

TABS: A database of molecular structures

Shamus A. Blair and Ajit J. Thakkar

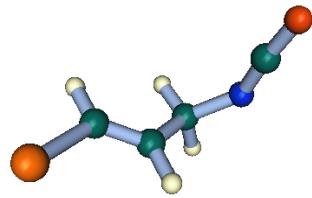
Department of Chemistry, University of New Brunswick,
Fredericton, New Brunswick E3B 5A3, Canada

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The Cartesian coordinates are in Å. The legend for the atoms in the molecular structure diagram is as defined below.



Molecule# 0001
(1E)-1-bromo-3-isocyanato-1-propene
PointGroup: C1
E= -2859.122678200 au
ZPE= 0.074649 au
LUMO_eps= -0.03691 au
HOMO_eps= -0.27228 au
Dipole= 2.633 debye



11

Br	-2.267871	-0.291954	-0.040277
O	3.663540	-1.567304	0.108174
N	2.809816	0.618208	-0.205898
C	1.638478	1.423302	0.082027
C	0.360464	0.765580	-0.357880
C	-0.627875	0.510467	0.482479
C	3.186038	-0.505612	-0.014415
H	1.767571	2.367862	-0.447493
H	1.606371	1.652917	1.148662
H	0.279107	0.508641	-1.406687
H	-0.597210	0.737527	1.537844

Molecule# 0002

(2-propyn-1-ylsulfonyl)benzene

PointGroup: C1

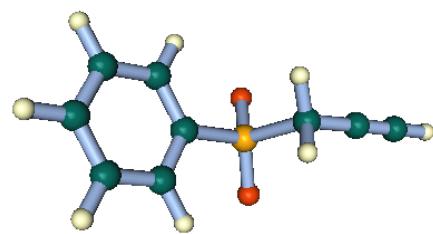
E= -896.517467806 au

ZPE= 0.147504 au

LUMO_eps= -0.06377 au

HOMO_eps= -0.28380 au

Dipole= 5.072 debye



20

O	1.156985	1.267774	1.230191
S	0.843996	0.000062	0.585576
C	1.650805	-0.000061	-1.080985
C	3.089778	-0.000082	-0.968083
C	4.283059	-0.000104	-0.864662
O	1.157003	-1.267545	1.230387
C	-0.900255	0.000015	0.152344
C	-1.559782	-1.213746	-0.004980
C	-2.908652	-1.207188	-0.338370
C	-3.579238	-0.000063	-0.507878
C	-2.908689	1.207101	-0.338507
C	-1.559819	1.213738	-0.005118
H	1.278876	0.889853	-1.588820
H	1.278846	-0.890027	-1.588706
H	5.340191	-0.000125	-0.768376
H	-1.026919	-2.140103	0.154686
H	-3.436604	-2.143231	-0.457340
H	-4.629833	-0.000093	-0.764710
H	-3.436669	2.143114	-0.457585
H	-1.026981	2.140129	0.154442

Molecule# 0003

(2R)-4-methylpentan-2-ol

PointGroup: C1

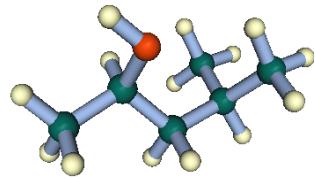
E= -312.422759949 au

ZPE= 0.192402 au

LUMO_eps= -0.01619 au

HOMO_eps= -0.27810 au

Dipole= 1.577 debye



21

C	1.757085	-1.091084	-0.817160
C	1.865711	1.150795	0.344263
C	-2.561944	-0.479494	0.222334
C	-0.108652	-0.438664	0.811498
C	1.383699	-0.300756	0.441026
C	-1.155311	-0.134494	-0.257223
O	-1.063482	1.259171	-0.592699
H	1.319591	-0.646459	-1.712763
H	1.420349	-2.128425	-0.757181
H	2.839293	-1.101666	-0.956361
H	1.631351	1.705127	1.254703
H	2.948329	1.182645	0.204223
H	1.395373	1.671994	-0.487552
H	-2.805836	0.079162	1.127243
H	-3.304011	-0.233062	-0.540810
H	-2.651586	-1.545510	0.436884
H	-0.321008	0.193554	1.678818
H	-0.280510	-1.470795	1.130737
H	1.924875	-0.758063	1.276660
H	-0.937758	-0.728497	-1.152861
H	-1.754119	1.468806	-1.228574

Molecule# 0004

(2S)-1,1,1-trifluoro-2-propanol

PointGroup: C1

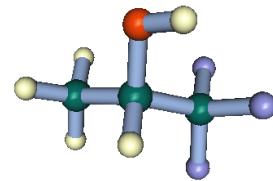
E= -492.294903682 au

ZPE= 0.084874 au

LUMO_eps= -0.01821 au

HOMO_eps= -0.31407 au

Dipole= 1.773 debye



12

C	1.691694	-1.059638	0.022200
C	0.834706	0.103985	-0.438962
C	-0.626301	-0.051282	-0.007120
O	1.377143	1.294553	0.099907
F	-1.202071	-1.107944	-0.616961
F	-0.772758	-0.215589	1.316667
F	-1.341353	1.047142	-0.354298
H	1.723765	-1.097280	1.109737
H	2.704918	-0.923400	-0.350521
H	1.303296	-2.003475	-0.356524
H	0.809896	0.144005	-1.533728
H	0.886012	2.052862	-0.233600

Molecule# 0005

(2Z)-(hydroxyimino)(1,2-oxazol-5-yl)acetic acid

PointGroup: C1

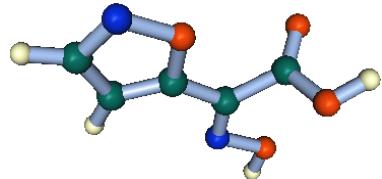
E= -603.460960761 au

ZPE= 0.098113 au

LUMO_eps= -0.08403 au

HOMO_eps= -0.26517 au

Dipole= 3.437 debye



15

O	-1.386694	-0.955842	-0.030927
O	1.673838	-1.363612	1.177598
O	1.760784	-1.318632	-1.074923
O	2.466034	1.540093	-0.013587
N	1.079600	1.577817	-0.028311
N	-2.776900	-0.886607	-0.040218
C	-0.883578	0.294634	0.005329
C	0.564807	0.409695	0.011606
C	1.394065	-0.855428	0.129539
C	-1.901139	1.199961	0.020623
C	-3.059097	0.390299	-0.009356
H	2.283422	-2.124288	-0.935669
H	2.715908	2.470145	-0.038919
H	-1.826555	2.270621	0.050855
H	-4.093711	0.694019	-0.008296

Molecule# 0006

(2Z,4E)-hexa-2,4-diene

PointGroup: Cs

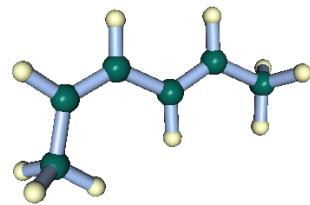
E= -234.722376697 au

ZPE= 0.141111 au

LUMO_eps= -0.02534 au

HOMO_eps= -0.22041 au

Dipole= 0.337 debye



16

C	0.295502	2.961166	0.000000
H	1.366295	2.756811	0.000000
H	0.066568	3.574997	0.875789
H	0.066568	3.574997	-0.875789
C	1.035454	-2.497577	0.000000
H	1.764853	-1.690390	0.000000
H	1.228827	-3.123576	-0.875540
H	1.228827	-3.123576	0.875540
C	-0.380018	-2.011080	0.000000
H	-1.135032	-2.790309	0.000000
C	-0.810657	-0.742182	0.000000
H	-1.883957	-0.578533	0.000000
C	0.000000	0.461923	0.000000
H	1.078980	0.347754	0.000000
C	-0.506126	1.700221	0.000000
H	-1.586860	1.816991	0.000000

Molecule# 0007

(2Z,4Z)-2,4-hexadiene

PointGroup: C2h

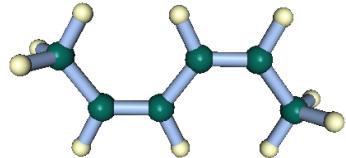
E= -234.720064893 au

ZPE= 0.141247 au

LUMO_eps= -0.02757 au

HOMO_eps= -0.22133 au

Dipole= 0.000 debye



16

H	0.310543	2.728828	0.000000
C	-0.313196	1.840812	0.000000
H	1.396218	0.676680	0.000000
C	0.313196	0.654900	0.000000
H	-1.396218	-0.676680	0.000000
C	-0.313196	-0.654900	0.000000
H	-0.310543	-2.728828	0.000000
C	0.313196	-1.840812	0.000000
H	2.383856	-1.194467	0.000000
H	2.072264	-2.692860	0.875470
H	2.072264	-2.692860	-0.875470
C	1.786306	-2.103254	0.000000
H	-2.383856	1.194467	0.000000
H	-2.072264	2.692860	0.875470
H	-2.072264	2.692860	-0.875470
C	-1.786306	2.103254	0.000000

Molecule# 0008

(3E)-2-methyl-1,3-pentadiene

PointGroup: C1

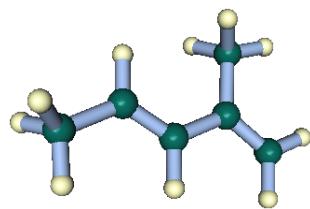
E= -234.722633756 au

ZPE= 0.141100 au

LUMO_eps= -0.03057 au

HOMO_eps= -0.22819 au

Dipole= 0.674 debye



16

C	2.066444	-1.078567	0.000000
C	1.117232	-0.133948	0.000001
C	-0.293736	-0.518951	0.000015
C	-1.341106	0.310850	0.000031
C	-2.772365	-0.122358	-0.000019
C	1.473859	1.328371	-0.000012
H	3.118414	-0.827682	-0.000025
H	1.813394	-2.130884	0.000014
H	-0.482710	-1.588989	-0.000013
H	-1.170199	1.382350	0.000073
H	-2.863802	-1.208498	-0.000060
H	-3.301379	0.263852	0.875706
H	-3.301329	0.263911	-0.875747
H	1.065954	1.834129	-0.878047
H	1.066119	1.834099	0.878118
H	2.553575	1.465330	-0.000111

Molecule# 0009

(3E)-3-methyl-1,3-pentadiene

PointGroup: C1

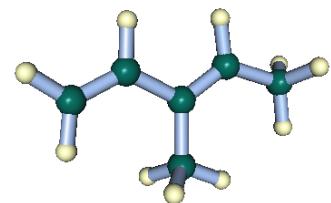
E= -234.720025267 au

ZPE= 0.141060 au

LUMO_eps= -0.02912 au

HOMO_eps= -0.22707 au

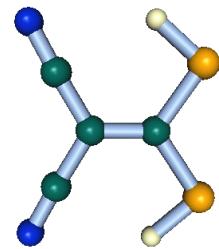
Dipole= 0.795 debye



16

C	2.526085	-0.224091	-0.000065
C	1.294342	-0.739554	0.000012
C	0.034400	0.006499	-0.000010
C	-1.115939	-0.688795	0.000099
C	-2.521058	-0.179706	0.000118
C	0.114883	1.508528	-0.000144
H	3.396043	-0.865751	-0.000039
H	2.711374	0.841312	-0.000153
H	1.189188	-1.820097	0.000100
H	-1.028922	-1.771727	0.000189
H	-3.063558	-0.549262	0.875060
H	-2.589482	0.905588	-0.000006
H	-3.063659	-0.549470	-0.874672
H	0.658431	1.866471	-0.877450
H	-0.864162	1.979015	-0.000164
H	0.658474	1.866628	0.877071

Molecule# 0010
(disulfanylmethylenemalononitrile
PointGroup: C1
E= -1059.618990000 au
ZPE= 0.048550 au
LUMO_eps= -0.10622 au
HOMO_eps= -0.27578 au
Dipole= 4.214 debye



10

S	-1.532660	-1.443390	-0.000144
S	-1.532666	1.443384	0.000144
N	2.115081	2.230324	0.000234
N	2.115090	-2.230316	-0.000233
C	0.830778	0.000002	0.000000
C	-0.544914	0.000000	0.000000
C	1.562090	1.217179	0.000129
C	1.562094	-1.217173	-0.000128
H	-0.513127	-2.326270	-0.000166
H	-0.513135	2.326268	0.000166

Molecule# 0011

(hydroxymethylene)malononitrile

PointGroup: C1

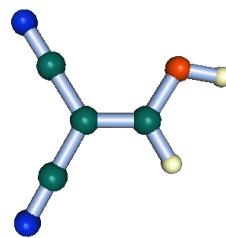
E= -338.422214657 au

ZPE= 0.054889 au

LUMO_eps= -0.09236 au

HOMO_eps= -0.29051 au

Dipole= 6.681 debye



9

O	1.964875	-1.028829	0.000000
N	-2.725203	-0.414146	0.000000
N	0.766731	2.336947	-0.000002
C	-0.171149	-0.063923	0.000000
C	0.638308	-1.147035	0.000000
C	-1.584579	-0.252310	0.000000
C	0.348128	1.264198	-0.000001
H	2.392732	-1.891508	0.000000
H	0.213330	-2.143050	0.000002

Molecule# 0012
(iminomethylene)malononitrile

PointGroup: C1

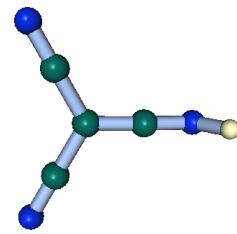
E= -317.305036213 au

ZPE= 0.042516 au

LUMO_eps= -0.09295 au

HOMO_eps= -0.29369 au

Dipole= 5.500 debye



8

N	-2.466280	-0.000132	-0.115548
N	1.326285	-2.243604	0.007368
N	1.326027	2.243752	0.007368
C	0.059128	0.000000	-0.004517
C	-1.277855	-0.000071	0.009938
C	0.760958	-1.239785	0.001005
C	0.760821	1.239864	0.001005
H	-3.120536	-0.000167	0.661103

Molecule# 0013

(methoxyimino)methanone

PointGroup: C1

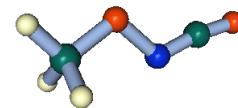
E= -283.244363463 au

ZPE= 0.054020 au

LUMO_eps= -0.06619 au

HOMO_eps= -0.26423 au

Dipole= 2.322 debye



8

O	-0.918919	0.545512	-0.000017
O	2.432931	0.084775	0.000018
N	0.106029	-0.423845	-0.000029
C	-2.173941	-0.133816	0.000020
C	1.278201	-0.072865	-0.000002
H	-2.914348	0.662738	0.000020
H	-2.282738	-0.749000	0.894011
H	-2.282772	-0.749032	-0.893944

Molecule# 0014

[(1Z)-2-chloroethanimidoyl]malononitrile

PointGroup: C1

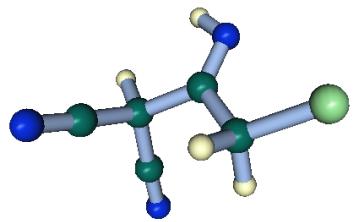
E= -817.486724238 au

ZPE= 0.085294 au

LUMO_eps= -0.07419 au

HOMO_eps= -0.31988 au

Dipole= 2.410 debye



13

C1	-2.745853	0.000000	-0.458741
N	-0.811909	-0.000003	1.816306
N	2.136126	2.181527	-0.641085
N	2.136127	-2.181525	-0.641088
C	-0.235309	0.000000	0.701571
C	1.323138	0.000000	0.550801
C	-0.970811	0.000001	-0.614246
C	1.796864	1.210768	-0.129504
C	1.796865	-1.210767	-0.129506
H	-0.172445	-0.000004	2.608644
H	1.744862	-0.000001	1.558684
H	-0.689901	0.880301	-1.191176
H	-0.689901	-0.880298	-1.191179

Molecule# 0015

[(5-chloro-2-furyl)methylidyne]azane oxide

PointGroup: C1

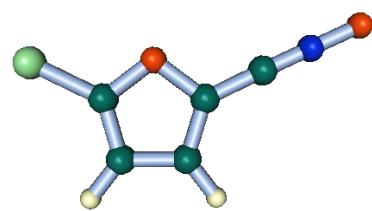
E= -857.193801589 au

ZPE= 0.063079 au

LUMO_eps= -0.06531 au

HOMO_eps= -0.23992 au

Dipole= 3.984 debye



11

C1	-2.933937	-0.850434	-0.000044
O	-0.346846	-0.549858	-0.000006
O	4.235353	-0.675671	-0.000125
N	3.080676	-0.335472	-0.000056
C	0.058308	1.657615	0.000110
C	0.637991	0.420462	0.000047
C	-1.349070	1.455584	0.000089
C	-1.524517	0.108140	0.000020
C	1.968174	-0.006252	0.000050
H	0.583129	2.596701	0.000164
H	-2.124310	2.199912	0.000120

Molecule# 0016

[(cyanomethyl)sulfanyl](hydroxy)acetic acid

PointGroup: C1

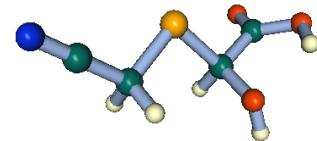
E= -834.233307762 au

ZPE= 0.094387 au

LUMO_eps= -0.05439 au

HOMO_eps= -0.27754 au

Dipole= 6.075 debye

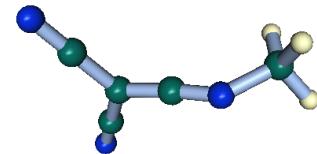


14

S	-0.536792	-0.543833	-0.276416
O	0.866478	1.705968	0.049598
O	2.489216	-1.419387	0.583107
O	2.845768	0.218453	-0.891343
N	-4.192497	-0.407208	-0.402880
C	0.859914	0.349946	0.489306
C	2.146941	-0.391213	0.076767
C	-1.899041	0.431745	0.492309
C	-3.177957	-0.037706	-0.008686
H	1.217959	2.266909	0.750986
H	2.393223	1.045651	-1.126008
H	0.773010	0.288303	1.574137
H	-1.868393	0.311523	1.575605
H	-1.770497	1.482491	0.239021

Molecule# 0017
[(methylimino)methylene]malononitrile
PointGroup: C1

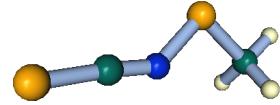
E= -356.633059110 au
ZPE= 0.070846 au
LUMO_eps= -0.07511 au
HOMO_eps= -0.27461 au
Dipole= 7.340 debye



11

N	1.861945	0.000000	-0.456084
N	-1.883795	-2.246172	0.097385
N	-1.883789	2.246175	0.097385
C	-0.633316	0.000000	-0.061156
C	0.702935	0.000000	-0.213424
C	-1.327965	-1.238667	0.025608
C	-1.327962	1.238668	0.025608
C	3.099732	-0.000002	0.296584
H	3.669604	0.881017	0.009638
H	3.669563	-0.881067	0.009698
H	2.919761	0.000038	1.370540

Molecule# 0018
[(methylsulfanyl)imino]methanethione
PointGroup: C1
E= -929.248327580 au
ZPE= 0.048868 au
LUMO_eps= -0.06885 au
HOMO_eps= -0.23163 au
Dipole= 3.167 debye



8

S	1.487854	-0.652185	0.000095
S	-2.683866	0.052343	-0.000262
N	0.082020	0.281815	0.000072
C	2.714170	0.680388	0.000283
C	-1.107551	0.131432	-0.000082
H	3.680142	0.176343	0.000324
H	2.621166	1.288815	-0.895396
H	2.621025	1.288688	0.896033

Molecule# 0019

[1,3]dioxolo[4,5-d]pyrimidine

PointGroup: Cs

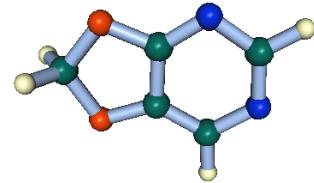
E= -453.025298214 au

ZPE= 0.092589 au

LUMO_eps= -0.04850 au

HOMO_eps= -0.25075 au

Dipole= 3.042 debye



13

C	-0.718665	-1.555127	0.000000
C	-2.163694	0.226359	0.000000
C	0.315607	-0.659942	0.000000
C	0.000000	0.695721	0.000000
C	2.228992	0.497352	0.000000
N	-1.985417	-1.080489	0.000000
N	-1.205174	1.183491	0.000000
O	1.668909	-0.830309	0.000000
O	1.140201	1.432865	0.000000
H	-0.576224	-2.627468	0.000000
H	-3.184942	0.584348	0.000000
H	2.824495	0.637742	0.902050
H	2.824495	0.637742	-0.902050

Molecule# 0020

[1,3]dithiolo[4,5-d]pyrimidine

PointGroup: C1

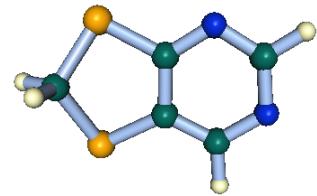
E= -1098.988719280 au

ZPE= 0.086233 au

LUMO_eps= -0.06151 au

HOMO_eps= -0.23608 au

Dipole= 2.825 debye



13

C	-1.485209	1.351731	0.043199
C	-2.539465	-0.658118	0.027515
C	-0.256809	0.716701	-0.007150
C	-0.286056	-0.686804	-0.018776
C	2.255116	-0.024473	0.324269
N	-2.633772	0.663232	0.061234
N	-1.410366	-1.376466	-0.006097
S	1.321935	1.487762	-0.135275
S	1.275421	-1.509989	-0.105022
H	-1.560648	2.432329	0.064669
H	-3.465024	-1.219915	0.032889
H	3.180774	-0.038600	-0.242667
H	2.470711	-0.019781	1.389566

Molecule# 0021

{[(1-chloroethyl)sulfanyl]imino}methanone

PointGroup: C1

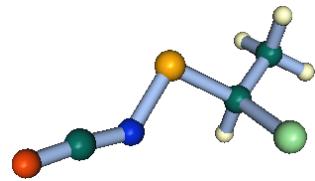
E= -1105.244569750 au

ZPE= 0.070538 au

LUMO_eps= -0.05858 au

HOMO_eps= -0.25085 au

Dipole= 3.210 debye



11

C1	1.561680	1.458583	-0.139280
S	-0.199332	-0.989403	-0.363561
O	-3.703891	0.379365	-0.024728
N	-1.406676	-0.052559	0.379697
C	1.249977	-0.250731	0.422674
C	-2.570828	0.137435	0.120568
C	2.453915	-1.127919	0.131443
H	1.049046	-0.158737	1.484752
H	2.308548	-2.119331	0.561143
H	3.342765	-0.681353	0.571677
H	2.619862	-1.225756	-0.940992

Molecule# 0022

acenaphthene

PointGroup: C2v

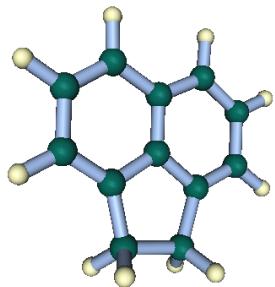
E= -463.473577225 au

ZPE= 0.182203 au

LUMO_eps= -0.04302 au

HOMO_eps= -0.21281 au

Dipole= 0.969 debye



22

C	0.000000	2.417403	1.181934
C	0.000000	-2.417403	1.181934
C	0.000000	1.271044	1.944423
C	0.000000	-1.271044	1.944423
C	0.000000	2.386884	-0.235954
C	0.000000	-2.386884	-0.235954
C	0.000000	0.000000	1.317592
C	0.000000	0.000000	-0.091156
C	0.000000	1.171139	-0.870305
C	0.000000	-1.171139	-0.870305
C	0.000000	0.782271	-2.334961
C	0.000000	-0.782271	-2.334961
H	0.000000	3.379258	1.678463
H	0.000000	-3.379258	1.678463
H	0.000000	1.338083	3.024941
H	0.000000	-1.338083	3.024941
H	0.000000	3.317350	-0.789309
H	0.000000	-3.317350	-0.789309
H	-0.874591	1.180702	-2.852112
H	0.874591	1.180702	-2.852112
H	0.874591	-1.180702	-2.852112
H	-0.874591	-1.180702	-2.852112

Molecule# 0023

acenaphthylene

PointGroup: C2v

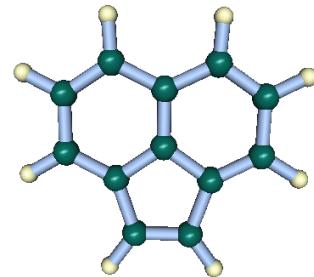
E= -462.246416366 au

ZPE= 0.159139 au

LUMO_eps= -0.08333 au

HOMO_eps= -0.22674 au

Dipole= 0.311 debye



20

C	0.000000	0.000000	-0.139949
C	0.000000	0.000000	1.250982
C	0.000000	1.278325	1.873143
C	0.000000	-1.278325	1.873143
C	0.000000	1.157671	-0.947530
C	0.000000	-1.157671	-0.947530
C	0.000000	2.419948	1.100100
C	0.000000	-2.419948	1.100100
C	0.000000	2.381426	-0.319988
C	0.000000	-2.381426	-0.319988
C	0.000000	0.679125	-2.336932
C	0.000000	-0.679125	-2.336932
H	0.000000	3.385258	1.589050
H	0.000000	-3.385258	1.589050
H	0.000000	1.356296	2.952947
H	0.000000	-1.356296	2.952947
H	0.000000	3.310213	-0.876427
H	0.000000	-3.310213	-0.876427
H	0.000000	1.311632	-3.211425
H	0.000000	-1.311632	-3.211425

Molecule# 0024

acetaldehyde

PointGroup: Cs

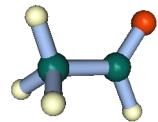
E= -153.896420318 au

ZPE= 0.055198 au

LUMO_eps= -0.04027 au

HOMO_eps= -0.26916 au

Dipole= 2.882 debye



7

C 0.000000 0.459417 0.000000

C 0.930231 -0.717880 0.000000

O -1.202256 0.385590 0.000000

H 0.496537 1.452118 0.000000

H 1.581867 -0.666234 0.876217

H 0.376396 -1.653588 0.000000

H 1.581867 -0.666234 -0.876217

Molecule# 0025

acetaldoxime

PointGroup: Cs

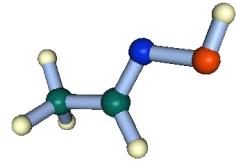
E= -209.225191302 au

ZPE= 0.072343 au

LUMO_eps= -0.01226 au

HOMO_eps= -0.26636 au

Dipole= 0.910 debye



9

C	-1.285321	1.316376	0.000000
C	0.000000	0.560718	0.000000
N	-0.003088	-0.706431	0.000000
O	1.307613	-1.225774	0.000000
H	1.160285	-2.176767	0.000000
H	-2.132483	0.633899	0.000000
H	-1.349609	1.963012	0.878124
H	-1.349609	1.963012	-0.878124
H	0.944054	1.105492	0.000000

Molecule# 0026

acetamide

PointGroup: C1

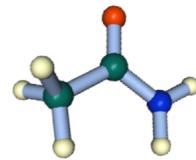
E= -209.307860987 au

ZPE= 0.073106 au

LUMO_eps= -0.02366 au

HOMO_eps= -0.26257 au

Dipole= 3.893 debye



9

C	-0.074379	0.144688	-0.000004
C	1.359129	-0.348132	-0.000001
N	-1.037040	-0.821835	0.000088
O	-0.350669	1.329673	-0.000014
H	1.862975	0.053389	-0.878184
H	1.862897	0.053119	0.878352
H	1.450574	-1.433310	-0.000159
H	-2.001439	-0.536727	-0.000165
H	-0.818878	-1.800341	-0.000316

Molecule# 0027

acetamidine

PointGroup: C1

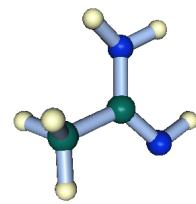
E= -189.408042286 au

ZPE= 0.085589 au

LUMO_eps= -0.02334 au

HOMO_eps= -0.25093 au

Dipole= 3.310 debye



10

C	-0.078977	0.122141	0.000466
C	1.411558	-0.089220	0.001120
N	-0.551941	1.306983	0.008721
N	-0.819020	-1.045938	-0.060148
H	1.910931	0.874016	0.006173
H	1.722528	-0.656817	0.881242
H	1.720667	-0.651513	-0.881909
H	-1.571784	1.312848	0.003132
H	-1.803738	-0.993258	0.139354
H	-0.377366	-1.910114	0.202483

Molecule# 0028

acetic acid

PointGroup: Cs

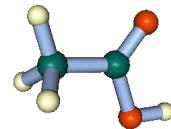
E= -229.185822548 au

ZPE= 0.061460 au

LUMO_eps= -0.01772 au

HOMO_eps= -0.29226 au

Dipole= 1.785 debye



8

C	0.000000	0.155267	0.000000
C	1.069204	-0.899341	0.000000
O	0.178356	1.345599	0.000000
O	-1.241854	-0.392584	0.000000
H	0.960614	-1.536194	0.877879
H	0.960614	-1.536194	-0.877879
H	2.046305	-0.427881	0.000000
H	-1.874777	0.340590	0.000000

Molecule# 0029

acetic anhydride

PointGroup: C2

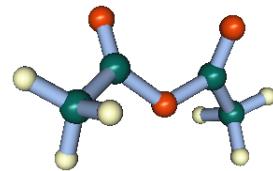
E= -381.883375051 au

ZPE= 0.097693 au

LUMO_eps= -0.04202 au

HOMO_eps= -0.29047 au

Dipole= 3.944 debye



13

C	0.000000	2.369460	0.740351
C	-0.343853	1.165080	-0.083876
O	-0.878029	1.154247	-1.148636
H	-0.405130	3.260516	0.271345
H	-0.391201	2.260041	1.751197
H	1.085006	2.452696	0.818365
O	0.000000	0.000000	0.602333
C	0.343853	-1.165080	-0.083876
C	0.000000	-2.369460	0.740351
O	0.878029	-1.154247	-1.148636
H	0.391201	-2.260041	1.751197
H	0.405130	-3.260516	0.271345
H	-1.085006	-2.452696	0.818365

Molecule# 0030

acetone

PointGroup: C1

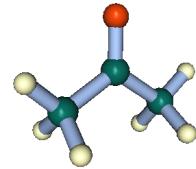
E= -193.236204798 au

ZPE= 0.083205 au

LUMO_eps= -0.02790 au

HOMO_eps= -0.25839 au

Dipole= 3.079 debye



10

C	0.000000	0.184262	-0.000004
C	1.287739	-0.611432	-0.001319
C	-1.287736	-0.611435	0.001318
O	-0.000003	1.394523	0.000000
H	1.360865	-1.200218	0.916077
H	1.300040	-1.319506	-0.832407
H	2.141095	0.057450	-0.072065
H	-2.141098	0.057436	0.072061
H	-1.300032	-1.319486	0.832420
H	-1.360868	-1.200234	-0.916065

Molecule# 0031

acetonitrile

PointGroup: C3

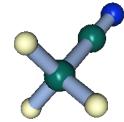
E= -132.808632064 au

ZPE= 0.045163 au

LUMO_eps= -0.02256 au

HOMO_eps= -0.33998 au

Dipole= 4.042 debye



6

C 0.000000 0.000000 0.280675

C 0.000000 0.000000 -1.174129

N 0.000000 0.000000 1.430070

H 0.000000 1.022452 -1.549923

H -0.885470 -0.511226 -1.549923

H 0.885470 -0.511226 -1.549923

Molecule# 0032

acetophenone

PointGroup: Cs

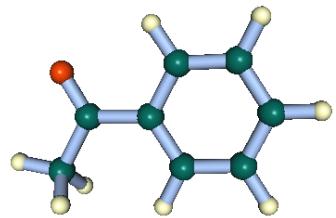
E= -385.039324962 au

ZPE= 0.137496 au

LUMO_eps= -0.07003 au

HOMO_eps= -0.26066 au

Dipole= 3.169 debye



17

C	0.597274	-2.517032	0.000000
C	-0.727051	-2.095954	0.000000
C	1.625447	-1.577546	0.000000
C	-1.024386	-0.738517	0.000000
C	1.328876	-0.224101	0.000000
C	0.000000	0.211798	0.000000
C	-0.267977	1.685966	0.000000
C	-1.703331	2.168928	0.000000
O	0.649584	2.482840	0.000000
H	0.828858	-3.573768	0.000000
H	-1.527758	-2.822994	0.000000
H	2.656502	-1.904437	0.000000
H	-2.058803	-0.426120	0.000000
H	2.113187	0.519223	0.000000
H	-2.237541	1.804546	0.879154
H	-2.237541	1.804546	-0.879154
H	-1.706692	3.255037	0.000000

Molecule# 0033

acetyl bromide

PointGroup: Cs

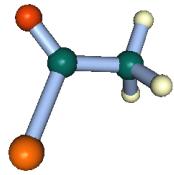
E= -2727.542994770 au

ZPE= 0.046537 au

LUMO_eps= -0.05663 au

HOMO_eps= -0.29436 au

Dipole= 2.905 debye



7

C	-1.141925	-1.709737	0.000000
C	0.191473	-1.029667	0.000000
O	1.263826	-1.514767	0.000000
H	-0.995380	-2.787715	0.000000
H	-1.706256	-1.398994	0.878078
H	-1.706256	-1.398994	-0.878078
Br	0.000000	0.975436	0.000000

Molecule# 0034

acetyl chloride

PointGroup: Cs

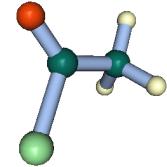
E= -613.548957579 au

ZPE= 0.047049 au

LUMO_eps= -0.05316 au

HOMO_eps= -0.30969 au

Dipole= 2.880 debye



7

C 0.000000 0.543632 0.000000

C 1.484355 0.734756 0.000000

O -0.843840 1.368109 0.000000

Cl -0.452456 -1.230552 0.000000

H 1.710473 1.798078 0.000000

H 1.912935 0.253054 0.877971

H 1.912935 0.253054 -0.877971

Molecule# 0035

acetyl fluoride

PointGroup: Cs

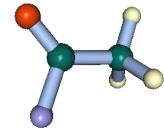
E= -253.203128201 au

ZPE= 0.048692 au

LUMO_eps= -0.03210 au

HOMO_eps= -0.32497 au

Dipole= 3.025 debye



7

C 0.000000 0.188237 0.000000

C 1.066414 -0.856833 0.000000

O 0.099012 1.365638 0.000000

F -1.237794 -0.393573 0.000000

H 2.044346 -0.386604 0.000000

H 0.952608 -1.492386 0.878134

H 0.952608 -1.492386 -0.878134

Molecule# 0036

acetylenamine

PointGroup: Cs

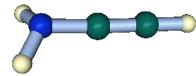
E= -132.745005040 au

ZPE= 0.044128 au

LUMO_eps= -0.02190 au

HOMO_eps= -0.23411 au

Dipole= 1.768 debye



6

N 0.090626 -1.183995 0.000000

C 0.000000 0.161705 0.000000

C -0.019053 1.362621 0.000000

H -0.239895 -1.640016 0.837356

H -0.239895 -1.640016 -0.837356

H -0.040274 2.422038 0.000000

Molecule# 0037

acetylenethiol

PointGroup: C1

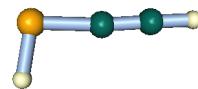
E= -475.591473367 au

ZPE= 0.027159 au

LUMO_eps= -0.02860 au

HOMO_eps= -0.25033 au

Dipole= 0.774 debye



5

S 1.039913 -0.088153 -0.000004

C -0.650468 0.025724 0.000041

C -1.852794 0.003642 -0.000042

H 1.294484 1.236611 -0.000009

H -2.913523 -0.002355 0.000079

Molecule# 0038

acrolein

PointGroup: Cs

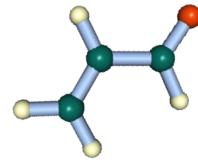
E= -191.992527724 au

ZPE= 0.061184 au

LUMO_eps= -0.08149 au

HOMO_eps= -0.27190 au

Dipole= 3.407 debye



8

C	-0.146975	-0.745307	0.000000
C	0.000000	0.717816	0.000000
C	1.203301	1.287661	0.000000
O	-1.208534	-1.324424	0.000000
H	0.808295	-1.308935	0.000000
H	-0.915368	1.296860	0.000000
H	1.332889	2.360924	0.000000
H	2.104499	0.685522	0.000000

