563602	-2.568107	C	-5.062463	1.126496	-5.825117
H	3.442425	5.282646	-3.777934	H	-4.516445	2.083193	-5.704903
H	4.735177	5.036208	-2.553425	H	-5.991096	1.326491	-6.396915
C	-0.556689	8.031327	1.296887	H	-4.438021	0.429104	-6.416020
H	-1.434382	7.458474	1.654233	C	-4.288490	-4.746382	-3.783987
H	-0.835461	9.103983	1.265103	H	-4.691580	-3.950952	-4.438879
H	0.271272	7.906419	2.022458	H	-5.030704	-4.971622	-2.991567
				H	-4.134942	-5.663210	-4.386727
	nation 34.						
	licity: 2						
Charge					mation 7.		
	Bc) = converged!)				licity: 2		
	def2-TZVP) = -3366 - D3(BJ)/def2-TZVP			Charge		242002 11	
					3c) = -3367.153670 def2-TZVP) = -3366		*****
	-3c) = -3362.56655	,	7447203 Haltiee		- D3(BJ)/def2-TZVF		
	= 73.79551  Kcal/m				- D3(BJ)/def2-TZV		
	= 105.72296 Kcal/				-3c) = $-3362.57129$		302/120 11020200
	K-V/def2-TZVP) = -		1 Hartree		= 71.42599 Kcal/m		
E (GFN1-	-xTB) = $-130.52590$	8425129 Hartree			= 116.51352 Kcal/		
E (GFN2-	-xTB) = $-127.36160$	9999001 Hartree		E(ωB97	X-V/def2-TZVP) = -	3368.99021392744	8 Hartree
E (GFN-	FF) = -15.76726656	4779 Hartree		E(GFN1	-xTB) = $-130.52758$	6939730 Hartree	
				E(GFN2	-xTB) = $-127.36461$	7110551 Hartree	
Coordi				E(GFN-	FF) = -15.76881797	9146 Hartree	
Со	0.456405	0.070127	0.070517				
N	1.984542	-1.028473	-0.496935	Coordi			
0	-0.438382	-2.865773	-5.192071	Co	0.400552	-0.228915	-0.264917
0	-2.012054	-4.079357	-4.202022	N	-0.959671	-1.457417	-0.982371
C	-1.817331	-0.097889	-1.934763	0	-2.530867	-2.954505	4.383151
С	3.702315	-0.319341	1.138175	0	-4.019901	-1.304826	4.273840
N	-1.020384	1.243376	0.594766	С	-0.169153	0.468378	2.626349
С	0.930639	-2.312123	-2.323452	С	-0.452600	-1.344767	-3.403847
H	1.084868	-3.077679	-3.095144	N	1.757504	1.002164	0.436007
C	-0.297935	-1.657618	-2.287332	C	-2.080851	-2.120614	1.116262
C	3.120146	0.837603	3.282104	H	-2.834015	-2.777874	1.571325
H	4.094634	0.709903	3.764053	C	-1.426632	-1.203269	1.935292
C	5.128125	-0.399012	1.570087	C	1.703981	-0.448136	-4.299980
N	1.466981	0.649969	1.648966	H	1.557179	-0.779649	-5.332770
C	5.916829	0.770340	1.631026	C	-0.859002	-1.733986	-4.786318
H	5.468366	1.732663	1.341560	N	1.240240	-0.132805	-2.036424
C H	7.049441 7.486792	-1.689004 -2.655492	2.358871 2.652363	C H	-0.863505 -0.556201	-3.085423 -3.862075	-5.194172 -4.477796
	1.400124		2.002303			-3.862075	-4.477796
C		-1 629554	1 9/2696	C	-1 606006	-1 095153	-7 02/075
C H	5.711444	-1.629554 -2.542847	1.942686 1.916557	C H	-1.606006 -1.898967	-1.095153 -0.310389	-7.024975 -7.739012
C H		-1.629554 -2.542847	1.942686 1.916557	C H	-1.606006 -1.898967	-1.095153 -0.310389	-7.024975 -7.739012

С	-1.230539	-0.743039	-5.720283	Н	-5.589749	-1.640392	-5.754567
Н	-1.227877	0.312526	-5.409063	C	-4.360474	-1.137307	-4.038685
C	-1.237602	-3.436429	-6.499594	Н	-3.463781	-0.931054	-4.642340
Н	-1.229906	-4.494392	-6.803214	C	-6.651746	-1.621813	-2.496151
С	4.651099	1.591013	-1.963142	Н	-7.547672	-1.813050	-1.886014
С	-1.612082	-2.442827	-7.418138	С	-2.161052	4.851878	0.637941
H	-1.905945	-2.718931	-8.442161	С	-6.703312	-1.776380	-3.890510
С	5.841574	1.093823	-1.390583	H	-7.640124	-2.085321	-4.378499
H	5.777063	0.332316	-0.598698	С	-1.458603	5.976837	0.155011
C	7.172244	2.522290	-2.842002	H	-0.517206	5.823991	-0.394041
H	8.153462	2.884111	-3.184811	C	-3.157309	7.464252	1.060219
C	4.743541	2.567528	-2.978220	H	-3.545365	8.480936	1.224448
H	3.819637	2.973440	-3.416968	C	-3.367764	5.056693	1.340842
C	5.994396	3.028720	-3.414093	H	-3.912348	4.185744	1.735562
H	6.048770	3.794592	-4.202794	C	-3.861676	6.352747	1.549703
C	7.091975	1.554531	-1.828249	H	-4.801241	6.495451	2.105054
H	8.010720	1.151427	-1.375588	C	-1.954058	7.272399	0.363008
C	-1.792917	-0.969154	3.310354	H	-1.396636	8.138422	-0.025258
C	-1.895654	-2.183619	-0.257388	C	3.356087	-1.880394	0.149587
C	2.492576	0.381769	-2.350829	C	0.151345	-2.135327	-1.823169
С	-1.225299	-1.759861	-2.309394	С	-2.318463	2.570026	-0.381173
С	-2.751579	-2.945808	-1.135124	С	-1.908211	-1.384318	-2.002035
H	-3.569448	-3.592490	-0.796311	С	-0.557831	-3.075126	-2.658295
С	0.746659	-0.636804	-3.232679	H	-0.112416	-3.977636	-3.093111
С	1.740377	1.652171	1.662543	С	-2.991104	0.724886	-1.382837
С	2.801364	0.153232	-3.744983	С	1.279730	1.973184	1.852620
H	3.743860	0.427827	-4.228529	C	-3.606700	2.859839	-0.970336
C	2.884888	2.522074	1.800773	H	-4.109072	3.830976	-0.924921
H	3.082054	3.148135	2.678707	C	1.251653	3.214962	2.589098
C C	2.920228	1.434673	-0.181405	H C	1.974617	3.487591	3.366678
Н	-2.363452 -2.791611	-2.650709 -3.007284	-2.414641 -3.356553	C	-0.438377 -1.850275	3.114463 -2.630191	1.090845 -2.739356
С	-1.014682	0.095767	3.746691	Н	-2.697946	-3.086687	-3.259769
C	3.632937	2.371425	0.664001	С	3.568160	-0.964891	1.170443
Н	4.574386	2.859728	0.392751	C	0.194744	3.936341	2.102609
C	0.823869	1.441325	2.683712	Н	-0.154717	4.929145	2.403566
Н	0.923240	2.001806	3.621966	C	2.295690	1.037382	1.989420
C	3.326562	1.100213	-1.481279	Н	3.095537	1.212483	2.720475
N	-0.439386	-0.322478	1.524877	C	-1.615781	3.479172	0.423021
C	-2.786560	-1.816653	4.046501	N	1.515924	-0.448089	0.189523
Č	-1.005643	0.713371	5.085223	C	4.258319	-2.958003	-0.375920
0	-0.305534	1.648864	5.449870	C	4.734679	-0.884035	2.068875
0	-1.910381	0.097924	5.896879	0	4.994660	0.017972	2.852028
С	-2.042127	0.610095	7.238548	0	5.518261	-1.986305	1.916778
H	-1.042470	0.929182	7.596181	С	6.740304	-2.031644	2.678559
H	-2.386698	-0.256674	7.835027	H	6.504556	-1.849232	3.748270
С	-4.378002	0.005123	3.791284	H	7.395102	-1.197095	2.347956
H	-4.228511	0.050706	2.690433	С	3.380421	-4.385755	1.381811
H	-3.716458	0.764692	4.254824	H	2.321143	-4.182869	1.111781
C	-3.032727	1.762179	7.296644	H	3.670055	-3.677385	2.184493
H	-2.666427	2.621982	6.702241	C	7.376490	-3.386090	2.441797
H	-3.161332	2.100741	8.344530	H	6.720533	-4.203685	2.802529
H	-4.025785	1.454975	6.910872	H	8.340948	-3.452430	2.982864
C	-5.826690	0.248751	4.164763	H	7.566273	-3.549799	1.362790
H	-6.488473	-0.516434	3.713415	C	3.571725	-5.823446	1.821890
H	-6.150007	1.246970	3.808764	H	3.296590	-6.526942	1.011465
H	-5.957761	0.210828	5.264699	H	2.937229	-6.040049	2.704002
				H	4.628775	-6.012014	2.096522
	mation 8.						
	licity: 2			YTK	LUC		
Charge		0275566 77 .					
	3c) = -3367.15411			05			
		6.985739053207 Ha			rmation 15.	0	
E (PBE	- na(Rn)/dei2-TZV	P) = -3365.962259	/0/300 Hartree	Multip	olicity: 2Charge:	U	

Conformation 8.

Multiplicity: 2
Charge: 0
E(B97-3c) = -3367.154119375566 Hartree
E(M06/def2-TZVP) = -3366.985739053207 Hartree
E(PBE - D3(BJ)/def2-TZVP) = -3365.962259767386 Hartree
E(PBEO - D3(BJ)/def2-TZVP) = -3366.027980937023 Hartree
E(PBEh-3c) = -326.572047966654 Hartree
E(PBEh-3c) = -323415 Kcal/mol
E(PM7) = 116.67385 Kcal/mol
E(PM7) = 116.67385 Kcal/mol
E(GFN1-xTB) = -130.526583704417 Hartree
E(GFN1-xTB) = -127.36466652091 Hartree
E(GFN2-xTB) = -127.36466652091 Hartree
E(M997X-V/def2-TZVP) = -2949.5366718861
E(M997X-V/def2-TZVP) = -2949.5366718861

Coordinates: Co -0.217741 0.406859 -0.238094

N	-0.681461	-1.099115	-1.420832
0	4.963679	-2.785479	-1.347956
0	4.223327	-4.167893	0.231610
C	2.422518	-0.073979	1.163685
C	-3.034765	-0.550293	-1.965944
N	0.229330	1.908412	0.947436
C	1.465009	-2.322431	-1.416202
Н	2.023251	-3.169828	-1.837340
C	2.079808	-1.549689	-0.434597
C	-4.038487	1.705101	-1.565093
Н	-4.966210	1.528037	-2.118214
C	-4.295954	-0.983148	-2.637040
N	-1.932913	1.264476	-0.663090
C	-5.458304	-1.226503	-1.874289
Н	-5.414855	-1.106416	-0.781253
C	-5.554784	-1.531071	-4.659874

E(M06/def2-TZVP) = -2948.910938074289 Hartree E(PBE - D3(BJ)/def2-TZVP) = -2947.690999370790 Hartree E(PBE0 - D3(BJ)/def2-TZVP) = -2947.965475922643 Hartree E(PBEh-3c) = -2944.948574562258 Hartree E(PBEh-3c) = -2944.948574562258 Hartree E(PM6) = -240.82987 Kcal/mol E(PM7) = -237.54253 Kcal/mol E(\omega B97X-V/def2-TZVP) = -2949.536671886141 Hartree E(GFN1-xTB) = -184.761142349843 Hartree E(GFN2-xTB) = -119.355662246845 Hartree E(GFN-FF) = -16.235874247916 Hartree Coordinates: -0.249646 -2.589284 Ti 0.084504 Si -1.741210 2.160932 Si -1.869116 1.344554 2.851139 1.088659 -1.166865 0 0.369543 -0.608686 1.368743 -0.923206 0 -1.870596 С -0.081500 1.597721 Н -2.584681 0.271314 0.806976 С 2.190835 -1.937049 0.202094 C C 3.066473 -2.128318 1.320159 1.121607 4.214227 -2.918016 Н 4.908695 -3.080191 1.954916 4.501742 -3.502719 -0.114222

-4.113213 -3.309910

-0.239942

-1.189050

5.408190

3.630435

Н	3.871768	-3.779144	-2.150795	E (B97	-3c) = -2948.79900	8603179 Hartree	
C	2.460663	-2.534569	-1.073157		/def2-TZVP) = -294		rtree
C	2.791324	-1.502470	2.706419		- D3(BJ)/def2-TZV		
С	3.868660	-1.896699	3.737898	E (PBE	0 - D3(BJ)/def2-TZ	VP) = -2947.96584	1782781 Hartree
H	3.921258	-2.993843	3.885548	E (PBE	h-3c) = -2944.9487	31135618 Hartree	
H	3.616088	-1.440441	4.716031	E(PM6	= -242.13411  Kca	l/mol	
H	4.876558	-1.533218	3.453147	,	) = -237.72387 Kca	, -	
С	2.807556	0.040522	2.615161		7X-V/def2-TZVP) =		5 Hartree
H	3.753685	0.399782	2.162840		1-xTB) = $-185.5250$		
H	2.720559	0.486169	3.627622		2-xTB) = $-119.3575$		
H	1.970853	0.430090	2.004676	E (GFN	-FF) = $-16.2381011$	60526 Hartree	
C	1.436381	-1.997178	3.261166	Q 1			
H H	0.590871 1.256198	-1.703410 -1.569457	2.614985 4.268689	Ti	inates: -0.193762	-0.234261	-0.368563
н	1.430517	-3.102263	3.350351	Si	-2.907316	-2.436706	-0.123707
C	1.523314	-2.376674	-2.292953	Si	-1.433031	-1.633432	-2.915310
C	2.019228	-3.181245	-3.512112	0	-1.050667	1.155490	0.461925
Н	3.012531	-2.840477	-3.867735	0	1.584841	-0.694562	-0.388553
H	1.305041	-3.043453	-4.348750	С	-1.367854	-1.806721	-1.022805
H	2.077459	-4.267635	-3.299934	H	-0.588973	-2.593033	-0.858280
C	1.449354	-0.900136	-2.737741	C	-1.262913	2.295643	1.163941
H	1.048923	-0.238173	-1.949968	С	-1.883367	3.407537	0.505737
H	0.783912	-0.791528	-3.618220	С	-2.034687	4.594832	1.246500
H	2.452161	-0.519980	-3.017497	H	-2.494969	5.471375	0.774512
C	0.115470	-2.909335	-1.950253 -1.630278	С	-1.620472	4.694043	2.577319
H H	0.162307 -0.549458	-3.969430 -2.843212	-1.630278	H C	-1.751032 -1.055030	5.637476 3.584419	3.128151 3.210060
н	-0.349438	-2.334373	-1.130807	Н	-0.754977	3.676278	4.261112
C	-0.526898	2.038195	-2.095447	C	-0.861729	2.362484	2.538323
C	-1.626843	1.934616	-3.014060	C	-2.418188	3.330528	-0.943770
C	-1.521558	2.616748	-4.237519	C	-3.087473	4.649712	-1.379161
H	-2.337570	2.551230	-4.968019	H	-3.950570	4.914413	-0.736162
С	-0.398791	3.390736	-4.553272	H	-3.467310	4.537941	-2.414518
H	-0.343242	3.919345	-5.516474	H	-2.377170	5.500855	-1.377028
C	0.646795	3.491017	-3.636752	C	-1.281289	3.057528	-1.952131
H	1.512243	4.119300	-3.891685	H	-0.501936	3.843128	-1.894173
C C	0.630847 -2.900782	2.818094 1.123339	-2.396138 -2.682538	H H	-1.682304 -0.793626	3.046226 2.081140	-2.986906 -1.773287
C	-3.574336	1.706251	-1.417724	C	-3.487054	2.221070	-1.038742
Н	-4.456426	1.095661	-1.131700	Н	-3.063923	1.229720	-0.804947
Н	-3.921383	2.742269	-1.605839	Н	-3.915040	2.186402	-2.062217
H	-2.877439	1.733422	-0.561751	H	-4.317266	2.410817	-0.329085
С	-2.566252	-0.372408	-2.485183	C	-0.235305	1.163411	3.288336
H	-1.890142	-0.547419	-1.626034	C	-0.033959	1.463788	4.787950
H	-2.072503	-0.787359	-3.386328	Н	0.677737	2.295931	4.958771
H	-3.492409	-0.955659	-2.302059	H	0.386015	0.565370	5.282993
C H	-3.938593	1.195587 0.616407	-3.821070 -3.530972	H C	-0.988636 1.162076	1.709986 0.848493	5.294348 2.710778
н Н	-4.838048 -3.555212	0.760383	-4.765873	Н	1.139953	0.848493	1.636026
H	-4.263774	2.235701	-4.023290	H	1.623242	-0.013469	3.234739
C	1.848831	3.073969	-1.467306	Н	1.837551	1.719868	2.823874
C	3.161801	2.868708	-2.263184	C	-1.160693	-0.072165	3.208542
Н	3.232675	1.828177	-2.639333	Н	-2.149243	0.151269	3.658123
H	4.034725	3.055234	-1.604759	H	-0.714705	-0.923547	3.763055
H	3.253770	3.548643	-3.131168	H	-1.334888	-0.400412	2.167673
С	1.760095	4.538985	-0.975417	С	2.887461	-0.783381	-0.030668
H	1.749295	5.253553	-1.821800	С	3.364303	-2.037216	0.486772
H	2.626580	4.786222	-0.327269	C	4.710221	-2.120587	0.877781
H C	0.833175 1.976311	4.697074 2.178447	-0.387647 -0.220629	H C	5.100052 5.577064	-3.062896 -1.028289	1.282083 0.762668
Н	1.155772	2.340232	0.504495	Н	6.628583	-1.118533	1.073366
Н	2.918771	2.427485	0.307726	C	5.098451	0.172008	0.241529
Н	2.045673	1.103120	-0.482143	Н	5.796509	1.015225	0.139899
С	-1.902705	-3.199942	1.159474	С	3.757267	0.342365	-0.165653
H	-2.146736	-3.093416	0.082920	C	2.443903	-3.269629	0.612987
H	-2.355301	-4.150033	1.513343	С	3.194998	-4.501566	1.157979
H	-0.801771	-3.291017	1.250209	H	2.494518	-5.359274	1.209713
C	-2.291189	-2.117339	3.997943	H	3.587132	-4.333183	2.180996
H	-1.212140	-2.177984 -3.098544	4.240822	H C	4.039560	-4.801489	0.505687
H H	-2.748309 -2.751466	-1.358248	4.243275 4.661701	Н	1.903272 2.733318	-3.660638 -4.007484	-0.783563 -1.431518
С	-4.465466	-1.686794	1.856244	Н	1.415927	-2.810572	-1.291311
Н	-4.944265	-0.872517	2.436681	Н	1.167875	-4.487823	-0.699284
Н	-4.948279	-2.644422	2.142782	C	1.301534	-2.982541	1.614270
Н	-4.680289	-1.506774	0.781734	Н	0.649826	-3.872683	1.723719
C	-3.593062	1.553739	3.625474	H	0.658065	-2.134869	1.309613
H	-4.354600	1.756372	2.844678	H	1.718419	-2.739461	2.612615
H	-3.596121	2.408393	4.333649	C	3.415385	1.725354	-0.782298
H	-3.910446	0.649597	4.182476	С	3.869124	2.850542	0.179845
C H	-1.460691	3.001242	2.004193	H H	3.334045	2.778763	1.148211
H H	-0.400624 -1.640725	3.065935 3.832568	1.684163 2.717881	H H	3.639550 4.955204	3.841199 2.825849	-0.263315 0.389601
н Н	-2.091870	3.178342	1.109937	н С	4.185704	1.844825	-2.120122
C	-0.605425	1.078232	4.236954	Н	5.278448	1.734016	-1.977372
Н	-0.807076	0.149966	4.805436	Н	4.000029	2.833870	-2.588829
H	-0.639469	1.930424	4.947053	H	3.858061	1.059914	-2.831748
H	0.423615	1.011717	3.832402	С	1.933432	2.000162	-1.087299
_				H	1.522008	1.304739	-1.842804
	mation 18.			H	1.837165	3.022390	-1.505212
	licity: 2			H	1.307133	1.981510	-0.173476
Charge	. 0			С	-2.373602	-3.326228	1.465368

