QUEST Database: Geometries

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S1 Geometries of closed-shell species

Below are given the Cartesian coordinates for all compounds investigated in the QUEST database. These are provided in atomic units (bohr).

Acetaldehyde

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	-0.00234503	0.00000000	0.87125063
C	-1.75847785	0.00000000	-1.34973671
O	2.27947397	0.00000000	0.71968028
H	-0.92904537	0.00000000	2.73929404
H	-2.97955463	1.66046488	-1.25209463
H	-2.97955463	-1.66046488	-1.25209463
H	-0.70043433	0.00000000	-3.11066412

Acetone

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	0.18807702
C	0.00000000	2.42007545	-1.31764698
C	0.00000000	-2.42007545	-1.31764698
O	0.00000000	0.00000000	2.48269094
H	0.00000000	4.03690733	-0.05185132
H	0.00000000	-4.03690733	-0.05185132
H	1.66061256	2.48420530	-2.53995285
H	-1.66061256	2.48420530	-2.53995285
H	1.66061256	-2.48420530	-2.53995285
H	-1.66061256	-2.48420530	-2.53995285

Acetylene

Level of theory: CC3(Full)/*aug*-cc-pVTZ

Ground state

C	0.00000000	0.00000000	1.14048351
C	0.00000000	0.00000000	-1.14048351
H	0.00000000	0.00000000	3.14009043
H	0.00000000	0.00000000	-3.14009043

Trans excited state (^1A_u state in the C_{2h} point group)

C	1.29567779	0.00000000	-0.01846047
C	-1.29567779	0.00000000	0.01846047
H	2.41938674	0.00000000	1.70881682
H	-2.41938674	0.00000000	-1.70881682

Cis excited state ($^1A_2$ state in the C_{2v} point group)

C	0.00000000	1.26834508	-0.11726146
C	0.00000000	-1.26834508	-0.11726146
H	0.00000000	2.67282325	1.39629264
H	0.00000000	-2.67282325	1.39629264

Acrolein

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	-1.11645072	-0.68348783	0.00000000
C	1.20647847	0.83714564	0.00000000
C	3.46831059	-0.28872636	0.00000000
O	-3.23666415	0.19187203	0.00000000
H	-0.80613858	-2.74747338	0.00000000
H	0.98699813	2.86613511	0.00000000
H	5.20930864	0.77443560	0.00000000
H	3.60951559	-2.33000749	0.00000000

Aminobenzonitrile

Level of theory: CC3(FC)/cc-pVTZ

C	0.00000000	0.00000000	-3.36820633
C	2.27829762	0.00000000	-2.01450309
C	-2.27829762	0.00000000	-2.01450309
C	0.00000000	0.00000000	1.93909521
C	2.27351166	0.00000000	0.59753796
C	-2.27351166	0.00000000	0.59753796
C	0.00000000	0.00000000	4.63257112
N	0.00000000	0.00000000	-5.94870080
N	0.00000000	0.00000000	6.83060124
H	4.04775542	0.00000000	-3.02611570
H	-4.04775542	0.00000000	-3.02611570
H	4.03704439	0.00000000	1.61551747

H	-4.03704439	0.00000000	1.61551747
H	-1.62177115	0.00000000	-6.91608217
H	1.62177115	0.00000000	-6.91608217

Ammonia

Level of theory: CC3(Full)/*aug*-cc-pVTZ

N	0.12804615	-0.00000000	0.00000000
H	-0.59303935	0.88580079	-1.53425197
H	-0.59303935	-1.77160157	-0.00000000
H	-0.59303935	0.88580079	1.53425197

Aniline

Level of theory: CC3(FC)/cc-pVTZ

C	0.00000000	0.00000000	-1.78643569
C	2.27316118	0.00000000	-0.43457234
C	-2.27316118	0.00000000	-0.43457234
C	0.00000000	0.00000000	3.53007775
C	2.26327651	0.00000000	2.18912925
C	-2.26327651	0.00000000	2.18912925
N	0.00000000	0.00000000	-4.38230793
H	4.03982526	0.00000000	3.18807501
H	-4.03982526	0.00000000	3.18807501
H	0.00000000	0.00000000	5.56493193
H	4.04200589	0.00000000	-1.45016965
H	-4.04200589	0.00000000	-1.45016965
H	-1.62137595	0.00000000	-5.34754284
H	1.62137595	0.00000000	-5.34754284

Anthracene

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	0.00000000	2.63580732	0.00000000
C	0.00000000	-2.63580732	0.00000000
C	-2.29791519	1.34956852	0.00000000
C	2.29791519	1.34956852	0.00000000
C	-2.29791519	-1.34956852	0.00000000
C	2.29791519	-1.34956852	0.00000000

C	-4.65745777	2.64726588	0.00000000
C	4.65745777	2.64726588	0.00000000
C	-4.65745777	-2.64726588	0.00000000
C	4.65745777	-2.64726588	0.00000000
C	-6.88218555	1.34593157	0.00000000
C	6.88218555	1.34593157	0.00000000
C	-6.88218555	-1.34593157	0.00000000
C	6.88218555	-1.34593157	0.00000000
H	-0.00000000	4.67946059	0.00000000
H	0.00000000	-4.67946059	0.00000000
H	-4.64776022	4.68790486	0.00000000
H	4.64776022	4.68790486	0.00000000
H	-4.64776022	-4.68790486	0.00000000
H	4.64776022	-4.68790486	0.00000000
H	-8.65488616	2.34873329	0.00000000
H	8.65488616	2.34873329	0.00000000
H	-8.65488616	-2.34873329	0.00000000
H	8.65488616	-2.34873329	0.00000000

Anthraquinone

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	0.00000000	2.77266798	0.00000000
C	0.00000000	-2.77266798	0.00000000
C	-2.39604276	1.31893403	0.00000000
C	2.39604276	1.31893403	0.00000000
C	-2.39604276	-1.31893403	0.00000000
C	2.39604276	-1.31893403	0.00000000
C	-4.67770721	2.63091924	0.00000000
C	4.67770721	2.63091924	0.00000000
C	-4.67770721	-2.63091924	0.00000000
C	4.67770721	-2.63091924	0.00000000
C	-6.94595480	1.31915183	0.00000000
C	6.94595480	1.31915183	0.00000000
C	-6.94595480	-1.31915183	0.00000000
C	6.94595480	-1.31915183	0.00000000
O	0.00000000	5.07701524	0.00000000
O	0.00000000	-5.07701524	0.00000000
H	-4.62532501	4.66594073	0.00000000
H	4.62532501	4.66594073	0.00000000
H	-4.62532501	-4.66594073	0.00000000
H	4.62532501	-4.66594073	0.00000000
H	-8.70925236	2.33764025	0.00000000

H	8.70925236	2.33764025	0.00000000
H	-8.70925236	-2.33764025	0.00000000
H	8.70925236	-2.33764025	0.00000000

Aza-BODIPY

Level of theory: CCSD(T)(FC)/cc-pVTZ

B	0.00000000	0.00000000	2.31704487
C	0.00000000	2.14450306	-2.14127722
C	0.00000000	-2.14450306	-2.14127722
C	0.00000000	4.63460750	-3.14651377
C	0.00000000	-4.63460750	-3.14651377
C	0.00000000	6.26996103	-1.12023173
C	0.00000000	-6.26996103	-1.12023173
C	0.00000000	4.75475012	1.08608078
C	0.00000000	-4.75475012	1.08608078
N	0.00000000	0.00000000	-3.41527163
N	0.00000000	2.31056089	0.47890837
N	0.00000000	-2.31056089	0.47890837
F	-2.14709422	0.00000000	3.76825470
F	2.14709422	0.00000000	3.76825470
H	0.00000000	5.07027917	-5.12686203
H	0.00000000	-5.07027917	-5.12686203
H	0.00000000	8.29623621	-1.15574338
H	0.00000000	-8.29623621	-1.15574338
H	0.00000000	5.33784503	3.03195696
H	0.00000000	-5.33784503	3.03195696

Azanaphthalene

Level of theory: CC3(Full)/cc-pVTZ

C	0.00000000	1.33735978	0.00000000
C	0.00000000	-1.33735978	0.00000000
C	4.26447087	1.34122299	0.00000000
C	-4.26447087	1.34122299	0.00000000
C	4.26447087	-1.34122299	0.00000000
C	-4.26447087	-1.34122299	0.00000000
N	2.18301381	2.68816340	0.00000000
N	-2.18301381	2.68816340	0.00000000
N	2.18301381	-2.68816340	0.00000000
N	-2.18301381	-2.68816340	0.00000000

H	6.03657953	2.35467535	0.00000000
H	-6.03657953	2.35467535	0.00000000
H	6.03657953	-2.35467535	0.00000000
H	-6.03657953	-2.35467535	0.00000000