Molecule# 0039

acrylamide

PointGroup: C1

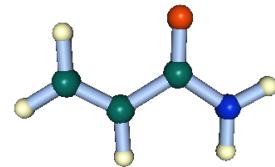
E= -247.400755857 au

ZPE= 0.078708 au

LUMO_eps= -0.05313 au

HOMO_eps= -0.26721 au

Dipole= 3.631 debye



10

C	-0.802490	-0.641917	-0.000049
C	0.476208	0.129519	-0.000019
N	1.603597	-0.640957	-0.000091
O	0.524695	1.347317	-0.000004
C	-1.976832	-0.024715	0.000041
H	-0.744777	-1.724573	-0.000141
H	2.497946	-0.182204	0.000312
H	1.570738	-1.643448	0.000506
H	-2.020997	1.056447	0.000120
H	-2.906961	-0.575387	0.000032

Molecule# 0040

acrylic acid

PointGroup: Cs

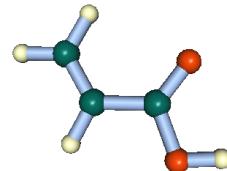
E= -267.278212043 au

ZPE= 0.067179 au

LUMO_eps= -0.06930 au

HOMO_eps= -0.29529 au

Dipole= 1.625 debye



9

C	0.434679	-1.920126	0.000000
C	-0.444755	-0.925478	0.000000
C	0.000000	0.486809	0.000000
O	1.141969	0.875860	0.000000
O	-1.059533	1.335003	0.000000
H	1.497057	-1.715390	0.000000
H	0.116437	-2.953067	0.000000
H	-1.511645	-1.100215	0.000000
H	-0.700884	2.234531	0.000000

Molecule# 0041

acrylonitrile

PointGroup: Cs

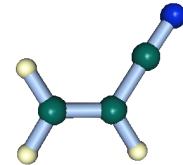
E= -170.899487870 au

ZPE= 0.050675 au

LUMO_eps= -0.07333 au

HOMO_eps= -0.30335 au

Dipole= 4.028 debye



7

C -0.574872 -0.536672 0.000000

N -1.065007 -1.579735 0.000000

C 0.000000 0.768522 0.000000

H -0.704356 1.590862 0.000000

C 1.313391 0.985354 0.000000

H 2.024361 0.171397 0.000000

H 1.703931 1.992659 0.000000

Molecule# 0042

adamantane

PointGroup: Td

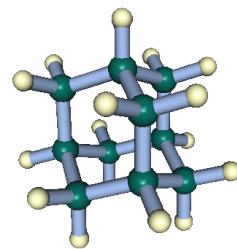
E= -390.859057164 au

ZPE= 0.243615 au

LUMO_eps= -0.01649 au

HOMO_eps= -0.27967 au

Dipole= 0.000 debye



26

C	-0.889735	0.889735	0.889735
C	0.000000	0.000000	1.775473
C	0.000000	1.775473	0.000000
C	0.889735	-0.889735	0.889735
C	-1.775473	0.000000	0.000000
C	-0.889735	-0.889735	-0.889735
C	0.000000	-1.775473	0.000000
C	0.889735	0.889735	-0.889735
C	0.000000	0.000000	-1.775473
C	1.775473	0.000000	0.000000
H	1.520690	-1.520690	1.520690
H	-1.520690	-1.520690	-1.520690
H	-1.520690	1.520690	1.520690
H	2.427208	-0.621055	-0.621055
H	1.520690	1.520690	-1.520690
H	-2.427208	0.621055	-0.621055
H	0.621055	-0.621055	-2.427208
H	2.427208	0.621055	0.621055
H	0.621055	-2.427208	-0.621055
H	0.621055	2.427208	0.621055
H	-0.621055	-2.427208	0.621055
H	0.621055	0.621055	2.427208
H	-0.621055	0.621055	-2.427208
H	-0.621055	2.427208	-0.621055
H	-2.427208	-0.621055	0.621055
H	-0.621055	-0.621055	2.427208

Molecule# 0043

alanine

PointGroup: C1

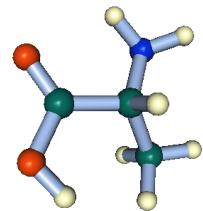
E= -323.875341508 au

ZPE= 0.107106 au

LUMO_eps= -0.03255 au

HOMO_eps= -0.26017 au

Dipole= 4.337 debye



13

H	-2.372022	1.258779	-0.041328
O	1.579853	0.982519	0.090040
H	1.029092	1.754950	0.261797
C	0.826544	-0.141556	0.027243
O	1.341664	-1.193160	-0.229770
C	-0.660281	0.015379	0.360045
H	-0.675584	0.146310	1.454547
C	-1.307277	1.254476	-0.272188
H	-0.900542	2.193255	0.114105
H	-1.199468	1.234270	-1.355735
H	-2.167312	-1.374487	0.506707
H	-0.734896	-1.985047	-0.035084
N	-1.357902	-1.187528	-0.068252

Molecule# 0044

allene

PointGroup: D2d

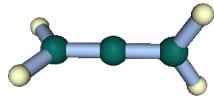
E= -116.707907734 au

ZPE= 0.054937 au

LUMO_eps= -0.00856 au

HOMO_eps= -0.27631 au

Dipole= 0.000 debye



7

C 0.000000 0.000000 0.000000

C 0.000000 0.000000 1.299944

C 0.000000 0.000000 -1.299944

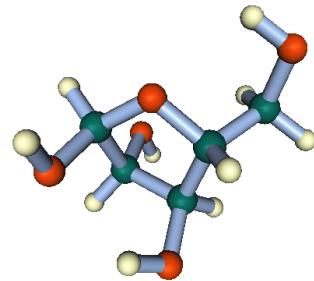
H 0.000000 0.925401 1.862995

H 0.000000 -0.925401 1.862995

H 0.925401 0.000000 -1.862995

H -0.925401 0.000000 -1.862995

Molecule# 0045
alpha-L-arabinofuranose
PointGroup: C1
E= -572.879157620 au
ZPE= 0.163064 au
LUMO_eps= -0.02028 au
HOMO_eps= -0.27122 au
Dipole= 2.206 debye



20

C	-0.379463	-0.952795	0.667838
C	-1.216504	-0.612725	-0.585325
C	0.778841	0.063866	0.600579
C	-0.988784	0.890637	-0.693430
C	2.095188	-0.498544	0.089983
O	0.349765	1.101351	-0.325741
O	-1.140863	-0.858323	1.860672
O	-0.699210	-1.200894	-1.771280
O	-1.886143	1.504898	0.226296
O	3.091379	0.506028	-0.023038
H	-0.014736	-1.978871	0.624883
H	-2.268903	-0.855465	-0.435326
H	0.930469	0.517790	1.580985
H	-1.123910	1.287185	-1.699521
H	1.930774	-0.998818	-0.869860
H	2.475020	-1.231156	0.803418
H	-1.576805	0.003890	1.866101
H	-0.895993	-2.142073	-1.764060
H	-1.658150	2.439069	0.286412
H	2.747131	1.191335	-0.606172

Molecule# 0046

aminoethylthiocyanate

PointGroup: C1

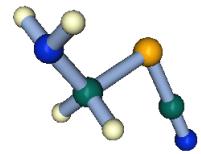
E= -586.397143033 au

ZPE= 0.064470 au

LUMO_eps= -0.04716 au

HOMO_eps= -0.26874 au

Dipole= 5.015 debye



9

S	-0.154598	0.797920	-0.000126
N	-2.619333	-0.626920	0.000187
N	2.422422	-0.270399	0.000050
C	-1.619108	-0.044584	0.000062
C	1.077109	-0.690019	-0.000032
H	2.715554	0.220385	0.831850
H	2.715654	0.220307	-0.831658
H	0.836423	-1.259219	-0.891167
H	0.836311	-1.259342	0.891152

Molecule# 0047

aminoethynol

PointGroup: C1

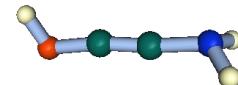
E= -207.982792028 au

ZPE= 0.049607 au

LUMO_eps= -0.02258 au

HOMO_eps= -0.22023 au

Dipole= 0.763 debye



7

O -1.938443 0.000039 -0.123358

N 1.923699 0.000027 0.086116

C 0.571151 -0.000066 -0.003646

C -0.628026 -0.000043 0.028755

H 2.378420 0.835039 -0.252203

H 2.378550 -0.834876 -0.252294

H -2.374067 -0.000010 0.737900

Molecule# 0048

aniline

PointGroup: Cs

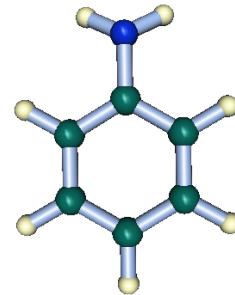
E= -287.717385806 au

ZPE= 0.116816 au

LUMO_eps= -0.01608 au

HOMO_eps= -0.21265 au

Dipole= 1.579 debye



14

C	-0.003357	-1.874982	0.000000
C	-0.003231	-1.167816	1.197776
C	-0.003231	-1.167816	-1.197776
C	-0.003231	0.219824	1.202965
C	-0.003231	0.219824	-1.202965
C	-0.002373	0.934694	0.000000
N	-0.059398	2.328540	0.000000
H	-0.002994	-2.955765	0.000000
H	-0.002518	-1.699840	2.140057
H	-0.002518	-1.699840	-2.140057
H	-0.008370	0.757854	2.143040
H	-0.008370	0.757854	-2.143040
H	0.276236	2.778796	-0.835682
H	0.276236	2.778796	0.835682

Molecule# 0049

anisole

PointGroup: Cs

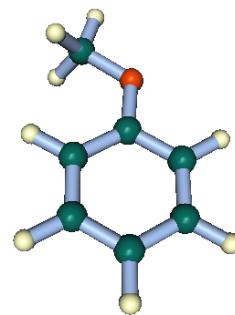
E= -346.903571453 au

ZPE= 0.132741 au

LUMO_eps= -0.01676 au

HOMO_eps= -0.22889 au

Dipole= 1.308 debye



16

C	0.893738	-2.119560	0.000000
C	-0.463564	-1.836161	0.000000
C	1.807314	-1.066569	0.000000
C	-0.921006	-0.519558	0.000000
C	1.369118	0.246605	0.000000
C	0.000000	0.526996	0.000000
C	-1.709890	2.199611	0.000000
O	-0.335558	1.848902	0.000000
H	1.239334	-3.143772	0.000000
H	-1.185110	-2.642410	0.000000
H	2.869659	-1.271259	0.000000
H	-1.982692	-0.326351	0.000000
H	2.067189	1.072124	0.000000
H	-2.218233	1.823281	0.891490
H	-2.218233	1.823281	-0.891490
H	-1.741707	3.285711	0.000000

Molecule# 0050

anthracene

PointGroup: C2

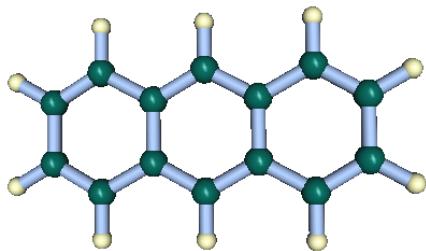
E= -539.716292676 au

ZPE= 0.193696 au

LUMO_eps= -0.07396 au

HOMO_eps= -0.20468 au

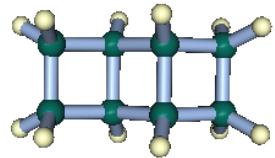
Dipole= 0.000 debye



24

C	0.000000	0.719869	1.218890
C	0.000000	-0.719869	1.218890
C	0.000000	1.398321	0.000000
C	0.000000	1.401530	2.470807
C	0.000000	-1.398321	0.000000
C	0.000000	-1.401530	2.470807
C	0.000000	0.719869	-1.218890
C	0.000000	0.710698	3.646151
C	0.000000	-0.719869	-1.218890
C	0.000000	-0.710698	3.646151
C	0.000000	1.401530	-2.470807
C	0.000000	-1.401530	-2.470807
C	0.000000	0.710698	-3.646151
C	0.000000	-0.710698	-3.646151
H	0.000000	2.481982	0.000000
H	0.000000	2.484308	2.470066
H	0.000000	-2.481982	0.000000
H	0.000000	-2.484308	2.470066
H	0.000000	1.241764	4.588686
H	0.000000	-1.241764	4.588686
H	0.000000	2.484308	-2.470066
H	0.000000	-2.484308	-2.470066
H	0.000000	1.241764	-4.588686
H	0.000000	-1.241764	-4.588686

Molecule# 0051
 anti-tricyclo-4,2,0,0-octane
 PointGroup: C2h
 E= -312.095066126 au
 ZPE= 0.179084 au
 LUMO_eps= -0.00781 au
 HOMO_eps= -0.26098 au
 Dipole= 0.000 debye



20

C	-0.418466	0.644989	0.791107
C	-0.418466	0.644989	-0.791107
C	0.418466	-0.644989	0.791107
C	0.418466	1.946235	0.777144
C	0.418466	-0.644989	-0.791107
C	0.418466	1.946235	-0.777144
C	-0.418466	-1.946235	-0.777144
C	-0.418466	-1.946235	0.777144
H	-1.320254	0.645883	1.403108
H	-1.320254	0.645883	-1.403108
H	1.320254	-0.645883	1.403108
H	-0.103896	2.800429	1.206129
H	1.394828	1.871332	1.257928
H	1.320254	-0.645883	-1.403108
H	1.394828	1.871332	-1.257928
H	-0.103896	2.800429	-1.206129
H	-1.394828	-1.871332	-1.257928
H	0.103896	-2.800429	-1.206129
H	0.103896	-2.800429	1.206129
H	-1.394828	-1.871332	1.257928

Molecule# 0052

arginine

PointGroup: C1

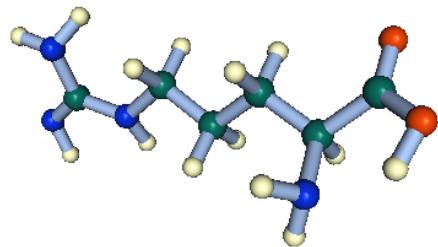
E= -606.787089447 au

ZPE= 0.221743 au

LUMO_eps= -0.03635 au

HOMO_eps= -0.23147 au

Dipole= 2.720 debye



26

N	-2.526983	1.644610	0.539401
C	-2.309574	0.430804	-0.263716
C	-3.543059	-0.493877	-0.155950
O	-3.559770	-1.614822	-0.589237
O	-4.602147	0.075386	0.430775
H	-4.303472	0.974710	0.689949
C	-1.025447	-0.342914	0.052142
C	0.250781	0.404006	-0.330854
C	1.510265	-0.390892	0.003386
N	2.702104	0.351444	-0.372440
C	3.997767	0.022671	-0.008400
N	4.099684	-0.984055	0.943541
N	5.063631	0.606486	-0.414314
H	-2.286412	0.732459	-1.314703
H	-1.014272	-0.576246	1.122559
H	-1.076507	-1.298385	-0.469583
H	0.232932	0.616099	-1.405631
H	0.304202	1.368500	0.179891
H	1.544459	-0.575336	1.078269
H	1.458323	-1.369138	-0.495193
H	2.638588	0.883680	-1.223524
H	3.488801	-1.778017	0.839937
H	5.061405	-1.240273	1.103040
H	4.860793	1.403058	-1.010069
H	-2.070153	1.586068	1.441314
H	-2.196817	2.480125	0.078473

Molecule# 0053

asparagine

PointGroup: C1

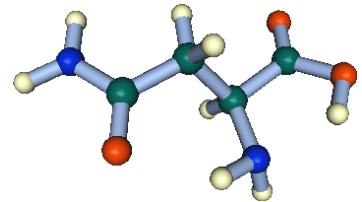
E= -492.658547033 au

ZPE= 0.135984 au

LUMO_eps= -0.02968 au

HOMO_eps= -0.26735 au

Dipole= 3.955 debye



17

N	-0.537636	1.634468	-0.311017
C	-0.506076	0.174773	-0.439687
C	-1.882737	-0.418460	-0.080577
O	-2.175140	-1.564324	-0.298926
O	-2.703547	0.449095	0.519188
H	-2.201073	1.295665	0.555522
C	0.530887	-0.449933	0.513055
C	1.954459	-0.058137	0.153171
O	2.308657	1.111421	0.104908
N	2.806159	-1.080562	-0.108786
H	-0.288369	-0.160572	-1.457832
H	0.343314	-0.088713	1.526973
H	0.392111	-1.529176	0.509676
H	2.517736	-2.040866	-0.075861
H	3.761371	-0.865241	-0.340502
H	0.386763	1.982426	-0.073290
H	-0.810476	2.070141	-1.183197

Molecule# 0054

aspartic acid

PointGroup: C1

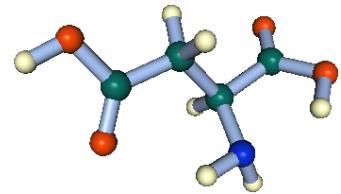
E= -512.532900801 au

ZPE= 0.123620 au

LUMO_eps= -0.03348 au

HOMO_eps= -0.27833 au

Dipole= 4.094 debye



16

N	-0.559751	1.671657	0.045915
C	-0.532972	0.280240	-0.418930
C	-1.890012	-0.388824	-0.132659
O	-2.226830	-1.423048	-0.641390
O	-2.644131	0.266174	0.760645
H	-2.137138	1.070719	1.003194
C	0.538406	-0.536571	0.312301
C	1.953822	-0.103384	0.017412
O	2.287312	0.951709	-0.465001
O	2.843745	-1.045709	0.388575
H	-0.363243	0.188219	-1.494723
H	0.398061	-0.461864	1.395187
H	0.431236	-1.589892	0.058200
H	0.385487	2.025817	0.133560
H	-1.022701	2.261966	-0.635773
H	3.730329	-0.698333	0.207579

Molecule# 0055

azetidine

PointGroup: Cs

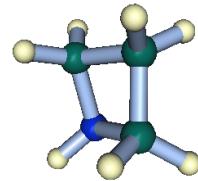
E= -173.308034221 au

ZPE= 0.099376 au

LUMO_eps= -0.01140 au

HOMO_eps= -0.23117 au

Dipole= 1.299 debye



11

C	0.082897	1.078427	0.000000
C	0.082897	-0.051210	1.054630
C	0.082897	-0.051210	-1.054630
N	-0.374490	-0.989590	0.000000
H	-0.845440	1.645623	0.000000
H	0.926741	1.763706	0.000000
H	1.090133	-0.261322	1.431487
H	-0.597396	0.043257	1.901760
H	-0.597396	0.043257	-1.901760
H	1.090133	-0.261322	-1.431487
H	0.062512	-1.902110	0.000000

Molecule# 0056

azidoethene

PointGroup: C1

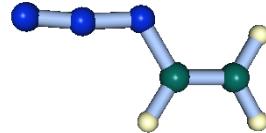
E= -242.275953292 au

ZPE= 0.055139 au

LUMO_eps= -0.04992 au

HOMO_eps= -0.24787 au

Dipole= 1.512 debye



8

N	-0.091593	-0.542859	-0.000002
N	-1.235025	-0.089021	0.000000
N	-2.326717	0.196979	0.000000
C	0.978435	0.373808	0.000000
C	2.241526	-0.037019	0.000000
H	0.716580	1.426207	0.000003
H	2.493945	-1.087536	-0.000002
H	3.043059	0.684904	0.000002

Molecule# 0057

aziridine

PointGroup: Cs

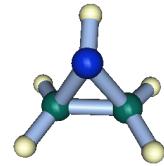
E= -133.977817006 au

ZPE= 0.070031 au

LUMO_eps= -0.01100 au

HOMO_eps= -0.25831 au

Dipole= 1.679 debye



8

N -0.037940 0.872541 0.000000

H 0.888780 1.282744 0.000000

C -0.037940 -0.397603 0.739990

C -0.037940 -0.397603 -0.739990

H -0.952512 -0.607514 1.278587

H 0.868549 -0.702138 1.248293

H -0.952512 -0.607514 -1.278587

H 0.868549 -0.702138 -1.248293

Molecule# 0058

azulene

PointGroup: C2v

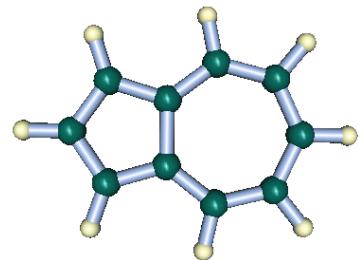
E= -385.975180319 au

ZPE= 0.145766 au

LUMO_eps= -0.08300 au

HOMO_eps= -0.20429 au

Dipole= 1.018 debye



18

C	0.000000	0.000000	-2.493269
C	0.000000	1.260954	-1.903510
C	0.000000	0.747825	0.551519
C	0.000000	1.588911	-0.550232
C	0.000000	0.000000	2.698578
C	0.000000	-1.145715	1.894921
C	0.000000	-0.747825	0.551519
C	0.000000	1.145715	1.894921
C	0.000000	-1.588911	-0.550232
C	0.000000	-1.260954	-1.903510
H	0.000000	0.000000	-3.577631
H	0.000000	2.098972	-2.589739
H	0.000000	2.650420	-0.323058
H	0.000000	0.000000	3.778585
H	0.000000	-2.167642	2.240201
H	0.000000	2.167642	2.240201
H	0.000000	-2.650420	-0.323058
H	0.000000	-2.098972	-2.589739

Molecule# 0059

benzaldehyde

PointGroup: Cs

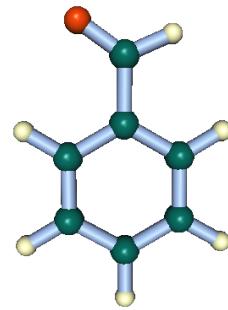
E= -345.702985879 au

ZPE= 0.109555 au

LUMO_eps= -0.07917 au

HOMO_eps= -0.26872 au

Dipole= 3.496 debye



14

C	0.571069	-2.149970	0.000000
C	1.611083	-1.227341	0.000000
C	-0.754728	-1.717051	0.000000
C	1.324206	0.131604	0.000000
C	-1.041517	-0.362317	0.000000
C	0.000000	0.570512	0.000000
C	-0.284070	2.020789	0.000000
O	-1.388905	2.512174	0.000000
H	0.790975	-3.209245	0.000000
H	2.637810	-1.566777	0.000000
H	-1.558218	-2.441065	0.000000
H	2.126678	0.859329	0.000000
H	-2.060939	-0.001955	0.000000
H	0.618676	2.664963	0.000000

Molecule# 0060

benzamide

PointGroup: C1

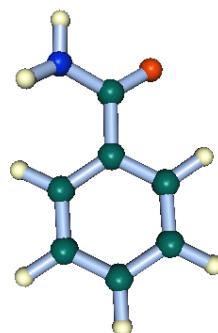
E= -401.109235668 au

ZPE= 0.127222 au

LUMO_eps= -0.05372 au

HOMO_eps= -0.26297 au

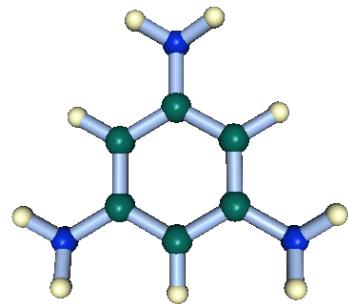
Dipole= 3.662 debye



16

C	-2.571902	0.046888	0.020768
C	-1.848389	1.223950	-0.131564
C	-1.902431	-1.166543	0.145550
C	-0.459401	1.189827	-0.147202
C	-0.515903	-1.202319	0.120287
C	0.218670	-0.023721	-0.016122
C	1.715052	-0.135921	-0.035243
N	2.416666	1.006941	0.237137
O	2.280280	-1.184451	-0.295323
H	-3.653148	0.074322	0.035323
H	-2.364586	2.167480	-0.245942
H	-2.462548	-2.084753	0.259361
H	0.086801	2.111464	-0.297061
H	0.020859	-2.136416	0.202736
H	1.984571	1.789885	0.692283
H	3.414974	0.912074	0.317082

Molecule# 0061
 benzene-1,3,5-triamine
 PointGroup: C3v
 E= -398.481202622 au
 ZPE= 0.149832 au
 LUMO_eps= -0.01649 au
 HOMO_eps= -0.19551 au
 Dipole= 2.663 debye



18

C	0.000000	1.396197	-0.005270
C	1.209142	-0.698099	-0.005270
C	-1.209142	-0.698099	-0.005270
C	1.208834	0.697921	-0.006832
C	-1.208834	0.697921	-0.006832
C	0.000000	-1.395841	-0.006832
N	2.416644	1.395250	-0.064461
N	-2.416644	1.395250	-0.064461
N	0.000000	-2.790500	-0.064461
H	0.000000	2.479119	-0.023214
H	2.146980	-1.239560	-0.023214
H	-2.146980	-1.239560	-0.023214
H	3.222171	0.895252	0.273528
H	2.386397	2.342856	0.273528
H	-2.386397	2.342856	0.273528
H	-3.222171	0.895252	0.273528
H	-0.835774	-3.238108	0.273528
H	0.835774	-3.238108	0.273528

Molecule# 0062

benzene

PointGroup: D6h

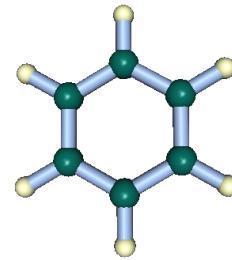
E= -232.335569946 au

ZPE= 0.100352 au

LUMO_eps= -0.01745 au

HOMO_eps= -0.26059 au

Dipole= 0.000 debye



12

C	0.000000	1.390589	0.000000
C	1.204285	0.695294	0.000000
C	-1.204285	0.695294	0.000000
C	1.204285	-0.695294	0.000000
C	-1.204285	-0.695294	0.000000
C	0.000000	-1.390589	0.000000
H	0.000000	2.472617	0.000000
H	0.000000	-2.472617	0.000000
H	-2.141349	1.236308	0.000000
H	2.141349	-1.236308	0.000000
H	2.141349	1.236308	0.000000
H	-2.141349	-1.236308	0.000000

Molecule# 0063

benzenethiol

PointGroup: Cs

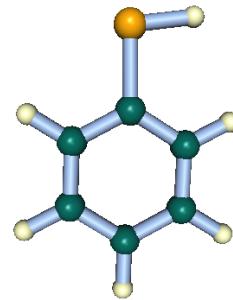
E= -630.558998029 au

ZPE= 0.099176 au

LUMO_eps= -0.02578 au

HOMO_eps= -0.22818 au

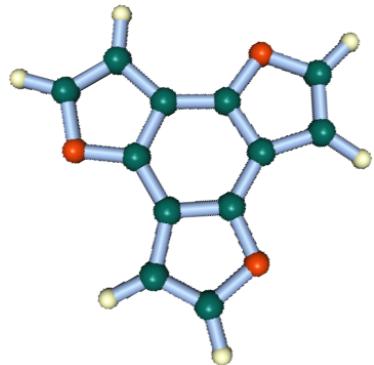
Dipole= 1.070 debye



13

C	0.007083	-2.289118	0.000000
C	1.204721	-1.583554	0.000000
C	-1.194960	-1.590256	0.000000
C	1.206584	-0.194173	0.000000
C	-1.203315	-0.201715	0.000000
C	0.000000	0.505241	0.000000
S	-0.086475	2.284006	0.000000
H	0.010418	-3.370141	0.000000
H	2.147471	-2.114249	0.000000
H	-2.134602	-2.126238	0.000000
H	2.146513	0.340962	0.000000
H	-2.144219	0.332370	0.000000
H	1.237336	2.514654	0.000000

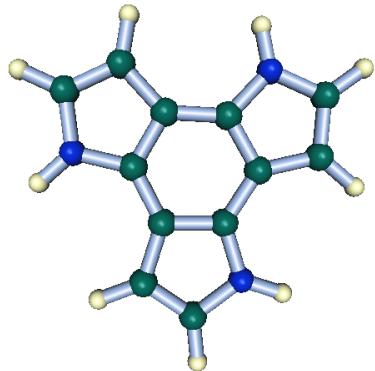
Molecule# 0064
benzo[1,2-b:3,4-b':5,6-b'']trifuran
PointGroup: Cs
E= -686.766010126 au
ZPE= 0.150739 au
LUMO_eps= -0.02261 au
HOMO_eps= -0.21934 au
Dipole= 0.000 debye



21

C	-2.229408	1.746979	0.000000
C	2.627632	1.057235	0.000000
C	-0.398224	-2.804213	0.000000
C	-1.554337	2.916926	0.000000
C	3.303300	-0.112368	0.000000
C	-1.748963	-2.804558	0.000000
C	-1.230229	0.713698	0.000000
C	1.233195	0.708561	0.000000
C	-0.002966	-1.422258	0.000000
C	0.000000	1.375748	0.000000
C	1.191433	-0.687874	0.000000
C	-1.191433	-0.687874	0.000000
O	-0.195326	2.723963	0.000000
O	2.456685	-1.192825	0.000000
O	-2.261359	-1.531139	0.000000
H	-3.298343	1.627719	0.000000
H	3.058818	2.042589	0.000000
H	0.239525	-3.670309	0.000000
H	-1.873962	3.943054	0.000000
H	4.351766	-0.348628	0.000000
H	-2.477803	-3.594426	0.000000

Molecule# 0065
 benzo[1,2-b:3,4-b':5,6-b'']tripyrrrole
 PointGroup: C3h
 E= -627.182303718 au
 ZPE= 0.188001 au
 LUMO_eps= -0.01380 au
 HOMO_eps= -0.18449 au
 Dipole= 0.000 debye



24

C	-2.260008	1.718793	0.000000
C	2.618522	1.097828	0.000000
C	-0.358514	-2.816621	0.000000
C	-1.636395	2.936436	0.000000
C	3.361226	-0.051059	0.000000
C	-1.724831	-2.885378	0.000000
C	-1.235698	0.719678	0.000000
C	1.241108	0.710307	0.000000
C	-0.005410	-1.429985	0.000000
C	0.000000	1.392828	0.000000
C	1.206225	-0.696414	0.000000
C	-1.206225	-0.696414	0.000000
N	-0.273028	2.739129	0.000000
N	2.508669	-1.133115	0.000000
N	-2.235641	-1.606014	0.000000
H	-3.326106	1.566758	0.000000
H	3.019905	2.097113	0.000000
H	0.306200	-3.663871	0.000000
H	-2.050289	3.929412	0.000000
H	4.428115	-0.189104	0.000000
H	-2.377826	-3.740308	0.000000
H	0.415105	3.468383	0.000000
H	2.796155	-2.093683	0.000000
H	-3.211260	-1.374700	0.000000

Molecule# 0066
benzocyclobutadiene

PointGroup: C2v

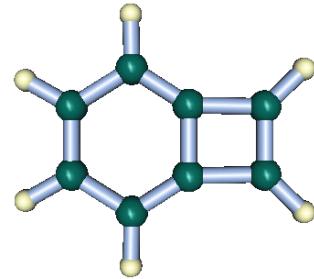
E= -308.469854822 au

ZPE= 0.110020 au

LUMO_eps= -0.06839 au

HOMO_eps= -0.20608 au

Dipole= 0.717 debye



14

C	0.000000	1.439760	-0.621675
C	0.000000	0.686345	-1.839508
C	0.000000	-0.686345	-1.839508
C	0.000000	-1.439760	-0.621675
C	0.000000	-0.673165	2.041672
C	0.000000	0.673165	2.041672
C	0.000000	0.709390	0.520531
C	0.000000	-0.709390	0.520531
H	0.000000	2.521064	-0.642939
H	0.000000	1.216563	-2.782280
H	0.000000	-1.216563	-2.782280
H	0.000000	-2.521064	-0.642939
H	0.000000	-1.421348	2.819103
H	0.000000	1.421348	2.819103

Molecule# 0067

benzofuran

PointGroup: Cs

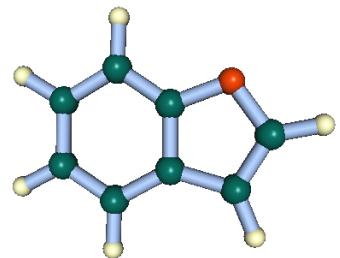
E= -383.813778331 au

ZPE= 0.117172 au

LUMO_eps= -0.03448 au

HOMO_eps= -0.23287 au

Dipole= 0.745 debye



15

C	1.747263	-1.406167	0.000000
C	2.223038	-0.087275	0.000000
C	0.389336	-1.682725	0.000000
C	1.351487	0.993360	0.000000
C	-1.940990	-0.463643	0.000000
C	-2.180642	0.864075	0.000000
C	-0.508089	-0.610981	0.000000
C	0.000000	0.695937	0.000000
O	-1.024824	1.601092	0.000000
H	2.457684	-2.221739	0.000000
H	3.289485	0.091942	0.000000
H	0.033887	-2.704379	0.000000
H	1.703212	2.015004	0.000000
H	-2.683681	-1.242643	0.000000
H	-3.090416	1.437594	0.000000

Molecule# 0068

benzoic acid

PointGroup: Cs

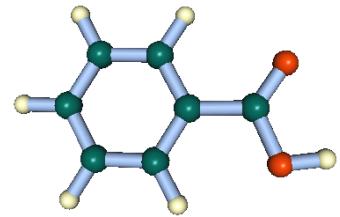
E= -420.988751615 au

ZPE= 0.115338 au

LUMO_eps= -0.06563 au

HOMO_eps= -0.27446 au

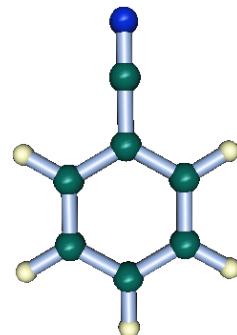
Dipole= 2.151 debye



15

C	0.307786	-2.544530	0.000000
C	1.429809	-1.720826	0.000000
C	-0.966751	-1.987681	0.000000
C	1.277760	-0.342753	0.000000
C	-1.123948	-0.608404	0.000000
C	0.000000	0.220374	0.000000
C	-0.110623	1.700856	0.000000
O	0.823931	2.465863	0.000000
O	-1.394622	2.140425	0.000000
H	0.427051	-3.619739	0.000000
H	2.420556	-2.154119	0.000000
H	-1.837930	-2.628373	0.000000
H	2.135639	0.314086	0.000000
H	-2.111190	-0.171656	0.000000
H	-1.352794	3.107284	0.000000