				_			
H	-1.722004	-4.193463	1.232421	C	-0.639851	3.684820	0.744341
H	-3.265441	-3.709506	2.003585	C	-1.932203	3.020552	1.268756
H	-1.818457	-2.660570	2.154568	H	-1.956947	3.055807	2.377812
С	-4.120327	-1.055799	0.332238	H	-2.012308	1.964143	0.958923
Н	-3.645715	-0.284761	0.971521	Н	-2.829171	3.549820	0.888301
H	-4.977521	-1.485291	0.891362	С	-0.628827	5.126371	1.293967
H	-4.523893	-0.549884	-0.567168	H	-1.493545	5.716783	0.930164
С	-3.871419	-3.726317	-1.140920	H	0.300728	5.670960	1.033278
H	-4.259820	-3.316690	-2.095074	H	-0.689421	5.092798	2.400357
Н	-4.741264	-4.089302	-0.554269	C	0.601829	2.974723	1.326466
H	-3.236815	-4.603985	-1.380394	Н	0.587520	3.018852	2.435342
C	-1.283777	-3.345615	-3.720205	H	1.536340	3.456649	0.977269
H	-0.345282	-3.841828	-3.396740	H	0.657348	1.909252	1.042872
H	-1.259072	-3.256101	-4.826352	С	-1.005403	1.178938	-3.823541
Н	-2.130661	-4.003914	-3.444531	C	0.162964	0.182827	-3.635285
С	0.039909	-0.616753	-3.588655	Н	1.119759	0.642188	-3.955594
H	-0.054106	0.467645	-3.370865	H	-0.003562	-0.727861	-4.246766
H	0.077553	-0.723221	-4.694324	H	0.291031	-0.146231	-2.584862
H	1.013729	-0.966823	-3.187538	С	-2.361210	0.547879	-3.422361
C	-3.016714	-0.768953	-3.488691	Н	-2.422303	0.346604	-2.338753
H	-3.926809	-1.315855	-3.170893	Н	-2.520485	-0.408644	-3.963103
H	-3.033333	-0.695248	-4.595680	H	-3.194117	1.230595	-3.685512
H	-3.078769	0.257754	-3.077069	C	-1.084682	1.473421	-5.335734
				H	-1.904561	2.177743	-5.581017
Confor	mation 19.			Н	-1.283635	0.528383	-5.880281
	licity: 2			H	-0.136485	1.889053	-5.732196
Charge				С	0.564035	-3.497461	-2.412238
E(B97-3	3c) = -2948.80018	6434236 Hartree		H	-0.047659	-3.358579	-3.328370
E(M06/	def2-TZVP) = -294	8.912489165615 Har	rtree	H	1.138975	-4.439555	-2.531426
E (PRE -	- D3(BJ)/def2-TZV	P) = -2947.6913538	350068 Hartree	H	1.287357	-2.661568	-2.360049
		VP) = -2947.966681		C	0.436084	-3.975957	0.672411
			1100020 Hartree				
	-3c) = -2944.9509			H	1.168046	-3.173065	0.892942
E(PM6)	= -242.72091 Kca	1/mol		H	0.990882	-4.929960	0.559364
E(PM7)	= -239.10820 Kca	1/mol		H	-0.233214	-4.078247	1.551473
E (@B97)	X-V/def2-TZVP) =	-2950.750865069244	Hartree	С	-1.720921	-5.070663	-1.227408
	-xTB) = $-184.9018$			Н	-2.442061	-5.259560	-0.407963
	-xTB) = $-119.3606$			Н	-1.114765	-5.991295	-1.360395
E (GFN-1	FF) = -16.2403787	44308 Hartree		H	-2.300199	-4.913283	-2.160290
				C	-3.235178	-3.145422	1.637879
Coordin	nates:			H	-3.024704	-4.199827	1.371756
Ti	-0.390808	-0.291344	-0.073004	Н	-4.246514	-3.109275	2.093178
				H			
Si	-0.568328	-3.592821	-0.890954		-2.506689	-2.838179	2.413529
Si	-3.188564	-2.000989	0.124707	С	-4.488608	-2.577730	-1.133646
0	1.119519	-0.512770	0.926182	H	-4.509797	-1.900594	-2.012864
0	-0.809368	1.264090	-0.926158	H	-5.501523	-2.574338	-0.679045
Ċ	-1.482006	-1.949682	-0.704704	Н	-4.278375	-3.602488	-1.498609
H	-1.695555	-1.587326	-1.741613	С	-3.746425	-0.278051	0.714516
C	2.176864	-0.322238	1.747527	H	-3.150237	0.086795	1.575709
С	1.986327	-0.380942	3.161136	H	-4.805580	-0.323329	1.045960
С	3.125164	-0.189591	3.972201	H	-3.682389	0.480094	-0.092876
Н	3.017020	-0.243453	5.065365		0.002003	0.100031	0.032070
				~ .			
С	4.386680	0.065707	3.436769		ormation 27.		
H	5.251035	0.216017	4.100715		iplicity: 2		
C	4.544653	0.130791	2.047670	Char	ge: 0		
H	5.542359	0.336453	1.640648	E(B9	7-3c) = -2948.803891	.329012 Hartree	
С	3.464638	-0.061047	1.169700		6/def2-TZVP) = -2948		rtree
С	0.659661	-0.673855	3.911861		E - D3(BJ)/def2-TZVE		
C	-0.620754	-0.743085	3.058665		E0 - D3(BJ)/def2-TZV		2993215 Hartree
H	-0.824944	0.216169	2.539375	E(PB	Eh-3c) = -2944.95295	55564924 Hartree	
H	-1.486059	-0.936597	3.725598	E (PM	6) = -241.69681  Kcal	./mol	
H	-0.588576	-1.566620	2.319971		7) = -239.68146  Kcal		
C	0.806330	-2.040872	4.623618		97X-V/def2-TZVP) = -		9 Hartree
Н							Juliareree
	0.971407	-2.850925	3.884280		N1-xTB) = $-184.82915$		
H	-0.112007	-2.279174	5.200007		N2-xTB) = -119.36411		
H	1.661861	-2.046831	5.326976	E (GFI	N-FF) = -16.23997709	6284 Hartree	
C	0.413043	0.439576	4.959895				
H	1.227896	0.513772	5.704595	Coor	dinates:		
H	-0.527558	0.239667	5.513588	Ti	-0.446714	-0.113517	0.145374
Н	0.316780	1.427543	4.464693	Si	-3.299243	1.362745	1.370323
С	3.687545	-0.001470	-0.358748	Si	-3.203310	-1.756519	0.509448
С	5.169801	0.230347	-0.716652	0	-0.201063	1.121250	-1.183512
H	5.549957	1.199219	-0.334909	0	0.821936	-1.181061	0.928959
Н	5.275538	0.246946	-1.819891	С	-2.279305	-0.209168	1.108601
Н	5.823706	-0.578319	-0.333117	Н	-1.890764	-0.503904	2.115017
C	2.893118	1.168291	-0.983356	C	0.493825	1.757680	-2.164881
H	1.802389	1.077874	-0.831742	С	0.251433	1.393883	-3.527856
H	3.069132	1.211834	-2.077531	C	1.024215	2.034615	-4.515153
Н	3.208181	2.136400	-0.546073	H	0.871435	1.777907	-5.570548
C	3.277725	-1.344039	-1.002979	C	1.989737	2.991739	-4.192130
H	3.881738	-2.177954	-0.591399	H	2.584700	3.466119	-4.986672
H	3.440274	-1.310674	-2.100289	С	2.181123	3.356999	-2.857023
H	2.214398	-1.578260	-0.822028	H	2.928400	4.126224	-2.626825
С	-0.730675	2.455129	-1.565689	С	1.439972	2.774024	-1.811179
C	-0.609404	3.660438	-0.802592	C	-0.822855	0.359735	-3.938900
C	-0.468946	4.862829	-1.521744	C	-0.948650	0.241151	-5.471393
H	-0.359905	5.808638	-0.976714	H	-1.232066	1.202852	-5.944231
С	-0.459486	4.892665	-2.919053	H	-1.740448	-0.495774	-5.713371
Н	-0.334511	5.848613	-3.449548	H	-0.011213	-0.115983	-5.942236
C	-0.623102	3.706608	-3.640493	C	-0.459270	-1.049150	-3.418689
H	-0.633672	3.753651	-4.736621	H	0.508864	-1.375479	-3.847339
C	-0.775082	2.464852	-2.997011	H	-1.234766	-1.784602	-3.717228