Azobenzene

Level of theory: CCSD(T)(FC)/cc-pVTZ

N	0.70983759	0.94706332	0.00000000
N	-0.70983759	-0.94706332	0.00000000
C	3.32897155	0.35325415	0.00000000
C	-3.32897155	-0.35325415	0.00000000
C	4.95331207	2.41934773	0.00000000
C	-4.95331207	-2.41934773	0.00000000
C	4.29774859	-2.10116089	0.00000000
C	-4.29774859	2.10116089	0.00000000
C	7.55507717	2.05070219	0.00000000
C	-7.55507717	-2.05070219	0.00000000
C	6.89206075	-2.45941610	0.00000000
C	-6.89206075	2.45941610	0.00000000
C	8.52712206	-0.38973890	0.00000000
C	-8.52712206	0.38973890	0.00000000
H	4.14639892	4.28913452	0.00000000
H	-4.14639892	-4.28913452	0.00000000
H	3.00966091	-3.67317406	0.00000000
H	-3.00966091	3.67317406	0.00000000
H	8.81009192	3.65424541	0.00000000
H	-8.81009192	-3.65424541	0.00000000
H	7.65006326	-4.35029611	0.00000000
H	-7.65006326	4.35029611	0.00000000
H	10.54199682	-0.68600884	0.00000000
H	-10.54199682	0.68600884	0.00000000

Azulene

Level of theory: CC3(FC)/cc-pVTZ

C	0.00000000	0.00000000	-5.08442654
C	2.16799436	0.00000000	-3.55850254
C	-2.16799436	0.00000000	-3.55850254
C	1.40560615	0.00000000	-1.02382432
C	-1.40560615	0.00000000	-1.02382432

C	0.00000000	0.00000000	4.72891515
C	2.38587647	0.00000000	3.61219185
C	-2.38587647	0.00000000	3.61219185
C	3.00158451	0.00000000	1.05184313
C	-3.00158451	0.00000000	1.05184313
H	0.00000000	0.00000000	-7.11850559
H	4.09656030	0.00000000	-4.20278074
H	-4.09656030	0.00000000	-4.20278074
H	0.00000000	0.00000000	6.77201689
H	3.96514987	0.00000000	4.90481753
H	-3.96514987	0.00000000	4.90481753
H	5.00047162	0.00000000	0.61482964
H	-5.00047162	0.00000000	0.61482964

Benzene

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	2.63144965	0.00000000
C	-2.27890225	1.31572483	0.00000000
C	-2.27890225	-1.31572483	0.00000000
C	0.00000000	-2.63144965	0.00000000
C	2.27890225	-1.31572483	0.00000000
C	2.27890225	1.31572483	0.00000000
H	-4.04725813	2.33668557	0.00000000
H	-4.04725813	-2.33668557	0.00000000
H	-0.00000000	-4.67337115	0.00000000
H	4.04725813	-2.33668557	0.00000000
H	4.04725813	2.33668557	0.00000000
H	0.00000000	4.67337115	0.00000000

Benzonitrile

Level of theory: CC3(FC)/cc-pVTZ

C	0.00000000	0.00000000	-3.73018216
C	0.00000000	0.00000000	-1.02720486
C	2.28760421	0.00000000	0.28592358
C	-2.28760421	0.00000000	0.28592358
C	0.00000000	0.00000000	4.22270922
C	2.28059554	0.00000000	2.90986462
C	-2.28059554	0.00000000	2.90986462
N	0.00000000	0.00000000	-5.92640038

H	4.03930466	0.00000000	-0.75078588
H	-4.03930466	0.00000000	-0.75078588
H	4.04556576	0.00000000	3.92452034
H	-4.04556576	0.00000000	3.92452034
H	0.00000000	0.00000000	6.25892556

Benzoquinone

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	2.71467427	0.00000000	0.00000000
C	-2.71467427	0.00000000	0.00000000
C	1.26645689	2.38719964	0.00000000
C	1.26645689	-2.38719964	0.00000000
C	-1.26645689	2.38719964	0.00000000
C	-1.26645689	-2.38719964	0.00000000
O	5.02607647	0.00000000	0.00000000
O	-5.02607647	0.00000000	0.00000000
H	2.37218673	4.10318853	0.00000000
H	2.37218673	-4.10318853	0.00000000
H	-2.37218673	4.10318853	0.00000000
H	-2.37218673	-4.10318853	0.00000000

Benzothiadiazole

Level of theory: CC3(FC)/cc-pVTZ

S	0.00000000	0.00000000	4.12782363
N	0.00000000	2.37994968	2.16794907
N	0.00000000	-2.37994968	2.16794907
C	0.00000000	1.35464582	-0.15090868
C	0.00000000	-1.35464582	-0.15090868
C	0.00000000	2.70608821	-2.46599859
C	0.00000000	-2.70608821	-2.46599859
C	0.00000000	1.34964552	-4.66429754
C	0.00000000	-1.34964552	-4.66429754
H	0.00000000	4.74051264	-2.44976392
H	0.00000000	-4.74051264	-2.44976392
H	0.00000000	2.32640888	-6.45161040
H	0.00000000	-2.32640888	-6.45161040

Benzoxadiazole

Level of theory: CC3(FC)/cc-pVTZ

O	0.00000000	0.00000000	4.23105351
N	0.00000000	2.15721782	2.80042430
N	0.00000000	-2.15721782	2.80042430
C	0.00000000	1.34474119	0.44505130
C	0.00000000	-1.34474119	0.44505130
C	0.00000000	2.73330026	-1.85469062
C	0.00000000	-2.73330026	-1.85469062
C	0.00000000	1.35965956	-4.03354365
C	0.00000000	-1.35965956	-4.03354365
H	0.00000000	4.76633138	-1.84544064
H	0.00000000	-4.76633138	-1.84544064
H	0.00000000	2.32124878	-5.82853313
H	0.00000000	-2.32124878	-5.82853313

Beryllium

Level of theory: N/A

Be	0.00000000	0.00000000	0.00000000

BF

Level of theory: CC3(Full)/*aug*-cc-pVTZ

B	0.00000000	0.00000000	0.00000000
F	0.00000000	0.00000000	2.39729626

BH

Level of theory: CC3(Full)/*aug*-cc-pVTZ

Ground state

B	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	2.31089693

Excited state

B	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	2.27596436

BODIPY

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	0.00000000	0.00000000	-3.45756235
C	0.00000000	2.28455780	-2.18740413
C	0.00000000	-2.28455780	-2.18740413
C	0.00000000	4.79788592	-3.09298460
C	0.00000000	-4.79788592	-3.09298460
C	0.00000000	6.36180283	-0.99687598
C	0.00000000	-6.36180283	-0.99687598
C	0.00000000	4.76869637	1.13918303
C	0.00000000	-4.76869637	1.13918303
B	0.00000000	0.00000000	2.22139632
F	2.14645956	0.00000000	3.68028136
F	-2.14645956	0.00000000	3.68028136
N	0.00000000	2.34821228	0.42497916
N	0.00000000	-2.34821228	0.42497916
H	0.00000000	5.33956943	-5.04999407
H	0.00000000	-5.33956943	-5.04999407
H	0.00000000	8.38849882	-0.96278552
H	0.00000000	-8.38849882	-0.96278552
H	0.00000000	5.26355675	3.10891537
H	0.00000000	-5.26355675	3.10891537
H	0.00000000	0.00000000	-5.49610864

Borole

Level of theory: CC3(Full)/*aug*-cc-pVTZ

B	0.00000000	0.00000000	2.44991435
C	0.00000000	2.35991046	0.62561328
C	0.00000000	-2.35991046	0.62561328
C	0.00000000	1.42526648	-1.74135978
C	0.00000000	-1.42526648	-1.74135978
H	0.00000000	0.00000000	4.69246473
H	0.00000000	4.35732912	1.03002724
H	0.00000000	-4.35732912	1.03002724
H	0.00000000	2.51021632	-3.47247633
H	0.00000000	-2.51021632	-3.47247633

Butadiene

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	1.14656244	0.00000000	0.75468820
C	-1.14656244	0.00000000	-0.75468820
C	3.48132647	0.00000000	-0.22482805
C	-3.48132647	0.00000000	0.22482805
H	0.90770978	0.00000000	2.78883925
H	-0.90770978	0.00000000	-2.78883925
H	3.77525814	0.00000000	-2.24895470
H	-3.77525814	0.00000000	2.24895470
H	5.13664967	0.00000000	0.96861890
H	-5.13664967	0.00000000	-0.96861890

Carbon dimer

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	1.17922927
C	0.00000000	0.00000000	-1.17922927

Carbon dioxide

Level of theory: CC3(FC)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	-2.20193016
O	0.00000000	0.00000000	2.20193016

Carbonic acid

Level of theory: CC3(FC)/*aug*-cc-pVTZ

O	0.00000000	0.00000000	2.46279243
C	0.00000000	0.00000000	0.18750328
O	0.00000000	2.04786599	-1.29140793
O	0.00000000	-2.04786599	-1.29140793
H	0.00000000	3.47810449	-0.16385522
H	0.00000000	-3.47810449	-0.16385522

Carbon monoxide

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	-1.24942055
O	0.00000000	0.00000000	0.89266692

Carbon trimer

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.45345613
C	0.00000000	0.00000000	-2.45345613

Carbonylfluoride

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	-0.30652633
O	0.00000000	0.00000000	-2.52469534
F	0.00000000	2.00254958	1.16003038
F	0.00000000	-2.00254958	1.16003038

CCl_2

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	-1.60920674
Cl	0.00000000	2.65360612	0.27602958
Cl	0.00000000	-2.65360612	0.27602958