Molecule# 0069
benzonitrile
PointGroup: C2v
E= -324.610166240 au
ZPE= 0.099052 au
LUMO_eps= -0.06718 au
HOMO_eps= -0.28011 au
Dipole= 4.711 debye



13

C	0.000000	0.000000	2.038408
C	0.000000	0.000000	-2.171450
C	0.000000	1.205362	-1.477349
C	0.000000	-1.205362	-1.477349
C	0.000000	1.211491	-0.090773
C	0.000000	-1.211491	-0.090773
C	0.000000	0.000000	0.608724
N	0.000000	0.000000	3.190989
H	0.000000	0.000000	-3.252992
H	0.000000	2.142437	-2.016824
H	0.000000	-2.142437	-2.016824
H	0.000000	2.143254	0.456544
H	0.000000	-2.143254	0.456544

Molecule# 0070

benzoquinone

PointGroup: D2h

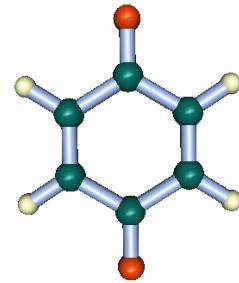
E= -381.597827226 au

ZPE= 0.084950 au

LUMO_eps= -0.14299 au

HOMO_eps= -0.28500 au

Dipole= 0.000 debye



12

C	0.000000	0.000000	1.438198
C	0.000000	0.000000	-1.438198
O	0.000000	0.000000	2.656988
O	0.000000	0.000000	-2.656988
C	0.000000	1.265716	0.667837
C	0.000000	-1.265716	0.667837
C	0.000000	-1.265716	-0.667837
C	0.000000	1.265716	-0.667837
H	0.000000	2.176019	1.252736
H	0.000000	-2.176019	1.252736
H	0.000000	-2.176019	-1.252736
H	0.000000	2.176019	-1.252736

Molecule# 0071

benzothiophene

PointGroup: Cs

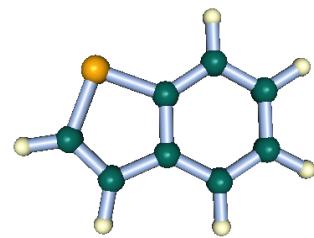
E= -706.800205277 au

ZPE= 0.113927 au

LUMO_eps= -0.03879 au

HOMO_eps= -0.22708 au

Dipole= 0.636 debye



15

C	2.419842	-0.781506	0.000000
C	2.384977	0.620139	0.000000
C	1.250934	-1.517608	0.000000
C	1.179130	1.298960	0.000000
C	-1.312092	-1.405181	0.000000
C	-2.275718	-0.456495	0.000000
C	0.014337	-0.856085	0.000000
C	0.000000	0.556152	0.000000
S	-1.639275	1.165435	0.000000
H	3.374674	-1.289610	0.000000
H	3.311216	1.178597	0.000000
H	1.282913	-2.599422	0.000000
H	1.154241	2.380060	0.000000
H	-1.519954	-2.465202	0.000000
H	-3.343153	-0.601646	0.000000

Molecule# 0072

benzyl alcohol

PointGroup: C1

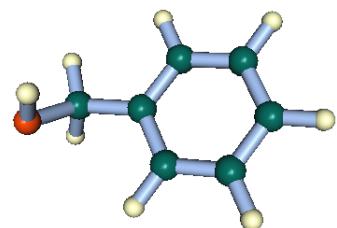
E= -346.910626996 au

ZPE= 0.133040 au

LUMO_eps= -0.02875 au

HOMO_eps= -0.25737 au

Dipole= 1.578 debye



16

C	2.295875	-0.194875	0.152817
C	1.760211	1.086177	0.147384
C	1.459304	-1.293258	-0.029852
C	0.392585	1.267430	-0.038587
C	0.097012	-1.108725	-0.219163
C	-0.452614	0.175941	-0.226405
C	-1.935484	0.370754	-0.429766
O	-2.736278	-0.345146	0.513236
H	3.357833	-0.339687	0.298826
H	2.403036	1.944269	0.291616
H	1.872130	-2.293318	-0.028077
H	-0.021144	2.268461	-0.038507
H	-0.552474	-1.963339	-0.357038
H	-2.174626	1.438864	-0.408291
H	-2.241931	-0.013856	-1.403463
H	-2.453932	-0.100885	1.400478

Molecule# 0073

benzyne

PointGroup: C2v

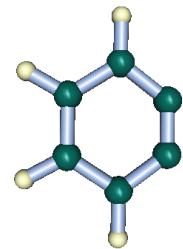
E= -230.996775461 au

ZPE= 0.075099 au

LUMO_eps= -0.08467 au

HOMO_eps= -0.27456 au

Dipole= 1.665 debye



10

C	0.000000	1.455634	-0.133697
C	0.000000	0.700529	1.053581
C	0.000000	-0.700529	1.053581
C	0.000000	-1.455634	-0.133697
C	0.000000	-0.620534	-1.230930
C	0.000000	0.620534	-1.230930
H	0.000000	2.535415	-0.135167
H	0.000000	1.224463	2.001444
H	0.000000	-1.224463	2.001444
H	0.000000	-2.535415	-0.135167

Molecule# 0074

beta-alanine

PointGroup: C1

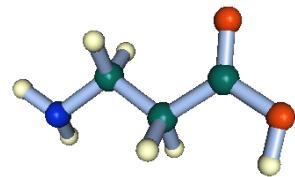
E= -323.875699906 au

ZPE= 0.107613 au

LUMO_eps= -0.02649 au

HOMO_eps= -0.25898 au

Dipole= 3.800 debye

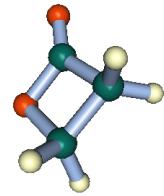


13

H	2.844792	-0.788170	0.777220
H	3.404575	0.345604	-0.245141
N	2.637944	-0.294370	-0.082906
H	1.280732	1.064160	0.901267
H	1.287489	1.091764	-0.849294
C	1.367895	0.430365	0.012626
H	0.282574	-1.185743	-0.904827
H	0.265487	-1.235933	0.844398
C	0.206748	-0.556935	-0.013182
O	-1.337293	1.297083	0.023560
C	-1.152003	0.113743	0.002622
H	-1.923395	-1.652577	-0.039753
O	-2.218170	-0.734777	-0.013051

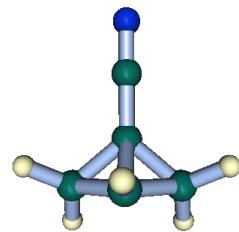
Molecule# 0075
beta-propiolactone
PointGroup: Cs

E= -267.261682036 au
ZPE= 0.068388 au
LUMO_eps= -0.01932 au
HOMO_eps= -0.29521 au
Dipole= 4.316 debye



9
O -1.034291 -0.277068 0.000000
C 0.000000 0.628638 0.000000
O -0.070941 1.813015 0.000000
C 1.084794 -0.444247 0.000000
H 1.709429 -0.440463 0.889880
H 1.709429 -0.440463 -0.889880
C -0.101764 -1.414106 0.000000
H -0.237589 -2.014177 -0.895897
H -0.237589 -2.014177 0.895897

Molecule# 0076
bicyclo-1,1,0-butane-1-carbonitrile
PointGroup: Cs
E= -248.284590005 au
ZPE= 0.085395 au
LUMO_eps= -0.01457 au
HOMO_eps= -0.27389 au
Dipole= 4.250 debye



11

H	-0.140619	0.678735	2.076979
H	1.129568	1.686573	1.231058
C	0.276344	1.019981	1.138037
H	-0.140619	0.678735	-2.076979
H	1.129568	1.686573	-1.231058
C	0.276344	1.019981	-1.138037
C	0.276344	0.034656	0.000000
H	-1.743752	1.161245	0.000000
C	-0.668943	1.198926	0.000000
N	-0.181839	-2.488939	0.000000
C	0.013033	-1.351758	0.000000

Molecule# 0077

bicyclo-1,1,0-butane

PointGroup: C2v

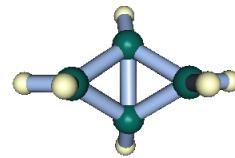
E= -156.007565891 au

ZPE= 0.086020 au

LUMO_eps= -0.00564 au

HOMO_eps= -0.24992 au

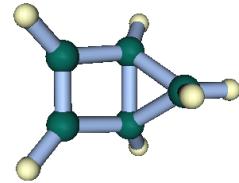
Dipole= 0.696 debye



10

C	-0.742813	0.000000	-0.317669
C	0.742813	0.000000	-0.317669
C	0.000000	1.134528	0.312889
C	0.000000	-1.134528	0.312889
H	0.000000	-1.232016	1.397188
H	0.000000	1.232016	1.397188
H	0.000000	-2.078551	-0.219647
H	0.000000	2.078551	-0.219647
H	-1.425483	0.000000	-1.148859
H	1.425483	0.000000	-1.148859

Molecule# 0078
bicyclo-2,1,0-pent-2-ene
PointGroup: Cs
E= -194.096782635 au
ZPE= 0.091436 au
LUMO_eps= -0.01390 au
HOMO_eps= -0.22774 au
Dipole= 0.459 debye



11

C	-0.266056	1.055248	0.669094
C	-0.266056	1.055248	-0.669094
C	-0.266056	-0.460196	0.760307
C	-0.266056	-0.460196	-0.760307
C	0.922329	-1.012414	0.000000
H	-0.135836	1.824369	1.417771
H	-0.135836	1.824369	-1.417771
H	-0.878809	-1.079524	1.397279
H	-0.878809	-1.079524	-1.397279
H	1.855860	-0.463241	0.000000
H	1.024808	-2.092588	0.000000

Molecule# 0079

bicyclo-2,1,0-pentane

PointGroup: Cs

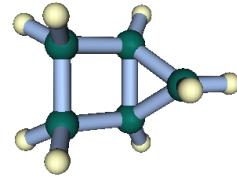
E= -195.352237221 au

ZPE= 0.115838 au

LUMO_eps= -0.00712 au

HOMO_eps= -0.26085 au

Dipole= 0.266 debye



13

C	-0.244446	-0.536702	0.764733
C	-0.244446	-0.536702	-0.764733
C	-0.244446	0.993902	0.781471
C	-0.244446	0.993902	-0.781471
C	0.939024	-1.048468	0.000000
H	-0.797183	-1.171910	1.441963
H	-0.797183	-1.171910	-1.441963
H	0.607058	1.464190	1.277074
H	0.607058	1.464190	-1.277074
H	-1.160667	1.417563	1.188390
H	-1.160667	1.417563	-1.188390
H	1.871038	-0.492128	0.000000
H	1.063120	-2.123147	0.000000

Molecule# 0080

bicyclo-2,1,1-hex-2-ene

PointGroup: C2v

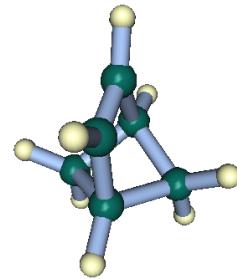
E= -233.449193811 au

ZPE= 0.122201 au

LUMO_eps= -0.00800 au

HOMO_eps= -0.23371 au

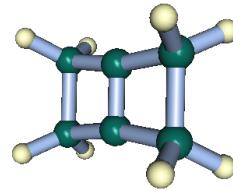
Dipole= 0.349 debye



14

C	0.000000	0.666639	1.212835
C	0.000000	-0.666639	1.212835
C	0.000000	-1.020958	-0.278406
C	0.000000	1.020958	-0.278406
C	1.063233	0.000000	-0.808697
C	-1.063233	0.000000	-0.808697
H	0.000000	1.359953	2.038801
H	0.000000	-1.359953	2.038801
H	0.000000	-2.068141	-0.567858
H	0.000000	2.068141	-0.567858
H	2.041135	0.000000	-0.329854
H	-2.041135	0.000000	-0.329854
H	-1.157060	0.000000	-1.895481
H	1.157060	0.000000	-1.895481

Molecule# 0081
 bicyclo-2,2,0-hex-1,4-ene
 PointGroup: D2h
 E= -233.399133383 au
 ZPE= 0.119853 au
 LUMO_eps= -0.00928 au
 HOMO_eps= -0.23749 au
 Dipole= 0.000 debye



14

C	-1.522244	0.801625	0.000000
H	-1.971604	1.251554	0.886835
H	-1.971604	1.251554	-0.886835
C	-1.522244	-0.801625	0.000000
H	-1.971604	-1.251554	-0.886835
H	-1.971604	-1.251554	0.886835
C	1.522244	-0.801625	0.000000
H	1.971604	-1.251554	0.886835
H	1.971604	-1.251554	-0.886835
C	0.000000	-0.656608	0.000000
C	0.000000	0.656608	0.000000
C	1.522244	0.801625	0.000000
H	1.971604	1.251554	-0.886835
H	1.971604	1.251554	0.886835

Molecule# 0082

bicyclo-2,2,0-hexane

PointGroup: C2v

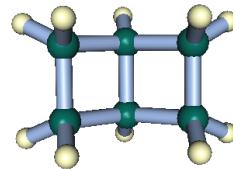
E= -234.681563766 au

ZPE= 0.144441 au

LUMO_eps= -0.00936 au

HOMO_eps= -0.27140 au

Dipole= 0.173 debye



16

C	1.306673	0.778578	-0.253085
C	1.306673	-0.778578	-0.253085
C	0.000000	-0.786260	0.577788
C	0.000000	0.786260	0.577788
C	-1.306673	0.778578	-0.253085
C	-1.306673	-0.778578	-0.253085
H	1.235314	1.258625	-1.230081
H	2.159674	1.206785	0.272012
H	2.159674	-1.206785	0.272012
H	1.235314	-1.258625	-1.230081
H	0.000000	-1.384950	1.486430
H	0.000000	1.384950	1.486430
H	-2.159674	1.206785	0.272012
H	-1.235314	1.258625	-1.230081
H	-1.235314	-1.258625	-1.230081
H	-2.159674	-1.206785	0.272012

Molecule# 0083

bicyclo-2,2,2-octane

PointGroup: D3

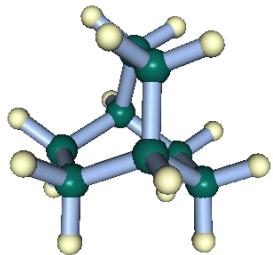
E= -313.400275644 au

ZPE= 0.205821 au

LUMO_eps= -0.01513 au

HOMO_eps= -0.28359 au

Dipole= 0.000 debye



22

C	0.000000	0.000000	1.295208
C	-0.017844	1.447195	0.777177
C	-1.244385	-0.739051	0.777177
C	0.017844	1.447195	-0.777177
C	0.000000	0.000000	-1.295208
C	-1.262230	-0.708144	-0.777177
C	1.262230	-0.708144	0.777177
C	1.244385	-0.739051	-0.777177
H	1.308838	-1.720784	1.182692
H	0.000000	0.000000	-2.387174
H	-2.149499	-0.186632	-1.142178
H	2.149499	-0.186632	1.142178
H	-1.308838	-1.720784	-1.182692
H	0.000000	0.000000	2.387174
H	-2.144662	-0.273094	1.182692
H	1.236378	-1.768205	-1.142178
H	0.835824	1.993879	1.182692
H	-0.835824	1.993879	-1.182692
H	2.144662	-0.273094	-1.182692
H	-0.913121	1.954837	1.142178
H	-1.236378	-1.768205	1.142178
H	0.913121	1.954837	-1.142178

Molecule# 0084

bicyclo-3,1,0-hex-2-ene

PointGroup: C1

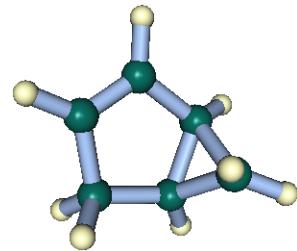
E= -233.484252379 au

ZPE= 0.121884 au

LUMO_eps= -0.00831 au

HOMO_eps= -0.23554 au

Dipole= 0.328 debye



14

C	0.645070	-0.770527	-0.387053
C	-0.789799	-1.153566	-0.033586
C	0.710734	0.747733	-0.438274
C	1.457988	-0.021657	0.630098
C	-1.464834	0.179434	0.203670
C	-0.653112	1.204214	-0.052761
H	1.177895	-1.366546	-1.113656
H	-1.269345	-1.698798	-0.852718
H	-0.844021	-1.804885	0.843900
H	1.275524	1.279992	-1.191271
H	1.092367	0.049534	1.646341
H	2.533970	-0.086125	0.538571
H	-2.482396	0.264631	0.559582
H	-0.920271	2.248412	0.036679

Molecule# 0085

bicyclo-3,1,0-hexane

PointGroup: Cs

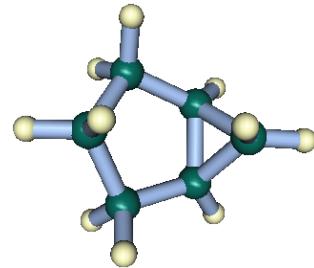
E= -234.716551958 au

ZPE= 0.145946 au

LUMO_eps= -0.00968 au

HOMO_eps= -0.26998 au

Dipole= 0.197 debye



16

H	-1.102142	-2.369592	0.000000
H	-1.825210	-0.706722	0.000000
C	-0.167576	1.451617	0.000000
H	-1.252508	1.558566	0.000000
H	0.244759	2.460062	0.000000
C	0.285460	0.631379	1.227651
H	-0.356020	0.801607	2.094810
H	1.301459	0.910417	1.518369
C	0.285460	0.631379	-1.227651
H	1.301459	0.910417	-1.518369
H	-0.356020	0.801607	-2.094810
C	-0.922260	-1.303615	0.000000
C	0.285460	-0.812956	0.755445
H	0.866098	-1.537728	1.309572
C	0.285460	-0.812956	-0.755445
H	0.866098	-1.537728	-1.309572

Molecule# 0086

bicyclo-3,3,1-nonane

PointGroup: Cs

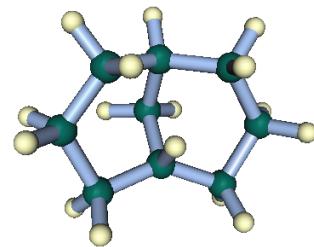
E= -352.648068166 au

ZPE= 0.234806 au

LUMO_eps= -0.01064 au

HOMO_eps= -0.26785 au

Dipole= 0.231 debye



25

C	-1.220553	0.008291	0.000000
C	0.018065	0.941134	0.000000
C	0.207716	1.430365	1.426632
C	0.207716	1.430365	-1.426632
C	-0.475923	-1.306583	0.000000
C	0.207716	0.053150	2.219513
C	0.207716	0.053150	-2.219513
C	0.362254	-1.260477	-1.348939
C	0.362254	-1.260477	1.348939
H	-1.853935	0.149273	0.874293
H	-1.853935	0.149273	-0.874293
H	0.882835	0.286335	0.000000
H	1.158855	1.951425	1.555610
H	-0.583800	2.082415	1.802671
H	-0.583800	2.082415	-1.802671
H	1.158855	1.951425	-1.555610
H	-1.113964	-2.193709	0.000000
H	1.006641	0.053850	2.962556
H	-0.719568	-0.025384	2.786768
H	-0.719568	-0.025384	-2.786768
H	1.006641	0.053850	-2.962556
H	1.419007	-1.432023	-1.131265
H	0.057484	-2.092626	-1.986451
H	0.057484	-2.092626	1.986451
H	1.419007	-1.432023	1.131265

Molecule# 0087

bicyclo-4,2,0-octane

PointGroup: C1

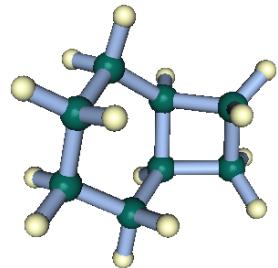
E= -313.375166867 au

ZPE= 0.204181 au

LUMO_eps= -0.01086 au

HOMO_eps= -0.27943 au

Dipole= 0.163 debye



22

C	-1.791427	-0.546342	-0.470725
C	-1.753453	0.902887	0.021944
C	-0.346099	1.484644	-0.136504
C	0.713967	0.691652	0.641171
C	2.060839	0.553545	-0.118966
C	1.570404	-0.813571	-0.662948
C	0.552087	-0.854996	0.508236
C	-0.849517	-1.436058	0.348591
H	-2.807213	-0.943727	-0.416752
H	-1.508563	-0.568405	-1.527994
H	-2.059618	0.940911	1.073243
H	-2.471421	1.510461	-0.533276
H	-0.099323	1.483279	-1.202799
H	-0.319965	2.530882	0.176897
H	0.774332	1.062996	1.665761
H	2.903852	0.434272	0.561752
H	2.304420	1.332097	-0.842353
H	2.293715	-1.626176	-0.723529
H	1.084176	-0.713631	-1.633483
H	1.040476	-1.331839	1.360944
H	-1.285091	-1.564400	1.345109
H	-0.790577	-2.437289	-0.088318

Molecule# 0088

bicyclo-5,1,0-octane

PointGroup: Cs

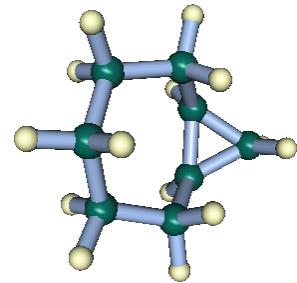
E= -313.372564201 au

ZPE= 0.203854 au

LUMO_eps= -0.00976 au

HOMO_eps= -0.26450 au

Dipole= 0.186 debye



22

C	0.322882	-1.211271	0.752902
C	0.322882	-1.211271	-0.752902
C	-0.466950	-2.251492	0.000000
C	-0.345255	-0.092908	1.527147
C	-0.345255	-0.092908	-1.527147
C	0.322882	1.274175	1.311568
C	0.322882	1.274175	-1.311568
C	-0.056876	1.976267	0.000000
H	1.240243	-1.564633	-1.210344
H	-0.116933	-3.274616	0.000000
H	-1.545089	-2.152272	0.000000
H	-1.402559	-0.021790	1.258165
H	-0.326225	-0.345142	2.590759
H	-0.326225	-0.345142	-2.590759
H	-1.402559	-0.021790	-1.258165
H	0.048720	1.937680	2.136366
H	1.410002	1.155998	1.365948
H	1.410002	1.155998	-1.365948
H	0.048720	1.937680	-2.136366
H	-1.139984	2.143490	0.000000
H	0.398488	2.970578	0.000000
H	1.240243	-1.564633	1.210344

Molecule# 0089

bicyclopropyl

PointGroup: C2h

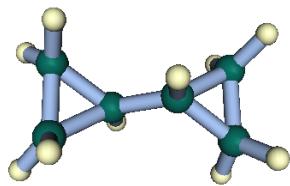
E= -234.683029321 au

ZPE= 0.143368 au

LUMO_eps= -0.00557 au

HOMO_eps= -0.25729 au

Dipole= 0.000 debye



16

C	0.000000	1.843020	0.753782
C	0.427743	0.611952	0.000000
C	0.000000	1.843020	-0.753782
C	-0.427743	-0.611952	0.000000
C	0.000000	-1.843020	0.753782
C	0.000000	-1.843020	-0.753782
H	0.754138	2.423213	1.266843
H	-0.956630	1.813429	1.257842
H	1.492677	0.407118	0.000000
H	-0.956630	1.813429	-1.257842
H	0.754138	2.423213	-1.266843
H	-1.492677	-0.407118	0.000000
H	-0.754138	-2.423213	1.266843
H	0.956630	-1.813429	1.257842
H	0.956630	-1.813429	-1.257842
H	-0.754138	-2.423213	-1.266843

Molecule# 0090

biphenyl

PointGroup: D2

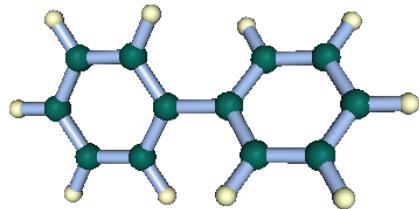
E= -463.470631646 au

ZPE= 0.181330 au

LUMO_eps= -0.04168 au

HOMO_eps= -0.23547 au

Dipole= 0.000 debye



22

C	0.000000	0.000000	-0.741117
C	-0.402579	1.130241	-1.461501
C	0.402579	-1.130241	-1.461501
C	0.403188	-1.130626	-2.850176
C	0.000000	0.000000	-3.551569
C	-0.403188	1.130626	-2.850176
C	0.000000	0.000000	0.741117
C	0.402579	1.130241	1.461501
C	0.403188	1.130626	2.850176
C	0.000000	0.000000	3.551569
C	-0.403188	-1.130626	2.850176
C	-0.402579	-1.130241	1.461501
H	-0.727357	-2.013375	3.385168
H	-0.727357	2.013375	-3.385168
H	0.000000	0.000000	4.633120
H	0.000000	0.000000	-4.633120
H	0.727357	-2.013375	-3.385168
H	0.727357	2.013375	3.385168
H	0.740949	2.008623	0.928761
H	0.740949	-2.008623	-0.928761
H	-0.740949	-2.008623	0.928761
H	-0.740949	2.008623	-0.928761

Molecule# 0091

biphenylene

PointGroup: D2

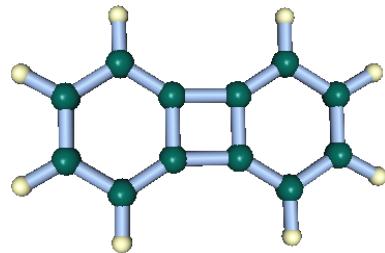
E= -462.190153805 au

ZPE= 0.158059 au

LUMO_eps= -0.05994 au

HOMO_eps= -0.21005 au

Dipole= 0.000 debye



20

C	3.111158	0.691977	0.000194
C	1.909382	1.439432	0.000379
C	0.753239	0.709064	-0.000071
C	-0.753239	0.709064	0.000071
C	-0.753239	-0.709064	-0.000071
C	0.753239	-0.709064	0.000071
C	1.909382	-1.439432	-0.000379
C	3.111158	-0.691977	-0.000194
C	-1.909382	-1.439432	0.000379
C	-3.111158	-0.691977	0.000194
C	-3.111158	0.691977	-0.000194
C	-1.909382	1.439432	-0.000379
H	4.056913	1.217403	0.000417
H	1.930044	2.520654	0.000453
H	1.930044	-2.520654	-0.000453
H	4.056913	-1.217403	-0.000417
H	-1.930044	-2.520654	0.000453
H	-4.056913	-1.217403	0.000417
H	-4.056913	1.217403	-0.000417
H	-1.930044	2.520654	-0.000453

Molecule# 0092

bromoacetic acid

PointGroup: C1

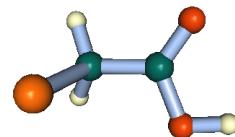
E= -2802.804028350 au

ZPE= 0.052793 au

LUMO_eps= -0.06681 au

HOMO_eps= -0.29314 au

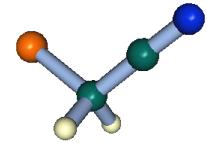
Dipole= 1.771 debye



8

Br	-1.318867	0.040683	-0.132375
O	2.187798	-0.953508	-0.501912
O	1.821768	1.191955	0.068190
C	1.529373	-0.124816	0.068151
C	0.298794	-0.427860	0.883869
H	2.605629	1.316076	-0.487285
H	0.244255	-1.489789	1.082828
H	0.264939	0.158301	1.795235

Molecule# 0093
bromoacetonitrile
PointGroup: Cs
E= -2706.424267630 au
ZPE= 0.036293 au
LUMO_eps= -0.07407 au
HOMO_eps= -0.31255 au
Dipole= 3.288 debye



6
Br 0.000000 1.021614 0.000000
N -0.960072 -2.658366 0.000000
C 0.820993 -0.769470 0.000000
C -0.180814 -1.812966 0.000000
H 1.439718 -0.826649 0.889758
H 1.439718 -0.826649 -0.889758

Molecule# 0094

bromobenzene

PointGroup: C2v

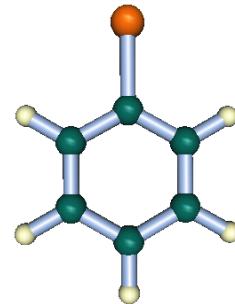
E= -2805.961499000 au

ZPE= 0.090291 au

LUMO_eps= -0.03211 au

HOMO_eps= -0.25393 au

Dipole= 1.822 debye

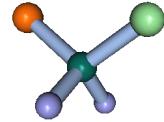


12

C	0.000000	0.000000	-2.873209
C	0.000000	1.202166	-2.175891
C	0.000000	-1.202166	-2.175891
C	0.000000	1.210301	-0.785384
C	0.000000	-1.210301	-0.785384
C	0.000000	0.000000	-0.106242
Br	0.000000	0.000000	1.807643
H	0.000000	0.000000	-3.954514
H	0.000000	2.142085	-2.711318
H	0.000000	-2.142085	-2.711318
H	0.000000	2.141988	-0.239178
H	0.000000	-2.141988	-0.239178

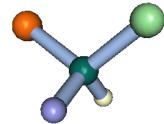
Molecule# 0095
bromochlorodifluoromethane
PointGroup: Cs

E= -3272.337180870 au
ZPE= 0.012156 au
LUMO_eps= -0.07306 au
HOMO_eps= -0.31918 au
Dipole= 0.481 debye



5
C 0.036531 0.683049 0.000000
F 0.550496 1.274721 1.079099
F 0.550496 1.274721 -1.079099
Cl -1.729146 0.889490 0.000000
Br 0.550496 -1.204703 0.000000

Molecule# 0096
bromochlorofluoromethane
PointGroup: C1
E= -3173.058859040 au
ZPE= 0.020713 au
LUMO_eps= -0.05846 au
HOMO_eps= -0.30958 au
Dipole= 1.214 debye



5
C 0.577564 0.464082 0.412192
H 0.617813 0.595487 1.486256
F 0.784837 1.645480 -0.202899
Cl 1.842585 -0.686603 -0.067367
Br -1.213448 -0.186201 -0.028231

Molecule# 0097

bromochloromethane

PointGroup: Cs

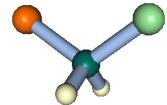
E= -3073.786816630 au

ZPE= 0.028610 au

LUMO_eps= -0.04890 au

HOMO_eps= -0.29879 au

Dipole= 1.581 debye



5

Br -0.845069 -0.732631 0.000000

Cl 1.778111 0.964335 0.000000

C 0.000000 1.029529 0.000000

H -0.325234 1.535603 0.898226

H -0.325234 1.535603 -0.898226

Molecule# 0098

bromocyanoacetamide

PointGroup: C1

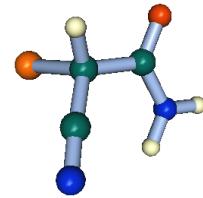
E= -2875.189169540 au

ZPE= 0.062948 au

LUMO_eps= -0.09414 au

HOMO_eps= -0.29753 au

Dipole= 1.626 debye

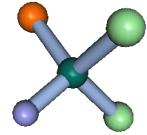


10

Br	-1.448897	-0.263707	0.144519
O	1.569901	-1.766738	-0.721307
N	2.035093	-0.351963	0.993793
N	0.811028	2.739524	-0.095712
C	0.299927	0.250807	-0.637089
C	1.379146	-0.731690	-0.124040
C	0.556447	1.646747	-0.350631
H	0.192365	0.085858	-1.703739
H	1.888477	0.539733	1.433247
H	2.735356	-0.970058	1.366768

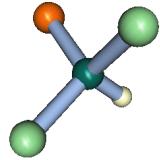
Molecule# 0099
bromodichlorofluoromethane
PointGroup: Cs

E= -3632.677845420 au
ZPE= 0.010285 au
LUMO_eps= -0.08420 au
HOMO_eps= -0.31230 au
Dipole= 0.407 debye



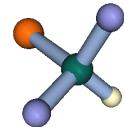
5
C -0.536473 0.132457 0.000000
F -1.077480 1.357510 0.000000
Br 1.415728 0.331072 0.000000
Cl -1.077480 -0.723524 1.463090
Cl -1.077480 -0.723524 -1.463090

Molecule# 0100
bromodichloromethane
PointGroup: Cs
E= -3533.407612560 au
ZPE= 0.019044 au
LUMO_eps= -0.07069 au
HOMO_eps= -0.30423 au
Dipole= 1.012 debye



5
C -0.674319 -0.145328 0.000000
H -1.576380 0.447271 0.000000
Br 0.815689 1.124019 0.000000
Cl -0.674319 -1.144587 1.468998
Cl -0.674319 -1.144587 -1.468998

Molecule# 0101
bromodifluoromethane
PointGroup: Cs
E= -2812.714013780 au
ZPE= 0.022500 au
LUMO_eps= -0.04356 au
HOMO_eps= -0.31675 au
Dipole= 1.401 debye



5
C -0.426419 -0.921785 0.000000
H -1.510576 -0.987137 0.000000
Br 0.076775 0.970226 0.000000
F 0.076775 -1.524448 1.088416
F 0.076775 -1.524448 -1.088416

Molecule# 0102

bromoethane

PointGroup: Cs

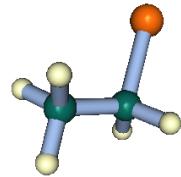
E= -2653.493066710 au

ZPE= 0.065672 au

LUMO_eps= -0.02347 au

HOMO_eps= -0.27954 au

Dipole= 2.239 debye



8

C	-0.571906	-2.045603	0.000000
C	0.597203	-1.087017	0.000000
Br	0.000000	0.801608	0.000000
H	-0.194783	-3.071850	0.000000
H	-1.194659	-1.912153	0.883211
H	-1.194659	-1.912153	-0.883211
H	1.216159	-1.182204	-0.886089
H	1.216159	-1.182204	0.886089

Molecule# 0103

bromoethene

PointGroup: Cs

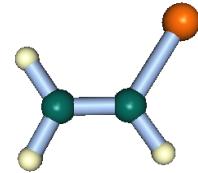
E= -2652.252237750 au

ZPE= 0.041972 au

LUMO_eps= -0.02688 au

HOMO_eps= -0.26698 au

Dipole= 1.483 debye



6

C	0.455162	-1.119119	0.000000
C	-0.440113	-2.087947	0.000000
Br	0.000000	0.729605	0.000000
H	1.522768	-1.275215	0.000000
H	-0.108956	-3.118613	0.000000
H	-1.504105	-1.899949	0.000000