## -2,738800	H C	-0.372934 -2.206810	-1.088210 0.792353	-2.314098 -3.406104	E (GFN	-FF) = $-16.2313555$	31878 Hartree	
Dec.   1,797163   1,797163   3,797261   31   -0.795502   -2.756929   2.316985   C.   1,777203   1,277273   -1.316304   -2.661174   -1.316102   2.316036   C.   1,77204   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75622   -2.75	H			-2.304224	Coord	inates:		
C 1.076720 3.257027 -0.35334 S -2.28117 -0.336303 C 2.35535 C 2.36120		-2.985221	0.079349	-3.748850		-0.300105	-0.208153	0.134316
C 2.034671 4.469677 -0.283992 D 1.130723 D 0.66338 C 3.866917 H 1.567674 A.167672 D 0.783935 -0.164189 -1.57678 D 1.28576 D 1.								
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C 2,139042 2,125754 0.770703 C 2,232360 1.403535 1.071260 C 1.671261 1.134940 C 3,271766 1.725568 0.02801 H 3,277662 1.725688 0.02801 H 3,672233 1.225696 1.22163 1.20163 C 0.339370 3.706888 0.026739 C 4.466062 1.295966 1.22163 1.20163 H 0.025370 C 4.466062 1.295966 1.20163 C 0.339370 3.706888 0.026739 C 4.466062 1.295966 1.20163 H 0.021754 C 2.395470 C 4.466062 1.295966 1.20163 C 2.395970 C 4.466062 1.295966 1.20163 C 2.301754 C 2.302470 C 4.466062 1.29696 1.20163 C 2.301754 C 2.302470 C 4.466062 1.296970 C 4.46062 1.296970 C 2.30246 C 4.47033 C 2.30546 C 4.47033 C 2.40546 C 4.47034 C 2.40546 C								
H 1.663407 1.235566 0.528129 C 3.541083 0.624139 1.104291 H 2.514594 C 4.514594 C 4.637419 1.716674 C 4.637419 1.706281 C 4.6367419 1.706281 C 4.6367419 1.706281 C 4.636741 C 4.6								
H 2.514594								
B								
C 0.334370 3.706888 0.2437399 C 4.486082 3.095948 1.209145								
## 0.489889	С	0.334370	3.706858	0.263759	С	4.486082	3.095984	1.204145
## -0.411754	H	-0.094629	4.548684	-0.316588	Н	5.367831	3.752790	1.240956
C 1.997380 -1.9898879 1.469763 C 2.052787 2.026876 1.120517 C 2.132464 -1.987100 2.895934 C 3.897909 -0.4680989 1.295218 C 3.3714030 -1.8851243 3.457723 C 4.1339073 -0.285127 2.723020 C 3.3714030 -1.8851243 3.457723 C 4.1339073 -0.285127 2.723020 C 2.523398 -2.2631283 3.457723 C 4.1339073 -0.285127 2.723020 C 4.253980 -2.2631297 3.135387 H 3.515908 -0.992294 3.425396 C 4.253498 -2.2631297 3.135387 H 3.515908 -0.992294 3.425396 C 4.254398 -2.2631297 3.135387 H 3.515908 -0.992294 3.425396 C 4.254398 -2.1675126 C 6.082735 H 3.515908 -0.992294 3.425396 C 6.254398 -1.085127 C 6.085213 C 7.085127 C 7.085	H	0.489589	4.054680	1.305950	С	3.198543	3.639968	1.191995
C 2.132646 -1.498710	H		2.894232	0.275769	H	3.087871	4.730350	1.229641
C 3,371493 -1,862245 3.459723 C 4,339073 -0,226427 2.723002 C H 3.518303 -1,786305 A 4547783 H 5.10802 -0,303162 C C 4.427033 -2,318007 2.167384 H 5.10802 -0,303162 C C 4.427033 -2,318007 2.167384 H 5.10802 -1,325299 2.865119 C 4.254398 -1,325299 2.865119 C 4.254398 -1,2254398 -1,2254398 -1,2254398 -1,2254398 -1,2254398 -1,2254398 -1,2254398 -1,2254398 -1,2254398 -1,2254398 -1,2254398 -1,2254398 -1,2254398 -1,2254398 -1,2254398 -1,2254398 -1,227366 C 3.050740 -2,120142 0.655949 H 3.154235 -2,702264 1.671216 C 3.050740 -1,20142 0.655949 H 3.154235 -1,225136 -0,0623338 C C 0.579450 -1,050774 S 3.18768 F 2.355078 -1,27136 -0,062333 H 1.65074 -2,143836 S 3.25774 H 4.791355 -0,041233 -0,041233 H 1.259457 H 1.259477 H 1.259477 H 1.25947 H 1.2		1.997180	-1.598879	1.469763	C	2.052787	2.828676	1.142517
## 3.519330		2.132646	-1.498710			3.897909		
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H	H	-1.086067	-1.665021	4.244041	H	-0.284312	5.427563	1.467612
H	C	0.588999	0.421446	3.562094	H	1.238837	5.515608	0.539913
H 1.457442 1.086551 3.740146 H -1.111608 3.408005 2.512743 C 2.902902 -2.312197 -0.873225 H 0.446010 3.163808 3.565841 C 2.747705 -0.939292 -1.561975 C -0.120332 3.255944 -0.103866 H 1.855588 -0.405020 -1.246141 H 0.445497 3.762195 -0.074504 H 3.661218 -1.059097 -2.663062 H 1.106749 3.762195 -0.074504 B 3.611278 -0.284167 -1.333929 H -0.3138499 3.762195 -0.074504 C 4.140634 -2.988550 -1.493566 C -0.933822 -0.200262 -2.988208 H 5.504800 -2.370978 -1.384555 C 0.172140 -0.678283 -5.204338 H 4.337457 -3.984924 -2.578716 C -0.013403 -0.689333 -5.204338 H 4.337457 -3.984924 -2.578716 C -0.013403 -0.689333 -5.204338 H 4.337457 -3.984924 -1.049224 H 0.16398 -0.930302 -5.85505 C 1.691149 -2.251274 C -0.200262 -2.988208 H 4.350457 -3.384924 -2.578716 C -0.013403 -0.689333 -5.204338 H 4.357457 -3.984924 -1.049224 H 0.16398 -0.930302 -0.805024 -5.85505 C -1.691299 -1.269209 -1.42075 H 1.532720 -3.332739 -2.255379 C -2.296196 -0.05045 -0.39294 -5.55502 H 1.69129 -3.332739 -2.255379 C -2.296196 -0.05045 -0.976279 H 0.762356 -2.832716 -0.714797 H -3.244600 0.32994 -5.451044 C -3.493859 2.318534 -0.246928 C -2.189700 0.091184 -3.573278 H -2.512474 2.616578 -0.664975 C 1.529066 -1.116197 -3.220312 H -4.031162 1.727816 -1.017853 H 3.499119 -1.797954 -3.832031 C -5.033736 1.041796 2.082862 H 2.775939 -0.643947 -3.1832031 D -0.078000 C 2.548456 -1.116197 -3.220312 H -5.566998 0.420826 1.417927 H 2.204343 -2.347011 -4.933659 H -5.554814 2.011627 2.228033 H 2.776393 -0.649397 -3.983822 H -5.566998 0.420826 1.417927 H 2.204343 -2.347011 -4.933659 H -5.554814 2.011627 2.228033 C 1.320300 -0.08035 H 2.775939 -0.649397 -3.832031 D -0.47962 B -2.282375 -2.743882 -2.041831 B -4.974981 0.543118 3.072011 H 0.939574 -3.197900 -2.988657 D -2.282332 D -2.282333	H	-0.233644	0.729796	4.238727	С	-0.111461	2.936058	2.435079
C 2.992902	H	0.233899	0.616024	2.530407	H	-0.250154	1.840805	2.387691
C 2.747705 -0.939292 -1.561975 C -0.120332 3.259944 -0.103826 H 1.835588 -0.405020 -1.246141 H 0.445497 3.648423 -0.972204 H 2.692118 -1.059097 -2.663062 H -1.106749 3.762195 -0.074504 C -1.106749 3.762195 -0.204504 C -1.333929 H -0.319849 3.762195 -0.280262 -2.988208 H 5.054800 -2.370978 -1.384555 C 0.172140 -0.678885 -3.809476 H 3.967095 -3.134124 -2.578716 C -0.013403 -0.689938 -5.204338 H 4.337457 -3.984924 -1.049927 H 0.816398 -0.980302 -5.855505 C 1.691147 -3.226376 -1.162314 C -1.228733 -0.332034 -5.790846 H 1.861929 -4.238350 -0.742075 H -1.344565 -0.55849 -6.888775 H 1.532720 -3.332739 -2.255379 C -2.296196 0.050450 -4.976279 H 0.762356 -2.822716 -0.714797 H -3.244600 0.329294 -5.451040 C -3.493859 2.318534 -0.246928 C -2.189700 0.991184 -3.573278 H -2.512474 2.616578 -0.664975 C 1.529066 -1.16197 -3.22031 H -4.098924 3.20210 -0.078000 C 2.548456 -1.194417 -3.32231 H -4.093173 (			1.086551				3.408805	
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H	H	-2.512474	2.616578	-0.664975	C	1.529066	-1.116197	-3.220312
C -5.033736	H	-4.098924	3.230210	-0.078000	C	2.548456	-1.494417	-4.314928
H -5.666998		-4.031162			H		-1.797954	
H -5.554814 2.011627 2.228033 C 1.320360 -2.385134 -2.362433 H -4.974981 0.543118 3.072011 H 0.893574 -3.197900 -2.983657 C -2.414211 2.453863 2.647437 H 0.622150 -2.216345 -1.519398 H -2.354124 1.937232 3.627339 H 2.282375 -2.743582 -1.944076 H -2.972094 3.401042 2.801449 C 2.166305 0.046907 -2.426636 H -1.383488 2.714103 2.337120 H 3.150530 -0.248633 -2.011891 C -4.395158 -1.367014 -0.911361 H 1.548395 0.400052 -1.581227 H -5.168669 -0.629733 -0.617183 H 2.326977 0.919029 -3.091307 H -4.914188 -2.292855 -1.234248 C -3.398756 0.556653 -2.734816 H -3.850759 -0.956489 -1.785029 C -4.153874 -2.531971 1.959670 H -4.436193 1.699743 -4.322631 H -3.465980 -2.750991 2.802624 H -5.464123 1.192417 -2.953464 H -4.949493 -1.861369 2.339838 C -3.828636 -0.553395 -1.750302 C -2.030213 -3.125915 -0.105448 H -4.114713 -1.470665 -2.303678 H -1.497339 -2.879355 -1.051793 H -4.171713 -1.470665 -2.303678 H -1.497339 -2.879355 -1.051793 H -4.171713 -1.470665 -2.303678 H -2.622707 -4.045796 -0.299538 H -3.020852 -0.818794 -1.156455 H -2.622707 -4.045796 -0.299538 H -3.020852 -0.818794 -1.156455 H -2.622707 -4.045796 -0.299538 H -3.020852 -0.818794 -1.047845 H -2.61613 -3.384228 0.651870 C -2.0308937 -3.820682 3.221646 E(BB7-3c) = -2948.99151379709 Hartree H -2.869973 -3.820682 3.221646 E(BB7-3c) = -2948.99551379709 Hartree H -2.86960 -4.385468 0.423097 E(BBD-3c) = -2944.99498985125730 Hartree H -2.619746 -3.260734 4.013373 E(BBD238.12200 Kcal/mol H -0.655029 -4.767746 1.660210 E(BM7) = -233.41507 Kcal/mol H -0.655029 -4.767746 1.660210 E(BM7)							-0.643947	
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C -2.030213			-3.488357				-0.009445	
H -1.497339	H	-4.949493	-1.861369	2.339838	С	-3.828636	-0.553395	-1.750302
H -1.497339								
H -1.261613 -3.384228 0.651870 C -3.024518 1.860496 -1.996708	H		-2.879355				-0.227448	
Conformation 29. H -2.187583 1.709896 -1.293393 Conformation 29. H -3.889109 2.248394 -1.420423 Multiplicity: 2 H -2.722970 2.639763 -2.725529 Charge: 0 C -2.082937 -3.820682 3.221646 E(B97-3c) = -2948.791163204811 Hartree H -2.619746 -3.260734 4.013373 E(M06/def2-TZVP) = -2948.905511797009 Hartree H -2.619746 -3.260734 4.013373 E(PBE - D3(BJ)/def2-TZVP) = -2947.683627294572 Hartree H -2.836961 -4.227523 2.517182 E(PBE0 - D3(BJ)/def2-TZVP) = -2947.958092797182 Hartree C 0.065975 -3.937705 1.108648 E(PBEh-3c) = -2944.943985125730 Hartree H -0.683690 -4.385468 0.423097 E(PM6) = -238.12200 Kcal/mol H 0.555029 -4.767746 1.660210 E(PM7) = -233.41507 Kcal/mol H 0.835925 -3.443289 0.486956 E(DM97X-V/def2-TZVP) = -2949.529129626508 Hartree C 0.410190 -2.095489 3.639321 E(GFN1-xTB) = -182.425733895070 Hartree H 0.815335 -1.098035 3.376761	H	-2.622707	-4.045796	-0.299538	H		-0.818794	
Conformation 29.  Multiplicity: 2  Charge: 0  E(B97-3c) = -2948.791163204811 Hartree  E(B97-3c) = -2948.905511797009 Hartree  E(B97-3c) = -2948.90551179709 Hartree  E(B97-3	H	-1.261613	-3.384228	0.651870				
Multiplicity: 2								
Charge: 0								
E (B97-3c) = -2948.791163204811 Hartree H -2.619746 -3.260734 4.013373 E (M06/def2-TZVP) = -2948.905511797009 Hartree H -1.572978 -4.680274 3.705737 E (PBE - D3 (BJ) /def2-TZVP) = -2947.683627294572 Hartree H -2.836961 -4.227523 2.517182 E (PBE0 - D3 (BJ) /def2-TZVP) = -2947.958092797182 Hartree C 0.065975 -3.937705 1.108648 E (PBEh-3c) = -2944.943985125730 Hartree H -0.683690 -4.385468 0.423097 E (PM6) = -238.12200 Kcal/mol H 0.555029 -4.767746 1.660210 E (PM7) = -233.41507 Kcal/mol H 0.835925 -3.443289 0.486956 E (0B97X-V/def2-TZVP) = -2949.529129626508 Hartree C 0.410190 -2.095489 3.639321 E (GFN1-xTB) = -182.425733895070 Hartree H 0.815335 -1.098035 3.376761								
E (M06/def2-TZVP) = -2948.905511797009 Hartree H -1.572978 -4.680274 3.705737 E(PBE - D3(BJ)/def2-TZVP) = -2947.683627294572 Hartree H -2.836961 -4.227523 2.517182 E(PBE0 - D3(BJ)/def2-TZVP) = -2947.958092797182 Hartree C 0.065975 -3.937705 1.108648 E(PBEh-3c) = -2944.943985125730 Hartree H -0.683690 -4.385468 0.423097 E(PM6) = -238.12200 Kcal/mol H 0.555029 -4.767746 1.660210 E(PM7) = -233.41507 Kcal/mol H 0.835925 -3.443289 0.486956 E(0B97X-V/def2-TZVP) = -2949.529129626508 Hartree C 0.410190 -2.095489 3.639321 E(GFN1-xTB) = -182.425733895070 Hartree H 0.815335 -1.098035 3.376761			320/011 110					
E(PBE - D3(BJ)/def2-TZVP) = -2947.683627294572 Hartree H -2.836961 -4.227523 2.517182 E(PBE0 - D3(BJ)/def2-TZVP) = -2947.958092797182 Hartree C 0.065975 -3.937705 1.108648 E(PBEh-3c) = -2944.943985125730 Hartree H -0.683690 -4.385468 0.423097 E(PM6) = -238.12200 Kcal/mol H 0.555029 -4.767746 1.660210 E(PM7) = -233.41507 Kcal/mol H 0.835925 -3.443289 0.486956 E(OB97X-V/def2-TZVP) = -2949.529129626508 Hartree C 0.410190 -2.095489 3.639321 E(GFN1-xTB) = -182.425733895070 Hartree H 0.815335 -1.098035 3.376761				rtroo				
E(PBE0 - D3(BJ)/def2-TZVP) = -2947.958092797182 Hartree C 0.065975 -3.937705 1.108648 E(PBEh-3c) = -2944.943985125730 Hartree H -0.683690 -4.385468 0.423097 E(PM6) = -238.12200 Kcal/mol H 0.555029 -4.767746 1.660210 E(PM7) = -233.41507 Kcal/mol H 0.835925 -3.443289 0.486956 E(MB97X-V/def2-TZVP) = -2949.529129626508 Hartree C 0.410190 -2.095489 3.639321 E(GFN1-xTB) = -182.425733895070 Hartree H 0.815335 -1.098035 3.376761								
E(PBEh-3c) = -2944.943985125730 Hartree H -0.683690 -4.385468 0.423097 E(PM6) = -238.12200 Kcal/mol H 0.555029 -4.767746 1.660210 E(PM7) = -233.41507 Kcal/mol H 0.835925 -3.443289 0.486956 E(GB97X-V/def2-TZVP) = -2949.529129626508 Hartree C 0.410190 -2.095489 3.639321 E(GFN1-xTB) = -182.425733895070 Hartree H 0.815335 -1.098035 3.376761								
E(PM6) = -238.12200 Kcal/mol H 0.555029 -4.767746 1.660210 E(PM7) = -233.41507 Kcal/mol H 0.835925 -3.443289 0.486956 E(ωB97X-V/def2-TzVP) = -2949.529129626508 Hartree C 0.410190 -2.095489 3.639321 E(GFN1-xTB) = -182.425733895070 Hartree H 0.815335 -1.098035 3.376761				2.7,102 HALLIEE				
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	0 104015	1 000010	4 61 5 61 5		1 050000	0.000064	2 106017	
H	-0.104215	-1.996916	4.615617	H	-1.052980	2.829364	-3.126817	
С	-3.333644	1.332946	1.529380	H	-0.862291	1.850212	-1.646994	
H	-2.457001	1.972752	1.315871	H	-2.131909	3.102499	-1.717230	
Н	-3.996105	1.890660	2.224939	C	-3.061753	-1.733454	1.334006	
Н	-3.888103	1.186253	0.583943	C	-2.159425	-2.846807	0.755696	
С	-2.288704	0.020252	4.082233	H	-2.723866	-3.487218	0.048351	
Н	-2.191506	-0.900855	4.690300	Н	-1.778875	-3.490274	1.575084	
Н	-3.022595	0.681073	4.588417	H	-1.282689	-2.442771	0.217106	
H	-1.307912	0.537259	4.090362	C	-2.266090	-0.853520	2.323537	
С	-4.513891	-1.305357	2.372703	H	-1.396617	-0.359050	1.854284	
H	-4.878018	-1.498049	1.342031	H	-1.881647	-1.467663	3.162977	
H	-5.292090	-0.714041	2.899483	H	-2.911582	-0.058766	2.746561	
Н	-4.414228	-2.280789	2.886093	C	-4.158925	-2.443917	2.154559	
				H	-4.816536	-1.728178	2.686845	
Confor	emation 30.			H	-3.677908	-3.080981	2.923379	
	olicity: 2			Н	-4.793291	-3.099465	1.524784	
Charge				C	3.360024	0.686849	-4.001863	
	-3c) = -2948.80227	CEOC770 H		Н				
	,				3.331662	-0.203207	-4.661462	
	def2-TZVP) = -294			H	4.318803	1.217452	-4.179149	
	- D3(BJ)/def2-TZV			H	2.537128	1.364966	-4.310827	
	) - D3(BJ)/def2-TZ		4251896 Hartree	C	3.354766	1.808324	-1.167217	
E (PBEł	1-3c) = -2944.9532	22712317 Hartree		H	2.598925	2.560614	-1.471057	
E(PM6)	= -241.84948 Kca	1/mol		H	4.356567	2.252718	-1.345614	
E(PM7)	= -239.71992 Kca	1/mol		H	3.247689	1.638717	-0.077165	
E (ωB97	7X-V/def2-TZVP) =	-2949.54060097573	7 Hartree	С	4.642290	-0.906808	-1.693309	
	L-xTB) = -183.8823			H	4.616261	-1.183990	-0.621832	
	2-xTB) = $-119.3634$			Н	5.587871	-0.354547	-1.874133	