CClF

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.29776085	0.00000000	1.47969075
F	2.16980264	0.00000000	-0.10569879
Cl	-2.46756349	0.00000000	-0.32822320

CF_2

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	-1.14170749
F	0.00000000	1.94810617	0.36114458
F	0.00000000	-1.94810617	0.36114458

Chlorobenzene

Level of theory: CC3(FC)/cc-pVTZ

Cl	0.00000000	0.00000000	-4.09694569
C	0.00000000	0.00000000	-0.80648356
C	2.28704058	0.00000000	0.47978453
C	-2.28704058	0.00000000	0.47978453
C	0.00000000	0.00000000	4.42840669
C	2.27492426	0.00000000	3.10862132
C	-2.27492426	0.00000000	3.10862132
H	4.03299260	0.00000000	-0.56250521
H	-4.03299260	0.00000000	-0.56250521
H	4.04398612	0.00000000	4.11768561
H	-4.04398612	0.00000000	4.11768561
H	0.00000000	0.00000000	6.46409111

Coumarin

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	-4.94880904	-1.94740654	0.00000000
C	-2.47093848	-2.79532569	0.00000000
C	-0.51937217	-1.03691944	0.00000000
C	-1.01215298	1.55096378	0.00000000
C	-3.52597295	2.36676114	0.00000000
C	-5.48705921	0.63898323	0.00000000
C	1.12079288	3.23364340	0.00000000
C	3.48627701	2.30671360	0.00000000
C	3.97501526	-0.40562242	0.00000000
O	1.88373948	-1.96225124	0.00000000
O	6.03004743	-1.37035420	0.00000000
H	-6.46892150	-3.30170531	0.00000000
H	-2.01507343	-4.77869214	0.00000000
H	-3.90920136	4.37002329	0.00000000

H	-7.41766766	1.28158133	0.00000000
H	0.79237605	5.24728088	0.00000000
H	5.13342919	3.49535270	0.00000000

Criegee's Intermediate

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	-2.14193693	0.46449461	0.00000000
O	-0.12214743	-0.85046436	0.00000000
O	2.09779397	0.38347786	0.00000000
H	-3.86593284	-0.61908241	0.00000000
H	-1.98533536	2.49983926	0.00000000

Cyanoacetylene

Level of theory: CC3(Full)/*aug*-cc-pVTZ

Ground state

C	0.00000000	0.00000000	-3.59120182
C	0.00000000	0.00000000	-1.30693904
C	0.00000000	0.00000000	1.28880240
N	0.00000000	0.00000000	3.48692211
H	0.00000000	0.00000000	-5.59619886

Lowest excited state

C	1.99411175	0.00000000	2.81781077
C	-0.07304269	0.00000000	1.33125774
C	-0.63630126	0.00000000	-1.14556678
N	-1.39755756	0.00000000	-3.26154643
H	1.90749857	0.00000000	4.87279180

Cyanoformaldehyde

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	-0.91561483	0.00000000	-1.22522833
C	-0.01092219	0.00000000	1.39523175
N	0.64170259	0.00000000	3.48820325
O	0.50833684	0.00000000	-3.00337867
H	-2.97202213	0.00000000	-1.42565674

Cyanogen

Level of theory: CC3(Full)/*aug*-cc-pVTZ

Ground state

C	0.00000000	0.00000000	1.30401924
C	0.00000000	0.00000000	-1.30401924
N	0.00000000	0.00000000	3.49784121
N	0.00000000	0.00000000	-3.49784121

Excited state

C	0.00000000	0.00000000	1.22784115
C	0.00000000	0.00000000	-1.22784115
N	0.00000000	0.00000000	3.56462559
N	0.00000000	0.00000000	-3.56462559

Cyclazine

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	0.00000000	-2.29619838	1.32571075
C	0.00000000	-4.57380843	-2.64068953
C	0.00000000	-0.00000000	-2.65142150
C	0.00000000	4.57380843	-2.64068953
C	0.00000000	2.29619838	1.32571075
C	0.00000000	0.00000000	5.28137906
C	0.00000000	-4.57334297	-0.03501138
C	0.00000000	2.31699223	-3.94312550
C	0.00000000	2.25635074	3.97813688
C	0.00000000	-2.25635074	3.97813688
C	0.00000000	-2.31699223	-3.94312550
C	0.00000000	4.57334297	-0.03501138
N	0.00000000	0.00000000	0.00000000
H	0.00000000	6.33829394	-3.65941571
H	0.00000000	0.00000000	7.31883143
H	0.00000000	-6.33829394	-3.65941571
H	0.00000000	-6.29930356	1.03947702
H	0.00000000	2.24943827	-5.97509542
H	0.00000000	4.04986529	4.93561840
H	0.00000000	-4.04986529	4.93561840
H	0.00000000	-2.24943827	-5.97509542
H	0.00000000	6.29930356	1.03947702

Cyclobutadiene

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	-1.47868321	-1.27004715	0.00000000
C	1.47868321	-1.27004715	0.00000000
C	-1.47868321	1.27004715	0.00000000
C	1.47868321	1.27004715	0.00000000
H	-2.91448237	-2.70994518	0.00000000
H	2.91448237	-2.70994518	0.00000000
H	-2.91448237	2.70994518	0.00000000
H	2.91448237	2.70994518	0.00000000

Cyclopentadiene

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	-2.33113051
C	0.00000000	2.22209092	-0.56871188
C	0.00000000	-2.22209092	-0.56871188
C	0.00000000	1.38514451	1.83772922
C	0.00000000	-1.38514451	1.83772922
H	1.66130504	0.00000000	-3.56414299
H	-1.66130504	0.00000000	-3.56414299
H	0.00000000	4.16550405	-1.18116624
H	0.00000000	-4.16550405	-1.18116624
H	0.00000000	2.54514584	3.51352303
H	0.00000000	-2.54514584	3.51352303

Cyclopentadienethione

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	0.54718884
C	0.00000000	2.23394142	-1.11648863
C	0.00000000	-2.23394142	-1.11648863
C	0.00000000	1.40618242	-3.52381930
C	0.00000000	-1.40618242	-3.52381930
S	0.00000000	0.00000000	3.63323789
H	0.00000000	4.14572930	-0.42732005
H	0.00000000	-4.14572930	-0.42732005
H	0.00000000	2.55090221	-5.20908210
H	0.00000000	-2.55090221	-5.20908210

Cyclopentadienone

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	1.45232781
C	0.00000000	2.26718523	-0.25413145
C	0.00000000	-2.26718523	-0.25413145
C	0.00000000	1.41557636	-2.63852689
C	0.00000000	-1.41557636	-2.63852689
O	0.00000000	0.00000000	3.74438847
H	0.00000000	4.18416912	0.42151096
H	0.00000000	-4.18416912	0.42151096
H	0.00000000	2.53760914	-4.33851399
H	0.00000000	-2.53760914	-4.33851399

Cyclopropene

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	-1.66820880
C	0.00000000	1.22523906	0.90681419
C	0.00000000	-1.22523906	0.90681419
H	1.72255446	0.00000000	-2.77881149
H	-1.72255446	0.00000000	-2.77881149
H	0.00000000	2.97844519	1.92076771
H	0.00000000	-2.97844519	1.92076771

Cyclopropenethione

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	1.26230744	-2.86571925
C	0.00000000	-1.26230744	-2.86571925
C	0.00000000	0.00000000	-0.49233236
S	0.00000000	0.00000000	2.57821680
H	0.00000000	2.97773331	-3.95114059
H	0.00000000	-2.97773331	-3.95114059

Cyclopropenone

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	1.27491826	-1.86930519
C	0.00000000	-1.27491826	-1.86930519
C	0.00000000	0.00000000	0.51814554
O	0.00000000	0.00000000	2.79326776
H	0.00000000	2.92791371	-3.05679837
H	0.00000000	-2.92791371	-3.05679837

Diacetylene

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	1.29447700
C	0.00000000	0.00000000	-1.29447700
C	0.00000000	0.00000000	3.58448429
C	0.00000000	0.00000000	-3.58448429
H	0.00000000	0.00000000	5.58943003
H	0.00000000	0.00000000	-5.58943003

Diazete

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	1.04088890	1.37023206	0.00000000
C	-1.04088890	-1.37023206	0.00000000
N	1.80420222	-0.93584807	0.00000000
N	-1.80420222	0.93584807	0.00000000
H	2.06402011	3.13844681	0.00000000
H	-2.06402011	-3.13844681	0.00000000

Diazirine

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	-0.26696099
H	0.00000000	1.75890895	-1.28616478
H	0.00000000	-1.75890895	-1.28616479
N	1.16058100	0.00000000	2.27183007
N	-1.16058100	0.00000000	2.27183007

Diazomethane

Level of theory: CC3(Full)/*aug*-cc-pVTZ

Ground state

C	0.00000000	0.00000000	-2.30830005
N	0.00000000	0.00000000	0.14457890
N	0.00000000	0.00000000	2.29923216
H	0.00000000	1.79875201	-3.24272317
H	0.00000000	-1.79875201	-3.24272317