Molecule# 0104

bromofluoromethane

PointGroup: Cs

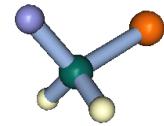
E= -2713.431850830 au

ZPE= 0.030233 au

LUMO_eps= -0.03469 au

HOMO_eps= -0.29752 au

Dipole= 1.786 debye



5

Br 0.000000 0.762073 0.000000

F -0.586982 -1.924918 0.000000

C 0.517543 -1.125903 0.000000

H 1.088790 -1.296442 0.906078

H 1.088790 -1.296442 -0.906078

Molecule# 0105

bromomethane

PointGroup: C3v

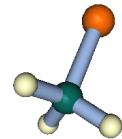
E= -2614.161825710 au

ZPE= 0.037017 au

LUMO_eps= -0.02963 au

HOMO_eps= -0.28378 au

Dipole= 1.929 debye



5

C 0.000000 0.000000 -1.536353

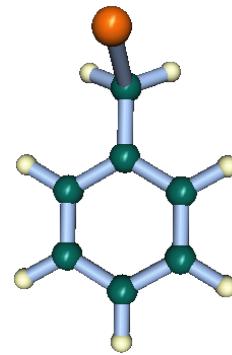
Br 0.000000 0.000000 0.423209

H 0.000000 1.032396 -1.864728

H 0.894081 -0.516198 -1.864728

H -0.894081 -0.516198 -1.864728

Molecule# 0106
 bromomethylbenzene
 PointGroup: Cs
 E= -2845.293894020 au
 ZPE= 0.118872 au
 LUMO_eps= -0.05353 au
 HOMO_eps= -0.26089 au
 Dipole= 2.299 debye



15
 C 0.747079 3.182018 0.000000
 C 0.748152 2.484260 1.203062
 C 0.748152 2.484260 -1.203062
 C 0.748152 1.095863 1.202097
 C 0.748152 1.095863 -1.202097
 C 0.748740 0.385906 0.000000
 C 0.766678 -1.101796 0.000000
 Br -1.077814 -1.889784 0.000000
 H 0.747714 4.263560 0.000000
 H 0.750769 3.021826 2.141614
 H 0.750769 3.021826 -2.141614
 H 0.745501 0.555942 2.140413
 H 0.745501 0.555942 -2.140413
 H 1.226311 -1.517461 0.889137
 H 1.226311 -1.517461 -0.889137

Molecule# 0107

bromonitroethane

PointGroup: C1

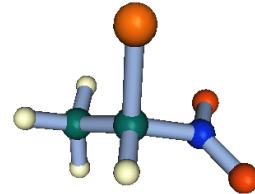
E= -2858.065468080 au

ZPE= 0.068320 au

LUMO_eps= -0.10489 au

HOMO_eps= -0.31058 au

Dipole= 3.463 debye



10

Br	-1.348107	-0.280154	0.061016
O	2.000045	-1.102787	-0.753014
O	1.771865	-0.160570	1.188419
N	1.470823	-0.327846	0.023462
C	0.335182	0.520755	-0.545999
C	0.468987	1.961630	-0.130102
H	0.374728	0.356066	-1.614458
H	-0.338882	2.539582	-0.573946
H	0.431069	2.059234	0.951329
H	1.420783	2.357962	-0.489362

Molecule# 0108

bromotrichloromethane

PointGroup: C3v

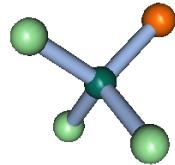
E= -3993.021028490 au

ZPE= 0.008540 au

LUMO_eps= -0.09197 au

HOMO_eps= -0.30967 au

Dipole= 0.077 debye



5

C 0.000000 0.000000 -0.422067

Br 0.000000 0.000000 1.546441

Cl 0.000000 1.681735 -1.011628

Cl 1.456425 -0.840867 -1.011628

Cl -1.456425 -0.840867 -1.011628

Molecule# 0109

bromotrifluoromethane

PointGroup: C3v

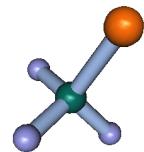
E= -2911.998444340 au

ZPE= 0.014091 au

LUMO_eps= -0.05799 au

HOMO_eps= -0.32976 au

Dipole= 0.492 debye



5

C 0.000000 0.000000 -0.821073

F 0.000000 1.248180 -1.280579

F 1.080956 -0.624090 -1.280579

F -1.080956 -0.624090 -1.280579

Br 0.000000 0.000000 1.128631

Molecule# 0110

but-2-ynamide

PointGroup: C1

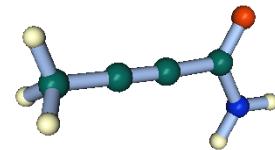
E= -285.480194259 au

ZPE= 0.082897 au

LUMO_eps= -0.03567 au

HOMO_eps= -0.26791 au

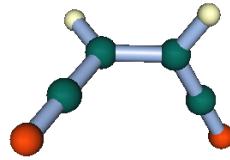
Dipole= 4.330 debye



11

C	-0.275084	-0.023840	0.000001
C	-1.476686	0.011199	-0.000006
C	1.173929	-0.141273	0.000002
C	-2.928915	0.034761	0.000001
N	1.835717	1.050955	0.000032
O	1.744529	-1.217101	-0.000005
H	-3.308404	0.552873	0.882157
H	-3.334521	-0.977755	-0.000225
H	-3.308412	0.553273	-0.881917
H	2.841046	1.040814	-0.000076
H	1.344570	1.925831	-0.000104

Molecule# 0111
buta-1,3-diene-1,4-dione
PointGroup: C2
E= -304.122370665 au
ZPE= 0.047239 au
LUMO_eps= -0.06830 au
HOMO_eps= -0.24765 au
Dipole= 1.880 debye



8

O	-0.115324	2.385771	-0.820827
O	0.115324	-2.385771	-0.820827
C	0.379356	0.637546	0.860073
C	-0.379356	-0.637546	0.860073
C	0.115324	1.569774	-0.030466
C	-0.115324	-1.569774	-0.030466
H	1.150733	0.853280	1.588973
H	-1.150733	-0.853280	1.588973

Molecule# 0112

buta-1,3-diyn-1,4-diol

PointGroup: C1

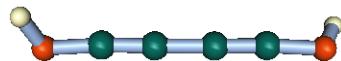
E= -304.032443670 au

ZPE= 0.046815 au

LUMO_eps= -0.03078 au

HOMO_eps= -0.23209 au

Dipole= 2.017 debye



8

O	3.189684	-0.076657	-0.064099
O	-3.189684	0.076659	-0.064103
C	0.681541	-0.006531	-0.008790
C	-0.681541	0.006524	-0.008791
C	1.886110	-0.000033	0.003758
C	-1.886111	0.000032	0.003757
H	3.604742	0.550174	0.542991
H	-3.604744	-0.550143	0.543017

Molecule# 0113

buta-1,3-diynyl fluoromethyl carbonate

PointGroup: C1

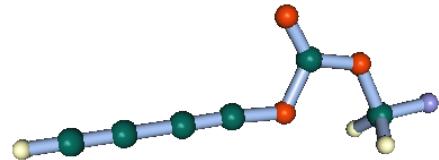
E= -556.018430401 au

ZPE= 0.077891 au

LUMO_eps= -0.04241 au

HOMO_eps= -0.26531 au

Dipole= 2.898 debye



13

F	3.940309	-0.700508	0.000001
O	0.078593	-0.377057	0.000001
O	2.113751	0.544697	0.000000
O	0.337726	1.902359	-0.000003
C	0.818126	0.821984	0.000000
C	-1.226279	-0.291508	0.000001
C	2.589453	-0.807507	0.000001
C	-2.427483	-0.308785	0.000000
C	-3.790073	-0.312892	0.000000
C	-4.994397	-0.317938	0.000000
H	2.268129	-1.318104	0.905799
H	2.268129	-1.318107	-0.905795
H	-6.055687	-0.319329	0.000000

Molecule# 0114

butanal

PointGroup: Cs

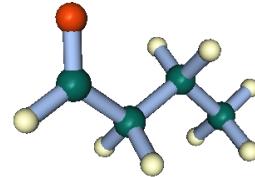
E= -232.552993098 au

ZPE= 0.112416 au

LUMO_eps= -0.03583 au

HOMO_eps= -0.26477 au

Dipole= 2.724 debye



13

C	-1.498796	0.606364	0.000000
C	2.286416	-0.364870	0.000000
C	0.000000	0.740162	0.000000
C	0.773358	-0.572830	0.000000
O	-2.103883	-0.435720	0.000000
H	-2.049279	1.570818	0.000000
H	2.612258	0.192076	0.881024
H	2.813086	-1.319587	0.000000
H	2.612258	0.192076	-0.881024
H	0.262254	1.359651	0.867455
H	0.262254	1.359651	-0.867455
H	0.476183	-1.160935	0.870082
H	0.476183	-1.160935	-0.870082

Molecule# 0115

butanamide

PointGroup: C1

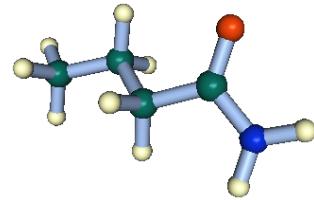
E= -287.963807516 au

ZPE= 0.130214 au

LUMO_eps= -0.02201 au

HOMO_eps= -0.26045 au

Dipole= 3.622 debye



15

C	-2.731329	-0.188210	0.027569
H	-2.896131	-0.208886	1.106914
H	-3.510969	0.433548	-0.413737
H	-2.869306	-1.205115	-0.346583
C	-1.343418	0.351342	-0.308883
H	-1.217269	0.398690	-1.393390
H	-1.233985	1.372797	0.054840
C	-0.221272	-0.497474	0.289364
H	-0.261557	-1.517699	-0.100776
H	-0.357479	-0.572869	1.373168
N	2.159806	-0.790578	-0.170020
H	3.099748	-0.446011	-0.265813
H	1.999084	-1.780108	-0.196024
C	1.158613	0.105753	0.066900
O	1.369207	1.303904	0.115231

Molecule# 0116

butane

PointGroup: C2

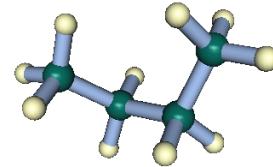
E= -158.519677430 au

ZPE= 0.131473 au

LUMO_eps= -0.00967 au

HOMO_eps= -0.32447 au

Dipole= 0.105 debye



14

C	-0.252798	0.723681	0.616235
C	0.252798	1.571360	-0.551646
C	0.252798	-0.723681	0.616235
C	-0.252798	-1.571360	-0.551646
H	-0.104388	2.599202	-0.473491
H	0.083428	-1.182319	-1.513402
H	-1.344623	-1.601548	-0.570383
H	-0.083428	1.182319	-1.513402
H	0.104388	-2.599202	-0.473491
H	1.344623	1.601548	-0.570383
H	-1.347442	0.719895	0.615666
H	0.047102	1.198634	1.554079
H	1.347442	-0.719895	0.615666
H	-0.047102	-1.198634	1.554079

Molecule# 0117

butanenitrile

PointGroup: Cs

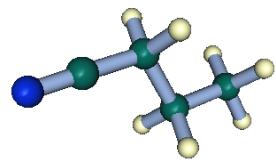
E= -211.465228055 au

ZPE= 0.102490 au

LUMO_eps= -0.02144 au

HOMO_eps= -0.33178 au

Dipole= 4.293 debye



12

C	1.454366	0.512277	0.000000
C	-2.231561	-0.577773	0.000000
C	0.000000	0.631202	0.000000
C	-0.713585	-0.731881	0.000000
N	2.598842	0.398853	0.000000
H	-2.575965	-0.034286	0.881826
H	-2.575965	-0.034286	-0.881826
H	-2.719763	-1.552135	0.000000
H	-0.295422	1.212550	0.876647
H	-0.295422	1.212550	-0.876647
H	-0.392342	-1.299658	0.874523
H	-0.392342	-1.299658	-0.874523

Molecule# 0118

butanethiol

PointGroup: C1

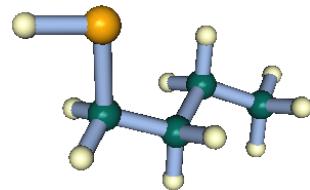
E= -556.741135455 au

ZPE= 0.131288 au

LUMO_eps= -0.01702 au

HOMO_eps= -0.23923 au

Dipole= 1.598 debye



15

C	2.784969	-0.371669	-0.128185
C	1.353327	-0.290285	0.397998
C	0.523956	0.782957	-0.309707
C	-0.898001	0.948281	0.219480
S	-1.902817	-0.567172	-0.109965
H	3.355821	-1.140150	0.394167
H	3.309752	0.577267	0.001618
H	2.800602	-0.614167	-1.192643
H	1.367691	-0.079826	1.471581
H	0.869424	-1.263165	0.287020
H	0.488279	0.573674	-1.382567
H	1.026483	1.749510	-0.202216
H	-0.887504	1.133147	1.293120
H	-1.385788	1.786314	-0.273539
H	-3.085182	-0.063565	0.285377

Molecule# 0119

butatriene

PointGroup: D2h

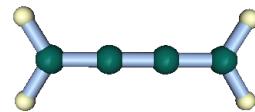
E= -154.793952401 au

ZPE= 0.059893 au

LUMO_eps= -0.06858 au

HOMO_eps= -0.25345 au

Dipole= 0.000 debye



8

C 0.000000 0.000000 0.631617

C 0.000000 0.000000 -0.631617

C 0.000000 0.000000 1.943149

C 0.000000 0.000000 -1.943149

H 0.000000 0.924533 2.508102

H 0.000000 -0.924533 2.508102

H 0.000000 0.924533 -2.508102

H 0.000000 -0.924533 -2.508102

Molecule# 0120

butyl acetate

PointGroup: C1

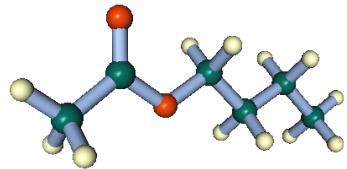
E= -386.489034434 au

ZPE= 0.174222 au

LUMO_eps= -0.01327 au

HOMO_eps= -0.28047 au

Dipole= 2.174 debye



20

C	2.202488	0.116111	-0.000012
C	3.288179	-0.927156	0.000005
C	-3.962455	-0.357641	-0.000017
C	-2.678902	0.470725	0.000022
C	-1.415543	-0.392205	-0.000009
C	-0.151969	0.444179	0.000021
O	2.380920	1.308789	-0.000020
O	0.980632	-0.454908	0.000000
H	3.191841	-1.565826	-0.877925
H	3.192067	-1.565518	0.878188
H	4.258416	-0.440768	-0.000192
H	-4.016737	-1.000104	-0.880951
H	-4.016742	-1.000179	0.880862
H	-4.846288	0.281106	0.000008
H	-2.669921	1.127959	-0.874214
H	-2.669927	1.127886	0.874314
H	-1.412843	-1.045046	0.876714
H	-1.412842	-1.044982	-0.876781
H	-0.090109	1.085203	-0.880362
H	-0.090117	1.085149	0.880444

Molecule# 0121

butylbenzene

PointGroup: Cs

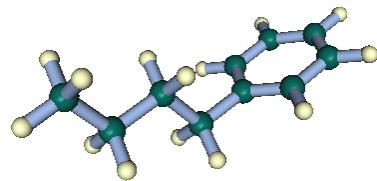
E= -389.650919067 au

ZPE= 0.212992 au

LUMO_eps= -0.01484 au

HOMO_eps= -0.24708 au

Dipole= 0.492 debye



24

C	0.680345	-3.295333	0.000000
C	0.681769	-2.594527	1.200390
C	0.681769	-2.594527	-1.200390
C	0.681769	-1.204878	1.197095
C	0.681769	-1.204878	-1.197095
C	0.679166	-0.487390	0.000000
C	-2.241322	3.689088	0.000000
C	0.640208	1.021053	0.000000
C	-0.822953	3.121120	0.000000
C	-0.786838	1.592902	0.000000
H	0.683708	-4.377103	0.000000
H	0.687861	-3.130232	2.140693
H	0.687861	-3.130232	-2.140693
H	0.689431	-0.667833	2.138051
H	0.689431	-0.667833	-2.138051
H	-2.797599	3.361340	0.880573
H	-2.797599	3.361340	-0.880573
H	-2.234070	4.779958	0.000000
H	1.173513	1.399551	0.875815
H	1.173513	1.399551	-0.875815
H	-0.280474	3.494116	0.873994
H	-0.280474	3.494116	-0.873994
H	-1.324598	1.213739	0.873915
H	-1.324598	1.213739	-0.873915

Molecule# 0122

butyric acid

PointGroup: Cs

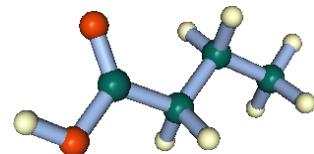
E= -307.842120721 au

ZPE= 0.118305 au

LUMO_eps= -0.01606 au

HOMO_eps= -0.28997 au

Dipole= 1.586 debye



14

C	-1.045329	-0.494601	0.000000
C	2.460708	1.198934	0.000000
C	0.000000	0.591852	0.000000
C	1.432695	0.069636	0.000000
O	-0.842076	-1.681341	0.000000
O	-2.300401	0.024009	0.000000
H	2.354021	1.835295	0.881002
H	2.354021	1.835295	-0.881002
H	3.476451	0.802896	0.000000
H	-0.189161	1.228211	0.869185
H	-0.189161	1.228211	-0.869185
H	1.580358	-0.571042	-0.870771
H	1.580358	-0.571042	0.870771
H	-2.915516	-0.724098	0.000000

Molecule# 0123

calicene

PointGroup: C2v

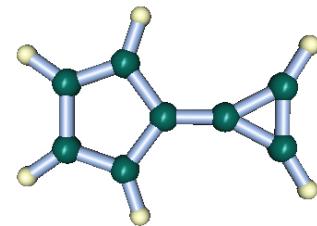
E= -308.428405123 au

ZPE= 0.107161 au

LUMO_eps= -0.05811 au

HOMO_eps= -0.19901 au

Dipole= 4.675 debye



14

C	0.000000	0.000000	-0.043798
C	0.000000	0.000000	1.304624
C	0.000000	0.659873	2.562756
C	0.000000	-0.659873	2.562756
C	0.000000	1.167314	-0.908995
C	0.000000	-1.167314	-0.908995
C	0.000000	0.725289	-2.197208
C	0.000000	-0.725289	-2.197208
H	0.000000	1.574226	3.129175
H	0.000000	-1.574226	3.129175
H	0.000000	2.191202	-0.569441
H	0.000000	-2.191202	-0.569441
H	0.000000	1.344285	-3.081535
H	0.000000	-1.344285	-3.081535

Molecule# 0124

carbodiimide

PointGroup: C2

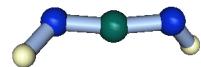
E= -148.849772344 au

ZPE= 0.032659 au

LUMO_eps= -0.02095 au

HOMO_eps= -0.29773 au

Dipole= 1.944 debye



5

C 0.000000 0.000000 0.018127

N 0.000000 1.215003 -0.079246

N 0.000000 -1.215003 -0.079246

H 0.613213 1.770339 0.500341

H -0.613213 -1.770339 0.500341

Molecule# 0125

carbon dioxide

PointGroup: D(infinity)h

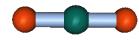
E= -188.663385641 au

ZPE= 0.011659 au

LUMO_eps= -0.02060 au

HOMO_eps= -0.38452 au

Dipole= 0.000 debye



3

C 0.000000 0.000000 0.000000

O 0.000000 0.000000 1.160386

O 0.000000 0.000000 -1.160386

Molecule# 0126

carbon disulfide

PointGroup: D(infinity)h

E= -834.572965659 au

ZPE= 0.006900 au

LUMO_eps= -0.08208 au

HOMO_eps= -0.28051 au

Dipole= 0.000 debye



3

C 0.000000 0.000000 0.000000

S 0.000000 0.000000 1.557501

S 0.000000 0.000000 -1.557501

Molecule# 0127

carbonic acid

PointGroup: C2v

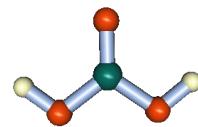
E= -265.121954733 au

ZPE= 0.039457 au

LUMO_eps= -0.02681 au

HOMO_eps= -0.31456 au

Dipole= 0.304 debye



6

C 0.000000 0.000000 0.101922

O 0.000000 0.000000 1.305118

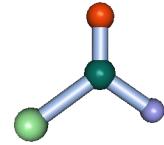
O 0.000000 1.088420 -0.679394

O 0.000000 -1.088420 -0.679394

H 0.000000 1.854503 -0.091082

H 0.000000 -1.854503 -0.091082

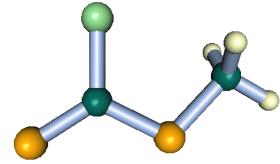
Molecule# 0128
carbonic chloride fluoride
PointGroup: Cs
E= -673.493643696 au
ZPE= 0.012081 au
LUMO_eps= -0.05728 au
HOMO_eps= -0.34934 au
Dipole= 1.271 debye



4
C 0.000000 0.510905 0.000000
O -0.797403 1.370426 0.000000
Cl -0.321200 -1.202070 0.000000
F 1.315513 0.711817 0.000000

Molecule# 0129
carbonochloridodithioic acid
PointGroup: C1

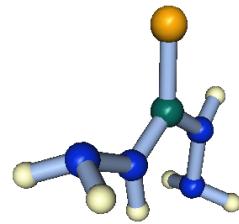
E= -1334.718513280 au
ZPE= 0.045989 au
LUMO_eps= -0.09386 au
HOMO_eps= -0.24972 au
Dipole= 3.406 debye



8

C1	-0.142353	1.682318	0.000006
S	0.908059	-1.112252	-0.000003
S	-1.983399	-0.651574	-0.000005
C	-0.475009	-0.060877	0.000000
C	2.395894	-0.059942	0.000003
H	2.437172	0.555719	0.893120
H	3.225785	-0.764724	0.000001
H	2.437174	0.555726	-0.893110

Molecule# 0130
carbonothioic dihydrazide
PointGroup: C1
E= -658.997044935 au
ZPE= 0.094845 au
LUMO_eps= -0.03286 au
HOMO_eps= -0.20037 au
Dipole= 6.420 debye



12

C	-0.008290	-0.208356	-0.024723
S	-1.217170	-1.356869	0.021420
N	-0.162614	1.134737	-0.015493
N	-1.417749	1.738272	0.008702
N	1.302148	-0.610414	-0.099972
N	2.364793	0.297605	0.049141
H	2.841583	0.157650	0.933495
H	3.025732	0.182703	-0.708975
H	-1.510815	2.327204	0.825721
H	-1.567518	2.280758	-0.832165
H	0.681476	1.689836	-0.040769
H	1.447958	-1.599522	0.031666

Molecule# 0131

carbonyl dibromide

PointGroup: C2v

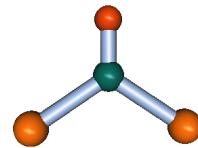
E= -5261.830399800 au

ZPE= 0.009238 au

LUMO_eps= -0.09320 au

HOMO_eps= -0.30821 au

Dipole= 1.180 debye



4

C 0.000000 0.000000 0.783861

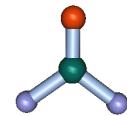
O 0.000000 0.000000 1.953708

Br 0.000000 1.613709 -0.290469

Br 0.000000 -1.613709 -0.290469

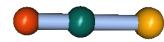
Molecule# 0132
carbonyl fluoride
PointGroup: C2v

E= -313.146349819 au
ZPE= 0.013916 au
LUMO_eps= -0.03508 au
HOMO_eps= -0.37475 au
Dipole= 1.033 debye



4
O 0.000000 0.000000 1.316315
C 0.000000 0.000000 0.145081
F 0.000000 1.065268 -0.633389
F 0.000000 -1.065268 -0.633389

Molecule# 0133
carbonyl sulfide
PointGroup: C(infinity)v
E= -511.619710462 au
ZPE= 0.009193 au
LUMO_eps= -0.04401 au
HOMO_eps= -0.31045 au
Dipole= 0.754 debye



3
C 0.000000 0.000000 -0.527573
O 0.000000 0.000000 -1.683489
S 0.000000 0.000000 1.039584

Molecule# 0134

chloro(chloromethyl)malononitrile

PointGroup: C1

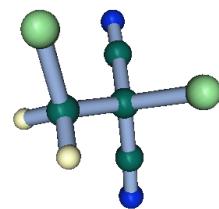
E= -1183.630044000 au

ZPE= 0.053839 au

LUMO_eps= -0.09825 au

HOMO_eps= -0.34093 au

Dipole= 2.870 debye



10

C1	0.454804	-1.139246	1.304813
C1	-2.281823	-0.133493	-0.404658
N	0.212304	2.469029	0.884988
N	2.741580	-0.189878	-1.346088
C	0.469741	0.052344	-0.074733
C	-0.644368	-0.282574	-1.092678
C	0.324537	1.401661	0.476873
C	1.759694	-0.075092	-0.761062
H	-0.569014	0.407136	-1.929326
H	-0.506489	-1.302670	-1.436011

Molecule# 0135
chloroacetaldehyde

PointGroup: C1

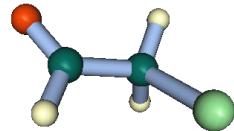
E= -613.522271979 au

ZPE= 0.046928 au

LUMO_eps= -0.06757 au

HOMO_eps= -0.28840 au

Dipole= 1.502 debye



7

C	0.028542	0.674903	0.133473
C	1.166085	-0.321837	0.199900
Cl	-1.550178	-0.167557	-0.077281
O	2.264073	-0.071400	-0.217240
H	-0.023974	1.228514	1.070602
H	0.172885	1.363727	-0.692610
H	0.923765	-1.290966	0.673464

Molecule# 0136

chloroacetonitrile

PointGroup: Cs

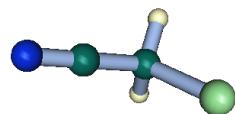
E= -592.427523419 au

ZPE= 0.036875 au

LUMO_eps= -0.05568 au

HOMO_eps= -0.33343 au

Dipole= 3.281 debye



6

C1 -1.385401 -0.338103 0.000000

N 2.297547 -0.400037 0.000000

C 0.000000 0.819137 0.000000

C 1.275830 0.126036 0.000000

H -0.092993 1.438487 0.887765

H -0.092993 1.438487 -0.887765

Molecule# 0137

chloroacetylene

PointGroup: C(infinity)v

E= -536.988364300 au

ZPE= 0.019197 au

LUMO_eps= -0.01247 au

HOMO_eps= -0.28622 au

Dipole= 0.374 debye



4

C 0.000000 0.000000 -0.615871

C 0.000000 0.000000 -1.813601

Cl 0.000000 0.000000 1.026530

H 0.000000 0.000000 -2.874172

Molecule# 0138

chloroaminoacetic acid

PointGroup: C1

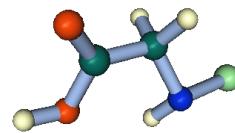
E= -744.143479312 au

ZPE= 0.069881 au

LUMO_eps= -0.05538 au

HOMO_eps= -0.26992 au

Dipole= 2.058 debye



10

C1	2.428631	-0.064395	0.032886
O	-1.730300	1.196583	0.115542
O	-2.527186	-0.891563	-0.130112
N	0.770338	0.388259	-0.379853
C	-0.158958	-0.592845	0.181441
C	-1.598551	-0.146064	0.017450
H	-0.003971	-0.777676	1.252540
H	-0.042747	-1.538938	-0.340394
H	0.644604	1.280659	0.086477
H	-2.672033	1.406156	0.024511

Molecule# 0139

chlorobenzene

PointGroup: C2v

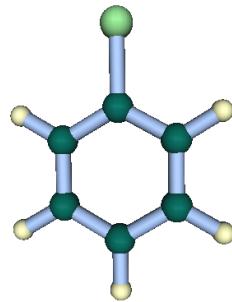
E= -691.967879754 au

ZPE= 0.090839 au

LUMO_eps= -0.03142 au

HOMO_eps= -0.25692 au

Dipole= 1.791 debye



12

C	0.000000	0.000000	-2.265776
C	0.000000	1.202168	-1.568121
C	0.000000	-1.202168	-1.568121
C	0.000000	1.209985	-0.178204
C	0.000000	-1.209985	-0.178204
C	0.000000	0.000000	0.501800
Cl	0.000000	0.000000	2.255827
H	0.000000	0.000000	-3.347036
H	0.000000	2.141915	-2.103741
H	0.000000	-2.141915	-2.103741
H	0.000000	2.139131	0.372605
H	0.000000	-2.139131	0.372605

Molecule# 0140

chlorodifluoromethane

PointGroup: Cs

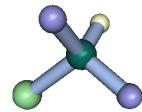
E= -698.721788858 au

ZPE= 0.023114 au

LUMO_eps= -0.01857 au

HOMO_eps= -0.34543 au

Dipole= 1.462 debye



5

C 0.570687 -0.092261 0.000000

F 0.570687 -0.879813 1.088316

F 0.570687 -0.879813 -1.088316

Cl -0.890989 0.932054 0.000000

H 1.450337 0.545289 0.000000

Molecule# 0141

chloroethane

PointGroup: Cs

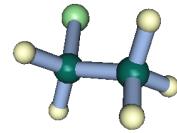
E= -539.497818224 au

ZPE= 0.066303 au

LUMO_eps= -0.01496 au

HOMO_eps= -0.29848 au

Dipole= 2.224 debye



8

C	1.506018	0.680611	0.000000
C	0.000000	0.820714	0.000000
H	1.961216	1.673866	0.000000
H	1.851632	0.145961	0.883624
H	1.851632	0.145961	-0.883624
Cl	-0.821829	-0.802430	0.000000
H	-0.364745	1.333788	0.885068
H	-0.364745	1.333788	-0.885068

Molecule# 0142

chloroethene

PointGroup: Cs

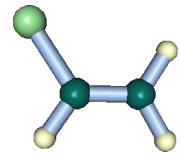
E= -538.258304997 au

ZPE= 0.042519 au

LUMO_eps= -0.02453 au

HOMO_eps= -0.27293 au

Dipole= 1.492 debye



6

C	1.289018	1.047846	0.000000
C	0.000000	0.763426	0.000000
Cl	-0.623753	-0.866823	0.000000
H	1.603767	2.082310	0.000000
H	2.051033	0.282196	0.000000
H	-0.785113	1.503855	0.000000

Molecule# 0143

chlorofluoromethane

PointGroup: Cs

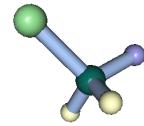
E= -599.438128946 au

ZPE= 0.030843 au

LUMO_eps= -0.01806 au

HOMO_eps= -0.31906 au

Dipole= 1.858 debye



5

C1 0.682538 -0.843775 0.000000

F -1.364381 0.762010 0.000000

C 0.000000 0.812042 0.000000

H 0.338141 1.306914 0.905061

H 0.338141 1.306914 -0.905061

Molecule# 0144

chloroketene

PointGroup: C1

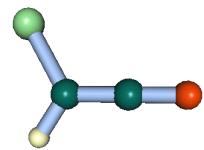
E= -612.282152834 au

ZPE= 0.023896 au

LUMO_eps= -0.08931 au

HOMO_eps= -0.25127 au

Dipole= 1.278 debye



5

C1 -1.452562 -0.235201 0.000013

O 2.214395 -0.375124 0.000033

C 0.002567 0.726842 -0.000115

C 1.175372 0.139924 -0.000030

H -0.089246 1.798809 0.000383

Molecule# 0145

chloromethane

PointGroup: C3v

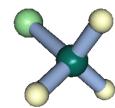
E= -500.165804121 au

ZPE= 0.037611 au

LUMO_eps= -0.01791 au

HOMO_eps= -0.30327 au

Dipole= 1.983 debye



5

C 0.000000 0.000000 -1.138108

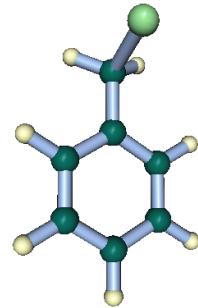
Cl 0.000000 0.000000 0.662444

H 0.000000 1.030124 -1.477634

H 0.892114 -0.515062 -1.477634

H -0.892114 -0.515062 -1.477634

Molecule# 0146
 chloromethylbenzene
 PointGroup: Cs
 E= -731.297565361 au
 ZPE= 0.119454 au
 LUMO_eps= -0.04323 au
 HOMO_eps= -0.26432 au
 Dipole= 2.249 debye



15

C	0.420637	2.644566	0.000000
C	0.421753	1.947096	1.203090
C	0.421753	1.947096	-1.203090
C	0.421753	0.558318	1.201822
C	0.421753	0.558318	-1.201822
C	0.421492	-0.150366	0.000000
C	0.426140	-1.643412	0.000000
Cl	-1.272788	-2.340959	0.000000
H	0.421639	3.726146	0.000000
H	0.424437	2.484779	2.141585
H	0.424437	2.484779	-2.141585
H	0.419754	0.018155	2.140045
H	0.419754	0.018155	-2.140045
H	0.897849	-2.052701	0.887296
H	0.897849	-2.052701	-0.887296

Molecule# 0147

chloromethyloxirane

PointGroup: C1

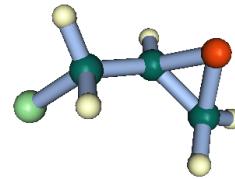
E= -652.818037873 au

ZPE= 0.076837 au

LUMO_eps= -0.01210 au

HOMO_eps= -0.29412 au

Dipole= 0.601 debye



10

C	0.385941	-0.723508	0.267146
Cl	1.900475	0.227545	-0.033923
C	-0.769906	-0.104546	-0.461481
C	-1.663184	0.846606	0.196657
O	-2.059013	-0.518958	0.002364
H	0.215602	-0.732869	1.339395
H	0.583531	-1.733301	-0.081694
H	-0.670754	-0.061183	-1.541492
H	-1.474553	1.128875	1.226754
H	-2.206901	1.570555	-0.399129

Molecule# 0148

chlorotrifluoromethane

PointGroup: C3v

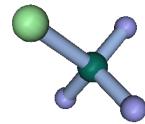
E= -798.006356459 au

ZPE= 0.014726 au

LUMO_eps= -0.02739 au

HOMO_eps= -0.36120 au

Dipole= 0.380 debye



5

C 0.000000 0.000000 -0.355296

Cl 0.000000 0.000000 1.420171

F 0.000000 1.248182 -0.815227

F 1.080957 -0.624091 -0.815227

F -1.080957 -0.624091 -0.815227

Molecule# 0149

cinnamaldehyde

PointGroup: Cs

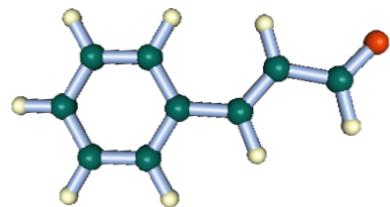
E= -423.135105750 au

ZPE= 0.142978 au

LUMO_eps= -0.09153 au

HOMO_eps= -0.25561 au

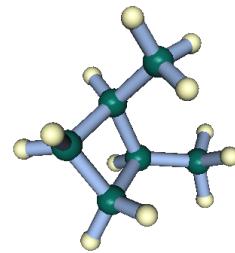
Dipole= 4.853 debye



18

C	-1.730590	-2.882390	0.000000
O	-1.562058	-4.083390	0.000000
C	-0.655985	-1.894403	0.000000
C	-0.933573	-0.580286	0.000000
C	0.000000	0.539524	0.000000
C	-0.511516	1.844139	0.000000
C	0.333448	2.945067	0.000000
C	1.710603	2.761404	0.000000
C	2.236083	1.470696	0.000000
C	1.393141	0.372360	0.000000
H	-2.755406	-2.457004	0.000000
H	0.353546	-2.285206	0.000000
H	-1.983825	-0.299778	0.000000
H	-1.584212	1.989985	0.000000
H	-0.081742	3.943603	0.000000
H	2.373203	3.616136	0.000000
H	3.307662	1.324322	0.000000
H	1.817575	-0.621621	0.000000