	-FF) = $-16.2427134$			Н	4.679709	-1.839940	-2.288688	
E (GEN-	-FF) = -10.242/134	00232 Hartree		C				
0	nator.				-0.348507	-3.066996	-2.667501	
	inates:	0 000100	0 054::=	H	-1.054891	-2.808298	-1.856222	
Ti	0.250663	-0.096100	-0.354447	H	-0.355634	-4.170759	-2.786521	
Si	3.181711	0.206908	-2.172044	H	-0.740592	-2.627772	-3.607084	
Si	1.429299	-2.485404	-2.337591	C	2.144702	-3.507666	-0.909562	
0	0.886681	0.597109	1.206376	H	3.191760	-3.224091	-0.685262	
0	-1.522391	-0.287852	-0.719506	H	2.129304	-4.587656	-1.164759	
Ċ	1.492161	-0.628305	-1.934626	Н	1.551805	-3.367962	0.017011	
Н	0.824733	-0.146007	-2.699048	C	2.381613	-2.909274	-3.930536	
C	1.107429	1.081858	2.452651	H	1.972767	-2.341602	-4.791678	
С	1.841966	0.272177	3.378277	H	2.265342	-3.990634	-4.153963	
С	2.048657	0.791451	4.669752	H	3.465845	-2.692951	-3.864323	
H	2.604586	0.200737	5.407950					
С	1.565865	2.047740	5.044468		mation 32.			
H	1.744173	2.427622	6.061541		licity: 2			
С	0.859367	2.821865	4.120856	Charge	: 0			
H	0.493690	3.806688	4.435277		3c) = -2948.795389			
H C	0.493690 0.606191				3c) = -2948.795389 def2-TZVP) = -2948		rtree	
		3.806688	4.435277	E(M06/		3.907235114917 Ha		
С	0.606191	3.806688 2.375938	4.435277 2.809405	E(M06/ E(PBE	def2-TZVP) = -2948	3.907235114917 Ha P) = -2947.687910	692649 Hartree	
C C	0.606191 2.393719	3.806688 2.375938 -1.124792	4.435277 2.809405 3.009099	E (M06/ E (PBE E (PBE0	def2-TZVP) = -2948 - D3(BJ)/def2-TZVI	3.907235114917 Ha P) = -2947.687910 JP) = -2947.96203	692649 Hartree	
C C	0.606191 2.393719 3.199393	3.806688 2.375938 -1.124792 -1.745581	4.435277 2.809405 3.009099 4.168657	E (M06/ E (PBE E (PBE0 E (PBEh	def2-TZVP) = -2948 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZV	3.907235114917 Ha P) = -2947.687910 JP) = -2947.96203 D1764185 Hartree	692649 Hartree	
C C H	0.606191 2.393719 3.199393 4.072178 3.584398	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991	4.435277 2.809405 3.009099 4.168657 4.451519	E (M06/ E (PBE E (PBE0 E (PBEh E (PM6)	def2-TZVP) = -2948 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI -3c) = -2944.94630 = -239.70165 Kca	3.907235114917 Ha P) = -2947.687910 VP) = -2947.96203 D1764185 Hartree 1/mol	692649 Hartree	
C C H H H	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237	E (M06/ E (PBE E (PBE0 E (PBEh E (PM6) E (PM7)	def2-TZVP) = -2948 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZV - C3C) = -2944.94630 = -239.70165 Kcai = -237.61489 Kcai	3.907235114917 Ha P) = -2947.687910 VP) = -2947.96203 01764185 Hartree 1/mol 1/mol	692649 Hartree 2391801 Hartree	
С С Н Н С	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960	E (M06/ E (PBE E (PBE0 E (PBEh E (PM6) E (PM7) E (ωB97	def2-TZVP) = -2946 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV -3c) = -2944.94636 = -239.70165 Kcai = -237.61489 Kcai X-V/def2-TZVP) = -	3.907235114917 Ha P) = -2947.687910 JPP) = -2947.96203 01764185 Hartree 1/mol 1/mol -2950.74654945518	692649 Hartree 2391801 Hartree	
С С Н Н С Н	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361	E (M06/ E (PBE E (PBE0 E (PBEh E (PM6) E (PM7) E (ωB97 E (GFN1	def2-TZVP) = -2946 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI -3c) = -2944.94636 = -239.70165 Kcai = -237.61489 Kcai X-V/def2-TZVP) = -xTB) = -183.2273	3.907235114917 Ha P) = -2947.687910 VP) = -2947.96203 01764185 Hartree 1/mol 1/mol -2950.74654945518 76004867 Hartree	692649 Hartree 2391801 Hartree	
С С Н Н С Н	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022	E (M06/ E (PBE E (PBE0 E (PBEh E (PM6) E (PM7) E (\omega B97 E (GFN1 E (GFN2	def2-TZVP) = -2946 - D3 (BJ)/def2-TZVI - D3 (BJ)/def2-TZVI -3c) = -2944.9463 = -239.70165 Kcai = -237.61489 Kcai X-V/def2-TZVP) = - -XTB) = -183.2273' -XTB) = -119.35616	3.907235114917 Ha P) = -2947.687910 VP) = -2947.96203 D1764185 Hartree 1/mol -2950.74654945518 76004867 Hartree 37457274 Hartree	692649 Hartree 2391801 Hartree	
С С Н Н С Н Н	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654	E (M06/ E (PBE E (PBE0 E (PBEh E (PM6) E (PM7) E (\omega B97 E (GFN1 E (GFN2	def2-TZVP) = -2946 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI -3c) = -2944.94636 = -239.70165 Kcai = -237.61489 Kcai X-V/def2-TZVP) = -xTB) = -183.2273	3.907235114917 Ha P) = -2947.687910 VP) = -2947.96203 D1764185 Hartree 1/mol -2950.74654945518 76004867 Hartree 37457274 Hartree	692649 Hartree 2391801 Hartree	
С С Н Н С Н Н С	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158 3.350270	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402 -1.029144	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654 1.800435	E (M06/ E (PBE E (PBE0 E (PBEh E (PM6) E (PM7) E (ωB97 E (GFN1 E (GFN2	def2-TZVP) = -2946 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZV -3c) = -2944.9463( = -237.61489 Kcai X-V/def2-TZVP) = -xxTB) = -183.2273' -xTB) = -119.35616 FFF) = -16.2348814'	3.907235114917 Ha P) = -2947.687910 VP) = -2947.96203 D1764185 Hartree 1/mol -2950.74654945518 76004867 Hartree 37457274 Hartree	692649 Hartree 2391801 Hartree	
С С Н Н С Н Н С Н	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158 3.350270 2.837118	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402 -1.029144 -0.673862	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654 1.800435 0.889760	E (M06/ E (PBE E (PBE0 E (PBEh E (PM6)) E (PM7) E (GB97 E (GFN1 E (GFN2 E (GFN-	def2-TZVP) = -2946 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV -3c) = -2944.94630 = -239.70165 Kcai = -237.61489 Kcai X-V/def2-TZVP) = -xTB) = -183.2273 -xTB) = -119.35618 FFF) = -16.23488143	3.907235114917 Ha P) = -2947.687910 PP) = -2947.96203 01764185 Hartree L/mol -/mol -2950.74654945518 76004867 Hartree 37457274 Hartree 33313 Hartree	692649 Hartree 2391801 Hartree 6 Hartree	
С С Н Н С Н Н Н С Н Н Н Н Н Н Н Н Н Н Н	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158 3.350270 2.837118 3.782837	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402 -1.029144 -0.673862 -2.025747	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654 1.800435 0.889760 1.577145	E (M06/ E (PBE E (PBE0 E (PBEh E (PM6)) E (PM7) E (GFN7) E (GFN1 E (GFN2 E (GFN- Coordi Ti	def2-TZVP) = -2946 - D3 (BJ)/def2-TZVI) - D3 (BJ)/def2-TZVI -3c) = -2944.9463 = -239.70165 Kcal = -237.61489 Kcal X-V/def2-TZVP) =XTB) = -183.2273' -XTB) = -119.35616 FF) = -16.2348814'  nates: 0.356914	3.907235114917 Ha P) = -2947.687910 VP) = -2947.96203 D1764185 Hartree 1/mol -2950.74654945518 76004867 Hartree 33313 Hartree -0.081411	692649 Hartree 2391801 Hartree 6 Hartree 0.367559	
С С С Н Н Н С Н Н Н С Н Н Н Н Н Н Н Н Н	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158 3.350270 2.837118 3.782837 4.185386	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402 -1.029144 -0.673862 -2.025747 -0.331210	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654 1.800435 0.889760 1.577145 2.012070	E (M06/ E (PBE E (PBE0 E (PBE0 E (PM6)) E (PM7) E (GB97 E (GFN1 E (GFN2 E (GFN- Coordi Ti Si	def2-TZVP) = -2946 - D3 (BJ)/def2-TZVI - D3 (BJ)/def2-TZVI - D3 (BJ)/def2-TZVI - D3 (BJ)/def2-TZVI - 239.70165 Kcal = -237.61489 Kcal X-V/def2-TZVP) =XTB) = -183.2273' -XTB) = -119.35616 FF) = -16.23488143'  nates:  0.356914 0.293980	3.907235114917 Ha P) = -2947.687910 VP) = -2947.96203 D1764185 Hartree 1/mol 1/mol 1/mol 1/mo1 1	692649 Hartree 2391801 Hartree 6 Hartree 0.367559 3.592250	
СССННСННСНН	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158 3.350270 2.837118 3.782837 4.185386 -0.184292	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402 -1.029144 -0.673862 -2.025747 -0.331210 3.279501	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654 1.800435 0.889760 1.577145 2.012070 1.832086	E (M06/ E (PBE E (PBE0) E (PBE0) E (PM7) E (GFM7) E (GFN1 E (GFN1- Coordi Ti Si	def2-TZVP) = -2946 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - 239.70165 Kcai = -239.70165 Kcai = -237.61489 Kcai X-V/def2-TZVP) = -xTB) = -183.2273' -xTB) = -119.35616 FF) = -16.2348814: nates:	3.907235114917 Ha P) = -2947.687910 PP) = -2947.96203 D1764185 Hartree L/mol L/mol -2950.74654945518 76004867 Hartree 33313 Hartree -0.081411 -1.068460 -1.484275	692649 Hartree 2391801 Hartree 6 Hartree 0.367559 3.592250 1.908412	
	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158 3.350270 2.837118 3.782837 4.185386 -0.184292 0.650852	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402 -1.029144 -0.673862 -2.025747 -0.331210 3.279501 3.575227	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654 1.800435 0.889760 1.577145 2.012070 1.832086 0.567606	E(M06/ E(PBE E(PBE0 E(PBE0 E(PBE0) E(PMT) E(GB97 E(GFN1 E(GFN2 E(GFN- Coordi Ti Si Si O	def2-TZVP) = -2946 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZV - D3(BJ)/def2-TZV -3c) = -2944.9463( = -237.61489 Kcai X-V/def2-TZVP) = -xXTB) = -183.2273' -xXTB) = -119.35616 FFF) = -16.2348814'  nates:  0.356914 0.293980 3.018437 -0.938803	3.907235114917 Ha P) = -2947.687910 PP) = -2947.96203 D1764185 Hartree L/mol L/mol -2950.74654945518 76004867 Hartree 33313 Hartree -0.081411 -1.068460 -1.484275 -1.236036	692649 Hartree 2391801 Hartree 6 Hartree 0.367559 3.592250 1.908412 -0.214424	
С С С Н Н С Н Н С С Н Н С С С Н	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158 3.350270 2.837118 3.782837 4.185386 -0.184292 0.650852 1.609293	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402 -1.029144 -0.673862 -2.025747 -0.331210 3.279501 3.575227 4.064825	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654 1.800435 0.889760 1.577145 2.012070 1.832086 0.567606 0.832958	E(M06/E(PBE) E(PBE) E(PBE) E(PBE) E(PBE) E(PM6) E(PM7) E(WB97 E(GFN1) E(GFN2) E(GFN2) Coordi Ti Si Si O O	def2-TZVP) = -2948 - D3 (BJ)/def2-TZVI) - D3 (BJ)/def2-TZVI - 3c) = -2944.94636 = -239.70165 Kcai = -237.61489 Kcai X-V/def2-TZVP) =xTB) = -183.2273' -xTB) = -119.35618 FF) = -16.2348814'  nates:  0.356914 0.293980 3.018437 -0.938803 0.758781	3.907235114917 Ha P) = -2947.687910 PP) = -2947.96203 01764185 Hartree 1/mol 1/mol -2950.74654945518 76004867 Hartree 33313 Hartree -0.081411 -1.068460 -1.484275 -1.236036 1.543663	692649 Hartree 2391801 Hartree 6 Hartree 0.367559 3.592250 1.908412 -0.214424 -0.374777	
С С С Н Н С С Н Н Н С С Н Н Н С С Н Н	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158 3.350270 2.837118 3.782837 4.185386 -0.184292 0.650852 1.609293 0.092617	3.806688 2.375938 -1.124792 -1.7745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402 -1.029144 -0.6673862 -2.025747 -0.331210 3.279501 3.575227 4.064825 4.251469	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654 1.800435 0.889760 1.577145 2.012070 1.832086 0.567606 0.832958 -0.112120	E(M06/E(PBE) E(PBE) E(PBE) E(PBE) E(PM6) E(PM7) E(GB97 E(GFN1) E(GFN2) E(GFN2) E(GFN3) Coordi Ti Si Si O C	def2-TZVP) = -2946 - D3 (BJ)/def2-TZVI - D3 (BJ)/def2-TZVI - D3 (BJ)/def2-TZVI - D3 (BJ)/def2-TZVI - 3c) = -2944.9463( = -239.70165 Kcal = -237.61489 Kcal X-V/def2-TZVP) = -183.2273' -XTB) = -183.2273' -XTB) = -119.35616 FF) = -16.23488143'  nates: 0.356914 0.293980 3.018437 -0.938803 0.758781 1.373867	3.907235114917 Ha P) = -2947.687910 VP) = -2947.96203 D1764185 Hartree 1/mol 1/mol 1/mol 1/mof 1	692649 Hartree 2391801 Hartree 6 Hartree 0.367559 3.592250 1.908412 -0.214424 -0.374777 2.120995	
С С С Н Н Н С Н Н Н С С Н Н Н Н С Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158 3.350270 2.837118 3.782837 4.185386 -0.184292 0.650852 1.609293 0.092617 0.893550	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402 -1.029144 -0.673862 -2.025747 -0.331210 3.279501 3.575227 4.064825 4.251469 2.655724	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654 1.800435 0.889760 1.577145 2.012070 1.832086 0.567606 0.832958 -0.112120 0.005914	E(M06/ E(PBE E(PBE0 E(PBE0 E(PBE0) E(PM7) E(GB97 E(GFN2 E(GFN2 Coordi Ti Si Si O O C	def2-TZVP) = -2946 - D3 (BJ)/def2-TZVI - D3 (BJ)/def2-TZVI - D3 (BJ)/def2-TZVI - D3 (BJ)/def2-TZVI - S244.9463( = -239.70165 Kcai = -237.61489 Kcai X-V/def2-TZVP) =xTB) = -183.2273' -xTB) = -119.35616 FF) = -16.23488143' nates:	3.907235114917 Ha P) = -2947.687910 VP) = -2947.96203 D1764185 Hartree L/mol L/mol -2950.74654945518 76004867 Hartree 33313 Hartree  -0.081411 -1.068460 -1.484275 -1.236036 1.543663 -0.557257 0.485621	692649 Hartree 2391801 Hartree 6 Hartree 0.367559 3.592250 1.908412 -0.214424 -0.374777 2.120995 2.347673	
С С С Н Н С Н Н Н С С Н Н Н С С Н Н Н С	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158 3.350270 2.837118 3.782837 4.185386 -0.184292 0.650852 1.609293 0.092617 0.893550 -0.528447	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402 -1.029144 -0.673862 -2.025747 -0.331210 3.279501 3.575227 4.064825 4.251469 2.655724 4.643738	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654 1.800435 0.889760 1.577145 2.012070 1.832086 0.567606 0.832958 -0.112120 0.005914 2.465658	E(M06/ E(PBE E(PBE0 E(PBE0 E(PBE0) E(PMT)) E(GFN1 E(GFN2 E(GFN- Coordi Ti Si Si O O C C	def2-TZVP) = -2946 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI = -239.70165 Kcai = -237.61489 Kcai X-V/def2-TZVP) = -xTB) = -183.2273* -xTB) = -119.35614 FF) = -16.2348814*  nates:	3.907235114917 Ha P) = -2947.687910 P) = -2947.96203 D1764185 Hartree P/mol Pmol Pmol Pmol Pmol Pmol Pmol Pmol P	692649 Hartree 2391801 Hartree  6 Hartree  0.367559 3.592250 1.908412 -0.214424 -0.374777 2.120995 2.347673 -1.048130	
СССНН СННСНН ССНН ССН	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158 3.350270 2.837118 3.782837 4.185386 -0.184292 0.650852 1.609293 0.092617 0.893550 -0.528447 -1.183396	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402 -1.029144 -0.673862 -2.025747 -0.331210 3.279501 3.575227 4.064825 4.251469 2.655724 4.643738 4.540356	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654 1.800435 0.889760 1.577145 2.012070 1.832086 0.567606 0.832958 -0.112120 0.005914 2.465658 3.353676	E (M06/ E (PBE) E (PBE) E (PBE) E (PM6) E (PM7) E (WB97 E (GFN1) E (GFN2) Coordi Ti Si O O C C H C	def2-TZVP) = -2946 - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI - D3(BJ)/def2-TZVI = -239.70165 Kcai = -237.61489 Kcai X-V/def2-TZVP) = -xTB) = -183.2273' -xTB) = -119.35616 FF) = -16.2348814'  nates:  0.356914 0.293980 3.018437 -0.938803 0.758781 1.373867 1.709618 -1.884530 -1.570194	3.907235114917 Ha P) = -2947.687910 P) = -2947.96203 D1764185 Hartree 1/mol 1/mol -2950.74654945518 76004867 Hartree 33313 Hartree -0.081411 -1.068460 -1.484275 -1.236036 1.543663 -0.557257 0.485621 -1.743396 -2.906151	692649 Hartree 2391801 Hartree  6 Hartree  0.367559 3.592250 1.908412 -0.214424 -0.374777 2.120995 2.347673 -1.048130 -1.823458	