Excited state

C	1.80206107	0.00000000	-1.03389466
N	-0.01743713	0.00000000	0.84742344
N	-2.25203764	0.00000000	0.54034983
H	3.74280590	0.00000000	-0.44375913
H	1.20115546	0.00000000	-2.98380249

Difluorodiazirine

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	-0.15283028
F	0.00000000	2.06077297	-1.57706828
F	0.00000000	-2.06077297	-1.57706828
N	1.20382241	0.00000000	2.20566821
N	-1.20382241	0.00000000	2.20566821

Diketopyrrolopyrrole

Level of theory: CC3(FC)/cc-pVTZ

C	-0.78095706	1.10654573	0.00000000
C	0.78095706	-1.10654573	0.00000000
C	0.75770683	3.16221974	0.00000000
C	-0.75770683	-3.16221974	0.00000000
C	-3.42805036	0.33490251	0.00000000
C	3.42805036	-0.33490251	0.00000000
N	-3.23354900	-2.34444494	0.00000000
N	3.23354900	2.34444494	0.00000000
O	-5.40649570	1.49154645	0.00000000

O	5.40649570	-1.49154645	0.00000000
H	-4.76571395	-3.46112039	0.00000000
H	4.76571395	3.46112039	0.00000000
H	0.30840723	5.14301221	0.00000000
H	-0.30840723	-5.14301221	0.00000000

Dimethylaminobenzonitrile

Level of theory: CCSD(T)(FC)/cc-pVTZ

Planar

C	0.00000000	0.00000000	-1.96083197
C	2.27891314	0.00000000	-0.58294740
C	-2.27891314	0.00000000	-0.58294740
C	0.00000000	0.00000000	3.37434994
C	2.26711046	0.00000000	2.02803761
C	-2.26711046	0.00000000	2.02803761
C	0.00000000	0.00000000	6.06798788
C	2.36485177	0.00000000	-5.90186899
C	-2.36485177	0.00000000	-5.90186899
N	0.00000000	0.00000000	-4.53733249
N	0.00000000	0.00000000	8.26382999
H	4.06469412	0.00000000	-1.55103579
H	-4.06469412	0.00000000	-1.55103579
H	4.03369195	0.00000000	3.04099978
H	-4.03369195	0.00000000	3.04099978
H	1.96836611	0.00000000	-7.91292844
H	-1.96836611	0.00000000	-7.91292844
H	3.49551175	-1.67111709	-5.47003452
H	3.49551175	1.67111709	-5.47003452
H	-3.49551175	1.67111709	-5.47003452
H	-3.49551175	-1.67111709	-5.47003452

Twisted

C	0.00000000	0.00000000	-1.92629020
C	2.27225178	0.00000000	-0.58317962
C	-2.27225178	0.00000000	-0.58317962
C	0.00000000	0.00000000	3.35560653
C	2.28330254	0.00000000	2.03752961
C	-2.28330254	0.00000000	2.03752961
C	0.00000000	0.00000000	6.05799119
C	0.00000000	2.39191725	-5.88267373

C	0.00000000	-2.39191725	-5.88267373
N	0.00000000	0.00000000	-4.58434634
N	0.00000000	0.00000000	8.25212738
H	4.02777860	0.00000000	-1.61674521
H	-4.02777860	0.00000000	-1.61674521
H	4.03804248	0.00000000	3.06961213
H	-4.03804248	0.00000000	3.06961213
H	0.00000000	2.05258096	-7.90903256
H	0.00000000	-2.05258096	-7.90903256
H	1.66857920	3.52919279	-5.43615170
H	-1.66857920	3.52919279	-5.43615170
H	-1.66857920	-3.52919279	-5.43615170
H	1.66857920	-3.52919279	-5.43615170

Dimethylaniline

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	0.00000000	0.00000000	4.89686867
C	2.25704297	0.00000000	3.55138467
C	-2.25704297	0.00000000	3.55138467
C	2.27412639	0.00000000	0.92841898
C	-2.27412639	0.00000000	0.92841898
C	0.00000000	0.00000000	-0.44595239
C	2.36139267	0.00000000	-4.39675011
C	-2.36139267	0.00000000	-4.39675011
N	0.00000000	0.00000000	-3.03916783
H	4.05922248	0.00000000	-0.04344476
H	-4.05922248	0.00000000	-0.04344476
H	4.03670718	0.00000000	4.54551891
H	-4.03670718	0.00000000	4.54551891
H	0.00000000	0.00000000	6.93154996
H	1.97020408	0.00000000	-6.40997108
H	-1.97020408	0.00000000	-6.40997108
H	3.49800498	-1.66955347	-3.96565000
H	3.49800498	1.66955347	-3.96565000
H	-3.49800498	1.66955347	-3.96565000
H	-3.49800498	-1.66955347	-3.96565000

Dinitrogen

Level of theory: CC3(Full)/*aug*-cc-pVTZ

N	0.00000000	0.00000000	1.04008632
N	0.00000000	0.00000000	-1.04008632

Ethylene

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	1.26026583	0.00000000
C	0.00000000	-1.26026583	0.00000000
H	0.00000000	2.32345976	1.74287672
H	0.00000000	-2.32345976	1.74287672
H	0.00000000	2.32345976	-1.74287672
H	0.00000000	-2.32345976	-1.74287672

Fluorobenzene

Level of theory: CC3(FC)/cc-pVTZ

F	0.00000000	0.00000000	-4.15873063
C	0.00000000	0.00000000	-1.61842149
C	2.29188824	0.00000000	-0.35805545
C	-2.29188824	0.00000000	-0.35805545
C	0.00000000	0.00000000	3.59063853
C	2.27621870	0.00000000	2.27153776
C	-2.27621870	0.00000000	2.27153776
H	4.02397454	0.00000000	-1.42355397
H	-4.02397454	0.00000000	-1.42355397
H	4.04329770	0.00000000	3.28356917
H	-4.04329770	0.00000000	3.28356917
H	0.00000000	0.00000000	5.62589878

Formaldehyde

Level of theory: CC3(Full)/*aug*-cc-pVTZ

Ground state

C	0.00000000	0.00000000	-1.13947666
O	0.00000000	0.00000000	1.14402883
H	0.00000000	1.76627623	-2.23398653
H	0.00000000	-1.76627623	-2.23398653

Excited state

C	-0.09942705	0.00000000	1.27071070
O	0.01987299	0.00000000	-1.23280536
H	0.42778855	1.76729629	2.18470884
H	0.42778855	-1.76729629	2.18470884

Formamide

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00183118	0.00000000	0.79313299
O	2.26817156	0.00000000	0.43918824
N	-1.76886033	0.00000000	-1.06219243
H	-0.84133459	0.00000000	2.68872485
H	-1.21254414	0.00000000	-2.87596907
H	-3.61627502	0.00000000	-0.65031317

Formylfluoride

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00536098	0.00000000	0.75320959
O	2.17369813	0.00000000	0.22287752
H	-0.83846350	0.00000000	2.62640974
F	-1.84051320	0.00000000	-0.99373750

Furan

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	2.06365826	-0.60051250
C	0.00000000	-2.06365826	-0.60051250
C	0.00000000	1.35348578	1.86336416
C	0.00000000	-1.35348578	1.86336416
O	0.00000000	0.00000000	-2.13945332
H	0.00000000	3.86337287	-1.53765695
H	0.00000000	-3.86337287	-1.53765695
H	0.00000000	2.59168789	3.47168051
H	0.00000000	-2.59168789	3.47168051

Furanofuran

Level of theory: CC3(FC)/cc-pVTZ

C	0.06548932	1.28240874	0.00000000
C	-0.06548932	-1.28240874	0.00000000
C	-2.43794558	2.25427215	0.00000000
C	2.43794558	-2.25427215	0.00000000
C	-3.90023785	0.12403225	0.00000000
C	3.90023785	-0.12403225	0.00000000
O	2.50066120	2.07485533	0.00000000
O	-2.50066120	-2.07485533	0.00000000
H	-3.10620733	4.16541687	0.00000000
H	3.10620733	-4.16541687	0.00000000
H	-5.90761266	-0.13384378	0.00000000
H	5.90761266	0.13384378	0.00000000

Glyoxal

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	1.21360282	0.75840215	0.00000000
C	-1.21360282	-0.75840215	0.00000000
O	3.25581408	-0.26453186	0.00000000
O	-3.25581408	0.26453186	0.00000000
H	0.96135276	2.81883243	0.00000000
H	-0.96135276	-2.81883243	0.00000000

HCCl

Level of theory: CC3(Full)/*aug*-cc-pVTZ

H	-1.88068369	0.00000000	-0.14323924
Cl	2.28559426	0.00000000	-0.43261163
C	-0.40491057	0.00000000	1.32161964

HCF

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	-0.13561085	0.00000000	1.20394474
F	1.85493976	0.00000000	-0.27610752
H	-1.71932891	0.00000000	-0.18206846