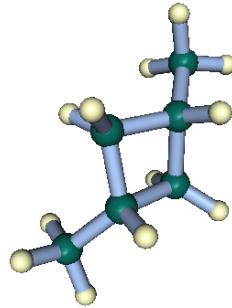
Molecule# 0150
 cis-1,2-dimethylcyclobutane
 PointGroup: C1
 E= -235.931460881 au
 ZPE= 0.166142 au
 LUMO_eps= -0.01081 au
 HOMO_eps= -0.28992 au
 Dipole= 0.163 debye



18

C	0.636065	0.415283	0.571630
C	-0.713037	-0.368475	0.430685
C	1.364965	-0.856683	0.052791
C	0.013200	-1.382989	-0.489869
C	0.802735	1.630562	-0.331113
C	-1.968744	0.323549	-0.068200
H	0.880376	0.697694	1.597241
H	-0.928293	-0.850203	1.387512
H	2.167047	-0.700311	-0.668994
H	-0.125626	-1.141655	-1.544800
H	1.747856	-1.473016	0.866030
H	-0.212001	-2.439705	-0.348512
H	0.603423	1.391862	-1.377604
H	-1.805638	0.816530	-1.027783
H	0.132470	2.442392	-0.042514
H	1.825302	2.008700	-0.271645
H	-2.318826	1.078652	0.639323
H	-2.777199	-0.398427	-0.203797

Molecule# 0151
 cis-1,3-dimethylcyclobutane
 PointGroup: C2v
 E= -235.934764879 au
 ZPE= 0.165861 au
 LUMO_eps= -0.00973 au
 HOMO_eps= -0.29179 au
 Dipole= 0.188 debye



18

C	-1.077960	0.000000	-0.148679
C	1.077960	0.000000	-0.148679
C	0.000000	1.086408	-0.403813
C	0.000000	-1.086408	-0.403813
C	0.000000	2.344796	0.443912
C	0.000000	-2.344796	0.443912
H	-1.394186	0.000000	0.897568
H	-1.966460	0.000000	-0.780419
H	1.394186	0.000000	0.897568
H	1.966460	0.000000	-0.780419
H	0.000000	1.356060	-1.462683
H	0.000000	-1.356060	-1.462683
H	0.000000	2.098731	1.508187
H	0.000000	-2.098731	1.508187
H	0.881667	2.958111	0.244413
H	-0.881667	2.958111	0.244413
H	-0.881667	-2.958111	0.244413
H	0.881667	-2.958111	0.244413

Molecule# 0152

cis-2,3,4-hexatriene

PointGroup: C2v

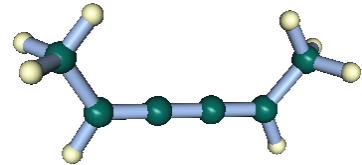
E= -233.460875403 au

ZPE= 0.116691 au

LUMO_eps= -0.04753 au

HOMO_eps= -0.22697 au

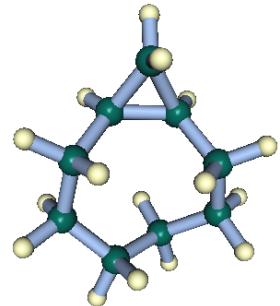
Dipole= 0.422 debye



14

H	0.000000	2.213829	1.634446
H	0.877402	3.463699	0.738497
H	-0.877402	3.463699	0.738497
H	0.000000	-2.213829	1.634446
H	0.877402	-3.463699	0.738497
H	-0.877402	-3.463699	0.738497
C	0.000000	2.811524	0.725249
C	0.000000	-2.811524	0.725249
H	0.000000	2.459711	-1.459498
H	0.000000	-2.459711	-1.459498
C	0.000000	-0.631593	-0.499294
C	0.000000	0.631593	-0.499294
C	0.000000	1.946711	-0.501278
C	0.000000	-1.946711	-0.501278

Molecule# 0153
 cis-bicyclo-6,1,0-nonane
 PointGroup: C1
 E= -352.696470296 au
 ZPE= 0.232561 au
 LUMO_eps= -0.00962 au
 HOMO_eps= -0.26783 au
 Dipole= 0.170 debye



25
 C 1.927322 0.636513 -0.258294
 C 1.743892 -0.637759 0.593827
 C 0.967529 1.802826 0.029936
 C 1.010427 -1.805008 -0.082822
 C -0.389151 -1.492307 -0.630603
 C -2.508959 -0.040026 -0.047710
 C -1.316135 0.696622 0.507138
 C -1.283474 -0.807165 0.375253
 C -0.501762 1.619138 -0.377467
 H 1.877073 0.382557 -1.322304
 H 2.940001 1.013596 -0.097779
 H 1.232847 -0.376497 1.523302
 H 2.727826 -1.006927 0.892208
 H 1.350022 2.683406 -0.493672
 H 1.017205 2.045069 1.097068
 H 0.931656 -2.621757 0.641307
 H 1.627908 -2.187488 -0.901162
 H -0.854124 -2.427139 -0.957440
 H -2.696494 0.053458 -1.110254
 H -1.427595 1.064908 1.521416
 H -0.986303 2.600318 -0.368695
 H -0.546416 1.282133 -1.416116
 H -3.404364 -0.117946 0.553456
 H -0.305848 -0.875995 -1.527448
 H -1.381530 -1.348693 1.310563

Molecule# 0154

crotonoic acid

PointGroup: C1

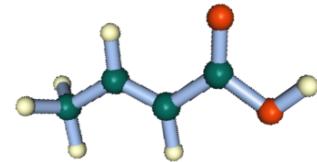
E= -306.614385096 au

ZPE= 0.095145 au

LUMO_eps= -0.05739 au

HOMO_eps= -0.28437 au

Dipole= 2.127 debye



12

C	-2.749597	-0.147991	0.000003
C	-1.333822	0.314316	0.000006
C	-0.264018	-0.479484	-0.000015
C	1.099386	0.081029	-0.000004
O	1.398388	1.251758	-0.000006
O	2.037208	-0.903645	0.000010
H	-2.827857	-1.234217	-0.000022
H	-3.278292	0.239886	0.874582
H	-3.278303	0.239927	-0.874551
H	-1.161440	1.385990	0.000028
H	-0.351243	-1.557948	-0.000032
H	2.900674	-0.465762	0.000017

Molecule# 0155

cubane

PointGroup: Oh

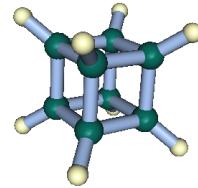
E= -309.560328341 au

ZPE= 0.133020 au

LUMO_eps= -0.00823 au

HOMO_eps= -0.26369 au

Dipole= 0.000 debye



16

C	0.783809	0.783809	0.783809
C	-0.783809	0.783809	0.783809
C	0.783809	0.783809	-0.783809
C	-0.783809	0.783809	-0.783809
C	0.783809	-0.783809	0.783809
C	-0.783809	-0.783809	0.783809
C	0.783809	-0.783809	-0.783809
C	-0.783809	-0.783809	-0.783809
H	1.410999	1.410999	1.410999
H	-1.410999	1.410999	1.410999
H	1.410999	1.410999	-1.410999
H	-1.410999	1.410999	-1.410999
H	1.410999	-1.410999	1.410999
H	-1.410999	-1.410999	1.410999
H	1.410999	-1.410999	-1.410999
H	-1.410999	-1.410999	-1.410999

Molecule# 0156

cyanamide

PointGroup: C1

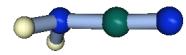
E= -148.848604164 au

ZPE= 0.033982 au

LUMO_eps= -0.03719 au

HOMO_eps= -0.28838 au

Dipole= 4.611 debye



5

N -1.375785 0.000002 0.012410

N 1.116606 0.000001 -0.079764

C -0.221237 -0.000004 -0.000219

H 1.570840 0.843614 0.236395

H 1.570840 -0.843611 0.236395

Molecule# 0157

cyanic acid

PointGroup: Cs

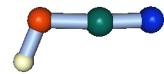
E= -168.709503108 au

ZPE= 0.021497 au

LUMO_eps= -0.05044 au

HOMO_eps= -0.32467 au

Dipole= 3.964 debye



4

N 0.042436 1.333654 0.000000

C 0.000000 0.181234 0.000000

O -0.128990 -1.109677 0.000000

H 0.734862 -1.545563 0.000000

Molecule# 0158

cyanic fluoride

PointGroup: C(infinity)v

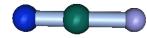
E= -192.713786764 au

ZPE= 0.010183 au

LUMO_eps= -0.03821 au

HOMO_eps= -0.36855 au

Dipole= 2.259 debye



3

C 0.000000 0.000000 -0.151984

F 0.000000 0.000000 1.114358

N 0.000000 0.000000 -1.302474

Molecule# 0159

cyanoacetyl isocyanate

PointGroup: C1

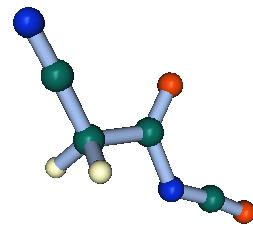
E= -413.721991744 au

ZPE= 0.059083 au

LUMO_eps= -0.08146 au

HOMO_eps= -0.32303 au

Dipole= 4.355 debye



10

O	-0.110702	1.322911	-0.000131
O	3.466618	0.112051	-0.000002
N	1.198390	-0.579867	0.000060
N	-3.543633	0.280825	-0.000038
C	-1.194850	-0.840419	0.000081
C	-0.022543	0.130129	-0.000013
C	-2.498057	-0.193546	0.000012
C	2.344250	-0.163499	0.000022
H	-1.101710	-1.491289	-0.872483
H	-1.101714	-1.491113	0.872777

Molecule# 0160

cyanogen

PointGroup: D(infinity)h

E= -185.724526963 au

ZPE= 0.016374 au

LUMO_eps= -0.10342 au

HOMO_eps= -0.38216 au

Dipole= 0.000 debye



4

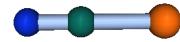
C 0.000000 0.000000 0.687813

C 0.000000 0.000000 -0.687813

N 0.000000 0.000000 1.839967

N 0.000000 0.000000 -1.839967

Molecule# 0161
cyanogen bromide
PointGroup: C(infinity)v
E= -2667.081539450 au
ZPE= 0.008212 au
LUMO_eps= -0.06135 au
HOMO_eps= -0.33248 au
Dipole= 3.295 debye



3
C 0.000000 0.000000 -1.140451
Br 0.000000 0.000000 0.654215
N 0.000000 0.000000 -2.293546

Molecule# 0162

cyanogen chloride

PointGroup: C(infinity)v

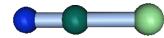
E= -553.085416766 au

ZPE= 0.008789 au

LUMO_eps= -0.03893 au

HOMO_eps= -0.34502 au

Dipole= 2.976 debye



3

Cl 0.000000 0.000000 0.978264

C 0.000000 0.000000 -0.658524

N 0.000000 0.000000 -1.811335

Molecule# 0163

cyclobutadiene

PointGroup: D2h

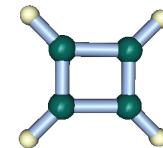
E= -154.736858884 au

ZPE= 0.061029 au

LUMO_eps= -0.06936 au

HOMO_eps= -0.19979 au

Dipole= 0.000 debye



8

C 0.000000 0.664652 0.787189

C 0.000000 0.664652 -0.787189

C 0.000000 -0.664652 0.787189

C 0.000000 -0.664652 -0.787189

H 0.000000 1.428618 1.548923

H 0.000000 1.428618 -1.548923

H 0.000000 -1.428618 1.548923

H 0.000000 -1.428618 -1.548923

Molecule# 0164

cyclobutane

PointGroup: D2d

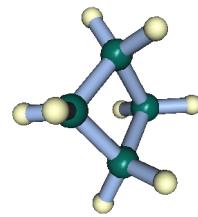
E= -157.272399200 au

ZPE= 0.110338 au

LUMO_eps= -0.00832 au

HOMO_eps= -0.30650 au

Dipole= 0.000 debye



12

C	0.000000	1.082580	0.123180
C	1.082580	0.000000	-0.123180
C	-1.082580	0.000000	-0.123180
C	0.000000	-1.082580	0.123180
H	0.000000	-1.957007	-0.526411
H	1.957007	0.000000	0.526411
H	-1.957007	0.000000	0.526411
H	0.000000	1.957007	-0.526411
H	0.000000	1.422103	1.159302
H	-1.422103	0.000000	-1.159302
H	1.422103	0.000000	-1.159302
H	0.000000	-1.422103	1.159302

Molecule# 0165

cyclobutanecarbonitrile

PointGroup: Cs

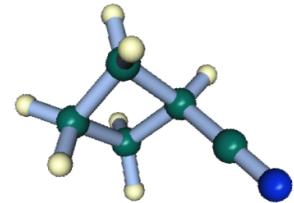
E= -249.546481767 au

ZPE= 0.109469 au

LUMO_eps= -0.02190 au

HOMO_eps= -0.31914 au

Dipole= 4.337 debye



13

H	1.757205	-0.189555	1.463765
H	0.080822	-0.525541	1.928692
C	0.759101	-0.406803	1.087809
H	-0.167443	-2.080157	0.000000
H	1.596662	-2.202628	0.000000
C	0.759101	-1.508440	0.000000
H	0.080822	-0.525541	-1.928692
H	1.757205	-0.189555	-1.463765
C	0.759101	-0.406803	-1.087809
H	0.914383	1.569711	0.000000
C	0.347469	0.639812	0.000000
N	-2.193925	1.206944	0.000000
C	-1.068470	0.964678	0.000000

Molecule# 0166

cyclobutanol

PointGroup: C1

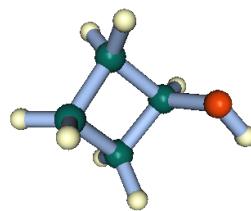
E= -232.521939619 au

ZPE= 0.114528 au

LUMO_eps= -0.01435 au

HOMO_eps= -0.27005 au

Dipole= 1.518 debye



13

H	-1.297824	0.008644	-1.543899
H	-2.422921	0.029181	-0.180212
C	-1.370643	0.014803	-0.458265
H	-0.900800	1.519610	1.097315
H	-0.113750	1.903984	-0.444735
C	-0.464979	1.093290	0.193316
H	0.987868	-0.008659	1.529152
C	0.579115	-0.009257	0.514978
H	-0.932014	-1.492737	1.105684
H	-0.141293	-1.892778	-0.431151
C	-0.487824	-1.078003	0.201469
H	2.214363	0.655067	-0.337686
O	1.634045	-0.105913	-0.437932

Molecule# 0167

cyclobutanone

PointGroup: Cs

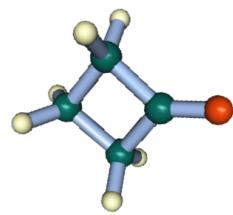
E= -231.318948732 au

ZPE= 0.090326 au

LUMO_eps= -0.03786 au

HOMO_eps= -0.25652 au

Dipole= 3.065 debye



11

H	-0.839567	-2.094249	0.000000
H	0.927182	-2.122428	0.000000
C	0.054138	-1.475036	0.000000
O	-0.153392	1.866794	0.000000
C	-0.034224	0.676084	0.000000
H	0.974306	-0.304588	1.688889
H	0.974306	-0.304588	-1.688889
H	-0.789114	-0.376716	1.798667
H	-0.789114	-0.376716	-1.798667
C	0.054138	-0.380113	1.107874
C	0.054138	-0.380113	-1.107874

Molecule# 0168

cyclobutene

PointGroup: C2v

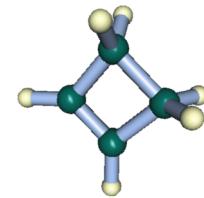
E= -156.032912020 au

ZPE= 0.086133 au

LUMO_eps= -0.00640 au

HOMO_eps= -0.25582 au

Dipole= 0.159 debye



10

C	0.000000	0.667446	0.812417
C	0.000000	-0.667446	0.812417
C	0.000000	0.784886	-0.698476
C	0.000000	-0.784886	-0.698476
H	0.000000	1.411038	1.598258
H	0.000000	-1.411038	1.598258
H	0.886543	1.242452	-1.140953
H	-0.886543	-1.242452	-1.140953
H	-0.886543	1.242452	-1.140953
H	0.886543	-1.242452	-1.140953

Molecule# 0169

cyclobutylamine

PointGroup: Cs

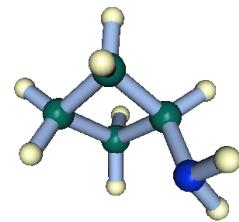
E= -212.645823108 au

ZPE= 0.127511 au

LUMO_eps= -0.01345 au

HOMO_eps= -0.24139 au

Dipole= 1.174 debye



14

N	-1.392026	0.964971	0.000000
H	-1.686104	1.489839	0.815536
H	-1.686104	1.489839	-0.815536
C	0.483446	-0.254439	-1.082525
H	-0.198668	-0.373542	-1.923807
H	1.483527	-0.047564	-1.463346
C	0.483446	-0.254439	1.082525
H	-0.198668	-0.373542	1.923807
H	1.483527	-0.047564	1.463346
C	0.057064	0.770920	0.000000
H	0.619951	1.711232	0.000000
C	0.483446	-1.364057	0.000000
H	1.324266	-2.055871	0.000000
H	-0.441946	-1.935530	0.000000

Molecule# 0170

cycloheptane

PointGroup: C2

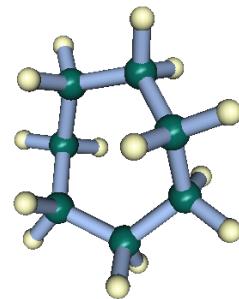
E= -275.284228349 au

ZPE= 0.198204 au

LUMO_eps= -0.01154 au

HOMO_eps= -0.30372 au

Dipole= 0.012 debye



21

C	0.000000	0.000000	1.772157
C	0.703601	1.107660	0.968327
C	-0.703601	-1.107660	0.968327
C	0.000000	1.576287	-0.314065
C	0.000000	-1.576287	-0.314065
C	0.302469	0.703389	-1.539522
C	-0.302469	-0.703389	-1.539522
H	-0.742021	0.456246	2.433052
H	0.742021	-0.456246	2.433052
H	1.710243	0.776893	0.696626
H	-1.710243	-0.776893	0.696626
H	0.847619	1.961484	1.634661
H	-0.847619	-1.961484	1.634661
H	0.331829	2.593009	-0.538454
H	-0.331829	-2.593009	-0.538454
H	-1.081166	1.642958	-0.154172
H	1.081166	-1.642958	-0.154172
H	1.390576	0.624307	-1.637984
H	-1.390576	-0.624307	-1.637984
H	-0.042785	1.221357	-2.438645
H	0.042785	-1.221357	-2.438645

Molecule# 0171

cycloheptanol

PointGroup: C1

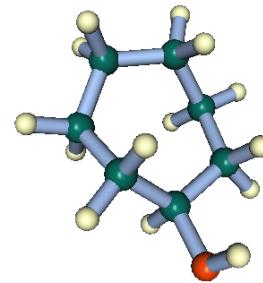
E= -350.534179325 au

ZPE= 0.202603 au

LUMO_eps= -0.01357 au

HOMO_eps= -0.27271 au

Dipole= 1.833 debye



22

C	1.737280	0.792495	-0.479503
C	2.019870	-0.672323	-0.100223
C	0.725512	1.538451	0.401741
C	0.827926	-1.495424	0.414755
C	-0.739200	1.302862	0.010037
C	-0.519506	-1.262644	-0.283540
C	-1.315360	-0.085645	0.291439
O	-2.684418	-0.139555	-0.132940
H	2.688253	1.329635	-0.472454
H	1.383423	0.840676	-1.513335
H	2.448382	-1.170470	-0.973960
H	2.799085	-0.698261	0.666057
H	0.880078	1.290425	1.456387
H	0.917245	2.610333	0.318106
H	1.092130	-2.551954	0.338093
H	0.690935	-1.308620	1.483722
H	-1.377340	2.026147	0.521809
H	-0.844172	1.505605	-1.063458
H	-0.381135	-1.129922	-1.362564
H	-1.146124	-2.147322	-0.159163
H	-1.374227	-0.226165	1.374425
H	-2.720326	0.039705	-1.078385

Molecule# 0172

cycloheptatriene

PointGroup: Cs

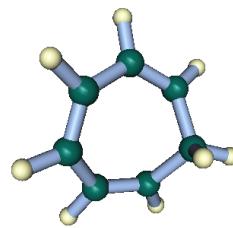
E= -271.612174001 au

ZPE= 0.127711 au

LUMO_eps= -0.04665 au

HOMO_eps= -0.22721 au

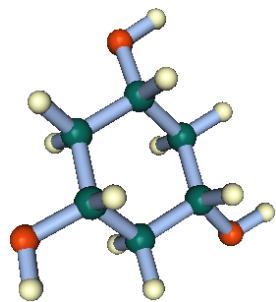
Dipole= 0.330 debye



15

C	-0.252782	-1.416887	0.679421
C	-0.252782	-1.416887	-0.679421
C	0.246301	-0.359998	1.524391
C	0.246301	-0.359998	-1.524391
C	0.246301	0.949673	1.219657
C	0.246301	0.949673	-1.219657
C	-0.452117	1.486050	0.000000
H	-0.530553	-2.340484	1.174711
H	-0.530553	-2.340484	-1.174711
H	0.673266	-0.666831	2.473189
H	0.673266	-0.666831	-2.473189
H	0.749061	1.649053	1.876836
H	0.749061	1.649053	-1.876836
H	-1.495770	1.152463	0.000000
H	-0.452905	2.574307	0.000000

Molecule# 0173
 cyclohexane-1,3,5-triol
 PointGroup: C1
 E= -461.714583349 au
 ZPE= 0.182086 au
 LUMO_eps= -0.02324 au
 HOMO_eps= -0.27583 au
 Dipole= 3.361 debye



21

C	-1.366891	0.474228	-0.146969
C	0.275353	-1.434457	-0.131432
C	1.099759	0.948113	-0.139858
C	-1.098479	-0.958309	0.321858
C	-0.269625	1.432558	0.319250
C	1.373754	-0.482882	0.325882
O	-2.056536	-1.879394	-0.204100
O	-0.446869	2.750757	-0.204758
O	2.605127	-0.984857	-0.196602
H	-1.412028	0.488864	-1.238475
H	-2.339459	0.812617	0.226852
H	0.466279	-2.436160	0.253202
H	0.288581	-1.495060	-1.222313
H	1.141058	0.982010	-1.231171
H	1.867909	1.627151	0.238193
H	-1.139106	-0.987591	1.419260
H	-0.278931	1.479268	1.416737
H	1.418949	-0.497589	1.423644
H	-2.934028	-1.628557	0.100071
H	-1.297930	3.093159	0.085131
H	3.321704	-0.405651	0.080163

Molecule# 0174

cyclohexane-1,4-dione

PointGroup: C2h

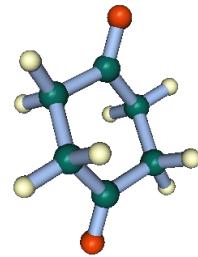
E= -384.047408232 au

ZPE= 0.130964 au

LUMO_eps= -0.05295 au

HOMO_eps= -0.26634 au

Dipole= 0.000 debye



16

C	-0.061344	1.463150	0.000000
C	0.061344	-1.463150	0.000000
C	-0.332830	0.695697	1.281972
C	-0.332830	0.695697	-1.281972
C	0.332830	-0.695697	1.281972
C	0.332830	-0.695697	-1.281972
O	0.332830	2.606139	0.000000
O	-0.332830	-2.606139	0.000000
H	-0.003435	1.294970	2.128181
H	-1.417638	0.571706	1.364952
H	-1.417638	0.571706	-1.364952
H	-0.003435	1.294970	-2.128181
H	0.003435	-1.294970	2.128181
H	1.417638	-0.571706	1.364952
H	1.417638	-0.571706	-1.364952
H	0.003435	-1.294970	-2.128181

Molecule# 0175

cyclohexane

PointGroup: S6

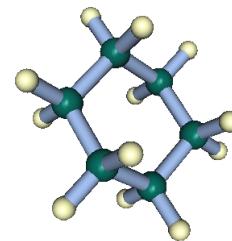
E= -235.966846189 au

ZPE= 0.169447 au

LUMO_eps= -0.01035 au

HOMO_eps= -0.29876 au

Dipole= 0.000 debye



18

C -1.267259 0.731652 0.227515

C 0.000000 1.463304 -0.227515

C -1.267259 -0.731652 -0.227515

C 0.000000 -1.463304 0.227515

C 1.267259 -0.731652 -0.227515

C 1.267259 0.731652 0.227515

H 2.155238 1.244327 -0.149267

H -2.155238 1.244327 -0.149267

H 0.000000 2.488655 0.149267

H 2.155238 -1.244327 0.149267

H 1.329045 -0.767324 -1.320511

H -1.329045 -0.767324 -1.320511

H 0.000000 1.534649 -1.320511

H 0.000000 -2.488655 -0.149267

H 0.000000 -1.534649 1.320511

H -2.155238 -1.244327 0.149267

H -1.329045 0.767324 1.320511

H 1.329045 0.767324 1.320511

Molecule# 0176

cyclohexanol

PointGroup: C1

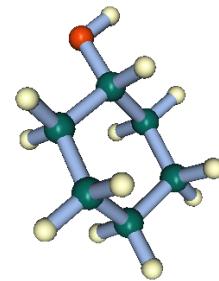
E= -311.217402044 au

ZPE= 0.173852 au

LUMO_eps= -0.01346 au

HOMO_eps= -0.27404 au

Dipole= 1.670 debye



19

C	1.868671	0.015665	-0.274924
C	1.165857	-1.254608	0.213738
C	1.143210	1.275650	0.207070
C	-0.316921	-1.266074	-0.173397
C	-0.338799	1.251562	-0.185476
C	-1.031529	-0.014315	0.318188
O	-2.389229	-0.097381	-0.127585
H	2.907050	0.026674	0.063303
H	1.897315	0.013456	-1.369367
H	1.659644	-2.140622	-0.189833
H	1.257836	-1.320104	1.302922
H	1.229487	1.346791	1.296330
H	1.621046	2.169628	-0.198474
H	-0.419613	-1.310640	-1.261741
H	-0.817792	-2.148289	0.228615
H	-0.850240	2.135483	0.207891
H	-0.437987	1.283978	-1.274557
H	-1.013629	-0.011453	1.417302
H	-2.862212	0.686872	0.167083

Molecule# 0177

cyclohexanone

PointGroup: Cs

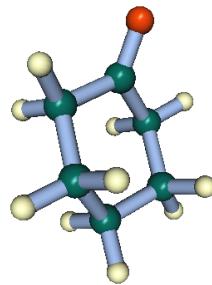
E= -310.009228824 au

ZPE= 0.150340 au

LUMO_eps= -0.03267 au

HOMO_eps= -0.24794 au

Dipole= 3.416 debye



17

C	-0.407739	1.083702	0.000000
C	0.155829	0.499472	1.282325
C	0.155829	0.499472	-1.282325
C	0.155829	-1.039311	1.263183
C	0.155829	-1.039311	-1.263183
C	0.820538	-1.590283	0.000000
O	-1.249483	1.954490	0.000000
H	1.188471	0.854961	1.375218
H	-0.408079	0.898882	2.123656
H	-0.408079	0.898882	-2.123656
H	1.188471	0.854961	-1.375218
H	0.657166	-1.415176	2.156695
H	-0.876952	-1.396180	1.313350
H	-0.876952	-1.396180	-1.313350
H	0.657166	-1.415176	-2.156695
H	1.882221	-1.322209	0.000000
H	0.775740	-2.681122	0.000000

Molecule# 0178

cyclohexene

PointGroup: C2

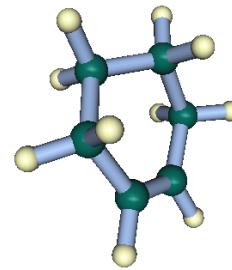
E= -234.735932677 au

ZPE= 0.145798 au

LUMO_eps= -0.01232 au

HOMO_eps= -0.24492 au

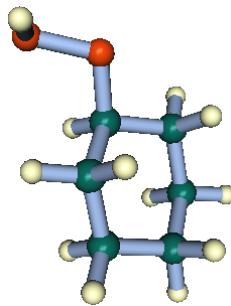
Dipole= 0.368 debye



16

C	0.005646	0.665273	1.302124
C	-0.005646	-0.665273	1.302124
C	-0.005646	1.497566	0.048624
C	0.005646	-1.497566	0.048624
C	-0.367769	0.670959	-1.190000
C	0.367769	-0.670959	-1.190000
H	0.020501	1.196537	2.247558
H	-0.020501	-1.196537	2.247558
H	-0.708445	2.326979	0.166811
H	0.977019	1.965639	-0.085347
H	0.708445	-2.326979	0.166811
H	-0.977019	-1.965639	-0.085347
H	-1.446378	0.487192	-1.195721
H	-0.141259	1.233380	-2.097788
H	1.446378	-0.487192	-1.195721
H	0.141259	-1.233380	-2.097788

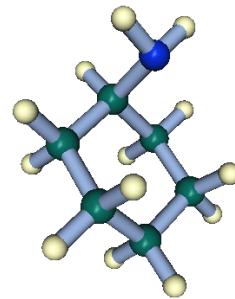
Molecule# 0179
 cyclohexyl hydroperoxide
 PointGroup: C1
 E= -386.378385545 au
 ZPE= 0.177087 au
 LUMO_eps= -0.01627 au
 HOMO_eps= -0.26509 au
 Dipole= 1.976 debye



20

C	2.273854	0.274215	-0.203952
C	1.762908	-1.084479	0.283467
C	0.328202	-1.357217	-0.186256
C	-0.603815	-0.222061	0.229009
C	-0.109581	1.129030	-0.279562
C	1.321941	1.404284	0.197425
O	-1.885928	-0.581152	-0.300631
O	-2.882481	0.292841	0.300204
H	3.273677	0.463179	0.192478
H	2.369370	0.253715	-1.294443
H	1.795630	-1.111497	1.377231
H	2.418338	-1.885041	-0.064459
H	-0.041640	-2.299048	0.220652
H	0.306159	-1.447044	-1.276226
H	-0.688027	-0.199332	1.321058
H	-0.139153	1.116756	-1.373872
H	-0.781503	1.918852	0.057557
H	1.326109	1.510541	1.287156
H	1.670130	2.357427	-0.205005
H	-3.202874	0.765346	-0.479497

Molecule# 0180
 cyclohexylamine
 PointGroup: Cs
 E= -291.338064686 au
 ZPE= 0.186679 au
 LUMO_eps= -0.01597 au
 HOMO_eps= -0.24021 au
 Dipole= 1.097 debye



20

C	-0.974235	1.501801	0.000000
C	-0.313710	0.943702	1.264192
C	-0.313710	0.943702	-1.264192
C	-0.313710	-0.588507	1.262787
C	-0.313710	-0.588507	-1.262787
C	0.322144	-1.187508	0.000000
N	1.768888	-0.919814	0.000000
H	-2.037859	1.237524	0.000000
H	-0.926534	2.593057	0.000000
H	0.714983	1.305090	1.322149
H	-0.829805	1.310092	2.154594
H	-0.829805	1.310092	-2.154594
H	0.714983	1.305090	-1.322149
H	0.204080	-0.970114	2.147778
H	-1.343580	-0.952418	1.329721
H	-1.343580	-0.952418	-1.329721
H	0.204080	-0.970114	-2.147778
H	0.112103	-2.266434	0.000000
H	2.210148	-1.329430	-0.814645
H	2.210148	-1.329430	0.814645

Molecule# 0181

cyclooctane

PointGroup: Cs

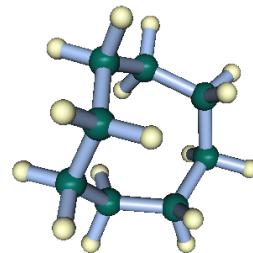
E= -314.605282735 au

ZPE= 0.227392 au

LUMO_eps= -0.01147 au

HOMO_eps= -0.29104 au

Dipole= 0.043 debye



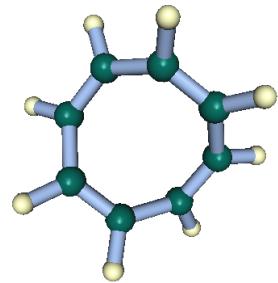
24

C	-0.924984	1.455665	0.000000
C	-0.134405	1.385461	1.310207
C	-0.134405	1.385461	-1.310207
C	0.629237	0.082662	1.610338
C	0.629237	0.082662	-1.610338
C	-0.134405	-1.227318	1.323869
C	-0.134405	-1.227318	-1.323869
C	0.207639	-1.929091	0.000000
H	-1.479369	2.398329	0.000000
H	0.570283	2.221967	1.352098
H	0.570283	2.221967	-1.352098
H	-0.845053	1.554786	2.124992
H	-0.845053	1.554786	-2.124992
H	-1.689785	0.675570	0.000000
H	0.902756	0.108766	2.667617
H	0.902756	0.108766	-2.667617
H	1.576536	0.069346	1.069122
H	1.576536	0.069346	-1.069122
H	-1.212799	-1.052435	1.383389
H	-1.212799	-1.052435	-1.383389
H	0.088126	-1.939415	2.121981
H	0.088126	-1.939415	-2.121981
H	1.281288	-2.147303	0.000000
H	-0.292875	-2.901727	0.000000

Molecule# 0182
cyclooctatetraene

PointGroup: D2d

E= -309.700993693 au
ZPE= 0.132416 au
LUMO_eps= -0.06151 au
HOMO_eps= -0.21894 au
Dipole= 0.000 debye



16

C	0.667787	1.563913	0.371103
C	-0.667787	1.563913	0.371103
C	0.667787	-1.563913	0.371103
C	-0.667787	-1.563913	0.371103
C	1.563913	0.667787	-0.371103
C	-1.563913	0.667787	-0.371103
C	1.563913	-0.667787	-0.371103
C	-1.563913	-0.667787	-0.371103
H	1.166556	2.358559	0.918777
H	-1.166556	2.358559	0.918777
H	1.166556	-2.358559	0.918777
H	-1.166556	-2.358559	0.918777
H	2.358559	1.166556	-0.918777
H	-2.358559	1.166556	-0.918777
H	2.358559	-1.166556	-0.918777
H	-2.358559	-1.166556	-0.918777