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СССНН НСНННСИННИСИННИСИННИСИН	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158 3.350270 2.837118 3.782837 4.185386 -0.184292 0.650852 1.609293 0.092617 0.893550 -0.528447 -1.183396 -1.075330 0.377924 -1.527234 -1.398624 -2.115723 -2.131346 -2.872140 -3.457415 -4.858156 -5.344943 -5.656182	3.806688 2.375938 -1.124792 -1.7745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402 -1.029144 -0.673862 -2.025747 -0.331210 3.279501 3.575227 4.064825 4.251469 2.655724 4.643738 4.540356 5.258170 5.208209 2.617897 1.666231 3.292317 2.406728 -0.171741 0.633614 0.767489 1.384986 0.127750	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654 1.800435 0.889760 1.577145 2.012070 1.832086 0.567606 0.832958 -0.112120 0.005914 2.465658 3.353676 1.722743 2.762808 1.451687 0.906820 0.796875 2.355967 -0.762807 -1.793112 -1.789361 -2.554155 -0.837185	E (M06/ E (PBE C (PBE) C (PBE) C (PBE) E (PM6) E (PM7) E (GB97 E (GFN1 E (GFN2	def2-TZVP) = -2948 - D3 (BJ)/def2-TZVI = -239.70165 Kcai = -237.61489 Kcai X-V/def2-TZVP) =	3.907235114917 Ha P) = -2947.687910 VP) = -2947.96203 D1764185 Hartree L/mol L/mol L/mol -2950.74654945518 76004867 Hartree 33313 Hartree  -0.081411 -1.068460 -1.484275 -1.236036 1.543663 -0.557257 0.485621 -1.743396 -2.906151 -3.344766 -4.221885 -2.694908 -3.055403 -1.600941 -1.124377 -1.099771 -3.692425 -4.973150 -5.659777 -5.515151	692649 Hartree 2391801 Hartree  6 Hartree  0.367559 3.592250 1.908412 -0.214424 -0.374777 2.120995 2.347673 -1.048130 -1.823458 -2.752194 -3.375767 -2.905783 -3.647590 -2.093756 -2.206254 -1.141075 -1.651573 -2.510667 -2.252522 -2.329609	
СССНН НСНННСНННССНННСНННСССН	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158 3.350270 2.837118 3.782837 4.185386 -0.184292 0.650852 1.609293 0.092617 0.893550 -0.528447 -1.183396 -1.075330 0.377924 -1.527234 -1.398624 -2.115723 -2.131346 -2.872140 -3.457415 -4.858156 -5.344943 -5.656182 -6.749359	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402 -1.029144 -0.673862 -2.025747 -0.331210 3.279501 3.575227 4.064825 4.251469 2.655724 4.643738 4.540356 5.258170 5.208209 2.617897 1.666231 3.292317 2.406728 -0.171741 0.633614 0.767489 1.384986 0.127750 0.250039	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654 1.800435 0.889760 1.577145 2.012070 1.832086 0.567606 0.832958 -0.112120 0.005914 2.465658 3.353676 1.722743 2.762808 1.451687 0.906820 0.796875 2.355967 -0.762807 -1.789361 -2.554155 -0.837185 -0.860724	E (M06/ E (PBE E (PBE0 E (PBE0 E (PBE0 E (PBE0 E (PBE0 E (PBE0 E (PM7)) E (GFN1 E (GFN2 E (GFN1 E (GFN2 E (GFN2 E (GFN E (PBE0 E (PBE0 E E (PBE0 E E (PBE0 E E E E E E E E E E E E E E E E E E	def2-TZVP) = -2946 - D3 (BJ)/def2-TZVI = -239.70165 Kcai = -237.61489 Kcai X-V/def2-TZVP) =	3.907235114917 Ha 2) = -2947.687910 VP) = -2947.96203 01764185 Hartree 1/mol 1/mol 1-2950.74654945518 76004867 Hartree 33313 Hartree -0.081411 -1.068460 -1.484275 -1.236036 1.543663 -0.557257 0.485621 -1.743396 -2.906151 -3.344766 -4.221885 -2.694908 -3.055403 -1.600941 -1.124377 -1.099771 -3.692425 -4.973150 -5.659777 -5.515151 -4.753715	692649 Hartree 2391801 Hartree  6 Hartree  0.367559 3.592250 1.908412 -0.214424 -0.374777 2.120995 2.347673 -1.048130 -1.823458 -2.752194 -3.375767 -2.905783 -3.647590 -2.093756 -2.206254 -1.141075 -1.651573 -2.510667 -2.252522 -2.329609 -3.595891	
СССНН НСНННСИНННСОНННСИННСИННСОСОНСНС	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158 3.350270 2.837118 3.782837 4.185386 -0.184292 0.650852 1.609293 0.092617 0.893550 -0.528447 -1.183396 -1.075330 0.377924 -1.527234 -1.398624 -2.115723 -2.131346 -2.872140 -3.457415 -4.858156 -5.344943 -5.656182 -6.749359 -5.062340	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402 -1.029144 -0.673862 -2.025747 -0.331210 3.279501 3.575227 4.064825 4.251469 2.655724 4.6643738 4.540356 5.258170 5.208209 2.617897 1.666231 3.292317 2.406728 -0.171741 0.633614 0.767489 1.384986 0.127750 0.250039 -0.676368	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654 1.800435 0.889760 1.577145 2.012070 1.832086 0.567606 0.832958 -0.112120 0.005914 2.465658 3.353676 1.722743 2.762808 1.451687 0.906820 0.796875 2.355967 -0.762807 -1.793112 -1.789361 -2.554155 -0.837185 -0.860724 0.138964	E (M06/E (PBE) E (PBE) E (PBE) E (PM6) E (PM7) E (GB71) E (GFN2) E (GFN- Coordi Ti Si O C C H C C C H C C H C C H C C H C C H C H C C H C C H C C H C C H C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C C H C C C C C C C C H C C C C C C C C C C C C C C C C C C C C	def2-TZVP) = -2948 - D3 (BJ)/def2-TZVI) - D3 (BJ)/def2-TZVI - D3 (BJ)/def2-TZVI - 3c) = -2944.9463 = -239.70165 Kcai = -237.61489 Kcai X-V/def2-TZVP) =xTB) = -183.2273 -xTB) = -119.35618 FF) = -16.23488143  nates:  0.356914 0.293980 3.018437 -0.938803 0.758781 1.373867 1.709618 -1.884530 -1.570194 -2.532542 -2.320498 -3.759656 -4.487838 -4.068037 -5.049386 -3.160319 -0.250653 -0.229568 -1.060418 0.720308 -0.281938 0.961841	3.907235114917 Ha 2) = -2947.687910 VP) = -2947.687910 VP) = -2947.96203 01764185 Hartree 1/mol -2950.74654945518 76004867 Hartree 33313 Hartree 33313 Hartree -0.081411 -1.068460 -1.484275 -1.236036 1.543663 -0.557257 0.485621 -1.743396 -2.906151 -3.344766 -4.221885 -2.694908 -3.055403 -1.600941 -1.124377 -1.099771 -3.692425 -4.973150 -5.659777 -5.515151 -4.753715 -2.843139	692649 Hartree 2391801 Hartree  6 Hartree  0.367559 3.592250 1.908412 -0.214424 -0.374777 2.120995 2.347673 -1.048130 -1.823458 -2.752194 -3.375767 -2.905783 -3.647590 -2.093756 -2.206254 -1.141075 -1.651573 -2.510667 -2.252522 -2.329609 -3.595891 -2.088783	
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СССНН НСНННСНННССНННСНННСНННСССНС	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158 3.350270 2.837118 3.782837 4.185386 -0.184292 0.650852 1.609293 0.092617 0.893550 -0.528447 -1.183396 -1.075330 0.377924 -1.527234 -1.398624 -2.115723 -2.131346 -2.872140 -3.457415 -4.858156 -5.344943 -5.656182 -6.749359 -5.062340	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402 -1.029144 -0.673862 -2.025747 -0.331210 3.279501 3.575227 4.064825 4.251469 2.655724 4.6643738 4.540356 5.258170 5.208209 2.617897 1.666231 3.292317 2.406728 -0.171741 0.633614 0.767489 1.384986 0.127750 0.250039 -0.676368	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654 1.800435 0.889760 1.577145 2.012070 1.832086 0.567606 0.832958 -0.112120 0.005914 2.465658 3.353676 1.722743 2.762808 1.451687 0.906820 0.796875 2.355967 -0.762807 -1.793112 -1.789361 -2.554155 -0.837185 -0.860724 0.138964	E (M06/ E (PBE) E (PBE) E (PM6) E (PM7) E (GFN7) E (GFN7) E (GFN2) Coordi Ti Si O C C H C C C C H C C C H C C H C C H C C H C C C H C C C H C C C H C C C H C C C C C H C C C C C C C C C C C C C C C C C C C C	def2-TZVP) = -2948 - D3 (BJ)/def2-TZVI) - D3 (BJ)/def2-TZVI - D3 (BJ)/def2-TZVI - 3c) = -2944.9463 = -239.70165 Kcai = -237.61489 Kcai X-V/def2-TZVP) =xTB) = -183.2273 -xTB) = -119.35618 FF) = -16.23488143  nates:  0.356914 0.293980 3.018437 -0.938803 0.758781 1.373867 1.709618 -1.884530 -1.570194 -2.532542 -2.320498 -3.759656 -4.487838 -4.068037 -5.049386 -3.160319 -0.250653 -0.229568 -1.060418 0.720308 -0.281938 0.961841	3.907235114917 Ha 2) = -2947.687910 VP) = -2947.687910 VP) = -2947.96203 01764185 Hartree 1/mol -2950.74654945518 76004867 Hartree 33313 Hartree 33313 Hartree -0.081411 -1.068460 -1.484275 -1.236036 1.543663 -0.557257 0.485621 -1.743396 -2.906151 -3.344766 -4.221885 -2.694908 -3.055403 -1.600941 -1.124377 -1.099771 -3.692425 -4.973150 -5.659777 -5.515151 -4.753715 -2.843139	692649 Hartree 2391801 Hartree  6 Hartree  0.367559 3.592250 1.908412 -0.214424 -0.374777 2.120995 2.347673 -1.048130 -1.823458 -2.752194 -3.375767 -2.905783 -3.647590 -2.093756 -2.206254 -1.141075 -1.651573 -2.510667 -2.252522 -2.329609 -3.595891 -2.088783	
СССНН НСНННСНННССНННСНННССНННССН	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158 3.350270 2.837118 3.782837 4.185386 -0.184292 0.650852 1.609293 0.092617 0.893550 -0.528447 -1.183396 -1.075330 0.377924 -1.52734 -1.398624 -2.115723 -2.131346 -2.872140 -3.457415 -4.858156 -5.344943 -5.656182 -6.749359 -5.062340 -5.709821	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402 -1.029144 -0.673862 -2.025747 -0.331210 3.279501 3.575227 4.064825 4.251469 2.655724 4.643738 4.540356 5.258170 5.208209 2.617897 1.666231 3.292317 2.406728 -0.171741 0.633614 0.767489 1.384986 0.127750 0.250039 -0.676368 -1.178517	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654 1.800435 0.889760 1.577145 2.012070 1.832086 0.567606 0.832958 -0.112120 0.005914 2.465658 3.353676 1.722743 2.762808 1.451687 0.906820 0.796875 2.355967 -0.762807 -1.793112 -1.789361 -2.554155 -0.837185 -0.860724 0.138964 0.867868	E (M06/ E (PBE E (PBE) E (PM6) E (PM7) E (GB97 E (GFN1) E (GFN2) E (GFN2) E (GFN2) E (GFN2) E (GFN2) E (GFN2) E (GFN3) E	def2-TZVP) = -2948 - D3 (BJ)/def2-TZVI) - D3 (BJ)/def2-TZVI - D3 (BJ)/def2-TZVI - D3 (BJ)/def2-TZVI - D3 (BJ)/def2-TZVI = -302944 .9463( = -239 .70165 Kcall = -237 .61489 Kcall X-V/def2-TZVP) = -183 .2273' -XTB) = -183 .2273' -XTB) = -119 .35618 FF) = -16 .23488143'  nates:	3.907235114917 Ha P) = -2947.687910 VP) = -2947.96203 D1764185 Hartree 1/mol 1	692649 Hartree 2391801 Hartree  6 Hartree  0.367559 3.592250 1.908412 -0.214424 -0.374777 2.120995 2.347673 -1.048130 -1.823458 -2.752194 -3.375767 -2.905783 -3.647590 -2.093756 -2.206254 -1.141075 -1.651573 -2.510667 -2.252522 -2.329609 -3.595891 -2.088783 -3.158175	
СССНН НСНННСНННССНННСНННСНННСССНСНСССС	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158 3.350270 2.837118 3.782837 4.185386 -0.184292 0.650852 1.609293 0.092617 0.893550 -0.528447 -1.183396 -1.075330 0.377924 -1.527234 -1.938624 -2.115723 -2.131346 -2.872140 -3.457415 -4.858156 -5.344943 -5.656182 -6.749359 -5.062340 -5.709821 -3.667131	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402 -1.029144 -0.673862 -2.025747 -0.331210 3.279501 3.575227 4.064825 4.251469 2.655724 4.643738 4.540356 5.258170 5.208209 2.617897 1.666231 3.292317 2.406728 -0.171741 0.633614 0.767489 1.384986 0.127750 0.250039 -0.676368 -1.178517 -0.852795 1.310101	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654 1.800435 0.889760 1.577145 2.012070 1.832086 0.567606 0.832958 -0.112120 0.005914 2.465658 3.353676 1.722743 2.762808 1.451687 0.906820 0.796875 2.355967 -0.762807 -1.793112 -1.789361 -2.554155 -0.837185 -0.860724 0.138964 0.867868 0.213710	E (M06/ E (PBE E (PBE0 E (PBE	def2-TZVP) = -2948 - D3 (BJ)/def2-TZVI) - D3 (BJ)/def2-TZVI = -239.70165 Kcai = -237.61489 Kcai X-V/def2-TZVP) =XTB) = -183.2273' -XTB) = -119.35618 FF) = -16.23488143'  nates:	3.907235114917 Ha 2) = -2947.687910 VP) = -2947.96203 D1764185 Hartree L/mol L/mol L/mol -2950.74654945518 76004867 Hartree 33313 Hartree  -0.081411 -1.068460 -1.484275 -1.236036 1.543663 -0.557257 0.485621 -1.743396 -2.906151 -3.344766 -4.221885 -2.694908 -3.055403 -1.124377 -1.099771 -3.692425 -4.973150 -5.659777 -5.515151 -4.753715 -2.843139 -2.563544 -3.414094 -1.906614	692649 Hartree 2391801 Hartree  6 Hartree  0.367559 3.592250 1.908412 -0.214424 -0.374777 2.120995 2.347673 -1.048130 -1.823458 -2.752194 -3.375767 -2.905783 -3.647590 -2.093756 -2.206254 -1.141075 -1.651573 -2.510667 -2.252522 -2.329609 -3.595891 -2.088783 -3.158175 -1.949498	
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СССНН НСНННСИНННСОНННСИНННСОСНСИСИСИСИ	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158 3.350270 2.837118 3.782837 4.185386 -0.184292 0.650852 1.609293 0.092617 0.893550 -0.528447 -1.183396 -1.075330 0.377924 -1.527234 -1.398624 -2.115723 -2.131346 -2.872140 -3.457415 -4.858156 -5.344943 -5.656182 -6.749359 -5.062340 -5.709821 -3.667131 -2.616246 -3.498930 -2.855762	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402 -1.029144 -0.673862 -2.025747 -0.331210 3.279501 3.575227 4.064825 4.251469 2.655724 4.643738 4.540356 5.258170 5.208209 2.617897 1.666231 3.292317 2.406728 -0.171741 0.633614 0.767489 1.384986 0.127750 0.250039 -0.676368 -1.178517 -0.852795 1.310101 2.094578 2.535825	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654 1.800435 0.889760 1.577145 2.012070 1.832086 0.567606 0.832958 -0.112120 0.005914 2.465658 3.353676 1.722743 2.762808 1.451687 0.906820 0.796875 2.355967 -0.762807 -1.793112 -1.789361 -2.554155 -0.837185 -0.860724 0.138964 0.867868 0.213710 -2.901319 -3.893422 -4.680953	E (M06/E (PBE) E (PBE) E (PPBC) E (PM6) E (PM7) E (GB91) E (GFN2) E (GFN2) Coordi Ti Si O C C H C C C H C C H C H C H C H C H C	def2-TZVP) = -2948 - D3 (BJ)/def2-TZVI) - D3 (BJ)/def2-TZVI = -239.70165 Kcal = -237.61489 Kcal X-V/def2-TZVP) = -183.2273 -XTB) = -183.2273 -XTB) = -119.35618 FF) = -16.23488143  nates:	3.907235114917 Ha P) = -2947.687910 VP) = -2947.96203 D1764185 Hartree 1/mol 1	692649 Hartree 2391801 Hartree 2391801 Hartree  6 Hartree  0.367559 3.592250 1.908412 -0.214424 -0.374777 2.120995 2.347673 -1.048130 -1.823458 -2.752194 -3.375767 -2.905783 -3.647590 -2.093756 -2.206254 -1.141075 -1.651573 -2.510667 -2.252522 -2.329609 -3.595891 -2.088783 -3.158175 -1.949498 -1.504764 -0.179516 0.506250	