HCN

Level of theory: CC3(FC)/*aug*-cc-pVTZ

H	0.00000000	0.00000000	3.06256364
C	0.00000000	0.00000000	1.05824145
N	0.00000000	0.00000000	-1.12728289

HCP

Level of theory: CC3(Full)/*aug*-cc-pVTZ

H	0.00000000	0.00000000	-4.03090449
C	0.00000000	0.00000000	-2.01691641
P	0.00000000	0.00000000	0.91401621

Heptazine

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	0.00000000	-2.28707566	1.32044375
C	0.00000000	-4.25961422	-2.45928942
C	0.00000000	0.00000000	-2.64088750
C	0.00000000	4.25961422	-2.45928942
C	0.00000000	2.28707566	1.32044375
C	0.00000000	0.00000000	4.91857884
N	0.00000000	0.00000000	0.00000000
N	0.00000000	-4.45372767	0.04447145
N	0.00000000	2.18835043	-3.87927703
N	0.00000000	2.26537724	3.83480558
N	0.00000000	-2.26537724	3.83480558
N	0.00000000	-2.18835043	-3.87927703
N	0.00000000	4.45372767	0.04447145
H	0.00000000	6.02612802	-3.47918663
H	0.00000000	0.00000000	6.95837327
H	0.00000000	-6.02612802	-3.47918663

Hexatriene

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	1.14024826	0.56596845	0.00000000
C	-1.14024826	-0.56596845	0.00000000
C	3.51540649	-0.78907931	0.00000000
C	-3.51540649	0.78907931	0.00000000
C	5.78668151	0.33754155	0.00000000
C	-5.78668151	-0.33754155	0.00000000
H	1.23448067	2.61584039	0.00000000
H	-1.23448067	-2.61584039	0.00000000
H	3.40773630	-2.83459321	0.00000000
H	-3.40773630	2.83459321	0.00000000
H	5.95047109	2.37626316	0.00000000
H	-5.95047109	-2.37626316	0.00000000
H	7.51470672	-0.74809921	0.00000000
H	-7.51470672	0.74809921	0.00000000

HNC

Level of theory: CC3(FC)/*aug*-cc-pVTZ

H	0.00000000	0.00000000	2.79539858
N	0.00000000	0.00000000	0.91469554
C	0.00000000	0.00000000	-1.30215184

HPO

Level of theory: CC3(Full)/*aug*-cc-pVTZ

H	0.31668637	0.00000000	0.14072725
P	-0.80573521	0.00000000	2.65136926
O	1.43391190	0.00000000	4.38886277

HPS

Level of theory: CC3(Full)/*aug*-cc-pVTZ

H	-2.56278959	0.00000000	2.36296006
P	0.09114182	0.00000000	1.82568543
S	0.07946992	0.00000000	-1.85778170

HSiF

Level of theory: CC3(Full)/*aug*-cc-pVTZ

Si	-0.06438136	0.00000000	1.67253150
F	2.24990164	0.00000000	-0.33928119
H	-2.18552027	0.00000000	-0.28748154

Hydrogen chloride

Level of theory: CC3(Full)/*aug*-cc-pVTZ

Cl	0.00000000	0.00000000	-0.02489783
H	0.00000000	0.00000000	2.38483140

Hydrogen peroxide

Level of theory: CC3(FC)/*aug*-cc-pVTZ

O	-1.37083247	-0.11183297	-0.05928025
O	1.37083247	0.11183297	-0.05928025
H	-1.80587866	1.34729428	0.94082062
H	1.80587866	-1.34729428	0.94082062

Hydrogen sulfide

Level of theory: CC3(Full)/*aug*-cc-pVTZ

S	0.00000000	0.00000000	-0.50365086
H	0.00000000	1.81828105	1.25212288
H	0.00000000	-1.81828105	1.25212288

Imidazole

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.41662795	2.06006259	0.00000000
C	-1.52618386	-1.62343163	0.00000000
C	1.04160471	-1.93007427	0.00000000
N	-1.90345764	0.94914956	0.00000000
N	2.24215443	0.38083431	0.00000000

H	0.65501634	4.07748278	0.00000000
H	-3.57500545	1.84103166	0.00000000
H	-3.06363894	-2.94559167	0.00000000
H	2.08673940	-3.67001102	0.00000000

Isobutene

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	2.70790758
C	0.00000000	0.00000000	0.18431282
C	0.00000000	2.39894572	-1.32482735
C	0.00000000	-2.39894572	-1.32482735
H	0.00000000	1.74848405	3.76691310
H	0.00000000	-1.74848405	3.76691310
H	0.00000000	4.05897160	-0.10582007
H	0.00000000	-4.05897160	-0.10582007
H	1.66026992	2.48337908	-2.55086178
H	-1.66026992	2.48337908	-2.55086178
H	1.66026992	-2.48337908	-2.55086178
H	-1.66026992	-2.48337908	-2.55086178

Ketene

Level of theory: CC3(Full)/*aug*-cc-pVTZ

Ground state

C	0.00000000	0.00000000	-2.44810151
C	0.00000000	0.00000000	0.03498545
O	0.00000000	0.00000000	2.23663914
H	0.00000000	1.77432079	-3.43705988
H	0.00000000	-1.77432079	-3.43705988

Excited state

C	2.04306304	0.00000000	-0.93056721
C	0.00400918	0.00000000	0.83531393
O	-2.23710378	0.00000000	0.46984584
H	1.63603518	0.00000000	-2.93687368
H	3.96212800	0.00000000	-0.26649149

Maleimide

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	2.17350401	0.25165554
C	0.00000000	-2.17350401	0.25165554
C	0.00000000	1.26218315	-2.42188951
C	0.00000000	-1.26218315	-2.42188951
N	0.00000000	0.00000000	1.72344743
O	0.00000000	4.32709218	1.01147397
O	0.00000000	-4.32709218	1.01147397
H	0.00000000	0.00000000	3.62206099
H	0.00000000	2.54941470	-3.99634348
H	0.00000000	-2.54941470	-3.99634348

Methanimine

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.10696646	0.00000000	1.11091130
N	0.10764012	0.00000000	-1.29677742
H	-1.59140953	0.00000000	2.27296652
H	1.90475160	0.00000000	2.09393982
H	-1.69956184	0.00000000	-1.96217482

Methylenecyclopropene

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	0.53512883
C	0.00000000	0.00000000	3.04739824
C	0.00000000	1.25042956	-1.88571561
C	0.00000000	-1.25042956	-1.88571561
H	0.00000000	2.96887531	-2.96270271
H	0.00000000	-2.96887531	-2.96270271
H	0.00000000	1.75335023	4.08608382
H	0.00000000	-1.75335023	4.08608382

Naphthalene

Level of theory: CC3(Full)/cc-pVTZ

C	0.00000000	1.33999524	0.00000000
C	0.00000000	-1.33999524	0.00000000
C	2.33779858	2.63841577	0.00000000
C	-2.33779858	2.63841577	0.00000000
C	2.33779858	-2.63841577	0.00000000
C	-2.33779858	-2.63841577	0.00000000
C	4.57964958	1.33587048	0.00000000
C	-4.57964958	1.33587048	0.00000000
C	4.57964958	-1.33587048	0.00000000
C	-4.57964958	-1.33587048	0.00000000
H	2.32888235	4.67949410	0.00000000
H	-2.32888235	4.67949410	0.00000000
H	2.32888235	-4.67949410	0.00000000
H	-2.32888235	-4.67949410	0.00000000
H	6.34884007	2.34551705	0.00000000
H	-6.34884007	2.34551705	0.00000000
H	6.34884007	-2.34551705	0.00000000
H	-6.34884007	-2.34551705	0.00000000

Naphthoquinone

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	0.00000000	1.31868219	5.07583353
C	0.00000000	-1.31868219	5.07583353
C	0.00000000	2.63328396	2.80719633
C	0.00000000	-2.63328396	2.80719633
C	0.00000000	1.31896773	0.52975242
C	0.00000000	-1.31896773	0.52975242
C	0.00000000	2.74649968	-1.88121997
C	0.00000000	-2.74649968	-1.88121997
C	0.00000000	1.26627836	-4.24808471
C	0.00000000	-1.26627836	-4.24808471
O	0.00000000	5.05039066	-1.94176133
O	0.00000000	-5.05039066	-1.94176133
H	0.00000000	2.33629038	6.83936996
H	0.00000000	-2.33629038	6.83936996
H	0.00000000	4.66861735	2.75798976
H	0.00000000	-4.66861735	2.75798976
H	0.00000000	2.35501749	-5.96917497
H	0.00000000	-2.35501749	-5.96917497

Nitroaniline

Level of theory: CC3(FC)/cc-pVTZ

C	0.00000000	0.00000000	-4.05915738
C	2.28068352	0.00000000	-2.70811066
C	-2.28068352	0.00000000	-2.70811066
C	0.00000000	0.00000000	1.19144079
C	2.28308329	0.00000000	-0.09681843
C	-2.28308329	0.00000000	-0.09681843
N	0.00000000	0.00000000	3.94052757
N	0.00000000	0.00000000	-6.63741535
O	2.04948184	0.00000000	5.01410797
O	-2.04948184	0.00000000	5.01410797
H	4.04799128	0.00000000	-3.72195018
H	-4.04799128	0.00000000	-3.72195018
H	4.02032559	0.00000000	0.95557275
H	-4.02032559	0.00000000	0.95557275
H	-1.62132329	0.00000000	-7.60488781
H	1.62132329	0.00000000	-7.60488781