Molecule# 0183

cyclopentanamine

PointGroup: Cs

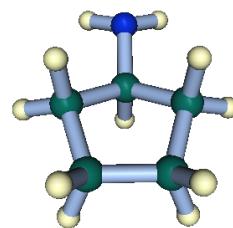
E= -252.003226490 au

ZPE= 0.157255 au

LUMO_eps= -0.01409 au

HOMO_eps= -0.24379 au

Dipole= 1.203 debye



17

N	0.137512	2.151652	0.000000
C	0.448122	0.721591	0.000000
H	1.532762	0.530144	0.000000
H	0.533560	2.608259	0.813100
H	0.533560	2.608259	-0.813100
C	-0.167084	-1.496898	0.778524
C	-0.167084	-1.496898	-0.778524
C	-0.167084	-0.013012	-1.194728
C	-0.167084	-0.013012	1.194728
H	-1.025406	-2.027487	-1.189237
H	-1.025406	-2.027487	1.189237
H	0.721946	-2.002668	1.157019
H	0.721946	-2.002668	-1.157019
H	-1.187175	0.355253	-1.326931
H	-1.187175	0.355253	1.326931
H	0.370046	0.165478	-2.127734
H	0.370046	0.165478	2.127734

Molecule# 0184

cyclopentane

PointGroup: C1

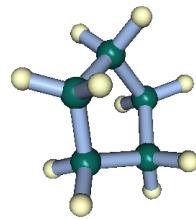
E= -196.630420411 au

ZPE= 0.140058 au

LUMO_eps= -0.01123 au

HOMO_eps= -0.31477 au

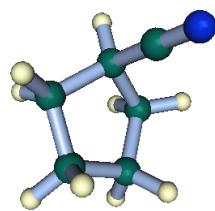
Dipole= 0.023 debye



15

C	-1.186192	0.423794	-0.243636
C	-0.796090	-0.975769	0.244802
C	0.027367	1.287285	0.136896
C	0.687806	-1.087600	-0.139625
C	1.257252	0.349375	0.001362
H	-2.118589	0.788232	0.188807
H	1.226616	-1.811506	0.471854
H	-1.407585	-1.769785	-0.185074
H	0.115243	2.182391	-0.478872
H	-1.314699	0.411348	-1.329698
H	1.864002	0.612109	-0.865357
H	1.906597	0.434583	0.872795
H	-0.909311	-1.030087	1.331284
H	-0.074596	1.623613	1.170697
H	0.771463	-1.423403	-1.175226

Molecule# 0185
 cyclopentanecarbonitrile
 PointGroup: C1
 E= -288.903576706 au
 ZPE= 0.139224 au
 LUMO_eps= -0.02324 au
 HOMO_eps= -0.32219 au
 Dipole= 4.247 debye



16

C	1.602438	0.009053	-0.031364
C	-1.371859	0.746330	-0.653168
C	-1.307418	-0.806205	-0.645590
C	-0.501396	1.220231	0.531175
C	-0.485334	-1.190374	0.598276
C	0.432357	0.028014	0.847230
N	2.515785	-0.006019	-0.731269
H	-0.984080	1.137519	-1.592694
H	-2.392524	1.113594	-0.555555
H	-2.295941	-1.262646	-0.625195
H	-0.810388	-1.165675	-1.546124
H	0.045306	2.137508	0.322211
H	-1.117683	1.398437	1.413455
H	-1.132932	-1.299095	1.469966
H	0.067826	-2.119975	0.478891
H	0.797203	0.060175	1.874581

Molecule# 0186

cyclopentanethiol

PointGroup: C1

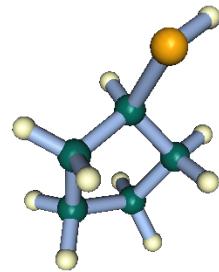
E= -594.853910396 au

ZPE= 0.139559 au

LUMO_eps= -0.01797 au

HOMO_eps= -0.23914 au

Dipole= 1.827 debye



16

H	-2.590075	1.232318	-0.681766
H	-2.238693	1.101270	1.028530
C	-1.912106	0.776892	0.039228
H	-2.427878	-1.128437	-0.935303
H	-2.435411	-1.206457	0.811001
C	-1.913085	-0.775183	-0.042566
H	-0.116781	-1.457884	-1.078076
H	-0.224491	-2.076259	0.562195
C	-0.425486	-1.206167	-0.060963
H	-0.202025	2.158408	0.251061
H	-0.233592	1.261134	-1.263701
C	-0.451026	1.195668	-0.195623
H	0.319079	0.094769	1.494721
C	0.345505	0.036292	0.405726
H	2.525374	1.067170	0.480115
S	2.110105	-0.075690	-0.096475

Molecule# 0187

cyclopentanol

PointGroup: C1

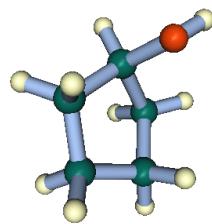
E= -271.880484872 au

ZPE= 0.144571 au

LUMO_eps= -0.01556 au

HOMO_eps= -0.27594 au

Dipole= 1.510 debye



16

C	1.478824	0.602081	-0.167602
C	1.131874	-0.871035	-0.441609
C	0.138007	1.266828	0.236745
C	-0.007005	-1.147497	0.545787
C	-0.865878	0.122768	0.481642
O	-1.764277	0.100355	-0.639892
H	2.191316	0.663706	0.657603
H	1.942541	1.089472	-1.024485
H	0.768396	-0.991211	-1.463462
H	1.983364	-1.539018	-0.312244
H	0.250934	1.884221	1.127542
H	-0.256769	1.906427	-0.551166
H	-0.583006	-2.047024	0.320771
H	0.393171	-1.259290	1.558075
H	-1.443380	0.274160	1.398057
H	-2.387285	-0.623160	-0.521332

Molecule# 0188

cyclopentanone

PointGroup: C2

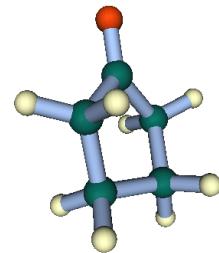
E= -270.677266613 au

ZPE= 0.120786 au

LUMO_eps= -0.03163 au

HOMO_eps= -0.25000 au

Dipole= 3.242 debye



14

C	0.000000	0.771638	-1.378323
H	-0.624422	1.190682	-2.165746
H	1.015837	1.139927	-1.539367
C	0.000000	-0.771638	-1.378323
H	0.624422	-1.190682	-2.165746
H	-1.015837	-1.139927	-1.539367
C	0.473205	-1.145341	0.031186
H	1.566143	-1.166083	0.089614
H	0.115834	-2.102523	0.407428
C	-0.473205	1.145341	0.031186
H	-0.115834	2.102523	0.407428
H	-1.566143	1.166083	0.089614
C	0.000000	0.000000	0.924314
O	0.000000	0.000000	2.129486

Molecule# 0189

cyclopentene

PointGroup: Cs

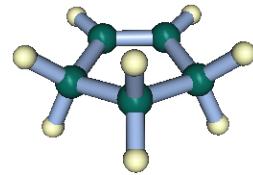
E= -195.401185459 au

ZPE= 0.116317 au

LUMO_eps= -0.01011 au

HOMO_eps= -0.24432 au

Dipole= 0.245 debye



13

C	-0.063692	1.072090	0.664505
C	-0.063692	1.072090	-0.664505
C	-0.063692	-0.324395	1.233989
C	-0.063692	-0.324395	-1.233989
C	0.247090	-1.207905	0.000000
H	-0.098837	1.958513	1.283789
H	-0.098837	1.958513	-1.283789
H	0.667358	-0.455946	2.034338
H	-1.041041	-0.560191	1.669221
H	-1.041041	-0.560191	-1.669221
H	0.667358	-0.455946	-2.034338
H	1.305988	-1.468869	0.000000
H	-0.314874	-2.140795	0.000000

Molecule# 0190

cyclopropane

PointGroup: D3h

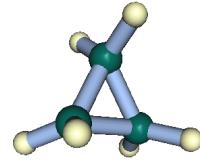
E= -117.943473498 au

ZPE= 0.081038 au

LUMO_eps= -0.00518 au

HOMO_eps= -0.29913 au

Dipole= 0.000 debye



9

C	0.000000	0.868264	0.000000
C	-0.751939	-0.434132	0.000000
C	0.751939	-0.434132	0.000000
H	1.260331	-0.727653	0.907443
H	0.000000	1.455305	0.907443
H	1.260331	-0.727653	-0.907443
H	-1.260331	-0.727653	0.907443
H	-1.260331	-0.727653	-0.907443
H	0.000000	1.455305	-0.907443

Molecule# 0191

cyclopropanecarbonitrile

PointGroup: Cs

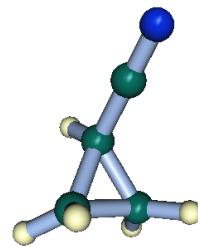
E= -210.218209450 au

ZPE= 0.080268 au

LUMO_eps= -0.02060 au

HOMO_eps= -0.30559 au

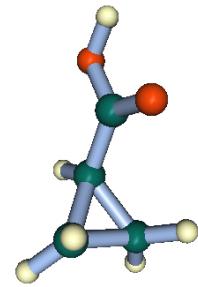
Dipole= 4.415 debye



10

H	0.336332	2.019953	1.266776
H	0.336332	2.019953	-1.266776
H	-1.118471	0.924048	-1.256429
H	-1.118471	0.924048	1.256429
H	1.651115	0.325415	0.000000
C	0.575980	0.213094	0.000000
N	-0.228299	-2.244511	0.000000
C	0.132495	-1.150808	0.000000
C	-0.228299	1.260370	0.746697
C	-0.228299	1.260370	-0.746697

Molecule# 0192
 cyclopropanecarboxylic acid
 PointGroup: Cs
 E= -306.598901283 au
 ZPE= 0.096642 au
 LUMO_eps= -0.01204 au
 HOMO_eps= -0.29072 au
 Dipole= 1.748 debye



12

C	-0.270459	-0.778426	0.000000
C	0.336510	1.596630	0.743093
C	0.336510	1.596630	-0.743093
C	0.710072	0.327080	0.000000
O	-1.472192	-0.658476	0.000000
O	0.336510	-1.992090	0.000000
H	1.135578	2.100682	1.266594
H	-0.620002	1.590351	1.244203
H	-0.620002	1.590351	-1.244203
H	1.135578	2.100682	-1.266594
H	1.746444	0.027754	0.000000
H	-0.367938	-2.656783	0.000000

Molecule# 0193

cyclopropanone

PointGroup: C2v

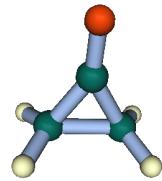
E= -191.958661218 au

ZPE= 0.060588 au

LUMO_eps= -0.04813 au

HOMO_eps= -0.25066 au

Dipole= 3.031 debye



8

C	0.000000	0.000000	0.381094
O	0.000000	0.000000	1.576449
C	0.000000	0.785897	-0.855963
C	0.000000	-0.785897	-0.855963
H	0.911746	1.287106	-1.156649
H	-0.911746	1.287106	-1.156649
H	-0.911746	-1.287106	-1.156649
H	0.911746	-1.287106	-1.156649

Molecule# 0194

cyclopropene

PointGroup: C2v

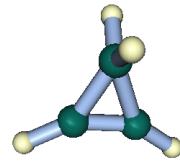
E= -116.666665302 au

ZPE= 0.055806 au

LUMO_eps= -0.01090 au

HOMO_eps= -0.25964 au

Dipole= 0.477 debye



7

C 0.000000 0.000000 0.861410

C 0.000000 0.643280 -0.499979

C 0.000000 -0.643280 -0.499979

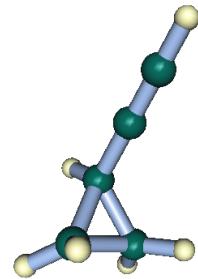
H 0.000000 1.571117 -1.041246

H 0.000000 -1.571117 -1.041246

H 0.910708 0.000000 1.456887

H -0.910708 0.000000 1.456887

Molecule# 0195
cyclopropylacetylene
PointGroup: Cs
E= -194.114861043 au
ZPE= 0.090494 au
LUMO_eps= -0.01007 au
HOMO_eps= -0.25678 au
Dipole= 1.007 debye



11

C	0.611276	0.150433	0.000000
C	-0.558771	0.979132	0.000000
H	1.547692	0.693190	0.000000
C	0.611276	-1.169532	0.748025
C	0.611276	-1.169532	-0.748025
C	-1.538704	1.673681	0.000000
H	-2.403449	2.288355	0.000000
H	1.520070	-1.440716	1.265675
H	-0.301248	-1.442601	1.256473
H	1.520070	-1.440716	-1.265675
H	-0.301248	-1.442601	-1.256473

Molecule# 0196

cyclopropylamine

PointGroup: Cs

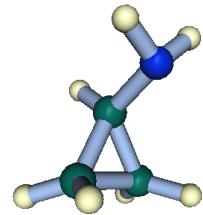
E= -173.317474428 au

ZPE= 0.098373 au

LUMO_eps= -0.01143 au

HOMO_eps= -0.24674 au

Dipole= 1.216 debye



11

C	-0.320050	0.416085	0.000000
H	-1.260116	0.962973	0.000000
N	0.903346	1.179214	0.000000
C	-0.320050	-0.882833	0.753840
C	-0.320050	-0.882833	-0.753840
H	0.970739	1.771825	0.818204
H	0.970739	1.771825	-0.818204
H	-1.223024	-1.176047	1.270152
H	-1.223024	-1.176047	-1.270152
H	0.601086	-1.155773	1.247962
H	0.601086	-1.155773	-1.247962

Molecule# 0197

cysteine

PointGroup: C1

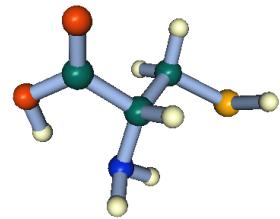
E= -722.106607503 au

ZPE= 0.108084 au

LUMO_eps= -0.03168 au

HOMO_eps= -0.26831 au

Dipole= 4.036 debye



14

N	0.132502	1.611883	0.297686
C	0.232379	0.161878	0.470580
C	1.642693	-0.320889	0.078786
O	2.061362	-1.407821	0.371619
O	2.340267	0.562288	-0.647593
H	1.773757	1.361340	-0.710982
C	-0.766023	-0.575233	-0.432100
S	-2.526785	-0.165977	-0.120311
H	0.072670	-0.163602	1.501691
H	-0.615582	-1.646562	-0.340585
H	-0.604235	-0.298474	-1.474310
H	-2.603154	-0.697517	1.114290
H	-0.830276	1.882258	0.128698
H	0.440533	2.104739	1.126558

Molecule# 0198

cytosine

PointGroup: C1

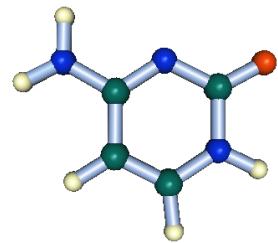
E= -395.091655091 au

ZPE= 0.098004 au

LUMO_eps= -0.04851 au

HOMO_eps= -0.24359 au

Dipole= 6.604 debye



13

N	-1.278679	0.891680	0.000794
C	-1.183279	-0.527836	-0.000005
O	-2.212368	-1.174968	0.000543
N	0.081477	-1.045063	0.000860
C	1.129520	-0.251037	-0.001356
N	2.350160	-0.839822	-0.016923
C	1.044869	1.182278	-0.000701
C	-0.202442	1.706311	0.000829
H	-2.216305	1.259538	0.001831
H	2.393103	-1.842117	0.040782
H	3.193278	-0.305790	0.070447
H	1.919772	1.812089	-0.004556
H	-0.393620	2.770157	0.001442

Molecule# 0199

decan-2-one

PointGroup: C1

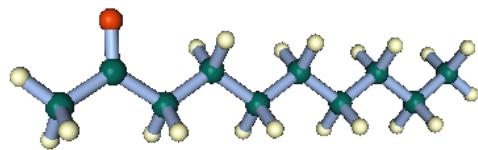
E= -468.532664261 au

ZPE= 0.281942 au

LUMO_eps= -0.02475 au

HOMO_eps= -0.25466 au

Dipole= 2.870 debye



31

C	-4.175993	0.207367	-0.005507
C	-5.448491	-0.614286	0.019396
C	6.054156	0.386362	0.006408
C	-2.871799	-0.571984	-0.012818
C	4.792505	-0.475092	-0.009332
C	-1.613136	0.286980	0.008336
C	3.501105	0.343620	0.008693
C	-0.327445	-0.540456	-0.008111
C	2.232016	-0.508852	-0.007095
C	0.941983	0.311836	0.009646
O	-4.204668	1.417596	-0.016635
H	-5.462714	-1.326538	-0.807857
H	-5.497683	-1.198360	0.941164
H	-6.314776	0.039007	-0.041572
H	6.089348	1.049308	-0.860580
H	6.956755	-0.226164	-0.008139
H	6.092680	1.012377	0.900299
H	-2.890569	-1.259757	0.840286
H	-2.883947	-1.221971	-0.895528
H	4.801833	-1.150837	0.851256
H	4.799527	-1.115634	-0.896480
H	-1.631210	0.927231	0.893082
H	-1.629208	0.965732	-0.846946
H	3.492536	1.020304	-0.852403
H	3.494509	0.985345	0.896184
H	-0.318063	-1.217877	0.852696
H	-0.317710	-1.181637	-0.896260
H	2.240008	-1.150711	-0.894489
H	2.241093	-1.184885	0.854517
H	0.932828	0.988464	-0.851005
H	0.932699	0.952874	0.897157

Molecule# 0200

decane

PointGroup: C2h

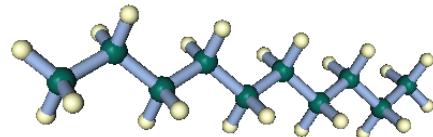
E= -394.489355879 au

ZPE= 0.301434 au

LUMO_eps= -0.01022 au

HOMO_eps= -0.29912 au

Dipole= 0.000 debye



32

C	2.789368	5.050688	0.000000
C	-2.789368	-5.050688	0.000000
C	2.800552	3.522861	0.000000
C	-2.800552	-3.522861	0.000000
C	1.400494	2.907631	0.000000
C	-1.400494	-2.907631	0.000000
C	1.400494	1.378640	0.000000
C	-1.400494	-1.378640	0.000000
C	-0.000057	0.764608	0.000000
C	0.000057	-0.764608	0.000000
H	3.801408	5.458123	0.000000
H	2.275152	5.441067	0.880579
H	2.275152	5.441067	-0.880579
H	-3.801408	-5.458123	0.000000
H	-2.275152	-5.441067	-0.880579
H	-2.275152	-5.441067	0.880579
H	3.351669	3.162311	0.873843
H	3.351669	3.162311	-0.873843
H	-3.351669	-3.162311	0.873843
H	-3.351669	-3.162311	-0.873843
H	0.848853	3.269313	-0.874391
H	0.848853	3.269313	0.874391
H	-0.848853	-3.269313	-0.874391
H	-0.848853	-3.269313	0.874391
H	1.952511	1.017990	0.874412
H	1.952511	1.017990	-0.874412
H	-1.952511	-1.017990	0.874412
H	-1.952511	-1.017990	-0.874412
H	-0.551998	1.125266	-0.874385
H	-0.551998	1.125266	0.874385
H	0.551998	-1.125266	0.874385
H	0.551998	-1.125266	-0.874385

Molecule# 0201

di-2-chloroethylether

PointGroup: Cs

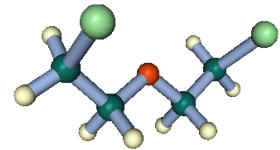
E= -1153.018117930 au

ZPE= 0.118946 au

LUMO_eps= -0.01950 au

HOMO_eps= -0.28328 au

Dipole= 4.516 debye



15

C	0.595129	1.129270	1.179795
C	0.595129	1.129270	-1.179795
C	-0.195354	0.681761	2.384225
C	-0.195354	0.681761	-2.384225
O	-0.097253	0.782414	0.000000
Cl	-0.195354	-1.116216	2.587045
Cl	-0.195354	-1.116216	-2.587045
H	0.715987	2.221674	1.242336
H	1.594518	0.679296	1.190046
H	1.594518	0.679296	-1.190046
H	0.715987	2.221674	-1.242336
H	0.235929	1.094093	3.292028
H	-1.235057	0.984758	2.300171
H	-1.235057	0.984758	-2.300171
H	0.235929	1.094093	-3.292028

Molecule# 0202

di-2-propyn-1-yltrioxidane

PointGroup: C1

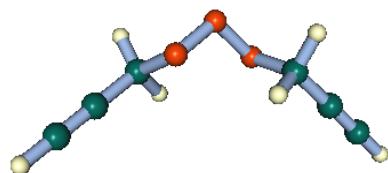
E= -457.763504667 au

ZPE= 0.104728 au

LUMO_eps= -0.03274 au

HOMO_eps= -0.28881 au

Dipole= 1.115 debye



15

O	0.000000	1.471034	0.000000
O	-1.045393	0.632131	0.498632
O	1.045393	0.632130	-0.498632
C	-1.857587	0.241250	-0.631137
C	1.857587	0.241251	0.631137
C	-2.930054	-0.597279	-0.127689
C	2.930054	-0.597279	0.127689
C	-3.820304	-1.289211	0.276887
C	3.820303	-1.289212	-0.276887
H	-2.252972	1.138284	-1.112154
H	-1.237646	-0.305795	-1.343916
H	2.252972	1.138285	1.112154
H	1.237646	-0.305794	1.343917
H	-4.609105	-1.902231	0.635967
H	4.609104	-1.902232	-0.635966

Molecule# 0203

di-t-butyl peroxide

PointGroup: C2

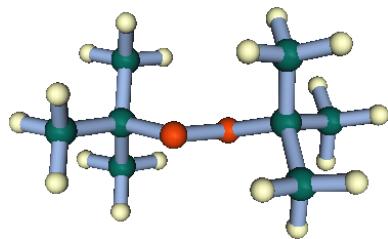
E= -466.249057195 au

ZPE= 0.249477 au

LUMO_eps= -0.01243 au

HOMO_eps= -0.23504 au

Dipole= 0.428 debye



28

O	0.573550	-0.456962	-0.218509
O	-0.573550	0.456962	-0.218509
C	-0.080170	1.796241	-0.003020
C	0.884776	2.195036	-1.121036
C	-1.367264	2.619106	-0.073034
C	0.573550	1.917363	1.374169
C	0.080170	-1.796241	-0.003020
C	-0.884776	-2.195036	-1.121036
C	1.367264	-2.619106	-0.073034
C	-0.573550	-1.917363	1.374169
H	0.409795	2.068957	-2.094034
H	1.176355	3.240428	-1.011020
H	1.784373	1.583641	-1.095314
H	-2.069771	2.304245	0.698415
H	-1.138092	3.673801	0.079206
H	-1.845273	2.506130	-1.045680
H	1.459710	1.289466	1.438562
H	0.871203	2.950204	1.559960
H	-0.124150	1.615244	2.155502
H	-0.409795	-2.068957	-2.094034
H	-1.176355	-3.240428	-1.011020
H	-1.784373	-1.583641	-1.095314
H	2.069771	-2.304245	0.698415
H	1.138092	-3.673801	0.079206
H	1.845273	-2.506130	-1.045680
H	-1.459710	-1.289466	1.438562
H	-0.871203	-2.950204	1.559960
H	0.124150	-1.615244	2.155502

Molecule# 0204

di-t-butyl sulfoxide

PointGroup: C1

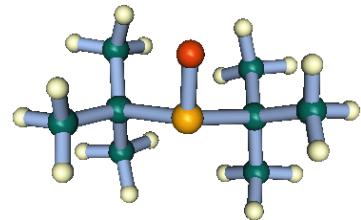
E= -789.267560972 au

ZPE= 0.247331 au

LUMO_eps= -0.01732 au

HOMO_eps= -0.22104 au

Dipole= 3.716 debye



28

C	2.663848	-0.782766	-0.312447
C	1.574850	0.243819	0.027897
S	0.003172	-0.652999	-0.591505
O	-0.020248	-1.977073	0.141990
C	1.557609	0.507360	1.528193
C	1.785704	1.512671	-0.796723
C	-1.573874	0.251467	0.029249
C	-1.560609	1.730836	-0.336792
C	-1.776120	0.006480	1.519693
C	-2.659747	-0.480531	-0.773418
H	2.509176	-1.714151	0.227716
H	2.686446	-1.005976	-1.380264
H	3.635357	-0.369465	-0.033555
H	1.255380	-0.384375	2.076591
H	0.895101	1.328817	1.794977
H	2.563900	0.776586	1.859022
H	1.684867	1.314388	-1.864966
H	2.799008	1.883799	-0.626678
H	1.096530	2.309355	-0.528584
H	-1.282606	1.890906	-1.379789
H	-0.889760	2.308180	0.296527
H	-2.565562	2.138481	-0.202592
H	-1.549414	-1.030527	1.766119
H	-2.819894	0.198857	1.778581
H	-1.156770	0.655303	2.134375
H	-2.534148	-0.333472	-1.846700
H	-2.647862	-1.549896	-0.566985
H	-3.638489	-0.088261	-0.489546

Molecule# 0205

diacetylene

PointGroup: D(infinity)h

E= -153.546820530 au

ZPE= 0.037399 au

LUMO_eps= -0.04203 au

HOMO_eps= -0.27472 au

Dipole= 0.000 debye



6

C 0.000000 0.000000 0.681680

C 0.000000 0.000000 -0.681680

C 0.000000 0.000000 1.885975

C 0.000000 0.000000 -1.885975

H 0.000000 0.000000 2.946942

H 0.000000 0.000000 -2.946942

Molecule# 0206

diaminoethyne

PointGroup: C1

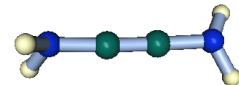
E= -188.122485462 au

ZPE= 0.061985 au

LUMO_eps= -0.01839 au

HOMO_eps= -0.21583 au

Dipole= 1.189 debye



8

N	-1.948870	-0.047511	0.054375
N	1.948870	-0.047536	-0.054353
C	-0.602828	0.001551	0.003804
C	0.602828	0.001550	-0.003806
H	-2.420980	-0.433572	-0.748716
H	-2.421589	0.756865	0.436515
H	2.420977	-0.433234	0.748914
H	2.421590	0.756668	-0.436853

Molecule# 0207

diaminomethane

PointGroup: C2v

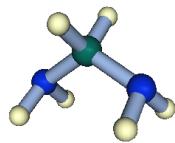
E= -151.281597287 au

ZPE= 0.081812 au

LUMO_eps= -0.01951 au

HOMO_eps= -0.23644 au

Dipole= 1.710 debye



9

C	0.000000	0.000000	0.550170
N	0.000000	1.261601	-0.185123
N	0.000000	-1.261601	-0.185123
H	0.876907	0.000000	1.198167
H	-0.876907	0.000000	1.198167
H	0.817663	1.348464	-0.776410
H	-0.817663	1.348464	-0.776410
H	-0.817663	-1.348464	-0.776410
H	0.817663	-1.348464	-0.776410

Molecule# 0208

diazenylacetic acid

PointGroup: C1

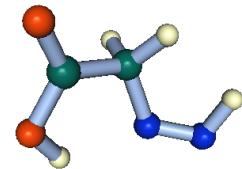
E= -338.657610905 au

ZPE= 0.071715 au

LUMO_eps= -0.09520 au

HOMO_eps= -0.28250 au

Dipole= 3.252 debye



10

O	-2.011808	-0.775896	-0.227722
O	-1.126265	1.260042	-0.024183
N	1.364084	0.336361	0.181249
N	2.444806	0.013050	-0.303623
C	-1.063326	-0.080407	-0.006367
C	0.305241	-0.661369	0.352535
H	-0.236965	1.621218	0.140319
H	2.475277	-1.001924	-0.544358
H	0.269739	-0.910304	1.417114
H	0.482809	-1.577382	-0.218226

Molecule# 0209

diaziridine

PointGroup: C2

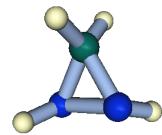
E= -149.998084439 au

ZPE= 0.058894 au

LUMO_eps= -0.00948 au

HOMO_eps= -0.26907 au

Dipole= 1.299 debye



7

C 0.000000 0.000000 0.794985

N 0.000000 0.748957 -0.440025

N 0.000000 -0.748957 -0.440025

H 0.911241 0.078114 1.376716

H -0.911241 -0.078114 1.376716

H -0.955168 0.999325 -0.681494

H 0.955168 -0.999325 -0.681494

Molecule# 0210

diazomethane

PointGroup: Cs

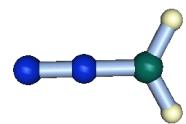
E= -148.801574364 au

ZPE= 0.031661 au

LUMO_eps= -0.05833 au

HOMO_eps= -0.23367 au

Dipole= 1.633 debye



5

C 0.000100 -1.136474 0.000000

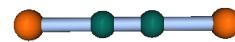
N 0.000000 0.155349 0.000000

N -0.000113 1.287404 0.000000

H 0.000095 -1.640214 0.950280

H 0.000095 -1.640214 -0.950280

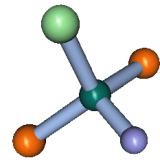
Molecule# 0211
dibromoacetylene
PointGroup: D(infinity)h
E= -5224.601886940 au
ZPE= 0.009967 au
LUMO_eps= -0.04241 au
HOMO_eps= -0.26718 au
Dipole= 0.000 debye



4
C 0.000000 0.000000 0.600713
C 0.000000 0.000000 -0.600713
Br 0.000000 0.000000 2.395760
Br 0.000000 0.000000 -2.395760

Molecule# 0212
dibromochlorofluoromethane
PointGroup: Cs

E= -5746.670910180 au
ZPE= 0.009674 au
LUMO_eps= -0.09373 au
HOMO_eps= -0.30371 au
Dipole= 0.436 debye



5
C -0.133365 0.516099 0.000000
F -1.254612 1.247561 0.000000
Cl 1.260427 1.617748 0.000000
Br -0.133365 -0.597519 1.611615
Br -0.133365 -0.597519 -1.611615

Molecule# 0213

dibromochloromethane

PointGroup: Cs

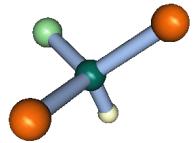
E= -5647.401662680 au

ZPE= 0.018456 au

LUMO_eps= -0.07975 au

HOMO_eps= -0.29642 au

Dipole= 0.938 debye



5

C -0.231638 0.598947 0.000000

H -1.159608 1.149214 0.000000

Cl 1.103771 1.765004 0.000000

Br -0.231638 -0.496400 1.614150

Br -0.231638 -0.496400 -1.614150

Molecule# 0214

dibromodichloromethane

PointGroup: C2v

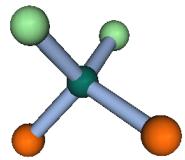
E= -6107.014661580 au

ZPE= 0.007928 au

LUMO_eps= -0.10022 au

HOMO_eps= -0.30041 au

Dipole= 0.096 debye



5

C 0.000000 0.000000 0.407165

Br 0.000000 1.601319 -0.729884

Br 0.000000 -1.601319 -0.729884

Cl -1.455405 0.000000 1.430851

Cl 1.455405 0.000000 1.430851

Molecule# 0215

dibromodifluoromethane

PointGroup: C2v

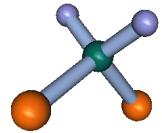
E= -5386.329782830 au

ZPE= 0.011530 au

LUMO_eps= -0.08467 au

HOMO_eps= -0.30918 au

Dipole= 0.522 debye



5

C 0.000000 0.000000 0.661772

F 0.000000 1.078609 1.445084

F 0.000000 -1.078609 1.445084

Br 1.622926 0.000000 -0.428316

Br -1.622926 0.000000 -0.428316

Molecule# 0216

dibromofluoromethane

PointGroup: Cs

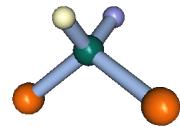
E= -5287.052009730 au

ZPE= 0.020107 au

LUMO_eps= -0.06892 au

HOMO_eps= -0.30077 au

Dipole= 1.148 debye



5

C -0.102173 0.789038 0.000000

H -1.009394 1.379452 0.000000

F 0.974951 1.598413 0.000000

Br -0.102173 -0.292848 1.621270

Br -0.102173 -0.292848 -1.621270

Molecule# 0217

dibromomethane

PointGroup: C2v

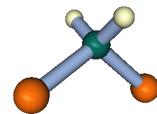
E= -5187.781650520 au

ZPE= 0.028009 au

LUMO_eps= -0.05857 au

HOMO_eps= -0.29291 au

Dipole= 1.479 debye



5

Br 0.000000 1.633181 -0.123859

Br 0.000000 -1.633181 -0.123859

C 0.000000 0.000000 0.933737

H 0.898343 0.000000 1.533842

H -0.898343 0.000000 1.533842

Molecule# 0218

dichloroacetaldehyde

PointGroup: Cs

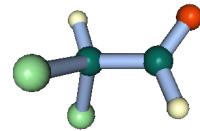
E= -1073.147695640 au

ZPE= 0.037998 au

LUMO_eps= -0.08211 au

HOMO_eps= -0.29849 au

Dipole= 1.003 debye



7

C 0.392398 -0.014823 0.000000

C -0.171128 1.398319 0.000000

H 1.474917 -0.012492 0.000000

Cl -0.171128 -0.843017 1.485142

Cl -0.171128 -0.843017 -1.485142

O 0.536130 2.365239 0.000000

H -1.273222 1.452187 0.000000

Molecule# 0219
dichloroacetylene
PointGroup: D(infinity)h
E= -996.610266629 au
ZPE= 0.011133 au
LUMO_eps= -0.01740 au
HOMO_eps= -0.27455 au
Dipole= 0.000 debye



4
C 0.000000 0.000000 0.599276
C 0.000000 0.000000 -0.599276
Cl 0.000000 0.000000 2.241149
Cl 0.000000 0.000000 -2.241149