СССНН НСНННСИНННСИНННСИНННСИННСООНОНСССИН	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158 3.350270 2.837118 3.782837 4.185386 -0.184292 0.650852 1.609293 0.092617 0.893550 -0.528447 -1.183396 -1.075330 0.377924 -1.527234 -1.398624 -2.115723 -2.131346 -2.872140 -3.457415 -4.858156 -5.344943 -5.656182 -6.749359 -5.062340 -5.709821 -3.667131 -2.616246 -3.498930 -2.855762 -4.043588	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402 -1.029144 -0.673862 -2.025747 -0.331210 3.279501 3.575227 4.064825 4.251469 2.655724 4.643738 4.540356 5.258170 5.208209 2.617897 1.666231 3.292317 2.406728 -0.171741 0.633614 0.767489 1.384986 0.127750 0.250039 -0.676368 -1.178517 -0.852795 1.310101 2.094578 2.535825 2.926358	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654 1.800435 0.889760 1.577145 2.012070 1.832086 0.567606 0.832958 -0.112120 0.005914 2.465658 3.353676 1.722743 2.762808 1.451687 0.906820 0.796875 2.355967 -0.762807 -1.793112 -1.789361 -2.554155 -0.837185 -0.860724 0.138964 0.867868 0.213710 -2.901319 -3.893422 -4.680953 -3.403024	E (M06/ E (PBE E (PBE) E (PM6) E (PM7) E (GB97 E (GFN1 E (GFN2	def2-TZVP) = -2948 - D3 (BJ)/def2-TZVI) - D3 (BJ)/def2-TZVI - D3 (BJ)/def2-TZVI - D3 (BJ)/def2-TZVI - D3 (BJ)/def2-TZVI = -3c) = -2944.9463( = -239.70165 Kcai = -237.61489 Kcai X-V/def2-TZVP) =XTB) = -183.2273' -XTB) = -119.35618 FF) = -16.23488143'  mates:	3.907235114917 Ha 2) = -2947.687910 VP) = -2947.96203 D1764185 Hartree 1/mol 1	692649 Hartree 2391801 Hartree 2391801 Hartree  6 Hartree  0.367559 3.592250 1.908412 -0.214424 -0.374777 2.120995 2.347673 -1.048130 -1.823458 -2.752194 -3.375767 -2.905783 -3.647590 -2.093756 -2.206254 -1.141075 -1.651573 -2.510667 -2.252522 -2.329609 -3.595891 -2.088783 -3.158175 -1.949498 -1.504764 -0.179516 0.506250 -0.059849	
СССНН НСНННСИННИСИННИСИННОИННСОСИСИСИСИСИИ	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158 3.350270 2.837118 3.782837 4.185386 -0.184292 0.650852 1.609293 0.092617 0.893550 -0.528447 -1.183396 -1.075330 0.377924 -1.527234 -1.398624 -2.115723 -2.131346 -2.872140 -3.457415 -4.858156 -5.344943 -5.656182 -6.749359 -5.062340 -5.709821 -3.667131 -2.616246 -3.498930 -2.855762 -4.043588 -4.238957	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402 -1.029144 -0.673862 -2.025747 -0.331210 3.279501 3.575227 4.064825 4.251469 2.655724 4.643738 4.540356 5.258170 5.208209 2.617897 1.666231 3.292317 2.406728 -0.171741 0.633614 0.767489 1.384986 0.127750 0.250039 -0.676368 -1.178517 -0.852795 1.310101 2.094578 2.535825 2.926358 1.441613	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654 1.800435 0.889760 1.577145 2.012070 1.832086 0.567606 0.832958 -0.112120 0.005914 2.465658 3.353676 1.722743 2.762808 1.451687 0.906820 0.796875 2.355967 -0.762807 -1.793112 -1.789361 -2.554155 -0.837185 -0.860724 0.138964 0.867868 0.213710 -2.901319 -3.893422 -4.680953 -3.403024 -4.397286	E (M06/ E (PBE C (PBE) E (PBE) E (PBE) E (PM6) E (PM7) E (GB97 E (GFN1 E (GFN2 E (GFN- C O C C C C C C C C C C C C C C C C C	def2-TZVP) = -2948 - D3 (BJ)/def2-TZVI = -30, 70165 Kcai = -237.61489 Kcai X-V/def2-TZVP) =	3.907235114917 Ha P) = -2947.687910 P) = -2947.96203 D1764185 Hartree L/mol L/mol L/mol -2950.74654945518 R6004867 Hartree 33313 Hartree -0.081411 -1.068460 -1.484275 -1.236036 1.543663 -0.557257 0.485621 -1.743396 -2.906151 -3.344766 -4.221885 -2.694908 -3.055403 -1.124377 -1.099771 -3.692425 -4.973150 -5.659777 -5.515151 -4.753715 -2.843139 -2.563544 -3.414094 -1.906614 -4.135008 -3.273440 -4.750915 -4.751069	692649 Hartree 2391801 Hartree  6 Hartree  0.367559 3.592250 1.908412 -0.214424 -0.374777 2.120995 2.347673 -1.048130 -1.823458 -2.752194 -3.375767 -2.905783 -3.647590 -2.905783 -3.647590 -2.093756 -2.206254 -1.141075 -1.651573 -2.510667 -2.252522 -2.329609 -3.595891 -2.088783 -3.158175 -1.949498 -1.504764 -0.179516 0.506250 -0.059849 0.134143	
СССНН НСНННСИН НСОНННОНННОНННССОНСНССССНННС	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158 3.350270 2.837118 3.782837 4.185386 -0.184292 0.650852 1.609293 0.092617 0.893550 -0.528447 -1.183396 -1.075330 0.377924 -1.527234 -1.398624 -2.115723 -2.131346 -2.872140 -3.457415 -4.858156 -5.344943 -5.656182 -6.749359 -5.062340 -5.709821 -3.667131 -2.616246 -3.498930 -2.855762 -4.238957 -1.876628	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402 -1.029144 -0.673862 -2.025747 -0.331210 3.279501 3.575227 4.064825 4.251469 2.655724 4.643738 4.540356 5.258170 5.208209 2.617897 1.666231 3.292317 2.406728 -0.171741 0.633614 0.767489 1.384986 0.127750 0.250039 -0.676368 -1.178517 -0.852795 1.310101 2.094578 2.535825 2.926358 1.441613 0.222806	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654 1.800435 0.889760 1.577145 2.012070 1.832086 0.567606 0.832958 -0.112120 0.005914 2.465658 3.353676 1.722743 2.762808 1.451687 0.906820 0.796875 2.355967 -0.762807 -1.793112 -1.789361 -2.554155 -0.837185 -0.860724 0.138964 0.867868 0.213710 -2.901319 -3.893422 -4.680953 -3.403024 -4.397286 -3.714218	E (M06/E (PBE) E (PBE) E (PPE) E (PM6) E (PM7) E (GFN1 E (GFN2 E (GFN2 COORDI Ti Si O C C H C C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C C C H C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C H C C C C H C C C H C C C C H C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C H C C C C C C H C C C C C C H C C C C C C C H C C C C C C C C C C C C C C C C C C C C	def2-TZVP) = -2948 - D3 (BJ)/def2-TZVI) - D3 (BJ)/def2-TZVI - D3 (BJ)/def2-TZVI - 3c) = -2944.9463 = -239.70165 Kcai = -237.61489 Kcai X-V/def2-TZVP) =xTB) = -183.2273 -xTB) = -119.35618 FF) = -16.23488143  nates:  0.356914 0.293980 3.018437 -0.938803 0.758781 1.373867 1.709618 -1.884530 -1.570194 -2.532542 -2.320498 -3.759656 -4.487838 -4.068037 -5.049386 -3.160319 -0.250653 -0.229568 -1.060418 0.720308 -0.281938 0.961841 0.885547 1.903100 1.048733 -0.099043 -0.030752 0.816043 -0.965663 -3.579229	3.907235114917 Ha 2) = -2947.687910 VP) = -2947.687910 VP) = -2947.96203 01764185 Hartree 1/mol -2950.74654945518 76004867 Hartree 33313 Hartree 33313 Hartree 33313 Hartree 34457274 Hartree 33313 Hartree 344575 -1.236036 -1.484275 -1.236036 -1.543663 -0.557257 0.485621 -1.743396 -2.906151 -3.344766 -4.221885 -2.694908 -3.055403 -1.600941 -1.124377 -1.099771 -3.692425 -4.973150 -5.659777 -5.515151 -4.753715 -2.843139 -2.563544 -3.414094 -1.906614 -4.135008 -3.273440 -4.750915 -4.751069 0.075809	692649 Hartree 2391801 Hartree  6 Hartree  0.367559 3.592250 1.908412 -0.214424 -0.374777 2.120995 2.347673 -1.048130 -1.823458 -2.752194 -3.375767 -2.905783 -3.647590 -2.093756 -2.206254 -1.141075 -1.651573 -2.510667 -2.252522 -2.329609 -3.595891 -2.088783 -3.158175 -1.949498 -1.504764 -0.179516 0.506250 -0.059849 0.134143 -0.226477	
СССНН НСНННСИНННСОНННСИНННСИННСОСНСНСИССИНННСИ	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158 3.350270 2.837118 3.782837 4.185386 -0.184292 0.650852 1.609293 0.092617 0.893550 -0.528447 -1.183396 -1.075330 0.377924 -1.527234 -1.398624 -2.115723 -2.131346 -2.872140 -3.457415 -4.858156 -5.344943 -5.656182 -6.749359 -5.062340 -5.709821 -3.667131 -2.616246 -3.498930 -2.855762 -4.043588 -4.238957 -1.876628 -2.602981	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402 -1.029144 -0.673862 -2.025747 -0.331210 3.279501 3.575227 4.064825 4.251469 2.655724 4.643738 4.540356 5.258170 5.208209 2.617897 1.666231 3.292317 2.406728 -0.171741 0.633614 0.767489 1.384986 0.127750 0.250039 -0.676368 -1.178517 -0.852795 1.310101 2.094578 2.535825 2.926358 1.441613 0.222806 -0.439247	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654 1.800435 0.889760 1.577145 2.012070 1.832086 0.567606 0.832958 -0.112120 0.005914 2.465658 3.353676 1.722743 2.762808 1.451687 0.906820 0.796875 2.355967 -0.762807 -1.793112 -1.789361 -2.554155 -0.837185 -0.860724 0.138964 0.867868 0.213710 -2.901319 -3.893422 -4.680953 -3.403024 -4.397286 -3.714218 -4.227158	E (M06/E (PBE) E (PBE) E (PPBE) E (PM6) E (PM7) E (GB71 E (GFN2 COORDITI Si Si O C C H C C C H C H C H C H C H C C H C C C H C C C H C C C C H C C C C C C C C C C C C C C C C C C C C	def2-TZVP) = -2948 - D3 (BJ)/def2-TZVI) - D3 (BJ)/def2-TZVI = -239.70165 Kcal = -237.61489 Kcal X-V/def2-TZVP) = -183.2273 -XTB) = -183.2273 -XTB) = -119.35618 FF) = -16.23488143  nates:	3.907235114917 Ha P) = -2947.687910 VP) = -2947.96203 D1764185 Hartree 1/mol 1	692649 Hartree 2391801 Hartree  6 Hartree  0.367559 3.592250 1.908412 -0.214424 -0.374777 2.120995 2.347673 -1.048130 -1.823458 -2.752194 -3.375767 -2.905783 -3.647590 -2.093756 -2.206254 -1.141075 -1.651573 -2.510667 -2.252522 -2.329609 -3.595891 -2.088783 -3.158175 -1.949498 -1.504764 -0.179516 0.506250 -0.059849 0.134143 -0.226477 1.254941	
СССНН НСНННСИНННСИНННСИНННСИННСОСИСИСОСИННСИН	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158 3.350270 2.837118 3.782837 4.185386 -0.184292 0.650852 1.609293 0.092617 0.893550 -0.528447 -1.183396 -1.075330 0.377924 -1.527234 -1.398624 -2.115723 -2.131346 -2.872140 -3.457415 -4.858156 -5.344943 -5.656182 -6.749359 -5.062340 -5.709821 -3.667131 -2.616246 -3.498930 -2.855762 -4.043588 -4.238957 -1.876628 -2.602981 -1.246942	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402 -1.029144 -0.673862 -2.025747 -0.331210 3.279501 3.575227 4.064825 4.251469 2.655724 4.643738 4.540356 5.258170 5.208209 2.617897 1.666231 3.292317 2.406728 -0.171741 0.633614 0.767489 1.384986 0.127750 0.250039 -0.676368 -1.178517 -0.852795 1.310101 2.094578 2.535825 2.926358 1.441613 0.222806 -0.439247 -0.411721	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654 1.800435 0.889760 1.577145 2.012070 1.832086 0.567606 0.832958 -0.112120 0.005914 2.465658 3.353676 1.722743 2.762808 1.451687 0.906820 0.796875 2.355967 -0.762807 -1.793112 -1.789361 -2.554155 -0.837185 -0.860724 0.138964 0.867868 0.213710 -2.901319 -3.893422 -4.680953 -3.403024 -4.397286 -3.714218 -4.227158 -3.068598	E (M06/E (PBE E (PBE)) E (PBE) E (PPM6) E (PM7) E (GB97 E (GFN1) Si Si O C H C C H C C H C H C H C H C H C H C	def2-TZVP) = -2948 - D3 (BJ)/def2-TZVI) - D3 (BJ)/def2-TZVI = -30, 70165 Kcai = -237.61489 Kcai X-V/def2-TZVP) = -183.2273 -XTB) = -183.2273 -XTB) = -16.23488143  nates:	3.907235114917 Ha 2) = -2947.687910 VP) = -2947.96203 D1764185 Hartree 1/mol 1	692649 Hartree 2391801 Hartree  6 Hartree  0.367559 3.592250 1.908412 -0.214424 -0.374777 2.120995 2.347673 -1.048130 -1.823458 -2.752194 -3.375767 -2.905783 -3.647590 -2.093756 -2.206254 -1.141075 -1.651573 -2.510667 -2.252522 -2.329609 -3.595891 -2.088783 -3.158175 -1.949498 -1.504764 -0.179516 0.506250 -0.059849 0.134143 -0.226477 1.254941 1.478140	
СССНН НСНННСИННИСИННИИНИИНИСИННИСИНИСИСИНИИИНИИ	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158 3.350270 2.837118 3.782837 4.185386 -0.184292 0.650852 1.609293 0.092617 0.893550 -0.528447 -1.183396 -1.075330 0.377924 -1.527234 -1.398624 -2.115723 -2.131346 -2.872140 -3.457415 -4.858156 -5.344943 -5.656182 -6.749359 -5.062340 -5.709821 -3.667131 -2.616246 -3.498930 -2.855762 -4.043588 -4.238957 -1.876628 -2.602981 -1.246942 -1.230830	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402 -1.029144 -0.673862 -2.025747 -0.331210 3.279501 3.575227 4.064825 4.251469 2.655724 4.643738 4.540356 5.258170 5.208209 2.617897 1.666231 3.292317 2.406728 -0.171741 0.633614 0.767489 1.384986 0.127750 0.250039 -0.676368 -1.178517 -0.852795 1.310101 2.094578 2.535825 2.926358 1.441613 0.222806 -0.439247 -0.411721 0.688920	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654 1.800435 0.889760 1.577145 2.012070 1.832086 0.567606 0.832958 -0.112120 0.005914 2.465658 3.353676 1.722743 2.762808 1.451687 0.906820 0.796875 2.355967 -0.762807 -1.793112 -1.789361 -2.554155 -0.837185 -0.860724 0.138964 0.867868 0.213710 -2.901319 -3.893422 -4.680953 -3.403024 -4.397286 -3.714218 -4.227158 -3.068598 -4.487559	E (M06/E (PBE E (PBE)) E (PBE) E (PPBE) E (PM6) E (PM7) E (GB97 E (GFN1 Ti Si Si O C C C C C C C C C C C C C C C C C C	def2-TZVP) = -2948 - D3 (BJ)/def2-TZVI) - D3 (BJ)/def2-TZVI = -30, 70165 Kcai = -237.61489 Kcai X-V/def2-TZVP) = -183.2273* -xTB) = -183.2273* -xTB) = -119.35618 FF) = -16.23488143*  nates:	3.907235114917 Ha P) = -2947.687910 P) = -2947.96203 D1764185 Hartree P/mol L/mol L/mol -2950.74654945518 R6004867 Hartree 33313 Hartree -0.081411 -1.068460 -1.484275 -1.236036 1.543663 -0.557257 0.485621 -1.743396 -2.906151 -3.344766 -4.221885 -2.694908 -3.055403 -1.600941 -1.124377 -1.099771 -3.692425 -4.973150 -5.6559777 -5.515151 -4.753715 -2.843139 -2.563544 -3.414094 -1.906614 -4.135008 -3.273440 -4.750915 -4.751069 0.075809 -0.341430 -1.206838 0.494229	692649 Hartree 2391801 Hartree  6 Hartree  0.367559 3.592250 1.908412 -0.214424 -0.374777 2.120995 2.347673 -1.048130 -1.823458 -2.752194 -3.375767 -2.905783 -3.647590 -2.905783 -3.647590 -2.093756 -2.206254 -1.141075 -1.651573 -2.510667 -2.252522 -2.329609 -3.595891 -2.088783 -3.158175 -1.949498 -1.504764 -0.179516 0.506250 -0.059849 0.134143 -0.226477 1.254941 1.478140 1.921263	
СССНН НСНННСИНННСИНННСИНННСИННСОСИСНССОСИННСИН	0.606191 2.393719 3.199393 4.072178 3.584398 2.577590 1.233456 0.551144 1.629800 0.629158 3.350270 2.837118 3.782837 4.185386 -0.184292 0.650852 1.609293 0.092617 0.893550 -0.528447 -1.183396 -1.075330 0.377924 -1.527234 -1.398624 -2.115723 -2.131346 -2.872140 -3.457415 -4.858156 -5.344943 -5.656182 -6.749359 -5.062340 -5.709821 -3.667131 -2.616246 -3.498930 -2.855762 -4.043588 -4.238957 -1.876628 -2.602981 -1.246942	3.806688 2.375938 -1.124792 -1.745581 -1.123473 -2.735991 -1.904499 -2.098824 -2.179997 -3.110757 -1.777402 -1.029144 -0.673862 -2.025747 -0.331210 3.279501 3.575227 4.064825 4.251469 2.655724 4.643738 4.540356 5.258170 5.208209 2.617897 1.666231 3.292317 2.406728 -0.171741 0.633614 0.767489 1.384986 0.127750 0.250039 -0.676368 -1.178517 -0.852795 1.310101 2.094578 2.535825 2.926358 1.441613 0.222806 -0.439247 -0.411721	4.435277 2.809405 3.009099 4.168657 4.451519 3.853408 5.072237 2.703960 3.573361 2.481022 1.833654 1.800435 0.889760 1.577145 2.012070 1.832086 0.567606 0.832958 -0.112120 0.005914 2.465658 3.353676 1.722743 2.762808 1.451687 0.906820 0.796875 2.355967 -0.762807 -1.793112 -1.789361 -2.554155 -0.837185 -0.860724 0.138964 0.867868 0.213710 -2.901319 -3.893422 -4.680953 -3.403024 -4.397286 -3.714218 -4.227158 -3.068598	E (M06/E (PBE E (PBE)) E (PBE) E (PPM6) E (PM7) E (GB97 E (GFN1) Si Si O C H C C H C C H C H C H C H C H C H C	def2-TZVP) = -2948 - D3 (BJ)/def2-TZVI) - D3 (BJ)/def2-TZVI = -30, 70165 Kcai = -237.61489 Kcai X-V/def2-TZVP) = -183.2273 -XTB) = -183.2273 -XTB) = -16.23488143  nates:	3.907235114917 Ha 2) = -2947.687910 VP) = -2947.96203 D1764185 Hartree 1/mol 1	692649 Hartree 2391801 Hartree  6 Hartree  0.367559 3.592250 1.908412 -0.214424 -0.374777 2.120995 2.347673 -1.048130 -1.823458 -2.752194 -3.375767 -2.905783 -3.647590 -2.093756 -2.206254 -1.141075 -1.651573 -2.510667 -2.252522 -2.329609 -3.595891 -2.088783 -3.158175 -1.949498 -1.504764 -0.179516 0.506250 -0.059849 0.134143 -0.226477 1.254941 1.478140	