Nitrobenzene

Level of theory: CC3(FC)/cc-pVTZ

C	0.00000000	0.00000000	-0.33719774
C	2.29667056	0.00000000	0.92138137
C	-2.29667056	0.00000000	0.92138137
C	0.00000000	0.00000000	4.85826496
C	2.28247086	0.00000000	3.54756893
C	-2.28247086	0.00000000	3.54756893
N	0.00000000	0.00000000	-3.11429157
O	-2.05476165	0.00000000	-4.18095202
O	2.05476165	0.00000000	-4.18095202
H	4.02347357	0.00000000	-0.14769848
H	-4.02347357	0.00000000	-0.14769848
H	4.04624818	0.00000000	4.56388578
H	-4.04624818	0.00000000	4.56388578
H	0.00000000	0.00000000	6.89454456

Nitrodimethylaniniline

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	0.00000000	0.00000000	-2.70893747
C	2.28286889	0.00000000	-1.33300281
C	-2.28286889	0.00000000	-1.33300281
C	0.00000000	0.00000000	2.57206374
C	2.27821428	0.00000000	1.27798588
C	-2.27821428	0.00000000	1.27798588
C	2.36504204	0.00000000	-6.64945038
C	-2.36504204	0.00000000	-6.64945038
N	0.00000000	0.00000000	-5.28314977
N	0.00000000	0.00000000	5.31851989
O	2.04957627	0.00000000	6.39360902
O	-2.04957627	0.00000000	6.39360902
H	4.06683325	0.00000000	-2.30372191
H	-4.06683325	0.00000000	-2.30372191
H	4.01906768	0.00000000	2.32551175
H	-4.01906768	0.00000000	2.32551175
H	1.96723800	0.00000000	-8.66013185
H	-1.96723800	0.00000000	-8.66013185
H	3.49498309	-1.67118066	-6.21739275
H	3.49498309	1.67118066	-6.21739275
H	-3.49498309	1.67118066	-6.21739275
H	-3.49498309	-1.67118066	-6.21739275

Nitropyridine N-oxide

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	0.00000000	0.00000000	-1.21738204
C	2.26825255	0.00000000	0.09038008
C	-2.26825255	0.00000000	0.09038008
C	2.22988276	0.00000000	2.68605086
C	-2.22988276	0.00000000	2.68605086
N	0.00000000	0.00000000	-3.96704616
N	0.00000000	0.00000000	4.00601244
O	0.00000000	0.00000000	6.38961931
O	-2.05398155	0.00000000	-5.02438491
O	2.05398155	0.00000000	-5.02438491
H	4.03491913	0.00000000	-0.90939267
H	-4.03491913	0.00000000	-0.90939267
H	3.88274506	0.00000000	3.86446617
H	-3.88274506	0.00000000	3.86446617

Nitrosomethane

Level of theory: CC3(Full)/*aug*-cc-pVTZ

Ground state

C	-1.78426612	0.00000000	-1.07224050
N	-0.00541753	0.00000000	1.08060391
O	2.18814985	0.00000000	0.43452135
H	-0.77343975	0.00000000	-2.86415606
H	-2.97471478	1.66801808	-0.86424584
H	-2.97471478	-1.66801808	-0.86424584

Excited state

C	1.86306273	0.00000000	-1.06035094
N	0.00638693	0.00000000	1.02546010
O	-2.26923072	0.00000000	0.47699489
H	3.72600129	0.00000000	-0.21094854
H	1.58491147	1.68964774	-2.20977225
H	1.58491147	-1.68964774	-2.20977225

Nitrous acid

Level of theory: CC3(FC)/*aug*-cc-pVTZ

H	-3.27788005	0.93588010	0.00000000
N	0.29308547	0.93895729	0.00000000
O	-2.05678600	-0.42335161	0.00000000
O	2.00673459	-0.45764664	0.00000000

Nitrous oxide

Level of theory: CC3(FC)/*aug*-cc-pVTZ

N	0.00000000	0.00000000	0.13652607
N	0.00000000	0.00000000	2.27480281
O	0.00000000	0.00000000	-2.11104702

Nitroxyl

Level of theory: CC3(Full)/*aug*-cc-pVTZ

O	0.21099695	0.00000000	2.15462460
N	-0.44776863	0.00000000	-0.03589263
H	1.18163475	0.00000000	-1.17386890

Octatetraene

Level of theory: CC3(Full)/cc-pVTZ

C	1.19649232	0.64794934	0.00000000
C	-1.19649232	-0.64794934	0.00000000
C	3.45745137	-0.52964709	0.00000000
C	-3.45745137	0.52964709	0.00000000
C	5.85705040	0.77625595	0.00000000
C	-5.85705040	-0.77625595	0.00000000
C	8.10525884	-0.39700663	0.00000000
C	-8.10525884	0.39700663	0.00000000
H	1.14813002	2.69304901	0.00000000
H	-1.14813002	-2.69304901	0.00000000
H	3.50962357	-2.57436634	0.00000000
H	-3.50962357	2.57436634	0.00000000
H	5.78969253	2.81832245	0.00000000
H	-5.78969253	-2.81832245	0.00000000
H	8.22516217	-2.43500100	0.00000000
H	-8.22516217	2.43500100	0.00000000
H	9.85247043	0.65022932	0.00000000
H	-9.85247043	-0.65022932	0.00000000

Oxalyl fluoride

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	-1.39903565	0.34476183	0.00000000
C	1.39903565	-0.34476183	0.00000000
O	-2.24825627	2.40855549	0.00000000
O	2.24825627	-2.40855549	0.00000000
F	-2.78737061	-1.74488227	0.00000000
F	2.78737061	1.74488227	0.00000000

Phenazine

Level of theory: CCSD(T)(FC)/cc-pVTZ

N	0.00000000	2.68425897	0.00000000
N	0.00000000	-2.68425897	0.00000000
C	-2.14725285	1.35123660	0.00000000
C	2.14725285	1.35123660	0.00000000
C	-2.14725285	-1.35123660	0.00000000
C	2.14725285	-1.35123660	0.00000000
C	-4.49864069	2.66174043	0.00000000
C	4.49864069	2.66174043	0.00000000
C	-4.49864069	-2.66174043	0.00000000
C	4.49864069	-2.66174043	0.00000000
C	-6.71414814	1.34756473	0.00000000
C	6.71414814	1.34756473	0.00000000
C	-6.71414814	-1.34756473	0.00000000
C	6.71414814	-1.34756473	0.00000000
H	-4.44549427	4.69771133	0.00000000
H	4.44549427	4.69771133	0.00000000
H	-4.44549427	-4.69771133	0.00000000
H	4.44549427	-4.69771133	0.00000000
H	-8.49075377	2.34322156	0.00000000
H	8.49075377	2.34322156	0.00000000
H	-8.49075377	-2.34322156	0.00000000
H	8.49075377	-2.34322156	0.00000000

Phenolate

Level of theory: CC3(FC)/cc-pVTZ

C	0.00000000	0.00000000	-1.94817868
C	2.27737723	0.00000000	-0.45104645
C	-2.27737723	0.00000000	-0.45104645
C	0.00000000	0.00000000	3.54287236
C	2.25856599	0.00000000	2.16672471
C	-2.25856599	0.00000000	2.16672471
O	0.00000000	0.00000000	-4.33677175
H	4.04811102	0.00000000	-1.47084405
H	-4.04811102	0.00000000	-1.47084405
H	4.04319440	0.00000000	3.17158878
H	-4.04319440	0.00000000	3.17158878
H	0.00000000	0.00000000	5.58190673

Phenyl-pyrrole

Level of theory: CCSD(T)(FC)/cc-pVTZ

Planar

C	0.00000000	0.00000000	0.78511855
C	2.26951425	0.00000000	2.12513335
C	-2.26951425	0.00000000	2.12513335
C	0.00000000	0.00000000	6.08505036
C	2.26188550	0.00000000	4.74952804
C	-2.26188550	0.00000000	4.74952804
C	2.11189435	0.00000000	-3.40622062
C	-2.11189435	0.00000000	-3.40622062
C	1.34457992	0.00000000	-5.87759851
C	-1.34457992	0.00000000	-5.87759851
N	0.00000000	0.00000000	-1.87596109
H	4.04529764	0.00000000	1.13844406
H	-4.04529764	0.00000000	1.13844406
H	4.03918748	0.00000000	5.74456463
H	-4.03918748	0.00000000	5.74456463
H	0.00000000	0.00000000	8.12006610
H	3.97993856	0.00000000	-2.63372956
H	-3.97993856	0.00000000	-2.63372956
H	2.56993408	0.00000000	-7.49221560
H	-2.56993408	0.00000000	-7.49221560

Twisted

C	0.00000000	0.00000000	0.80351712
C	2.28073444	0.00000000	2.10816686
C	-2.28073444	0.00000000	2.10816686
C	0.00000000	0.00000000	6.05091031
C	2.27731959	0.00000000	4.73583348
C	-2.27731959	0.00000000	4.73583348
C	0.00000000	2.11496090	-3.38187966
C	0.00000000	-2.11496090	-3.38187966
C	0.00000000	1.34265418	-5.86240596
C	0.00000000	-1.34265418	-5.86240596
N	0.00000000	0.00000000	-1.87814812
H	4.02558097	0.00000000	1.05801658
H	-4.02558097	0.00000000	1.05801658
H	4.04316226	0.00000000	5.75023395
H	-4.04316226	0.00000000	5.75023395
H	0.00000000	0.00000000	8.08702673
H	0.00000000	3.96297102	-2.54995976
H	0.00000000	-3.96297102	-2.54995976
H	0.00000000	2.56243264	-7.48144109
H	0.00000000	-2.56243264	-7.48144109