Molecule# 0220

dichlorodifluoromethane

PointGroup: C2v

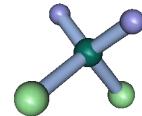
E= -1158.344649800 au

ZPE= 0.012773 au

LUMO_eps= -0.05213 au

HOMO_eps= -0.33976 au

Dipole= 0.423 debye



5

C 0.000000 0.000000 0.342340

F 0.000000 1.079325 1.126414

F 0.000000 -1.079325 1.126414

Cl 1.472567 0.000000 -0.656750

Cl -1.472567 0.000000 -0.656750

Molecule# 0221

dichlorofluoromethane

PointGroup: Cs

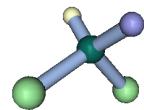
E= -1059.065792640 au

ZPE= 0.021322 au

LUMO_eps= -0.03861 au

HOMO_eps= -0.32915 au

Dipole= 1.280 debye



5

C -0.178150 0.524281 0.000000

H -1.074887 1.131933 0.000000

F 0.911211 1.319595 0.000000

Cl -0.178150 -0.475117 1.474553

Cl -0.178150 -0.475117 -1.474553

Molecule# 0222

dichloromethane

PointGroup: C2v

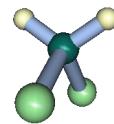
E= -959.792079637 au

ZPE= 0.029228 au

LUMO_eps= -0.03205 au

HOMO_eps= -0.31445 au

Dipole= 1.677 debye



5

C1 0.000000 1.489376 -0.216532

C1 0.000000 -1.489376 -0.216532

C 0.000000 0.000000 0.769333

H -0.896869 0.000000 1.373046

H 0.896869 0.000000 1.373046

Molecule# 0223

dicyanomethane

PointGroup: C2v

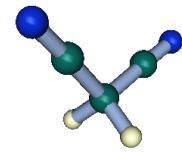
E= -225.063513310 au

ZPE= 0.044540 au

LUMO_eps= -0.03898 au

HOMO_eps= -0.36274 au

Dipole= 3.843 debye



7

C 0.000000 0.000000 0.828233

C 0.000000 1.221205 0.021726

C 0.000000 -1.221205 0.021726

H 0.879349 0.000000 1.476388

H -0.879349 0.000000 1.476388

N 0.000000 2.195867 -0.584492

N 0.000000 -2.195867 -0.584492

Molecule# 0224

dicyanomethanol

PointGroup: C1

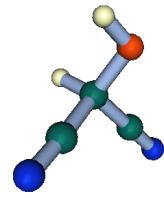
E= -300.296958708 au

ZPE= 0.048620 au

LUMO_eps= -0.06919 au

HOMO_eps= -0.35784 au

Dipole= 4.083 debye



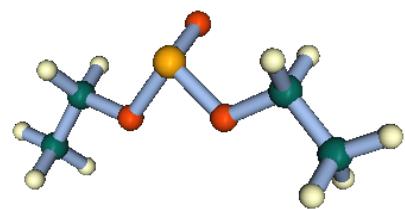
8

O	-0.023151	1.622923	-0.280281
N	-2.199831	-0.919309	-0.166719
N	2.157942	-0.992833	-0.172002
C	-0.002614	0.387114	0.400860
C	-1.233688	-0.342601	0.060384
C	1.190268	-0.419958	0.063748
H	0.756685	2.130316	-0.026335
H	-0.002056	0.523963	1.489685

Molecule# 0225
diethoxysulfoxide

PointGroup: Cs

E= -782.464435688 au
ZPE= 0.145420 au
LUMO_eps= -0.01802 au
HOMO_eps= -0.27195 au
Dipole= 1.782 debye



18

C	0.150438	-1.090521	3.446524
C	0.085296	0.101402	2.517436
O	0.150438	-0.404858	1.160874
S	0.167579	0.766272	0.000000
O	-1.132613	1.441502	0.000000
O	0.150438	-0.404858	-1.160874
C	0.085296	0.101402	-2.517436
C	0.150438	-1.090521	-3.446524
H	-0.680200	-1.769479	3.258074
H	1.082937	-1.637650	3.313150
H	0.092076	-0.751674	4.481673
H	0.923392	0.782173	2.691692
H	-0.846294	0.654026	2.644175
H	-0.846294	0.654026	-2.644175
H	0.923392	0.782173	-2.691692
H	1.082937	-1.637650	-3.313150
H	-0.680200	-1.769479	-3.258074
H	0.092076	-0.751674	-4.481673

Molecule# 0226

diethyl butanedioate

PointGroup: C2

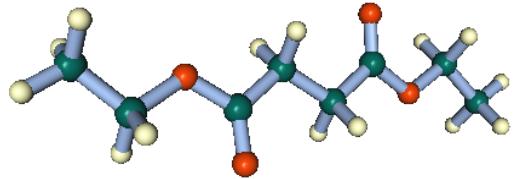
E= -614.457706103 au

ZPE= 0.217278 au

LUMO_eps= -0.01451 au

HOMO_eps= -0.28136 au

Dipole= 0.398 debye



26

C	0.188348	1.924575	-0.056731
C	-0.188348	-1.924575	-0.056731
C	-1.353289	5.221305	0.159863
C	1.353289	-5.221305	0.159863
C	-0.494217	0.577874	-0.004149
C	0.494217	-0.577874	-0.004149
C	-0.188348	4.271183	0.002037
C	0.188348	-4.271183	0.002037
O	1.374196	2.105516	-0.191402
O	-1.374196	-2.105516	-0.191402
O	-0.708999	2.921630	0.057961
O	0.708999	-2.921630	0.057961
H	-0.993955	6.250306	0.122700
H	-2.082017	5.084576	-0.638821
H	-1.856365	5.069159	1.114540
H	0.993955	-6.250306	0.122700
H	2.082017	-5.084576	-0.638821
H	1.856365	-5.069159	1.114540
H	-1.172064	0.507988	-0.856621
H	-1.139461	0.549023	0.874561
H	1.139461	-0.549023	0.874561
H	1.172064	-0.507988	-0.856621
H	0.548903	4.392492	0.795533
H	0.323949	4.406624	-0.950483
H	-0.548903	-4.392492	0.795533
H	-0.323949	-4.406624	-0.950483

Molecule# 0227

diethyl disulfide

PointGroup: C2

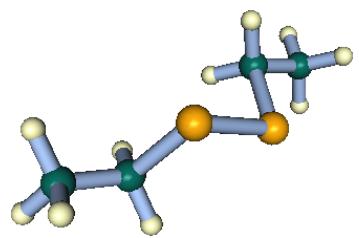
E= -954.976119364 au

ZPE= 0.133957 au

LUMO_eps= -0.02703 au

HOMO_eps= -0.23770 au

Dipole= 2.206 debye



16

C	0.340762	3.287075	0.629973
C	-0.340762	-3.287075	0.629973
C	0.695762	1.806304	0.586711
C	-0.695762	-1.806304	0.586711
S	-0.340762	0.974925	-0.694192
S	0.340762	-0.974925	-0.694192
H	0.525276	3.767942	-0.330968
H	-0.707346	3.438737	0.889650
H	0.949124	3.792561	1.381474
H	-0.525276	-3.767942	-0.330968
H	0.707346	-3.438737	0.889650
H	-0.949124	-3.792561	1.381474
H	0.508220	1.330131	1.547298
H	1.739469	1.654869	0.319514
H	-0.508220	-1.330131	1.547298
H	-1.739469	-1.654869	0.319514

Molecule# 0228

diethyl malonate

PointGroup: C1

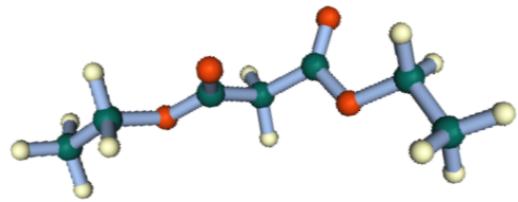
E= -575.124205720 au

ZPE= 0.189011 au

LUMO_eps= -0.01529 au

HOMO_eps= -0.28558 au

Dipole= 2.905 debye



23

C	1.306354	0.956233	-0.134176
C	-1.044968	0.127302	0.167328
C	3.886887	-1.608049	-0.254851
C	-4.599276	-0.443312	-0.394492
C	-0.088316	0.906240	-0.718617
C	3.316527	-0.269540	0.153530
C	-3.305169	-0.571942	0.375011
O	1.744359	1.881556	0.499819
O	-0.757253	-0.411532	1.203966
O	1.990697	-0.161001	-0.420971
O	-2.276334	0.126892	-0.371097
H	4.887123	-1.722217	0.164487
H	3.266466	-2.424893	0.112600
H	3.960144	-1.689656	-1.339244
H	-5.395469	-0.960067	0.142386
H	-4.886137	0.601847	-0.507648
H	-4.512178	-0.886897	-1.386071
H	-0.462283	1.922798	-0.825864
H	-0.078310	0.440983	-1.704161
H	3.919903	0.562400	-0.209284
H	3.228446	-0.173746	1.235219
H	-2.999534	-1.611161	0.493470
H	-3.372156	-0.128302	1.367982

Molecule# 0229

diethyl peroxide

PointGroup: C2h

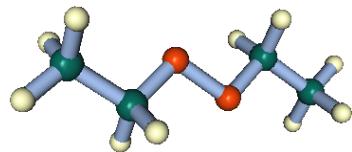
E= -308.925960914 au

ZPE= 0.139089 au

LUMO_eps= -0.00813 au

HOMO_eps= -0.24096 au

Dipole= 0.000 debye



16

O	-0.015813	0.731327	0.000000
O	0.015813	-0.731327	0.000000
C	-1.344283	-1.140143	0.000000
H	-1.844417	-0.742104	0.887786
C	1.344283	1.140143	0.000000
H	1.844417	0.742104	-0.887786
H	1.844417	0.742104	0.887786
C	1.344283	2.657005	0.000000
C	-1.344283	-2.657005	0.000000
H	-1.844417	-0.742104	-0.887786
H	0.842512	3.047916	-0.884749
H	0.842512	3.047916	0.884749
H	2.372433	3.019890	0.000000
H	-0.842512	-3.047916	-0.884749
H	-0.842512	-3.047916	0.884749
H	-2.372433	-3.019890	0.000000

Molecule# 0230

diethyl sulfide

PointGroup: C2v

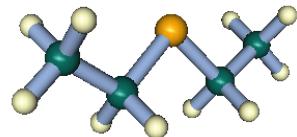
E= -556.741946515 au

ZPE= 0.132380 au

LUMO_eps= -0.01149 au

HOMO_eps= -0.22051 au

Dipole= 1.639 debye



15

C	0.000000	2.726159	0.135205
C	0.000000	-2.726159	0.135205
C	0.000000	1.403492	-0.620064
C	0.000000	-1.403492	-0.620064
S	0.000000	0.000000	0.556153
H	-0.882330	2.818735	0.768807
H	0.882330	2.818735	0.768807
H	0.000000	3.560604	-0.567621
H	0.882330	-2.818735	0.768807
H	-0.882330	-2.818735	0.768807
H	0.000000	-3.560604	-0.567621
H	0.883227	1.323432	-1.255033
H	-0.883227	1.323432	-1.255033
H	-0.883227	-1.323432	-1.255033
H	0.883227	-1.323432	-1.255033

Molecule# 0231

diethyl sulfone

PointGroup: Cs

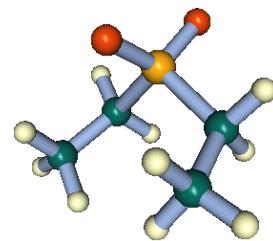
E= -707.215310248 au

ZPE= 0.141592 au

LUMO_eps= -0.02376 au

HOMO_eps= -0.28899 au

Dipole= 4.865 debye



17

O	0.424779	2.021733	0.000000
S	0.358890	0.561255	0.000000
C	-0.613205	0.101793	1.471297
C	-0.613205	-1.376626	1.826915
C	-0.613205	0.101793	-1.471297
C	-0.613205	-1.376626	-1.826915
O	1.592893	-0.223650	0.000000
H	-1.610423	0.511825	1.314449
H	-0.127133	0.701508	2.241547
H	0.402605	-1.766402	1.849066
H	-1.195297	-1.970903	1.125329
H	-1.053100	-1.509402	2.815892
H	-0.127133	0.701508	-2.241547
H	-1.610423	0.511825	-1.314449
H	0.402605	-1.766402	-1.849066
H	-1.053100	-1.509402	-2.815892
H	-1.195297	-1.970903	-1.125329

Molecule# 0232

diethyl sulfoxide

PointGroup: C1

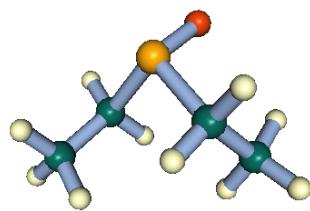
E= -631.962163267 au

ZPE= 0.136176 au

LUMO_eps= -0.01923 au

HOMO_eps= -0.23188 au

Dipole= 4.247 debye



16

C	1.610605	1.384300	0.549759
H	2.332239	2.160342	0.292049
H	0.860212	1.834406	1.198917
H	2.129278	0.606001	1.108397
C	-2.280666	0.756806	-0.091466
H	-2.643528	0.312964	-1.019464
H	-3.146309	0.940646	0.545887
H	-1.838910	1.724439	-0.328261
C	-1.298769	-0.163282	0.619431
H	-1.776187	-1.092001	0.931530
H	-0.846975	0.288433	1.501243
C	0.999535	0.803974	-0.714910
H	0.322444	1.489329	-1.225847
S	0.072252	-0.774645	-0.452665
O	0.937001	-1.633899	0.435963
H	1.771453	0.510148	-1.426400

Molecule# 0233

diethylamine

PointGroup: Cs

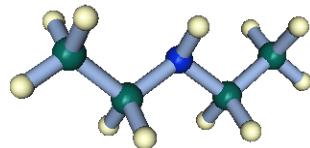
E= -213.884725985 au

ZPE= 0.148610 au

LUMO_eps= -0.01094 au

HOMO_eps= -0.22662 au

Dipole= 0.874 debye



16

C	-0.008620	-0.371616	2.458950
C	-0.008620	-0.371616	-2.458950
C	-0.008620	0.517598	1.223905
C	-0.008620	0.517598	-1.223905
N	-0.059012	-0.273364	0.000000
H	-0.896650	-1.003443	2.479604
H	0.868669	-1.022627	2.474208
H	0.011382	0.229192	3.368838
H	0.868669	-1.022627	-2.474208
H	-0.896650	-1.003443	-2.479604
H	0.011382	0.229192	-3.368838
H	0.867606	1.187009	1.250354
H	-0.889411	1.165441	1.236824
H	-0.889411	1.165441	-1.236824
H	0.867606	1.187009	-1.250354
H	0.696784	-0.949384	0.000000

Molecule# 0234

diethylhydroxylamine

PointGroup: Cs

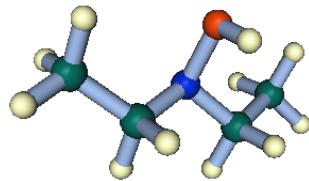
E= -289.084920024 au

ZPE= 0.151937 au

LUMO_eps= -0.01655 au

HOMO_eps= -0.24256 au

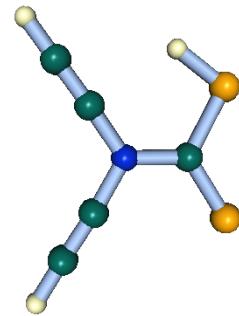
Dipole= 2.256 debye



17

N	-0.135879	-0.159469	0.000000
O	1.161592	-0.759998	0.000000
H	1.809832	-0.031424	0.000000
C	-0.288759	-0.230429	2.472841
C	-0.288759	-0.230429	-2.472841
C	-0.288759	0.629302	1.218177
C	-0.288759	0.629302	-1.218177
H	0.647697	-0.775732	2.573295
H	0.647697	-0.775732	-2.573295
H	0.502431	1.398690	-1.280754
H	0.502431	1.398690	1.280754
H	-1.239354	1.157946	-1.127847
H	-1.239354	1.157946	1.127847
H	-1.101796	-0.955280	2.437155
H	-1.101796	-0.955280	-2.437155
H	-0.419577	0.394984	3.356866
H	-0.419577	0.394984	-3.356866

Molecule# 0235
diethynylcarbamodithioic acid
PointGroup: C1
E= -1043.447751980 au
ZPE= 0.060203 au
LUMO_eps= -0.08196 au
HOMO_eps= -0.24193 au
Dipole= 3.446 debye



11

S	1.785669	1.142219	0.000055
S	1.219674	-1.735364	-0.000051
N	-0.725832	0.098897	-0.000008
C	0.657309	-0.199787	-0.000005
C	-1.229803	1.357918	-0.000005
C	-1.636455	-0.913125	-0.000051
C	-1.716879	2.453129	-0.000088
C	-2.495073	-1.745684	0.000145
H	0.900322	2.162085	0.000064
H	-2.142646	3.424997	-0.000013
H	-3.236933	-2.503747	-0.000019

Molecule# 0236

difluoroacetylene

PointGroup: D(infinity)h

E= -275.860432290 au

ZPE= 0.013486 au

LUMO_eps= -0.01372 au

HOMO_eps= -0.29682 au

Dipole= 0.000 debye



4

C 0.000000 0.000000 0.591567

C 0.000000 0.000000 -0.591567

F 0.000000 0.000000 1.877004

F 0.000000 0.000000 -1.877004

Molecule# 0237

difluoroaminomethyl acetate

PointGroup: C1

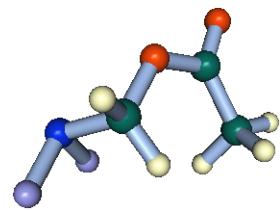
E= -522.287672221 au

ZPE= 0.089213 au

LUMO_eps= -0.02844 au

HOMO_eps= -0.30430 au

Dipole= 3.863 debye



13

F	2.734032	-0.044650	0.294765
F	1.181883	0.979329	-0.865319
O	-0.624931	-0.986352	0.049400
O	-2.650125	-0.501223	-0.660014
N	1.562213	-0.308934	-0.435957
C	0.589833	-0.642433	0.639320
C	-1.709038	-0.127949	-0.029755
C	-1.645992	1.182508	0.711998
H	0.536070	0.185170	1.344177
H	1.001583	-1.530166	1.114473
H	-0.840166	1.812068	0.338768
H	-2.596239	1.685000	0.564689
H	-1.488346	1.026194	1.780109

Molecule# 0238

difluoromethane

PointGroup: C2v

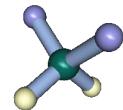
E= -239.088376863 au

ZPE= 0.032588 au

LUMO_eps= -0.00975 au

HOMO_eps= -0.36001 au

Dipole= 1.957 debye



5

F 0.000000 1.105295 -0.290293

F 0.000000 -1.105295 -0.290293

C 0.000000 0.000000 0.502981

H 0.909963 0.000000 1.103692

H -0.909963 0.000000 1.103692

Molecule# 0239

difuro[3,2-b:2',3'-d]furan

PointGroup: C2v

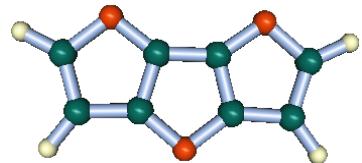
E= -533.018488058 au

ZPE= 0.103390 au

LUMO_eps= -0.03400 au

HOMO_eps= -0.20546 au

Dipole= 0.764 debye



15

C	0.000000	2.489253	0.832738
C	0.000000	-2.489253	0.832738
C	0.000000	2.874720	-0.476647
C	0.000000	-2.874720	-0.476647
C	0.000000	1.073622	0.774661
C	0.000000	-1.073622	0.774661
C	0.000000	0.706341	-0.549010
C	0.000000	-0.706341	-0.549010
O	0.000000	1.799140	-1.343744
O	0.000000	-1.799140	-1.343744
O	0.000000	0.000000	1.629823
H	0.000000	3.143332	1.686236
H	0.000000	-3.143332	1.686236
H	0.000000	3.840540	-0.946024
H	0.000000	-3.840540	-0.946024

Molecule# 0240

dihydro-2(3H)-thiophenone

PointGroup: C1

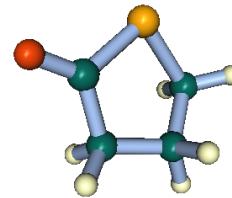
E= -629.586974799 au

ZPE= 0.094640 au

LUMO_eps= -0.03342 au

HOMO_eps= -0.26037 au

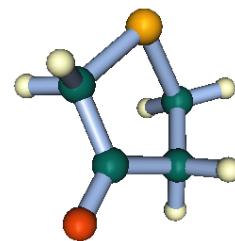
Dipole= 4.278 debye



12

C	-0.123642	1.418300	0.182281
H	-0.576061	2.246214	-0.360785
H	-0.140157	1.675948	1.245871
C	1.285993	1.069039	-0.279367
H	2.029750	1.761665	0.115463
H	1.337092	1.113708	-1.368217
C	1.580762	-0.362867	0.182655
H	1.863237	-0.398574	1.234120
H	2.363223	-0.838008	-0.403468
C	-1.005756	0.186332	0.018862
O	-2.202205	0.172101	-0.051174
S	0.019776	-1.300161	-0.042511

Molecule# 0241
dihydro-3(2H)-thiophenone
PointGroup: C1
E= -629.571524024 au
ZPE= 0.093613 au
LUMO_eps= -0.04586 au
HOMO_eps= -0.23990 au
Dipole= 1.977 debye



12

C	-1.173933	-0.086028	-0.010331
C	-0.518527	1.277829	-0.187572
H	-1.108936	2.034769	0.327755
H	-0.554216	1.502662	-1.257211
C	0.925632	1.196028	0.287908
H	1.002801	1.342170	1.364887
H	1.581138	1.908061	-0.205713
C	-0.148546	-1.207971	0.168542
S	1.503686	-0.500212	-0.148246
H	-0.361635	-2.019932	-0.522700
O	-2.361719	-0.281087	-0.009054
H	-0.232119	-1.594793	1.186057

Molecule# 0242

diisobutyl sulfone

PointGroup: C1

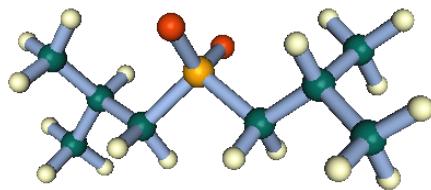
E= -864.527860875 au

ZPE= 0.254386 au

LUMO_eps= -0.02100 au

HOMO_eps= -0.28369 au

Dipole= 4.094 debye



29

C	-1.420834	0.793414	-0.007311
S	0.000000	-0.346947	-0.000010
C	-2.762715	0.095086	0.252798
C	1.420834	0.793414	0.007287
O	-0.034424	-1.089441	1.260830
O	0.034424	-1.089442	-1.260849
C	-3.806859	1.145917	0.648578
C	-3.239642	-0.730464	-0.945570
C	2.762718	0.095073	-0.252778
C	3.806866	1.145882	-0.648603
C	3.239634	-0.730417	0.945635
H	-1.201428	1.513412	0.781999
H	-1.403435	1.302515	-0.971723
H	-2.618202	-0.575090	1.103169
H	1.201441	1.513390	-0.782045
H	1.403420	1.302541	0.971685
H	-4.763693	0.667778	0.861289
H	-3.504390	1.699334	1.539005
H	-3.969663	1.865389	-0.157619
H	-3.398705	-0.091329	-1.817765
H	-2.520753	-1.498674	-1.222382
H	-4.188123	-1.215944	-0.712598
H	2.618210	-0.575147	-1.103115
H	4.763704	0.667732	-0.861274
H	3.504408	1.699247	-1.539066
H	3.969659	1.865400	0.157555
H	3.398692	-0.091241	1.817801
H	2.520742	-1.498613	1.222481
H	4.188116	-1.215910	0.712694

Molecule# 0243

diisopropylamine

PointGroup: C1

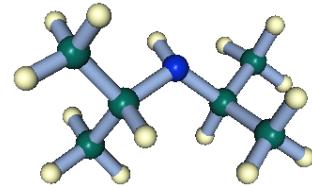
E= -292.542290189 au

ZPE= 0.204316 au

LUMO_eps= -0.01278 au

HOMO_eps= -0.22309 au

Dipole= 0.863 debye



22

C	-1.682099	0.843342	1.108925
C	-2.329448	-0.758201	-0.729885
C	1.677526	1.040130	-0.932617
C	2.330696	-0.886661	0.546317
C	-1.240487	0.173905	-0.201334
C	1.245402	0.137972	0.223722
N	0.012917	-0.583301	-0.108885
H	-2.599081	1.417126	0.962026
H	-1.878405	0.091069	1.877487
H	-0.925163	1.527203	1.493070
H	-2.033698	-1.190788	-1.684763
H	-3.272260	-0.225869	-0.861804
H	-2.508153	-1.577776	-0.028379
H	2.612240	1.547255	-0.688563
H	1.827598	0.448053	-1.836881
H	0.936364	1.809119	-1.150478
H	2.039406	-1.518516	1.388533
H	3.264720	-0.390727	0.811648
H	2.513905	-1.532110	-0.314411
H	-1.083299	0.957612	-0.946157
H	1.117881	0.773535	1.113812
H	-0.112018	-1.354992	0.536287

Molecule# 0244

dimethoxymethane

PointGroup: C2

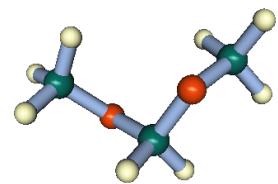
E= -269.666323870 au

ZPE= 0.112868 au

LUMO_eps= -0.00917 au

HOMO_eps= -0.28025 au

Dipole= 0.188 debye



13

C	0.000000	1.856169	-0.553318
C	0.000000	-1.856169	-0.553318
C	0.000000	0.000000	0.918263
O	-0.768127	0.891716	0.154870
O	0.768127	-0.891716	0.154870
H	0.611878	2.448681	0.135651
H	-0.705463	2.511536	-1.058607
H	0.653146	1.386863	-1.291849
H	-0.653146	-1.386863	-1.291849
H	-0.611878	-2.448681	0.135651
H	0.705463	-2.511536	-1.058607
H	0.718837	0.541142	1.540958
H	-0.718837	-0.541142	1.540958

Molecule# 0245

dimethoxysulfoxide

PointGroup: C1

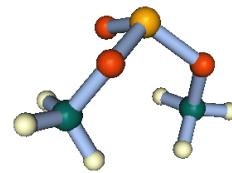
E= -703.801621019 au

ZPE= 0.088811 au

LUMO_eps= -0.01719 au

HOMO_eps= -0.29353 au

Dipole= 2.416 debye



12

S	0.000000	-0.857107	-0.318004
O	0.000000	-1.053613	1.137761
O	1.279962	0.121780	-0.679264
O	-1.279962	0.121780	-0.679265
C	1.785232	1.045978	0.304035
C	-1.785232	1.045978	0.304035
H	2.837899	1.182815	0.071216
H	-2.837900	1.182815	0.071215
H	1.263493	1.999548	0.224505
H	1.675420	0.638837	1.307173
H	-1.675421	0.638836	1.307172
H	-1.263493	1.999547	0.224506

Molecule# 0246

dimethyl carbonotrithioate

PointGroup: C2v

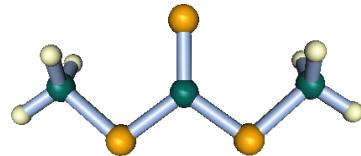
E= -1312.651789520 au

ZPE= 0.084175 au

LUMO_eps= -0.07388 au

HOMO_eps= -0.23221 au

Dipole= 0.379 debye



12

C	0.000000	0.000000	0.036614
S	0.000000	0.000000	1.679557
S	0.000000	1.427910	-0.995436
S	0.000000	-1.427910	-0.995436
C	0.000000	2.795841	0.193673
C	0.000000	-2.795841	0.193673
H	0.889349	2.757958	0.816057
H	0.889349	-2.757958	0.816057
H	0.000000	3.699161	-0.413472
H	-0.889349	2.757958	0.816057
H	-0.889349	-2.757958	0.816057
H	0.000000	-3.699161	-0.413472

Molecule# 0247

dimethyl trisulfide

PointGroup: C2

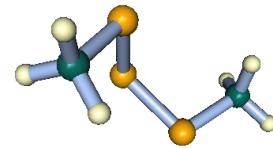
E= -1274.554253990 au

ZPE= 0.078576 au

LUMO_eps= -0.04908 au

HOMO_eps= -0.24364 au

Dipole= 1.205 debye



11

S	0.000000	0.000000	1.056821
S	0.000000	1.684277	-0.162632
S	0.000000	-1.684277	-0.162632
C	1.760232	1.865036	-0.616415
C	-1.760232	-1.865036	-0.616415
H	1.824265	2.768057	-1.223005
H	-1.824265	-2.768057	-1.223005
H	2.373978	1.976752	0.273229
H	2.086891	1.011010	-1.204189
H	-2.373978	-1.976752	0.273229
H	-2.086891	-1.011010	-1.204189

Molecule# 0248

dimethylamine

PointGroup: Cs

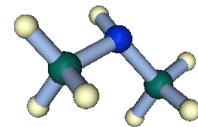
E= -135.222784347 au

ZPE= 0.091940 au

LUMO_eps= -0.01152 au

HOMO_eps= -0.22743 au

Dipole= 0.962 debye



10

C	0.026505	-0.221412	1.216049
C	0.026505	-0.221412	-1.216049
N	0.026505	0.577608	0.000000
H	-0.798102	-0.949693	1.270491
H	-0.034174	0.431778	2.086295
H	0.962937	-0.778731	1.284180
H	-0.034174	0.431778	-2.086295
H	-0.798102	-0.949693	-1.270491
H	0.962937	-0.778731	-1.284180
H	-0.764915	1.206982	0.000000

Molecule# 0249

dimethylcarbamodithioic acid

PointGroup: C1

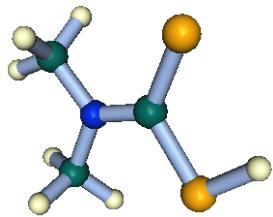
E= -969.796357375 au

ZPE= 0.099206 au

LUMO_eps= -0.04007 au

HOMO_eps= -0.21721 au

Dipole= 4.105 debye



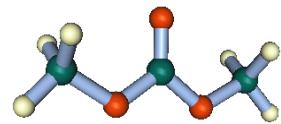
13

C	-1.974833	0.997968	0.019134
N	-1.035538	-0.121579	-0.049562
C	-1.596834	-1.468210	0.005922
C	0.285310	0.130885	-0.019832
S	1.322882	-1.336523	0.009919
S	0.951587	1.656130	0.001950
H	-1.857982	1.544153	0.955692
H	-1.791240	1.695551	-0.795852
H	-2.985427	0.605274	-0.050728
H	-0.950304	-2.175190	-0.507850
H	-1.737185	-1.803323	1.037130
H	-2.560576	-1.471415	-0.497443
H	2.458114	-0.621579	-0.015256

Molecule# 0250
dimethylcarbonate

PointGroup: C2v

E= -343.750985722 au
ZPE= 0.094998 au
LUMO_eps= -0.01092 au
HOMO_eps= -0.30049 au
Dipole= 0.441 debye

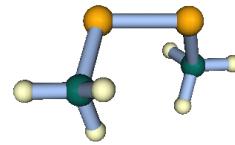


12

C	0.000000	0.000000	0.075891
C	0.000000	2.340391	-0.016158
C	0.000000	-2.340391	-0.016158
O	0.000000	0.000000	1.281653
O	0.000000	1.081938	-0.709482
O	0.000000	-1.081938	-0.709482
H	-0.887790	2.432734	0.606454
H	0.000000	3.096867	-0.794390
H	0.887790	2.432734	0.606454
H	0.000000	-3.096867	-0.794390
H	-0.887790	-2.432734	0.606454
H	0.887790	-2.432734	0.606454

Molecule# 0251
dimethyldisulfide
PointGroup: C2

E= -876.317999973 au
ZPE= 0.076851 au
LUMO_eps= -0.02775 au
HOMO_eps= -0.24175 au
Dipole= 2.023 debye



10

C	-0.975094	1.648785	0.791622
C	0.975094	-1.648785	0.791622
S	-0.975094	0.343346	-0.490829
S	0.975094	-0.343346	-0.490829
H	-0.781660	1.231798	1.776638
H	-1.975350	2.081790	0.775132
H	-0.243016	2.415025	0.551763
H	0.781660	-1.231798	1.776638
H	1.975350	-2.081790	0.775132
H	0.243016	-2.415025	0.551763

Molecule# 0252

dimethylether

PointGroup: C2v

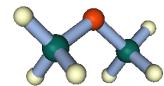
E= -155.093122517 au

ZPE= 0.079278 au

LUMO_eps= -0.01043 au

HOMO_eps= -0.26576 au

Dipole= 1.266 debye



9

C	0.000000	1.175422	-0.194884
C	0.000000	-1.175422	-0.194884
O	0.000000	0.000000	0.586687
H	0.890246	1.231929	-0.833515
H	0.000000	2.021254	0.489588
H	-0.890246	1.231929	-0.833515
H	0.890246	-1.231929	-0.833515
H	-0.890246	-1.231929	-0.833515
H	0.000000	-2.021254	0.489588

Molecule# 0253

dimethylnitroamine

PointGroup: Cs

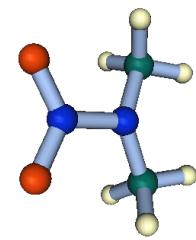
E= -339.795357625 au

ZPE= 0.094553 au

LUMO_eps= -0.05580 au

HOMO_eps= -0.28342 au

Dipole= 4.753 debye



12

O	-0.037714	-1.357944	1.090603
O	-0.037714	-1.357944	-1.090603
H	-1.093723	1.213482	1.547438
H	0.276620	2.273597	1.142183
H	0.546613	0.777805	2.052059
C	-0.037714	1.240481	1.264007
H	-1.093723	1.213482	-1.547438
H	0.546613	0.777805	-2.052059
H	0.276620	2.273597	-1.142183
C	-0.037714	1.240481	-1.264007
N	0.022482	-0.802092	0.000000
N	0.205657	0.560886	0.000000

Molecule# 0254

dimethylperoxide

PointGroup: C2h

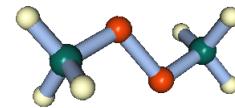
E= -230.260034507 au

ZPE= 0.082526 au

LUMO_eps= -0.00664 au

HOMO_eps= -0.24610 au

Dipole= 0.000 debye



10

O	-0.437201	0.587681	0.000000
O	0.437201	-0.587681	0.000000
C	-0.437201	-1.696109	0.000000
H	-1.064231	-1.705853	0.894667
C	0.437201	1.696109	0.000000
H	1.064231	1.705853	-0.894667
H	1.064231	1.705853	0.894667
H	-0.218746	2.566214	0.000000
H	0.218746	-2.566214	0.000000
H	-1.064231	-1.705853	-0.894667

Molecule# 0255

dimethylsulfide

PointGroup: C2v

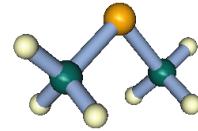
E= -478.084634783 au

ZPE= 0.075287 au

LUMO_eps= -0.01224 au

HOMO_eps= -0.22401 au

Dipole= 1.603 debye



9

C	0.000000	1.391186	-0.512622
C	0.000000	-1.391186	-0.512622
S	0.000000	0.000000	0.659277
H	0.891412	1.376095	-1.138641
H	0.000000	2.304501	0.078799
H	-0.891412	1.376095	-1.138641
H	0.891412	-1.376095	-1.138641
H	-0.891412	-1.376095	-1.138641
H	0.000000	-2.304501	0.078799

Molecule# 0256

dimethylsulfone

PointGroup: C2v

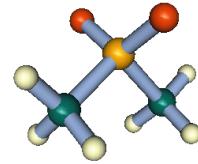
E= -628.559493926 au

ZPE= 0.084589 au

LUMO_eps= -0.02465 au

HOMO_eps= -0.30195 au

Dipole= 4.722 debye



11

C	0.000000	1.419305	-0.919648
C	0.000000	-1.419305	-0.919648
O	-1.263521	0.000000	0.917477
O	1.263521	0.000000	0.917477
S	0.000000	0.000000	0.188195
H	0.000000	2.292780	-0.271559
H	0.900388	1.399538	-1.527965
H	-0.900388	1.399538	-1.527965
H	0.900388	-1.399538	-1.527965
H	0.000000	-2.292780	-0.271559
H	-0.900388	-1.399538	-1.527965