С	-5.054687	0.470850	-0.446444	С	-1.141709	2.635909	1.003867
Н	-5.239677	0.853759	-1.470027	C	-0.999992	3.188084	2.317429
Н	-5.321460	1.280614	0.261814	C	-1.867937	4.237536	2.671533
H	-5.743868	-0.376739	-0.260380	H	-1.795701	4.686036	3.669668
C	-2.742348	1.341441	-0.513914	C	-2.826093	4.733668	1.783606
H	-1.674408	1.233196	-0.242288	H	-3.489217	5.556362	2.089891
H	-3.132543	2.198161	0.073027	C	-2.937943	4.182947	0.504453
H	-2.780060	1.617251	-1.585993	Н	-3.695291	4.590380	-0.176046
С	0.709229	2.714553	-1.059431	С	-2.113321	3.126265	0.073117
C	0.834122	2.691160	-2.492711	C	0.059335	2.680796	3.323807
C	0.705873			C	-0.172497		3.660040
		3.909062	-3.181872			1.191387	
H	0.791460	3.921929	-4.274987	H	-1.193620	1.027094	4.057631
С	0.457114	5.113418	-2.516844	H	0.555133	0.853071	4.426508
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C	0.372022	5.117444	-1.126816	C	1.477339	2.881869	2.743970
H	0.184861	6.071661	-0.614673	Н	1.609188	2.345621	1.789169
С	0.520556	3.945983	-0.353929	Н	2.241047	2.513130	3.459858
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H	2.494818	-0.275862	-3.372705	H	0.191014	4.535625	4.523927
H	2.253161	0.372877	-1.724102	H	0.784091	3.060481	5.337671
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C	1.308939	1.674801	-4.795041	C	-2.294816	2.537673	-1.348025
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H	1.076098	6.274317	1.143235	Н	-3.082375	4.383269	-2.280007
С	-1.042488	4.495304	1.541259	С	-1.309348	-2.548730	-0.363288
Н	-1.389184	5.399945	1.003849	C	-2.095455	-3.071308	0.719875
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H	-1.722676	3.661766	1.274647	Н	-3.434807	-4.677706	1.286889
С	0.838043	2.937867	2.038680	С	-2.815131	-4.885587	-0.762895
H	0.121522	2.100065	1.955885	H	-3.392684	-5.808999	-0.917437
H	0.855200	3.240820	3.105835	С	-2.071810	-4.337853	-1.806548
H	1.847054	2.569547	1.771359	H	-2.078126	-4.845435	-2.781818
C	-0.711940	-2.634263	3.232630	C	-1.312816	-3.157700	-1.654836
H	-1.397460	-2.503439	2.372121	C	-2.158759	-2.387243	2.105867
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H	-0.053867	-3.497845	3.011466	H	-0.819883	-1.900156	3.772883
С	1.314005	-1.390597	5.166457	Н	-0.030660	-1.782695	2.171812
H	2.017565	-2.239686	5.053241	Н	-0.363590	-3.390235	2.878041
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H	-1.551200		3.188714	H	-2.842287	-0.490845	2.969318
C	2.845701	-3.349320	2.195524	H	-3.728652	-0.981038	1.488696
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Н	3.975120	-0.931753	4.187627	C	0.514600	-3.729398	-3.282249
C	3.770145	-1.225571	0.181407	Н	1.244999	-3.850645	-2.457254
Н		-1.225571				-3.850645	
	3.154136		-0.621743	H	1.072099		-4.191881
H	4.775373	-1.695749	0.135459	H	0.064419	-4.721992	-3.479094
Н	3.896619	-0.147248	-0.048388	С	-1.567512	-2.538438	-4.085123
				H	-2.078384	-3.491786	-4.318021
	mation 33.			H	-1.045435	-2.205411	-5.005650
Multip	licity: 2			H	-2.347128	-1.788207	-3.841515
Charge	: 0			C	3.959452	-2.059147	-1.836411
E(B97-	3c) = -2948.79789	7032777 Hartree		Н	3.091351	-2.155250	-2.517969
		8.911673040435 Hai	rtree	Н	4.455948	-3.050345	-1.787155
		P) = -2947.6901769		Н	4.674254	-1.346488	-2.293068
		VP) = -2947.965346			4.968422	-1.408041	1.015545
	-3c) = -2944.9501		DIIZIIO NGICICC	Н	5.665158	-0.623162	0.661177
	= -243.08368 Kca			H	5.517389	-2.372450	1.041367
	= -239.63652 Kca		2 77	H	4.676443	-1.158857	2.057047
		-2950.749844454588	d Hartree	С	2.384847	-2.963456	0.616050
	-xTB) = $-183.9220$			H	2.061722	-2.755816	1.656491
	-xTB) = $-119.3590$			H	2.996272	-3.890148	0.637381
E (GFN-	FF) = -16.2422956	14269 Hartree		H	1.475197	-3.170573	0.017880
				C	2.598041	3.187905	-0.735255
Coordi	nates:			H	1.497289	3.265971	-0.645706
Ti	0.441880	0.048089	0.141416	H	2.934201	3.927025	-1.492281
Si	3.428986	-1.540195	-0.088390	H	3.038527	3.483354	0.238139
Si	3.183687	1.457676	-1.251333	C	2.641027	1.164395	-3.045736
0	-0.321179	1.624142	0.632865	Н	2.936446	0.163095	-3.414454
Ö	-0.544562	-1.457561	-0.140713	Н	3.115199	1.923267	-3.702529
C	2.508642	0.121297	-0.081053	Н	1.542961	1.259456	-3.159978
Н	2.649524	0.541980	0.954145	C	5.085666	1.538263	-1.222823
11	2.047724	0.041700	0.734143	_	5.005000	1.000200	1.222023