Phthalazine

Level of theory: CC3(FC)/cc-pVTZ

C	0.00000000	1.32459443	-0.07132677
C	0.00000000	-1.32459443	-0.07132677
C	0.00000000	2.65486490	-2.37693013
C	0.00000000	-2.65486490	-2.37693013
C	0.00000000	1.33510515	-4.61541123
C	0.00000000	-1.33510515	-4.61541123
C	0.00000000	2.49806192	2.33813333
C	0.00000000	-2.49806192	2.33813333
N	0.00000000	1.29575320	4.50170701
N	0.00000000	-1.29575320	4.50170701
H	0.00000000	4.69409431	-2.36246981
H	0.00000000	-4.69409431	-2.36246981
H	0.00000000	2.33538579	-6.38945264
H	0.00000000	-2.33538579	-6.38945264
H	0.00000000	4.53863166	2.46976178
H	0.00000000	-4.53863166	2.46976178

Phthalimide

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	0.00000000	2.20210348	2.25054900
C	0.00000000	-2.20210348	2.25054900
C	0.00000000	1.31050301	-0.41254468
C	0.00000000	-1.31050301	-0.41254468
C	0.00000000	2.68001925	-2.63336829
C	0.00000000	-2.68001925	-2.63336829
C	0.00000000	1.32018039	-4.89183006
C	0.00000000	-1.32018039	-4.89183006
N	0.00000000	0.00000000	3.69708218
O	0.00000000	4.33361053	3.05657131
O	0.00000000	-4.33361053	3.05657131
H	0.00000000	0.00000000	5.59565443
H	0.00000000	4.71538263	-2.60774609
H	0.00000000	-4.71538263	-2.60774609
H	0.00000000	2.31561890	-6.66791824
H	0.00000000	-2.31561890	-6.66791824

Propynal

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	-0.78051115	0.00000000	-1.38900384
C	-0.17873562	0.00000000	1.27825868
C	0.23763714	0.00000000	3.52644798
O	0.80143996	0.00000000	-3.04628328
H	-2.80713069	0.00000000	-1.82768750
H	0.64026209	0.00000000	5.48853193

Pyranone

Level of theory: CC3(FC)/cc-pVTZ

C	0.00000000	0.00000000	-2.03875103
C	2.29857501	0.00000000	-0.50612872
C	-2.29857501	0.00000000	-0.50612872
C	2.18356567	0.00000000	2.02781371
C	-2.18356567	0.00000000	2.02781371
O	0.00000000	0.00000000	3.36810442
O	0.00000000	0.00000000	-4.35224344
H	3.80117763	0.00000000	3.26042029
H	-3.80117763	0.00000000	3.26042029
H	4.10758504	0.00000000	-1.43183287
H	-4.10758504	0.00000000	-1.43183287

Pyrazine

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	2.13188686	1.31510863
C	0.00000000	-2.13188686	1.31510863
C	0.00000000	2.13188686	-1.31510863
C	0.00000000	-2.13188686	-1.31510863
N	0.00000000	0.00000000	2.66620111
N	0.00000000	0.00000000	-2.66620111
H	0.00000000	3.88751412	2.35234226
H	0.00000000	-3.88751412	2.35234226
H	0.00000000	3.88751412	-2.35234226
H	0.00000000	-3.88751412	-2.35234226

Pyridazine

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	1.30150855	-2.31552865
C	0.00000000	-1.30150855	-2.31552865
C	0.00000000	2.49271907	0.03513416
C	0.00000000	-2.49271907	0.03513416
N	0.00000000	1.26228251	2.23104685
N	0.00000000	-1.26228251	2.23104685
H	0.00000000	4.52804172	0.19299731
H	0.00000000	-4.52804172	0.19299731
H	0.00000000	2.39011496	-4.03967703
H	0.00000000	-2.39011496	-4.03967703

Pyridine

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	-2.66451139
C	0.00000000	2.25494985	-1.32069889
C	0.00000000	-2.25494985	-1.32069889
C	0.00000000	2.15398594	1.30669632
C	0.00000000	-2.15398594	1.30669632
N	0.00000000	0.00000000	2.62778932
H	0.00000000	0.00000000	-4.70641516
H	0.00000000	4.05768507	-2.27625442
H	0.00000000	-4.05768507	-2.27625442
H	0.00000000	3.88059079	2.40341581
H	0.00000000	-3.88059079	2.40341581

Pyridinium

Level of theory: CC3(FC)/cc-pVTZ

C	0.00000000	0.00000000	-2.66667191
C	2.28175579	0.00000000	-1.35203950
C	-2.28175579	0.00000000	-1.35203950
C	2.23916852	0.00000000	1.25404098
C	-2.23916852	0.00000000	1.25404098
N	0.00000000	0.00000000	2.46287949
H	0.00000000	0.00000000	-4.70272202
H	4.06725168	0.00000000	-2.32197291

```
H   -4.06725168          0.00000000         -2.32197291
H    3.90684584          0.00000000          2.41825457
H   -3.90684584          0.00000000          2.41825457
H    0.00000000          0.00000000          4.37535718
```

Pyrimidine

Level of theory: CC3(Full)/*aug*-cc-pVTZ

```
C    0.00000000          0.00000000          2.41518350
C    0.00000000          0.00000000         -2.60410885
C    0.00000000          2.23272561         -1.22869402
C    0.00000000         -2.23272561         -1.22869402
N    0.00000000          2.26214196          1.29619742
N    0.00000000         -2.26214196          1.29619742
H    0.00000000          0.00000000          4.45780256
H    0.00000000          0.00000000         -4.64120942
H    0.00000000          4.05149341         -2.16351748
H    0.00000000         -4.05149341         -2.16351748
```

Pyrrole

Level of theory: CC3(Full)/*aug*-cc-pVTZ

```
C    0.00000000          2.11924634          0.62676569
C    0.00000000         -2.11924634          0.62676569
C    0.00000000          1.34568862         -1.85506908
C    0.00000000         -1.34568862         -1.85506908
N    0.00000000          0.00000000          2.10934391
H    0.00000000          0.00000000          4.00257355
H    0.00000000          3.97648410          1.44830201
H    0.00000000         -3.97648410          1.44830201
H    0.00000000          2.56726559         -3.47837232
H    0.00000000         -2.56726559         -3.47837232
```

Pyrrolopyrrole

Level of theory: CC3(FC)/cc-pVTZ

```
C    0.01987029          1.31191436          0.00000000
C   -0.01987029         -1.31191436          0.00000000
C   -2.50055820          2.23026347          0.00000000
```

C	2.50055820	-2.23026347	0.00000000
C	-3.99867844	0.09474099	0.00000000
C	3.99867844	-0.09474099	0.00000000
N	2.50780926	2.04699311	0.00000000
N	-2.50780926	-2.04699311	0.00000000
H	-3.17172573	4.14262242	0.00000000
H	3.17172573	-4.14262242	0.00000000
H	-6.02037705	-0.05658473	0.00000000
H	6.02037705	0.05658473	0.00000000
H	3.16071224	3.82066088	0.00000000
H	-3.16071224	-3.82066088	0.00000000

Quinoxaline

Level of theory: CC3(FC)/cc-pVTZ

C	0.00000000	1.33833541	0.04624026
C	0.00000000	-1.33833541	0.04624026
C	0.00000000	2.65319151	-2.27752466
C	0.00000000	-2.65319151	-2.27752466
C	0.00000000	1.33717941	-4.51073479
C	0.00000000	-1.33717941	-4.51073479
C	0.00000000	1.33936683	4.32768896
C	0.00000000	-1.33936683	4.32768896
N	0.00000000	2.68409862	2.24219152
N	0.00000000	-2.68409862	2.24219152
H	0.00000000	4.68915946	-2.22328575
H	0.00000000	-4.68915946	-2.22328575
H	0.00000000	2.33972888	-6.28367426
H	0.00000000	-2.33972888	-6.28367426
H	0.00000000	2.35369837	6.10018213
H	0.00000000	-2.35369837	6.10018213

$SiCl_2$

Level of theory: CC3(Full)/*aug*-cc-pVTZ

Si	0.00000000	0.00000000	-1.78528322
Cl	0.00000000	3.04414528	0.71619419
Cl	0.00000000	-3.04414528	0.71619419

Silylidene

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	-2.09539928
Si	0.00000000	0.00000000	1.14992930
H	0.00000000	1.70929524	-3.22894481
H	0.00000000	-1.70929524	-3.22894481

Streptocyanine-C1

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	0.80488833
N	0.00000000	2.19423463	-0.33580561
N	0.00000000	-2.19423463	-0.33580561
H	0.00000000	0.00000000	2.84436959
H	0.00000000	2.36978315	-2.23371976
H	0.00000000	-2.36978315	-2.23371976
H	0.00000000	3.79412648	0.69399206
H	0.00000000	-3.79412648	0.69399206