Н	5.456895	1.751252	-0.199329	Н	-4.034875	0.383943	1.415647
Н	5.431849	2.359329	-1.885127	Н	-4.419528	0.357518	-0.338640
Н	5.564993	0.601290	-1.569341	C	-4.765196	-2.113024	0.848174
	3.301333	0.001290	1.000011	Н	-5.603784	-1.855377	0.170868
Confor	mation 34.			H	-5.028203	-1.743156	1.859270
							0.908071
	olicity: 2			H	-4.691013	-3.217218	
Charge				C	2.909542	2.568401	1.223824
	3c) = -2948.79360			H	2.383454	3.223406	1.949643
	def2-TZVP) = -294			H	3.992094	2.804652	1.288200
	- D3(BJ)/def2-TZV			H	2.766264	1.519776	1.549908
	- D3(BJ)/def2-TZ		6829451 Hartree	C	3.317663	1.859221	-1.757976
E (PBEh	(-3c) = -2944.9460	18581296 Hartree		H	3.243664	0.772884	-1.553094
E(PM6)	= -241.79341 Kca	1/mol		H	4.386384	2.147408	-1.674810
E(PM7)	= -238.47640 Kca	1/mol		H	3.001353	2.028141	-2.806066
E(ωB97	X-V/def2-TZVP) =	-2949.53337930620	7 Hartree	С	2.610865	4.719834	-0.902847
E (GFN1	-xTB) = $-184.3214$	34540650 Hartree		H	2.345867	4.999703	-1.942355
E (GFN2	-xTB) = $-119.3552$	82959582 Hartree		H	3.687721	4.947281	-0.756627
E (GFN-	FF) = -16.2392705	60723 Hartree		H	2.030632	5.371269	-0.217456
				С	-2.154366	2.240781	-2.451978
Coordi	nates:			Н	-2.005910	1.166044	-2.674617
Ti	-0.020270	0.524757	-0.014373	Н	-2.683997	2.702265	-3.311722
Si	2.279271	2.881064	-0.542367	Н	-2.826789	2.308164	-1.572098
Si	-0.516942	3.154804	-2.145403	C	0.487665	3.076762	-3.754793
0	0.727286	-0.069710	1.534704	Н	1.412070	3.686040	-3.700737
0	-1.057999	-0.566998	-1.025009	H	-0.127172	3.472415	-4.589660
C	0.436812	2.451505	-0.665384	H	0.777764	2.039677	-4.015164
Н	-0.038745	2.923543	0.239274	C	-0.970221	4.968206	-1.804275
C	1.102536	-0.684409	2.678865	Н	-1.588349	5.051866	-0.886002
C	1.928937	-1.856255	2.592700	H	-1.559116	5.389486	-2.645788
C	2.310140	-2.471585	3.797020	н	-0.069538		
				п	-0.069538	5.597982	-1.664513
H	2.942728	-3.367069	3.770844	~ .			
С	1.902291	-1.976195	5.040617		rmation 9.		
H	2.215032	-2.479909	5.967279		olicity: 2		
С	1.098026	-0.839403	5.095099	Charge			
H	0.786335	-0.460744	6.079457		-3c) = -2948.80485		
C	0.674419	-0.156906	3.934797		def2-TZVP) = -294		
C	2.387443	-2.454175	1.241307		- D3(BJ)/def2-TZV		
С	3.326258	-3.661941	1.441444	E(PBEC	) - D3(BJ)/def2-TZ	VP) = -2947.97099	9992164 Hartree
H	4.245689	-3.388646	1.997082	E (PBEh	n-3c) = -2944.9547	22030579 Hartree	
H	3.638564	-4.045641	0.449579	E(PM6)	= -242.88212 Kca.	l/mol	
H	2.830167	-4.496217	1.976371	E(PM7)	= -240.24007 Kca.	l/mol	
С	1.165359	-2.968548	0.445928	E(ωB97	7X-V/def2-TZVP) =	-2950.75388613385	5 Hartree
H	0.614819	-3.735869	1.025962	E(GFN1	1-xTB) = $-184.6767$	67207757 Hartree	
			0 500004	F (CENC	2-xTB) = $-119.3648$	70040051	
H	1.494456	-3.432963	-0.506934	E (GEN2	- MID) - IJ. JOIO	/U949251 Hartree	
H	0.445224	-2.170087	0.192610		-FF) = $-16.2411078$		
H C	0.445224 3.181372	-2.170087 -1.413950	0.192610 0.419050	E (GFN-	-FF) = -16.2411078		
H C H	0.445224 3.181372 2.568968	-2.170087 -1.413950 -0.535212	0.192610 0.419050 0.147095	E (GFN- Coordi	-FF) = -16.2411078 inates:	33530 Hartree	-0.234362
H C H H	0.445224 3.181372 2.568968 3.550241	-2.170087 -1.413950 -0.535212 -1.869780	0.192610 0.419050 0.147095 -0.522901	E (GFN- Coordi Ti	-FF) = -16.2411078 inates: 0.382302	-0.113896	-0.234362 -1.694703
Н С Н Н	0.445224 3.181372 2.568968 3.550241 4.058264	-2.170087 -1.413950 -0.535212 -1.869780 -1.047063	0.192610 0.419050 0.147095 -0.522901 0.989452	E (GFN- Coordi Ti Si	-FF) = -16.2411078 inates: 0.382302 2.987610	-0.113896 1.634351	-1.694703
Н С Н Н С	0.445224 3.181372 2.568968 3.550241 4.058264 -0.205982	-2.170087 -1.413950 -0.535212 -1.869780 -1.047063 1.099506	0.192610 0.419050 0.147095 -0.522901 0.989452 4.175453	E (GFN- Coordi Ti Si Si	-FF) = -16.2411078 inates:	-0.113896 1.634351 -1.578517	-1.694703 -1.310113
H C H H C C	0.445224 3.181372 2.568968 3.550241 4.058264 -0.205982 -0.693362	-2.170087 -1.413950 -0.535212 -1.869780 -1.047063 1.099506 1.858341	0.192610 0.419050 0.147095 -0.522901 0.989452 4.175453 2.926930	E (GFN-Coordi Ti Si Si	-FF) = -16.2411078 inates: 0.382302 2.987610 3.058992 0.367039	-0.113896 1.634351 -1.578517 0.892064	-1.694703 -1.310113 1.289678
H C H H C C	0.445224 3.181372 2.568968 3.550241 4.058264 -0.205982 -0.693362 0.149290	-2.170087 -1.413950 -0.535212 -1.869780 -1.047063 1.099506 1.858341 2.246661	0.192610 0.419050 0.147095 -0.522901 0.989452 4.175453 2.926930 2.326640	E (GFN-Coordi	-FF) = -16.2411078 inates: 0.382302 2.987610 3.058992 0.367039 -1.039142	-0.113896 1.634351 -1.578517 0.892064 -1.040786	-1.694703 -1.310113 1.289678 -0.926181
Н С Н Н С С Н	0.445224 3.181372 2.568968 3.550241 4.058264 -0.205982 -0.693362 0.149290 -1.298523	-2.170087 -1.413950 -0.535212 -1.869780 -1.047063 1.099506 1.858341 2.246661 2.729354	0.192610 0.419050 0.147095 -0.522901 0.989452 4.175453 2.926930 2.326640 3.253517	E (GFN-Coordi Ti Si Si O C	-FF) = -16.2411078 inates: 0.382302 2.987610 3.058992 0.367039 -1.039142 2.034670	-0.113896 1.634351 -1.578517 0.892064 -1.040786 0.013480	-1.694703 -1.310113 1.289678 -0.926181 -1.484187
Н С Н Н С С Н Н	0.445224 3.181372 2.568968 3.550241 4.058264 -0.205982 -0.693362 0.149290 -1.298523 -1.345623	-2.170087 -1.413950 -0.535212 -1.869780 -1.047063 1.099506 1.858341 2.246661 2.729354 1.236507	0.192610 0.419050 0.147095 -0.522901 0.989452 4.175453 2.926930 2.326640 3.253517 2.280569	E (GFN-Coordi Ti Si Si O C H	-FF) = -16.2411078 inates: 0.382302 2.987610 3.058992 0.367039 -1.039142 2.034670 1.476937	-0.113896 1.634351 -1.578517 0.892064 -1.040786 0.013480 -0.132437	-1.694703 -1.310113 1.289678 -0.926181 -1.484187 -2.442613
Н С Н Н С С Н Н С	0.445224 3.181372 2.568968 3.550241 4.058264 -0.205982 -0.693362 0.149290 -1.298523 -1.345623 0.616554	-2.170087 -1.413950 -0.535212 -1.869780 -1.047063 1.099506 1.858341 2.246661 2.729354 1.236507 2.113576	0.192610 0.419050 0.147095 -0.522901 0.989452 4.175453 2.926930 2.326640 3.253517 2.280569 5.009135	E (GFN-Coordi	-FF) = -16.2411078 inates: 0.382302 2.987610 3.058992 0.367039 -1.039142 2.034670 1.476937 -0.071879	-0.113896 1.634351 -1.578517 0.892064 -1.040786 0.013480 -0.132437 1.407400	-1.694703 -1.310113 1.289678 -0.926181 -1.484187 -2.442613 2.466064
Н С Н Н С С Н Н С Н Н С Н	0.445224 3.181372 2.568968 3.550241 4.058264 -0.205982 -0.693362 0.149290 -1.298523 -1.345623 0.616554 0.945285	-2.170087 -1.413950 -0.535212 -1.869780 -1.047063 1.099506 1.858341 2.246661 2.729354 1.236507 2.113576 1.691972	0.192610 0.419050 0.147095 -0.522901 0.989452 4.175453 2.926930 2.326640 3.253517 2.280569 5.009135 5.978532	E (GFN-Coordi	-FF) = -16.2411078 inates:	-0.113896 1.634351 -1.578517 0.892064 -1.040786 0.013480 -0.132437 1.407400 0.860267	-1.694703 -1.310113 1.289678 -0.926181 -1.484187 -2.442613 2.466064 3.689451
Н С Н Н С С Н Н С Н Н Н С Н Н Н Н Н Н Н	0.445224 3.181372 2.568968 3.550241 4.058264 -0.205982 -0.693362 0.149290 -1.298523 -1.345623 0.616554 0.945285	-2.170087 -1.413950 -0.535212 -1.869780 -1.047063 1.099506 1.858341 2.246661 2.729354 1.236507 2.113776 1.691972 3.018638	0.192610 0.419050 0.147095 -0.522901 0.989452 4.175453 2.926930 2.326640 3.253517 2.280569 5.009135 5.978532 5.222204	E (GFN-Coordi	-FF) = -16.2411078 inates: 0.382302 2.987610 3.058992 0.367039 -1.039142 2.034670 1.476937 -0.071879 0.432396 -0.096499	-0.113896 1.634351 -1.578517 0.892064 -1.040786 0.013480 -0.132437 1.407400 0.860267 1.369013	-1.694703 -1.310113 1.289678 -0.926181 -1.484187 -2.442613 2.466064 3.689451 4.890545
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Н С Н Н Н С С Н Н Н С Н Н Н С С	0.445224 3.181372 2.568968 3.550241 4.058264 -0.205982 -0.693362 0.149290 -1.298523 -1.345623 0.616554 0.945285 0.010571 1.523054 -1.470781 -2.073242 -2.105066 -1.227242 -1.808182 -1.397006	-2.170087 -1.413950 -0.535212 -1.869780 -1.047063 1.099506 1.858341 2.246661 2.729354 1.236507 2.113576 1.691972 3.018638 2.427370 0.678437 -0.045548 1.565020 0.204982 -1.502190 -2.000756	0.192610 0.419050 0.147095 -0.522901 0.989452 4.175453 2.926930 2.326640 3.253517 2.280569 5.009135 5.978532 5.222204 4.452882 4.962007 4.376135 5.169444 5.932600 -1.645082 -2.918016	E (GFN- Coordi Ti Si Si O C C H C C C H C C H C C H C C H C C C H C C C C C C C C C C C C C C C C C C C C	-FF) = -16.2411078  inates:	-0.113896 1.634351 -1.578517 0.892064 -1.040786 0.013480 -0.132437 1.407400 0.860267 1.369013 0.968741 2.377630 2.750019 2.924466 3.731121 2.471459 -0.235938	-1.694703 -1.310113 1.289678 -0.926181 -1.484187 -2.442613 2.466064 3.689451 4.890545 5.848887 4.902033 5.857497 3.695563 3.726755 2.451423 3.726734
Н С Н Н Н С С Н Н Н С Н Н Н С С С	0.445224 3.181372 2.568968 3.550241 4.058264 -0.205982 -0.693362 0.149290 -1.298523 -1.345623 0.616554 0.945285 0.010571 1.523054 -1.470781 -2.073242 -2.105066 -1.227242 -1.808182 -1.397006 -2.261993	-2.170087 -1.413950 -0.535212 -1.869780 -1.047063 1.099506 1.858341 2.246661 2.729354 1.236507 2.113576 1.691972 3.018638 2.427370 0.678437 -0.045548 1.565020 0.204982 -1.502190 -2.000756 -2.915697	0.192610 0.419050 0.147095 -0.522901 0.989452 4.175453 2.926930 2.326640 3.253517 2.280569 5.009135 5.978532 5.222204 4.452882 4.962007 4.376135 5.169444 5.932600 -1.645082 -2.918016 -3.554783	E (GFN- Coordi Ti Si Si O C C H C C H C C H C C C H C C C C C C	-FF) = -16.2411078 inates: 0.382302 2.987610 3.058992 0.367039 -1.039142 2.034670 1.476937 -0.071879 0.432396 -0.096499 0.256381 -1.063552 -1.462178 -1.508108 -2.250609 -1.029603 1.522435 1.967257	-0.113896 1.634351 -1.578517 0.892064 -1.040786 0.013480 -0.132437 1.407400 0.860267 1.369013 0.968741 2.377630 2.750019 2.924466 3.731121 2.471459 -0.235938 -0.553408	-1.694703 -1.310113 1.289678 -0.926181 -1.484187 -2.442613 2.466064 3.689451 4.890545 5.848887 4.902033 5.857497 3.695563 3.726755 2.451423 3.726734 5.169171
Н С Н Н Н С С Н Н Н С Н Н Н С С С Н	0.445224 3.181372 2.568968 3.550241 4.058264 -0.205982 -0.693362 0.149290 -1.298523 -1.345623 0.616554 0.945285 0.010571 1.523054 -1.470781 -2.073242 -2.105066 -1.227242 -1.808182 -1.397006 -2.261993 -1.993420	-2.170087 -1.413950 -0.535212 -1.869780 -1.047063 1.099506 1.858341 2.246661 2.729354 1.236507 2.113576 1.691972 3.018638 2.427370 0.678437 -0.045548 1.565020 0.204982 -1.502190 -2.000756 -2.915697 -3.300233	0.192610 0.419050 0.147095 -0.522901 0.989452 4.175453 2.926930 2.326640 3.253517 2.280569 5.009135 5.978532 5.222204 4.452882 4.962007 4.376135 5.169444 5.932600 -1.645082 -2.918016 -3.554783 -4.549059	E (GFN- Coordi Ti Si Si O C H C C H C C H C H C H C H C H C H C	-FF) = -16.2411078 inates: 0.382302 2.987610 3.058992 0.367039 -1.039142 2.034670 1.476937 -0.071879 0.432396 -0.096499 0.256381 -1.063552 -1.462178 -1.508108 -2.250609 -1.029603 1.522435 1.967257 2.379299	-0.113896 1.634351 -1.578517 0.892064 -1.040786 0.013480 -0.132437 1.407400 0.860267 1.369013 0.968741 2.377630 2.750019 2.924466 3.731121 2.471459 -0.235938 -0.553408 0.338116	-1.694703 -1.310113 1.289678 -0.926181 -1.484187 -2.442613 2.466064 3.689451 4.890545 5.848887 4.902033 5.857497 3.695563 3.726755 2.451423 3.726734 5.169171 5.682885
Н С Н Н Н С С Н Н Н С Н Н Н С С С Н С	0.445224 3.181372 2.568968 3.550241 4.058264 -0.205982 -0.693362 0.149290 -1.298523 -1.345623 0.616554 0.945285 0.010571 1.523054 -1.470781 -2.073242 -2.105066 -1.227242 -1.808182 -1.397006 -2.261993 -1.993420 -3.450387	-2.170087 -1.413950 -0.535212 -1.869780 -1.047063 1.099506 1.858341 2.246661 2.729354 1.236507 2.113576 1.691972 3.018638 2.427370 0.678437 -0.045548 1.565020 0.204982 -1.502190 -2.000756 -2.915697 -3.300233 -3.348800	0.192610 0.419050 0.147095 -0.522901 0.989452 4.175453 2.926930 2.326640 3.253517 2.280569 5.009135 5.978532 5.222204 4.452882 4.962007 4.376135 5.169444 5.932600 -1.645082 -2.918016 -3.554783 -4.549059 -2.968612	E (GFN- Coordi Ti Si Si O C H C C H C C C H C H C H C H C H C H	-FF) = -16.2411078 inates: 0.382302 2.987610 3.058992 0.367039 -1.039142 2.034670 1.476937 -0.071879 0.432396 -0.096499 0.256381 -1.063552 -1.462178 -1.508108 -2.250609 -1.029603 1.522435 1.967257 2.379299 2.765355	-0.113896 1.634351 -1.578517 0.892064 -1.040786 0.013480 -0.132437 1.407400 0.860267 1.369013 0.968741 2.377630 2.750019 2.924466 3.731121 2.471459 -0.235938 -0.553408 0.338116 -1.322020	-1.694703 -1.310113 1.289678 -0.926181 -1.484187 -2.442613 2.466064 3.689451 4.890545 5.84887 4.902033 5.857497 3.695563 3.726755 2.451423 3.726734 5.169171 5.682885 5.140567
Н С Н Н Н С С Н Н Н С Н Н Н С С С Н С Н	0.445224 3.181372 2.568968 3.550241 4.058264 -0.205982 -0.693362 0.149290 -1.298523 -1.345623 0.616554 0.945285 0.010571 1.523054 -1.470781 -2.073242 -2.105066 -1.227242 -1.808182 -1.397006 -2.261993 -1.993420 -3.450387 -4.100759	-2.170087 -1.413950 -0.535212 -1.869780 -1.047063 1.099506 1.888341 2.246661 2.729354 1.236507 2.113576 1.691972 3.018638 2.427370 0.678437 -0.045548 1.565020 0.204982 -1.502190 -2.000756 -2.915697 -3.300233 -3.348800 -4.062332	0.192610 0.419050 0.147095 -0.522901 0.989452 4.175453 2.926930 2.326640 3.253517 2.280569 5.009135 5.978532 5.222204 4.452882 4.962007 4.376135 5.169444 5.932600 -1.645082 -2.918016 -3.554783 -4.549059 -2.968612 -3.496058	E (GFN- Coordi Ti Si Si O C C H C C C H C C H C H H H	-FF) = -16.2411078  inates:	-0.113896 1.634351 -1.578517 0.892064 -1.040786 0.013480 -0.132437 1.407400 0.860267 1.369013 0.968741 2.377630 2.750019 2.924466 3.731121 2.471459 -0.235938 -0.553408 0.338116 -1.322020 -0.959925	-1.694703 -1.310113 1.289678 -0.926181 -1.484187 -2.442613 2.466064 3.689451 4.890545 5.848887 4.902033 5.857497 3.695563 3.726755 2.451423 3.726734 5.169171 5.682885 5.140567 5.785385
Н С Н Н Н С С Н Н Н С Н Н Н С С С Н С Н	0.445224 3.181372 2.568968 3.550241 4.058264 -0.205982 -0.693362 0.149290 -1.298523 -1.345623 0.616554 0.945285 0.010571 1.523054 -1.470781 -2.073242 -2.105066 -1.227242 -1.808182 -1.397006 -2.261993 -1.993420 -3.450387 -4.100759 -3.807376	-2.170087 -1.413950 -0.535212 -1.869780 -1.047063 1.099506 1.858341 2.246661 2.7729354 1.236507 2.113576 1.691972 3.018638 2.427370 0.678437 -0.045548 1.565020 0.204982 -1.502190 -2.000756 -2.915697 -3.300233 -3.348800 -4.062332 -2.876643	0.192610 0.419050 0.147095 -0.522901 0.989452 4.175453 2.926930 2.326640 3.253517 2.280569 5.009135 5.978532 5.222204 4.452882 4.962007 4.376135 5.169444 5.932600 -1.645082 -2.918016 -3.554783 -4.549059 -2.968612 -3.496058 -1.700196	E (GFN- Coordi Ti Si Si O C H C C H C C H C H C H C H C C H C H	-FF) = -16.2411078  inates:	-0.113896 1.634351 -1.578517 0.892064 -1.040786 0.013480 -0.132437 1.407400 0.860267 1.369013 0.968741 2.377630 2.750019 2.924466 3.731121 2.471459 -0.235938 -0.553408 0.338116 -1.322020 -0.959925 -1.555139	-1.694703 -1.310113 1.289678 -0.926181 -1.484187 -2.442613 2.466064 3.689451 4.890545 5.848887 4.902033 5.857497 3.695563 3.726755 2.451423 3.726734 5.169171 5.682885 5.140567 5.785385 3.125040
Н С Н Н Н С С Н Н Н С Н Н Н С С С Н С Н	0.445224 3.181372 2.568968 3.550241 4.058264 -0.205982 -0.693362 0.149290 -1.298523 -1.345623 0.616554 0.945285 0.010571 1.523054 -1.470781 -2.073242 -2.105066 -1.227242 -1.808182 -1.397006 -2.261993 -1.993420 -3.450387 -4.100759 -3.807376 -4.738041	-2.170087 -1.413950 -0.535212 -1.869780 -1.047063 1.099506 1.858341 2.246661 2.729354 1.236507 2.113576 1.691972 3.018638 2.427370 0.678437 -0.045548 1.565020 0.204982 -1.502190 -2.000756 -2.915697 -3.300233 -3.348800 -4.062332 -2.876643 -3.240395	0.192610 0.419050 0.147095 -0.522901 0.989452 4.175453 2.926930 2.326640 3.253517 2.280569 5.009135 5.978532 5.222204 4.452882 4.962007 4.376135 5.169444 5.932600 -1.645082 -2.918016 -3.554783 -4.549059 -2.968612 -3.496058 -1.700196 -1.248184	E (GFN- Coordi Ti Si Si O C H C C H C C H C H C H C H C H C H H H H H H H H H H C H	-FF) = -16.2411078  inates:	-0.113896     1.634351     -1.578517     0.892064     -1.040786     0.013480     -0.132437     1.407400     0.860267     1.369013     0.968741     2.377630     2.750019     2.924466     3.731121     2.471459     -0.235938     -0.553408     0.338116     -1.322020     -0.959925     -1.555139     -1.922573	-1.694703 -1.310113 1.289678 -0.926181 -1.484187 -2.442613 2.466064 3.689451 4.890545 5.848887 4.902033 5.857497 3.695563 3.726755 2.451423 3.726734 5.169171 5.682885 5.140567 5.785385 3.125040 3.691225
Н С Н Н Н С С Н Н Н С Н Н Н С С С Н С Н	0.445224 3.181372 2.568968 3.550241 4.058264 -0.205982 -0.693362 0.149290 -1.298523 -1.345623 0.616554 0.945285 0.010571 1.523054 -1.470781 -2.073242 -2.105066 -1.227242 -1.808182 -1.397006 -2.261993 -1.993420 -3.450387 -4.100759 -3.807376 -4.738041 -3.010443	-2.170087 -1.413950 -0.535212 -1.869780 -1.047063 1.099506 1.858341 2.246661 2.729354 1.236507 2.113576 1.691972 3.018638 2.427370 0.678437 -0.045548 1.565020 0.204982 -1.502190 -2.000756 -2.915697 -3.300233 -3.348800 -4.062332 -2.876643 -3.240395 -1.952831	0.192610 0.419050 0.147095 -0.522901 0.989452 4.175453 2.926930 2.326640 3.253517 2.280569 5.009135 5.978532 5.222204 4.452882 4.962007 4.376135 5.169444 5.932600 -1.645082 -2.918016 -3.554783 -4.549059 -2.968612 -3.496058 -1.700196 -1.248184 -1.002829	E (GFN- Coordi Ti Si Si O C H C C H C C H C H C H C H C H C H H H H	-FF) = -16.2411078  inates:	-0.113896 1.634351 -1.578517 0.892064 -1.040786 0.013480 -0.132437 1.407400 0.860267 1.369013 0.968741 2.377630 2.750019 2.924466 3.731121 2.471459 -0.235938 -0.553408 0.338116 -1.322020 -0.959925 -1.555139 -1.922573 -2.339024	-1.694703 -1.310113 1.289678 -0.926181 -1.484187 -2.442613 2.466064 3.689451 4.890545 5.848887 4.902033 5.857497 3.695563 3.726755 2.451423 3.726734 5.169171 5.682885 5.140567 5.785385 3.125040 3.691225 3.155438
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Н С Н Н Н С С Н Н Н С Н Н Н С С С Н С Н	0.445224 3.181372 2.568968 3.550241 4.058264 -0.205982 -0.693362 0.149290 -1.298523 -1.345623 0.616554 0.945285 0.010571 1.523054 -1.470781 -2.073242 -2.105066 -1.227242 -1.808182 -1.397006 -2.261993 -1.993420 -3.450387 -4.100759 -3.807376 -4.738041 -3.010443 -0.108965 0.947048 1.842751 1.274689 0.595822 -0.522798 -1.025847 -1.220767 0.370053 0.611200 1.532821 -0.010424 0.903950 -3.436775 -2.377335 -2.204690 -2.723618	-2.170087 -1.413950 -0.535212 -1.869780 -1.047063 1.099506 1.858341 2.246661 2.729354 1.236507 2.113576 1.691972 3.018638 2.427370 0.678437 -0.045548 1.565020 0.204982 -1.565020 0.204982 -1.565020 0.204982 -1.502190 -2.000756 -2.915697 -3.300233 -3.348800 -4.062332 -2.876643 -3.240395 -1.952831 -1.615480 -0.799249 -0.675609 -1.311298 0.216252 -0.793034 0.148427 -1.355113 -0.526789 -2.910038 -2.651624 -3.542755 -3.522938 -1.465420 -1.863940 -2.988494 -1.581494	0.192610 0.419050 0.147095 -0.522901 0.989452 4.175453 2.926930 2.326640 3.253517 2.280569 5.009135 5.978532 5.222204 4.452882 4.962007 4.376135 5.169444 5.932600 -1.645082 -2.918016 -3.554783 -4.549059 -2.968612 -3.496058 -1.700196 -1.248184 -1.002829 -3.696795 -2.924686 -3.567400 -2.000113 -2.667226 -4.940528 -4.641717 -5.592196 -5.544187 -4.150075 -4.710902 -4.811744 -3.273308 0.404292 1.458322 1.449773 2.474247	E (GFN-Coordinate of the coordinate of the coord	-FF) = -16.2411078  inates:	-0.113896 1.634351 -1.578517 0.892064 -1.040786 0.013480 -0.132437 1.407400 0.860267 1.369013 0.968741 2.377630 2.750019 2.924466 3.731121 2.471459 -0.235938 -0.553408 0.338116 -1.322020 -0.959525 -1.555139 -1.922573 -2.339024 -1.440371 0.236089 0.414701 -0.527974 1.181858 3.138483 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.355242 4.812641 5.122793 2.150623 1.254224 2.643606 1.794782 3.673658 4.416901 4.171346	-1.694703 -1.310113 1.289678 -0.926181 -1.484187 -2.442613 2.466064 3.689451 4.890545 5.848887 4.902033 5.857497 3.695563 3.726755 2.451423 3.726755 2.451423 3.726734 5.169171 5.682885 5.140567 5.785385 3.125040 3.691225 3.155438 2.068359 2.962570 1.893945 3.039286 3.389813 1.145289 1.429773 1.951847 0.467774 2.034518 0.295480 -0.014595 -0.633206 0.856966 0.339425 0.931973 -0.588012
Н С Н Н Н С С Н Н Н С Н Н Н С Н Н Н С С С Н С Н С С С Н Н Н С Н Н Н С Н Н Н С С Н Н Н	0.445224 3.181372 2.568968 3.550241 4.058264 -0.205982 -0.693362 0.149290 -1.298523 -1.345623 0.616554 0.945285 0.010571 1.523054 -1.470781 -2.073242 -2.105066 -1.227242 -1.808182 -1.397006 -2.261993 -1.993420 -3.450387 -4.100759 -3.807376 -4.738041 -3.010443 -0.108965 0.947048 1.842751 1.274689 0.595822 -0.522798 -1.025847 -1.220767 0.370053 0.611200 1.532821 -0.010424 0.903950 -3.436775 -2.377335 -2.204690 -2.773618 -1.400950	-2.170087 -1.413950 -0.535212 -1.869780 -1.047063 1.099506 1.888341 2.246661 2.729354 1.236507 2.113576 1.691972 3.018638 2.427370 0.678437 -0.045548 1.565020 0.204982 -1.502190 -2.000756 -2.915697 -3.300233 -3.348800 -4.062332 -2.876643 -3.240395 -1.952831 -1.615480 -0.799249 -0.675609 -1.311298 0.216252 -0.793034 0.148427 -1.355113 -0.526789 -2.910038 -2.651624 -3.542755 -3.522938 -1.465420 -1.863940 -2.958494 -1.581494 -1.581494 -1.581494	0.192610 0.419050 0.147095 -0.522901 0.989452 4.175453 2.926930 2.326640 3.253517 2.280569 5.009135 5.978532 5.222204 4.452882 4.962007 4.376135 5.169444 5.932600 -1.645082 -2.918016 -3.554783 -4.549059 -2.968612 -3.496058 -1.700196 -1.248184 -1.002829 -3.696795 -2.924686 -3.567400 -2.000113 -2.667226 -4.940528 -4.641717 -5.592196 -5.544187 -4.150075 -4.710902 -4.811744 -3.273308 0.404292 1.458322 1.449773 2.474247 1.298167	E (GFN-Coordinate of the coordinate of the coord	-FF) = -16.2411078  inates:	-0.113896 1.634351 -1.578517 0.892064 -1.040786 0.013480 -0.132437 1.407400 0.860267 1.369013 0.968741 2.377630 2.750019 2.924466 3.731121 2.471459 -0.235938 -0.553408 0.338116 -1.322020 -0.959925 -1.555139 -1.922573 -2.339024 -1.440371 0.236089 0.414701 -0.527974 1.181858 3.138483 4.346983 4.055242 4.812641 5.122793 2.150623 1.254224 2.643606 1.794782 3.673658 4.416901 4.171346 2.868308	-1.694703 -1.310113 1.289678 -0.926181 -1.484187 -2.442613 2.466064 3.689451 4.890545 5.848887 4.902033 5.857497 3.695563 3.726755 2.451423 3.726755 2.451423 3.726734 5.169171 5.682885 5.140567 5.785385 3.125040 3.691225 3.155438 2.068359 2.962570 1.893945 3.039286 3.389813 1.145289 1.429773 1.951847 0.467774 2.034518 0.295480 -0.014595 -0.633206 0.856966 0.339425 0.931973 -0.588012 0.050678
Н С Н Н Н С С Н Н Н С Н Н Н С С С Н С Н	0.445224 3.181372 2.568968 3.550241 4.058264 -0.205982 -0.693362 0.149290 -1.298523 -1.345623 0.616554 0.945285 0.010571 1.523054 -1.470781 -2.073242 -2.105066 -1.227242 -1.808182 -1.397006 -2.261993 -1.993420 -3.450387 -4.100759 -3.807376 -4.738041 -3.010443 -0.108965 0.947048 1.842751 1.274689 0.595822 -0.522798 -1.025847 -1.220767 0.370053 0.611200 1.532821 -0.010424 0.903950 -3.436775 -2.377335 -2.204690 -2.723618	-2.170087 -1.413950 -0.535212 -1.869780 -1.047063 1.099506 1.858341 2.246661 2.729354 1.236507 2.113576 1.691972 3.018638 2.427370 0.678437 -0.045548 1.565020 0.204982 -1.565020 0.204982 -1.565020 0.204982 -1.502190 -2.000756 -2.915697 -3.300233 -3.348800 -4.062332 -2.876643 -3.240395 -1.952831 -1.615480 -0.799249 -0.675609 -1.311298 0.216252 -0.793034 0.148427 -1.355113 -0.526789 -2.910038 -2.651624 -3.542755 -3.522938 -1.465420 -1.863940 -2.988494 -1.581494	0.192610 0.419050 0.147095 -0.522901 0.989452 4.175453 2.926930 2.326640 3.253517 2.280569 5.009135 5.978532 5.222204 4.452882 4.962007 4.376135 5.169444 5.932600 -1.645082 -2.918016 -3.554783 -4.549059 -2.968612 -3.496058 -1.700196 -1.248184 -1.002829 -3.696795 -2.924686 -3.567400 -2.000113 -2.667226 -4.940528 -4.641717 -5.592196 -5.544187 -4.150075 -4.710902 -4.811744 -3.273308 0.404292 1.458322 1.449773 2.474247	E (GFN-Coordinate of the coordinate of the coord	-FF) = -16.2411078  inates:	-0.113896 1.634351 -1.578517 0.892064 -1.040786 0.013480 -0.132437 1.407400 0.860267 1.369013 0.968741 2.377630 2.750019 2.924466 3.731121 2.471459 -0.235938 -0.553408 0.338116 -1.322020 -0.959525 -1.555139 -1.922573 -2.339024 -1.440371 0.236089 0.414701 -0.527974 1.181858 3.138483 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.346983 4.355242 4.812641 5.122793 2.150623 1.254224 2.643606 1.794782 3.673658 4.416901 4.171346	-1.694703 -1.310113 1.289678 -0.926181 -1.484187 -2.442613 2.466064 3.689451 4.890545 5.848887 4.902033 5.857497 3.695563 3.726755 2.451423 3.726755 2.451423 3.726734 5.169171 5.682885 5.140567 5.785385 3.125040 3.691225 3.155438 2.068359 2.962570 1.893945 3.039286 3.389813 1.145289 1.429773 1.951847 0.467774 2.034518 0.295480 -0.014595 -0.633206 0.856966 0.339425 0.931973 -0.588012

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