Streptocyanine-C3

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	0.65419136
C	0.00000000	2.24294899	-0.68901318
C	0.00000000	-2.24294899	-0.68901318
N	0.00000000	4.52279187	0.30876781
N	0.00000000	-4.52279187	0.30876781
H	0.00000000	0.00000000	2.69658250
H	0.00000000	2.18484165	-2.73430592
H	0.00000000	-2.18484165	-2.73430592
H	0.00000000	6.07453303	-0.78935070
H	0.00000000	-6.07453303	-0.78935070
H	0.00000000	4.78699964	2.19452692
H	0.00000000	-4.78699964	2.19452692

Streptocyanine-C5

Level of theory: CC3(Full)/cc-pVTZ

C	0.00000000	0.00000000	0.46857445
C	0.00000000	2.33439812	-0.72581892
C	0.00000000	-2.33439812	-0.72581892
C	0.00000000	4.51630408	0.70773577
C	0.00000000	-4.51630408	0.70773577
N	0.00000000	6.84533147	-0.19544059
N	0.00000000	-6.84533147	-0.19544059
H	0.00000000	0.00000000	2.51676448
H	0.00000000	2.44956750	-2.76140399
H	0.00000000	-2.44956750	-2.76140399
H	0.00000000	4.36770843	2.74488884
H	0.00000000	-4.36770843	2.74488884
H	0.00000000	8.34616080	0.96591148
H	0.00000000	-8.34616080	0.96591148
H	0.00000000	7.18140877	-2.06656349
H	0.00000000	-7.18140877	-2.06656349

Tetrathiafulvalene

Level of theory: CC3(FC)/cc-pVTZ

C	-1.27140171	0.00000000	0.00000000
C	1.27140171	0.00000000	0.00000000
C	-5.98994256	1.26331812	0.00000000
C	-5.98994256	-1.26331812	0.00000000
C	5.98994256	-1.26331812	0.00000000
C	5.98994256	1.26331812	0.00000000
S	-3.07078317	2.82030107	0.00000000
S	-3.07078317	-2.82030107	0.00000000
S	3.07078317	-2.82030107	0.00000000
S	3.07078317	2.82030107	0.00000000
H	-7.66536437	2.41057807	0.00000000
H	-7.66536437	-2.41057807	0.00000000
H	7.66536437	-2.41057807	0.00000000
H	7.66536437	2.41057807	0.00000000

Tetrazine

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	2.38208164
C	0.00000000	0.00000000	-2.38208164
N	2.25673244	0.00000000	1.24973261

N	-2.25673244	0.00000000	1.24973261
N	2.25673244	0.00000000	-1.24973261
N	-2.25673244	0.00000000	-1.24973261
H	0.00000000	0.00000000	4.41850901
H	0.00000000	0.00000000	-4.41850901

Thienothienyl

Level of theory: CC3(FC)/cc-pVTZ

C	0.41618901	1.24091123	0.00000000
C	-0.41618901	-1.24091123	0.00000000
C	-1.56128826	3.05660382	0.00000000
C	1.56128826	-3.05660382	0.00000000
C	-3.86882315	1.90421786	0.00000000
C	3.86882315	-1.90421786	0.00000000
S	3.68518133	1.37661050	0.00000000
S	-3.68518133	-1.37661050	0.00000000
H	-1.30761309	5.07161572	0.00000000
H	1.30761309	-5.07161572	0.00000000
H	-5.68944011	2.79705270	0.00000000
H	5.68944011	-2.79705270	0.00000000

Thioacetone

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	0.00000000	0.68476030
C	0.00000000	2.38541696	2.20685096
C	0.00000000	-2.38541696	2.20685096
S	0.00000000	0.00000000	-2.39920303
H	0.00000000	4.04609254	1.00090614
H	0.00000000	-4.04609254	1.00090614
H	1.65894780	2.42602225	3.43712000
H	-1.65894780	2.42602225	3.43712000
H	1.65894780	-2.42602225	3.43712000
H	-1.65894780	-2.42602225	3.43712000

Thioacrolein

Level of theory: CC3(Full)/*aug*-cc-pVTZ

```
C     4.27693176           0.00000000          -0.88320133
C     1.76449030           0.00000000          -1.23998444
C     0.00891877           0.00000000           0.85393278
S    -3.06510749           0.00000000           0.58558716
H     5.57642075           0.00000000          -2.45571463
H     5.06950243           0.00000000           1.00139499
H     0.96616458           0.00000000          -3.11935314
H     0.87110201           0.00000000           2.71756937
```

Thioformaldehyde

Level of theory: CC3(Full)/*aug*-cc-pVTZ

Ground state

```
C     0.00000000           0.00000000          -2.08677304
S     0.00000000           0.00000000           0.97251194
H     0.00000000           1.73657773          -3.17013507
H     0.00000000          -1.73657773          -3.17013507
```

Excited state

```
C     0.00000000           0.00000000          -2.20256705
S     0.00000000           0.00000000           1.02717172
H     0.00000000           1.76634191          -3.21909384
H     0.00000000          -1.76634191          -3.21909384
```

Thioformaldehyde-S-oxide

Level of theory: CC3(Full)/*aug*-cc-pVTZ

```
C    -2.60499135           0.77983525           0.00000000
O     2.33211975           0.83760351           0.00000000
S     0.03093612          -0.78961636           0.00000000
H    -4.30439246          -0.34582852           0.00000000
H    -2.67226676           2.81674398           0.00000000
```

Thiophene

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	2.33342542	-0.09858421
C	0.00000000	-2.33342542	-0.09858421
C	0.00000000	1.34371718	-2.48297725
C	0.00000000	-1.34371718	-2.48297725
S	0.00000000	0.00000000	2.17250692
H	0.00000000	4.29028016	0.44577296
H	0.00000000	-4.29028016	0.44577296
H	0.00000000	2.48760051	-4.16768392
H	0.00000000	-2.48760051	-4.16768392

Thiopropynal

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	-0.00382924	0.00000000	-1.25249909
C	-2.27832423	0.00000000	0.15152736
C	-4.26309583	0.00000000	1.29548793
S	2.81920288	0.00000000	-0.00828974
H	-0.23056990	0.00000000	-3.28862183
H	-5.97712967	0.00000000	2.33206931

Tolan

Level of theory: CCSD(T)(FC)/cc-pVTZ

C	-1.14632202	0.00000000	0.00000000
C	1.14632202	0.00000000	0.00000000
C	-3.83802475	0.00000000	0.00000000
C	3.83802475	0.00000000	0.00000000
C	-5.17616712	-2.27953873	0.00000000
C	-5.17616712	2.27953873	0.00000000
C	5.17616712	2.27953873	0.00000000
C	5.17616712	-2.27953873	0.00000000
C	-7.79943938	-2.27513115	0.00000000
C	-7.79943938	2.27513115	0.00000000
C	7.79943938	2.27513115	0.00000000
C	7.79943938	-2.27513115	0.00000000
C	-9.12002539	0.00000000	0.00000000
C	9.12002539	0.00000000	0.00000000
H	-4.14659821	-4.03713330	0.00000000
H	-4.14659821	4.03713330	0.00000000
H	4.14659821	4.03713330	0.00000000
H	4.14659821	-4.03713330	0.00000000

H	-8.81141954	-4.04290254	0.00000000
H	-8.81141954	4.04290254	0.00000000
H	8.81141954	4.04290254	0.00000000
H	8.81141954	-4.04290254	0.00000000
H	-11.15613663	0.00000000	0.00000000
H	11.15613663	0.00000000	0.00000000

Triazapentalene

Level of theory: CC3(FC)/cc-pVTZ

C	-2.50499953	2.11638523	0.00000000
C	-3.96445816	-0.07303868	0.00000000
C	-2.35355924	-2.15265577	0.00000000
C	3.83593935	-0.03073106	0.00000000
C	2.43560744	2.16757403	0.00000000
N	0.04006152	-1.21957559	0.00000000
N	-0.04182459	1.35780418	0.00000000
N	2.39603035	-2.14324663	0.00000000
H	-3.00087038	4.07607227	0.00000000
H	-5.98766760	-0.14484657	0.00000000
H	-2.68330099	-4.14581320	0.00000000
H	5.85502782	-0.19299220	0.00000000
H	2.92994089	4.12450552	0.00000000

Triazine

Level of theory: CC3(Full)/*aug*-cc-pVTZ

C	0.00000000	-2.11414732	-1.22060353
C	0.00000000	0.00000000	2.44120705
C	0.00000000	2.11414732	-1.22060353
N	0.00000000	-2.24624733	1.29687150
N	0.00000000	2.24624733	1.29687150
N	0.00000000	0.00000000	-2.59374300
H	0.00000000	3.88296710	-2.24183210
H	0.00000000	-3.88296710	-2.24183210
H	0.00000000	0.00000000	4.48366420

Water

Level of theory: CC3(Full)/*aug*-cc-pVTZ

O	0.00000000	0.00000000	-0.13209669
H	0.00000000	1.43152878	0.97970006
H	0.00000000	-1.43152878	0.97970006