Molecule# 0257

dimethylsulfoxide

PointGroup: Cs

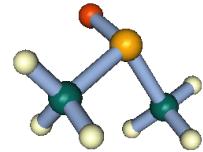
E= -553.306018178 au

ZPE= 0.078879 au

LUMO_eps= -0.01797 au

HOMO_eps= -0.23905 au

Dipole= 4.125 debye



10

C	-0.259600	-0.785887	1.366100
C	-0.259600	-0.785887	-1.366100
O	1.100868	1.072126	0.000000
S	-0.259600	0.429008	0.000000
H	-0.208786	-0.213648	2.289139
H	0.618458	-1.422179	1.270379
H	-1.178748	-1.369415	1.337781
H	-1.178748	-1.369415	-1.337781
H	0.618458	-1.422179	-1.270379
H	-0.208786	-0.213648	-2.289139

Molecule# 0258

dioxathiolane

PointGroup: C1

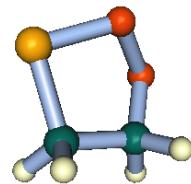
E= -627.258256445 au

ZPE= 0.063700 au

LUMO_eps= -0.05372 au

HOMO_eps= -0.23926 au

Dipole= 3.327 debye



9

S	1.236970	0.049907	-0.108638
O	0.170344	-1.178406	0.365430
O	-1.065349	-0.869992	-0.353876
C	-0.081416	1.306104	0.072269
C	-1.371008	0.445059	0.086653
H	-0.029247	1.976188	-0.782424
H	0.016390	1.873792	0.994257
H	-2.117419	0.815604	-0.614952
H	-1.786663	0.416113	1.095372

Molecule# 0259

dioxirane

PointGroup: C2v

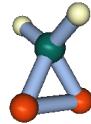
E= -189.697504399 au

ZPE= 0.032458 au

LUMO_eps= -0.05377 au

HOMO_eps= -0.29241 au

Dipole= 2.551 debye



5

C 0.000000 0.000000 0.731328

H 0.926417 0.000000 1.301629

H -0.926417 0.000000 1.301629

O 0.000000 0.749219 -0.436952

O 0.000000 -0.749219 -0.436952

Molecule# 0260

diphenylsulfoxide

PointGroup: C1

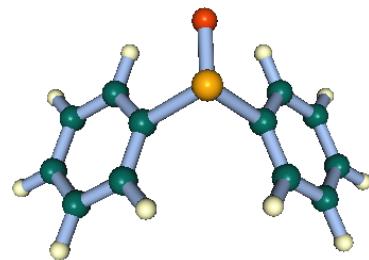
E= -936.901315118 au

ZPE= 0.185635 au

LUMO_eps= -0.04918 au

HOMO_eps= -0.24036 au

Dipole= 4.022 debye



24

S	0.000000	1.198969	-1.022088
O	-0.000019	2.525292	-0.313898
C	-1.379883	0.233902	-0.310543
C	-1.827639	-0.916094	-0.948304
C	-2.903944	-1.613131	-0.411977
C	-3.530081	-1.148516	0.740491
C	-3.084519	0.016906	1.355299
C	-2.005880	0.718377	0.827890
C	1.379888	0.233926	-0.310531
C	2.005793	0.718340	0.827976
C	3.084431	0.016873	1.355398
C	3.530079	-1.148482	0.740528
C	2.904037	-1.613032	-0.412019
C	1.827738	-0.915998	-0.948359
H	-1.351533	-1.264663	-1.855542
H	-3.259487	-2.510929	-0.899140
H	-4.371765	-1.688895	1.151883
H	-3.580077	0.384290	2.243835
H	-1.652216	1.637972	1.273661
H	1.652066	1.637890	1.273792
H	3.579920	0.384210	2.243992
H	4.371760	-1.688857	1.151931
H	3.259655	-2.510772	-0.899234
H	1.351714	-1.264502	-1.855665

Molecule# 0261

dipropargylnitrosamine

PointGroup: C1

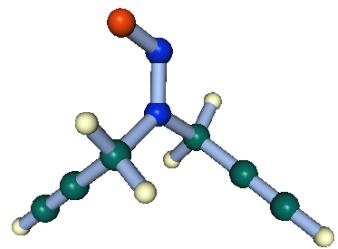
E= -416.907116721 au

ZPE= 0.107925 au

LUMO_eps= -0.05915 au

HOMO_eps= -0.24996 au

Dipole= 3.534 debye



15

O	1.240989	2.316707	-0.287642
N	0.074392	0.539266	0.153552
N	0.338574	1.835872	0.364116
C	-1.018081	-0.017513	0.938595
C	0.805026	-0.270810	-0.823168
C	-2.168330	-0.409668	0.125287
C	1.525451	-1.378278	-0.205251
C	-3.106676	-0.740595	-0.542391
C	2.105048	-2.294984	0.304845
H	-0.653615	-0.880360	1.501749
H	-1.300451	0.756689	1.652149
H	1.494721	0.413664	-1.317408
H	0.099799	-0.648227	-1.567386
H	-3.943385	-1.027237	-1.129310
H	2.629621	-3.103060	0.750177

Molecule# 0262

dipropyl sulfoxide

PointGroup: C1

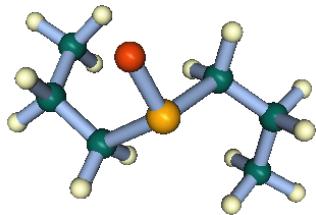
E= -710.612179804 au

ZPE= 0.193015 au

LUMO_eps= -0.01694 au

HOMO_eps= -0.22803 au

Dipole= 4.047 debye



22

C	-2.486191	-0.072064	0.552450
C	-1.024223	0.142152	0.935317
S	-0.047098	0.993348	-0.402402
O	0.947086	1.893124	0.293391
C	-2.714523	-1.122271	-0.534399
C	0.925143	-0.441946	-1.093699
C	2.275145	-0.662317	-0.419059
C	2.229720	-1.279940	0.977069
H	-2.917557	0.881786	0.239294
H	-3.024646	-0.367002	1.456918
H	-0.533523	-0.786746	1.217820
H	-0.928225	0.849831	1.758194
H	-2.255162	-0.831273	-1.480484
H	-2.300045	-2.089896	-0.243556
H	-3.779511	-1.261717	-0.720802
H	1.067876	-0.172666	-2.140309
H	0.277509	-1.317972	-1.055491
H	2.793803	0.296174	-0.372767
H	2.859562	-1.304564	-1.083624
H	1.774757	-0.601276	1.697093
H	1.672070	-2.219643	0.985066
H	3.239545	-1.495279	1.327871

Molecule# 0263

dipropylamine

PointGroup: Cs

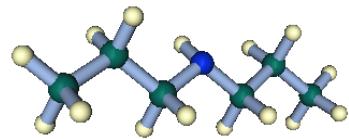
E= -292.540366159 au

ZPE= 0.205334 au

LUMO_eps= -0.01100 au

HOMO_eps= -0.22569 au

Dipole= 0.799 debye



22

C	0.002905	-0.287931	3.765494
C	0.002905	-0.287931	-3.765494
C	0.002905	0.516132	2.466843
C	0.002905	0.516132	-2.466843
C	0.019045	-0.366124	1.223486
C	0.019045	-0.366124	-1.223486
N	0.041090	0.425929	0.000000
H	-0.869191	-0.941707	3.829272
H	0.892625	-0.916399	3.840202
H	-0.011524	0.368209	4.636319
H	0.892625	-0.916399	-3.840202
H	-0.869191	-0.941707	-3.829272
H	-0.011524	0.368209	-4.636319
H	0.868617	1.180978	2.434926
H	-0.882182	1.160098	2.437277
H	-0.882182	1.160098	-2.437277
H	0.868617	1.180978	-2.434926
H	-0.839000	-1.059882	1.257260
H	0.917482	-0.990937	1.233278
H	0.917482	-0.990937	-1.233278
H	-0.839000	-1.059882	-1.257260
H	-0.739557	1.072851	0.000000

Molecule# 0264

dispiro[2.0.2.1]heptane

PointGroup: C2v

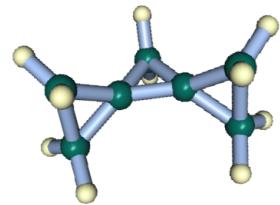
E= -272.748147336 au

ZPE= 0.147816 au

LUMO_eps= -0.00774 au

HOMO_eps= -0.26924 au

Dipole= 0.012 debye



17

C	0.000000	0.728728	0.184208
C	-0.763274	1.830763	-0.441725
C	0.763274	1.830763	-0.441725
C	0.000000	-0.728728	0.184208
C	0.000000	0.000000	1.493939
C	-0.763274	-1.830763	-0.441725
C	0.763274	-1.830763	-0.441725
H	-1.265756	2.542902	0.199945
H	-1.265398	1.641386	-1.381956
H	1.265756	2.542902	0.199945
H	1.265398	1.641386	-1.381956
H	-0.913191	0.000000	2.077660
H	0.913191	0.000000	2.077660
H	-1.265398	-1.641386	-1.381956
H	-1.265756	-2.542902	0.199945
H	1.265398	-1.641386	-1.381956
H	1.265756	-2.542902	0.199945

Molecule# 0265

disulfanylacetic acid

PointGroup: C1

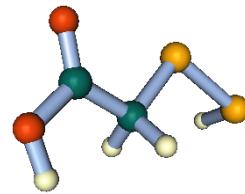
E= -1025.623332800 au

ZPE= 0.062588 au

LUMO_eps= -0.05108 au

HOMO_eps= -0.26299 au

Dipole= 4.545 debye



10

S	-0.802200	0.738403	0.006465
S	-2.555014	-0.375391	-0.096171
O	2.866754	-0.880415	-0.028233
O	2.068290	1.188928	0.002883
C	0.458292	-0.598704	0.045623
C	1.844967	0.013992	0.003269
H	0.311493	-1.260107	-0.808448
H	0.346394	-1.185656	0.958254
H	2.539718	-1.788027	-0.031196
H	-2.782096	-0.534219	1.226126

Molecule# 0266

dithiolane-3,5-diimine

PointGroup: C1

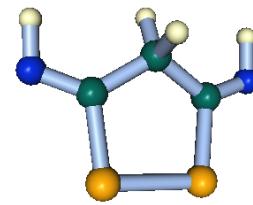
E= -1022.736538050 au

ZPE= 0.072649 au

LUMO_eps= -0.06805 au

HOMO_eps= -0.23403 au

Dipole= 3.186 debye



11

S	-1.060866	-1.182537	0.010069
S	1.060865	-1.182537	0.010062
N	-2.426341	1.041613	-0.216817
N	2.426343	1.041611	-0.216812
C	0.000000	1.355502	0.314245
C	-1.267395	0.594687	-0.001788
C	1.267396	0.594686	-0.001787
H	0.000000	1.557660	1.390467
H	0.000000	2.314713	-0.204060
H	-2.461028	2.058497	-0.168561
H	2.461031	2.058496	-0.168554

Molecule# 0267

dithiooxamide

PointGroup: C1

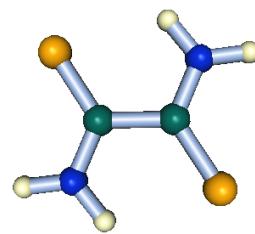
E= -984.666681744 au

ZPE= 0.069238 au

LUMO_eps= -0.10748 au

HOMO_eps= -0.23158 au

Dipole= 0.000 debye



10

S	2.159288	0.225879	-0.000022
S	-2.159288	-0.225879	-0.000022
N	0.380905	-1.736090	0.000033
N	-0.380905	1.736090	0.000033
C	0.630428	-0.433440	0.000013
C	-0.630428	0.433440	0.000008
H	1.142640	-2.391307	0.000019
H	-0.586716	-2.040345	0.000035
H	0.586717	2.040345	0.000036
H	-1.142640	2.391307	0.000026

Molecule# 0268

divinylsulfide

PointGroup: C2

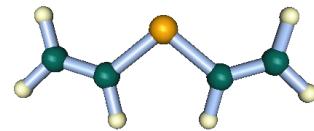
E= -554.272686284 au

ZPE= 0.084967 au

LUMO_eps= -0.01717 au

HOMO_eps= -0.21791 au

Dipole= 1.056 debye



11

S	0.000000	0.000000	0.622694
C	0.000000	1.368102	-0.488687
C	0.000000	-1.368102	-0.488687
C	0.070431	2.637301	-0.102333
C	-0.070431	-2.637301	-0.102333
H	-0.074147	1.103676	-1.536088
H	0.074147	-1.103676	-1.536088
H	0.052949	3.429596	-0.836759
H	0.143817	2.926289	0.937418
H	-0.052949	-3.429596	-0.836759
H	-0.143817	-2.926289	0.937418

Molecule# 0269

E-1-chloro-1-butene

PointGroup: C1

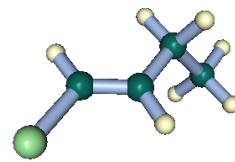
E= -616.919507369 au

ZPE= 0.099213 au

LUMO_eps= -0.01727 au

HOMO_eps= -0.25651 au

Dipole= 2.123 debye



12

H	0.284273	-0.845671	1.087487
C	0.403159	-0.010172	0.405810
H	-0.632701	1.282616	-0.927159
Cl	-2.268012	-0.194803	-0.026317
C	-0.658000	0.458163	-0.230058
H	1.762492	1.394082	-0.449259
H	2.138737	0.922123	1.195638
C	1.787551	0.540851	0.231531
H	3.784823	-0.084931	-0.358058
H	2.833963	-1.363785	0.395683
H	2.491345	-0.877346	-1.263208
C	2.782835	-0.508081	-0.279571

Molecule# 0270

E-1-chloro-1-propene

PointGroup: Cs

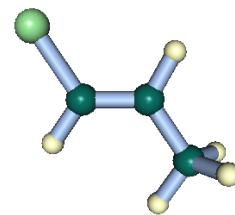
E= -577.591590938 au

ZPE= 0.070616 au

LUMO_eps= -0.01230 au

HOMO_eps= -0.25688 au

Dipole= 2.059 debye



9

C	0.000000	0.452712	0.000000
C	0.928558	-0.489343	0.000000
C	2.397943	-0.202796	0.000000
Cl	-1.714743	0.109952	0.000000
H	0.209814	1.512034	0.000000
H	0.622206	-1.529082	0.000000
H	2.601687	0.867563	0.000000
H	2.878957	-0.641565	0.877384
H	2.878957	-0.641565	-0.877384

Molecule# 0271

E-1-chloro-3-(chloroamino)oxyprop-1-ene

PointGroup: C1

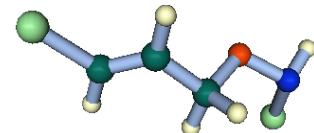
E= -1167.754905640 au

ZPE= 0.082865 au

LUMO_eps= -0.06858 au

HOMO_eps= -0.27617 au

Dipole= 0.974 debye



12

C1	-3.711306	-0.250025	-0.222443
C1	3.245768	-0.766998	-0.070147
O	1.080001	0.724444	-0.457102
N	2.390823	0.873305	-0.035920
C	0.233303	0.411497	0.671316
C	-1.182193	0.586458	0.237594
C	-2.040512	-0.420694	0.228155
H	0.492240	1.094323	1.483319
H	0.434639	-0.612867	0.990518
H	-1.495582	1.578817	-0.060378
H	-1.781946	-1.432223	0.504925
H	2.825450	1.289086	-0.858485

Molecule# 0272

E-1,2-dichloroethene

PointGroup: C2h

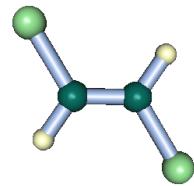
E= -997.887689596 au

ZPE= 0.033683 au

LUMO_eps= -0.03670 au

HOMO_eps= -0.26689 au

Dipole= 0.000 debye



6

C -0.364902 0.550673 0.000000

C 0.364902 -0.550673 0.000000

Cl 0.364902 2.127712 0.000000

Cl -0.364902 -2.127712 0.000000

H -1.443008 0.559873 0.000000

H 1.443008 -0.559873 0.000000

Molecule# 0273

E-1,2-difluoroethene

PointGroup: C2h

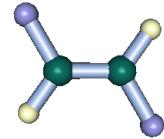
E= -277.167587660 au

ZPE= 0.036558 au

LUMO_eps= -0.01136 au

HOMO_eps= -0.27476 au

Dipole= 0.000 debye



6

C -0.332378 0.570025 0.000000

C 0.332378 -0.570025 0.000000

F 0.332378 1.740937 0.000000

F -0.332378 -1.740937 0.000000

H -1.407427 0.668528 0.000000

H 1.407427 -0.668528 0.000000

Molecule# 0274

E-1,2,3-trifluoropropene

PointGroup: C1

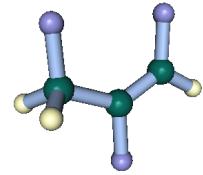
E= -415.768193812 au

ZPE= 0.057343 au

LUMO_eps= -0.01359 au

HOMO_eps= -0.27179 au

Dipole= 1.532 debye



9

C	0.146734	-1.257992	-0.001003
F	1.486654	-1.231502	0.002109
H	-0.279000	-2.250688	-0.004801
C	-0.595977	-0.163277	0.000497
F	-1.944444	-0.328243	-0.001783
C	-0.254498	1.291824	0.004837
F	1.109404	1.503367	-0.004948
H	-0.674434	1.763787	0.897350
H	-0.688638	1.770979	-0.876947

Molecule# 0275

E-1,3-hexadiene

PointGroup: Cs

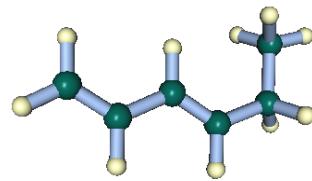
E= -234.718192786 au

ZPE= 0.141661 au

LUMO_eps= -0.03035 au

HOMO_eps= -0.22969 au

Dipole= 0.844 debye



16

H	-0.081998	3.962781	0.000000
H	1.401922	2.867737	0.000000
C	0.322716	2.960628	0.000000
H	-1.546765	2.025344	0.000000
C	-0.469613	1.886059	0.000000
H	1.076131	0.373269	0.000000
C	0.000000	0.512043	0.000000
H	-1.883157	-0.373116	0.000000
C	-0.810602	-0.551298	0.000000
H	-0.872163	-2.479687	0.867089
H	-0.872163	-2.479687	-0.867089
C	-0.407996	-1.995454	0.000000
H	1.273015	-3.356046	0.000000
H	1.577427	-1.862279	-0.881724
H	1.577427	-1.862279	0.881724
C	1.090549	-2.281317	0.000000

Molecule# 0276

E-1,3-pentadiene

PointGroup: Cs

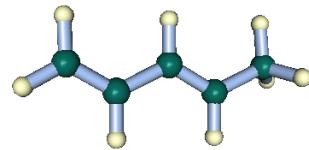
E= -195.391230495 au

ZPE= 0.112877 au

LUMO_eps= -0.03230 au

HOMO_eps= -0.23091 au

Dipole= 0.705 debye



13

C	-2.410690	0.780868	0.000000
C	-1.408259	-0.101026	0.000000
C	0.000000	0.249530	0.000000
C	0.998002	-0.639690	0.000000
C	2.453681	-0.304012	0.000000
H	-2.224937	1.847997	0.000000
H	-3.443962	0.464039	0.000000
H	-1.639093	-1.162269	0.000000
H	0.236275	1.310487	0.000000
H	0.747222	-1.697270	0.000000
H	2.617556	0.773488	0.000000
H	2.955266	-0.725245	0.875717
H	2.955266	-0.725245	-0.875717

Molecule# 0277

E-1,3,3-trifluoropropene

PointGroup: Cs

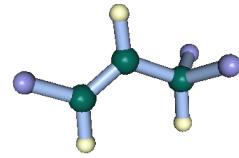
E= -415.791324898 au

ZPE= 0.057730 au

LUMO_eps= -0.03461 au

HOMO_eps= -0.30380 au

Dipole= 1.858 debye



9

C	-0.154478	1.510212	0.000000
H	-1.217229	1.713662	0.000000
F	0.576176	2.632653	0.000000
C	0.400564	0.312634	0.000000
H	1.474625	0.185038	0.000000
C	-0.438047	-0.911202	0.000000
H	-1.510614	-0.713266	0.000000
F	-0.154478	-1.686065	1.097573
F	-0.154478	-1.686065	-1.097573

Molecule# 0278

E-1,3,5-hexatriene

PointGroup: C2h

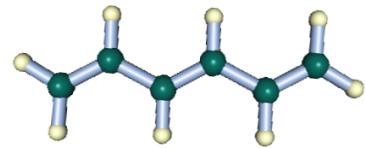
E= -233.492530042 au

ZPE= 0.118367 au

LUMO_eps= -0.06086 au

HOMO_eps= -0.22348 au

Dipole= 0.000 debye



14

C	1.188032	2.829092	0.000000
C	-1.188032	-2.829092	0.000000
C	1.188032	1.492100	0.000000
C	-1.188032	-1.492100	0.000000
C	-0.002470	0.672860	0.000000
C	0.002470	-0.672860	0.000000
H	2.108575	3.395117	0.000000
H	0.264255	3.394397	0.000000
H	-2.108575	-3.395117	0.000000
H	-0.264255	-3.394397	0.000000
H	2.137085	0.964589	0.000000
H	-2.137085	-0.964589	0.000000
H	-0.955353	1.194813	0.000000
H	0.955353	-1.194813	0.000000

Molecule# 0279

E-1,4-hexadiene

PointGroup: C1

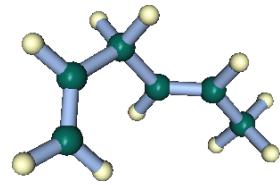
E= -234.710350945 au

ZPE= 0.141021 au

LUMO_eps= -0.00862 au

HOMO_eps= -0.25133 au

Dipole= 0.482 debye



16

C	2.774263	0.471453	0.018406
H	3.025428	1.225242	-0.732402
H	2.694425	0.968642	0.985285
H	3.620197	-0.219765	0.061021
C	1.508736	-0.244855	-0.337967
H	1.506561	-0.764857	-1.293079
C	0.414083	-0.292101	0.413417
H	0.408451	0.231044	1.366497
C	-0.843677	-1.027566	0.061292
H	-0.699053	-1.585556	-0.870041
H	-1.042235	-1.789762	0.825223
C	-2.083249	-0.179059	-0.069246
H	-3.009282	-0.738490	-0.164929
C	-2.134346	1.146986	-0.084084
H	-3.075965	1.668839	-0.188328
H	-1.243382	1.755515	-0.000158

Molecule# 0280

E-2-butene

PointGroup: C2h

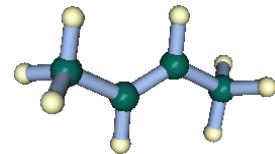
E= -157.290798030 au

ZPE= 0.107440 au

LUMO_eps= -0.00657 au

HOMO_eps= -0.24682 au

Dipole= 0.000 debye



12

C	-0.323065	0.580595	0.000000
C	0.323065	-0.580595	0.000000
C	0.323065	1.931514	0.000000
C	-0.323065	-1.931514	0.000000
H	-1.410554	0.569817	0.000000
H	1.410554	-0.569817	0.000000
H	0.024557	2.513142	0.876335
H	1.410604	1.854162	0.000000
H	0.024557	2.513142	-0.876335
H	-0.024557	-2.513142	0.876335
H	-1.410604	-1.854162	0.000000
H	-0.024557	-2.513142	-0.876335

Molecule# 0281

E-2-butenenitrile

PointGroup: Cs

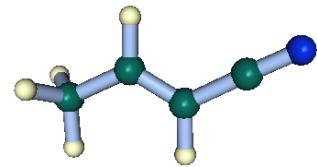
E= -210.235723059 au

ZPE= 0.078658 au

LUMO_eps= -0.05920 au

HOMO_eps= -0.28523 au

Dipole= 4.846 debye



10

H	2.655683	0.401193	0.000000
H	2.622682	-1.138527	0.875361
H	2.622682	-1.138527	-0.875361
C	2.242257	-0.606309	0.000000
H	0.256482	-1.562903	0.000000
C	0.752473	-0.598413	0.000000
H	0.451575	1.489847	0.000000
C	0.000000	0.504802	0.000000
N	-2.576635	0.473241	0.000000
C	-1.423506	0.472625	0.000000

Molecule# 0282

E-2-chloro-2-butene

PointGroup: Cs

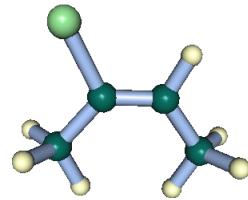
E= -616.924505665 au

ZPE= 0.098608 au

LUMO_eps= -0.01422 au

HOMO_eps= -0.24816 au

Dipole= 2.179 debye



12

C	-2.219388	-1.031508	0.000000
H	-2.709797	-0.060794	0.000000
H	-2.567570	-1.583635	0.876540
H	-2.567570	-1.583635	-0.876540
C	0.000000	0.174336	0.000000
H	-0.192077	-1.881945	0.000000
C	-0.724178	-0.938568	0.000000
H	-0.067567	2.120550	0.878325
H	-0.067567	2.120550	-0.878325
C	-0.449589	1.597487	0.000000
Cl	1.768594	0.022859	0.000000
H	-1.535021	1.669819	0.000000

Molecule# 0283

E-2-diazino-1,2-methylprop-2-enoxy-ethenolate

PointGroup: C1

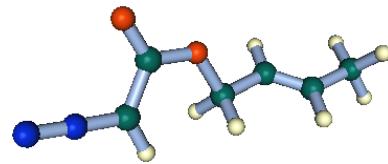
E= -493.522127924 au

ZPE= 0.136992 au

LUMO_eps= -0.07960 au

HOMO_eps= -0.26039 au

Dipole= 5.416 debye



18

O	-0.050156	0.740035	0.079572
O	1.936027	1.687629	-0.182327
N	3.213504	-0.696582	-0.044778
N	4.330864	-0.709304	-0.134489
C	1.298833	0.673982	-0.023993
C	1.909663	-0.650513	0.057625
C	-0.856529	-0.436953	0.311416
C	-2.276948	-0.004647	0.447772
C	-3.260722	-0.448114	-0.326484
C	-4.699726	-0.063453	-0.200434
H	1.420216	-1.598861	0.184598
H	-0.512068	-0.920689	1.230337
H	-0.746910	-1.133819	-0.522395
H	-2.482030	0.705676	1.242038
H	-3.020014	-1.148491	-1.122413
H	-5.062145	0.389855	-1.126289
H	-4.856995	0.645101	0.612065
H	-5.325023	-0.940694	-0.016433

Molecule# 0284

E-2-pentene

PointGroup: C1

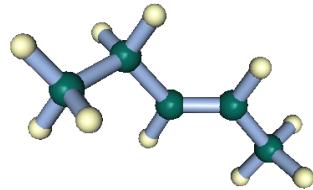
E= -196.618583381 au

ZPE= 0.136010 au

LUMO_eps= -0.00809 au

HOMO_eps= -0.24715 au

Dipole= 0.050 debye



15

C	1.170211	0.338779	0.232071
C	0.066000	-0.045993	-0.399570
C	2.527893	-0.268148	0.055662
C	-2.338851	-0.455053	0.271000
C	-1.295746	0.556611	-0.220194
H	1.103462	1.163582	0.937874
H	0.129624	-0.873234	-1.104350
H	3.251170	0.475143	-0.290413
H	2.510259	-1.084591	-0.666589
H	2.912006	-0.659771	1.001395
H	-3.323952	0.006212	0.354652
H	-2.066008	-0.853268	1.249121
H	-2.423715	-1.297719	-0.417841
H	-1.635193	0.971610	-1.175306
H	-1.234696	1.394857	0.477641

Molecule# 0285

E-2-pentenenitrile

PointGroup: Cs

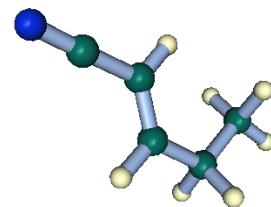
E= -249.563230594 au

ZPE= 0.107418 au

LUMO_eps= -0.05577 au

HOMO_eps= -0.28283 au

Dipole= 5.084 debye



13

N	-1.442941	2.799964	0.000000
C	-0.809520	1.836292	0.000000
H	1.068858	0.833466	0.000000
C	0.000000	0.664830	0.000000
H	-1.596381	-0.669835	0.000000
C	-0.516510	-0.567384	0.000000
H	-0.069250	-2.431965	0.866379
H	-0.069250	-2.431965	-0.866379
C	0.258117	-1.846322	0.000000
H	2.237470	-2.709684	0.000000
H	2.135946	-1.190903	-0.882660
H	2.135946	-1.190903	0.882660
C	1.777455	-1.722075	0.000000

Molecule# 0286

E-3-amino-3-oxo-1-propen-1-yl thiocyanate

PointGroup: C1

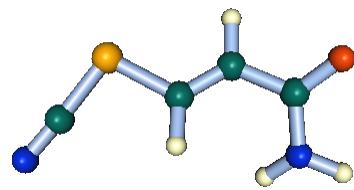
E= -737.884773926 au

ZPE= 0.078727 au

LUMO_eps= -0.07917 au

HOMO_eps= -0.27532 au

Dipole= 1.716 debye



12

S	-1.676534	-0.926064	0.051194
O	3.331516	-0.631562	-0.252865
N	2.397628	1.405048	0.103813
N	-3.577023	1.191000	-0.109127
C	1.020168	-0.608219	0.179875
C	2.350109	0.042718	0.002223
C	-0.149655	-0.019457	-0.048702
C	-2.785853	0.351530	-0.044843
H	1.086429	-1.657050	0.439278
H	-0.254458	1.009404	-0.361619
H	1.678256	1.917370	0.581658
H	3.309355	1.828033	0.050389

Molecule# 0287

E-3-bromoacrylic acid

PointGroup: Cs

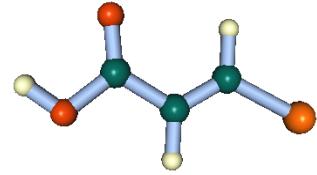
E= -2840.904875060 au

ZPE= 0.057561 au

LUMO_eps= -0.07929 au

HOMO_eps= -0.28427 au

Dipole= 1.137 debye



9

Br	-1.882364	0.535029	0.000000
O	2.696637	-1.863890	0.000000
O	2.849176	0.381701	0.000000
C	0.691544	-0.667087	0.000000
C	2.169010	-0.615182	0.000000
C	0.000000	0.465322	0.000000
H	0.218899	-1.637846	0.000000
H	0.473941	1.435314	0.000000
H	3.660057	-1.764272	0.000000

Molecule# 0288

E-3-chloroacryloyl chloride

PointGroup: Cs

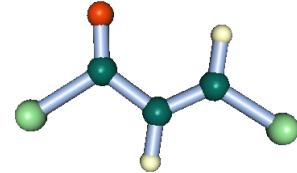
E= -1111.273086110 au

ZPE= 0.043642 au

LUMO_eps= -0.10567 au

HOMO_eps= -0.30588 au

Dipole= 2.368 debye



8

C1	2.462394	-0.834112	0.000000
C1	-2.210865	1.860330	0.000000
O	0.141352	-2.060501	0.000000
C	0.651704	-0.988993	0.000000
C	0.000000	0.327350	0.000000
C	-1.330710	0.383125	0.000000
H	0.617498	1.210825	0.000000
H	-1.950271	-0.501414	0.000000

Molecule# 0289

E-3-chloroprop-2-enenitrile

PointGroup: C1

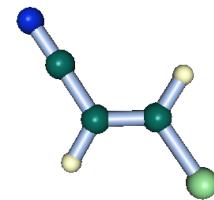
E= -630.530785680 au

ZPE= 0.041725 au

LUMO_eps= -0.08243 au

HOMO_eps= -0.29376 au

Dipole= 2.995 debye



7

C1 -2.048706 0.016035 -0.000004

N 3.079563 -0.194242 0.000006

C 0.597673 0.488341 0.000004

C -0.380235 -0.415943 -0.000003

C 1.964239 0.097426 0.000005

H 0.384661 1.548887 0.000008

H -0.203660 -1.480729 -0.000008

Molecule# 0290

E-3-methyl-2-pentene

PointGroup: C1

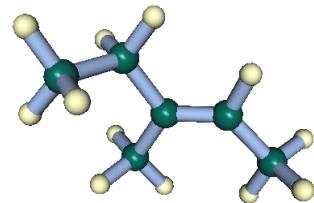
E= -235.947305876 au

ZPE= 0.163893 au

LUMO_eps= -0.01183 au

HOMO_eps= -0.23624 au

Dipole= 0.175 debye



18

C	-2.527968	-0.340410	0.248367
H	-2.845198	-0.840786	1.167646
H	-3.212398	-0.673991	-0.536560
H	-2.678013	0.728124	0.387385
C	-0.091832	1.594432	-0.057239
H	-1.098162	1.981097	0.081533
H	0.337517	2.085539	-0.935154
H	0.504466	1.914750	0.800675
C	2.353687	-0.333741	0.539518
H	2.021622	-0.818646	1.458831
H	2.559701	0.712205	0.768285
C	1.300293	-0.481395	-0.567402
H	1.676589	0.006126	-1.473854
H	1.184446	-1.539282	-0.809716
C	-1.113898	-0.703078	-0.090968
H	-0.948822	-1.766018	-0.246586
C	-0.053177	0.098298	-0.222235
H	3.295617	-0.793751	0.237267

Molecule# 0291

E-3-penten-1-yne

PointGroup: Cs

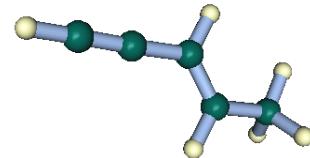
E= -194.134156418 au

ZPE= 0.088962 au

LUMO_eps= -0.03534 au

HOMO_eps= -0.24362 au

Dipole= 1.150 debye



11

C	-2.320917	-0.461628	0.000000
H	-2.746079	-0.959757	0.875622
H	-2.746079	-0.959757	-0.875622
H	-2.655927	0.575371	0.000000
C	-0.831837	-0.562138	0.000000
H	-0.407944	-1.560710	0.000000
C	0.000000	0.484435	0.000000
H	-0.409236	1.490531	0.000000
C	1.415974	0.385941	0.000000
C	2.618043	0.340629	0.000000
H	3.677687	0.290883	0.000000

Molecule# 0292

E-3-pentenenitrile

PointGroup: C1

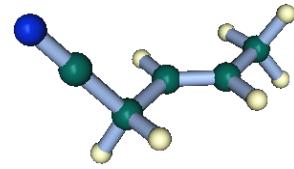
E= -249.560389100 au

ZPE= 0.106926 au

LUMO_eps= -0.01997 au

HOMO_eps= -0.27788 au

Dipole= 4.434 debye



13

H	3.609044	0.273076	0.113372
H	3.098636	-1.103376	-0.844452
H	2.741762	-1.060175	0.886842
C	2.803885	-0.454173	-0.016457
H	1.487319	0.854078	-1.202776
C	1.507467	0.229794	-0.313018
H	0.395283	-0.497491	1.305299
C	0.405132	0.126989	0.418299
C	-0.883366	0.846575	0.103693
N	-2.901787	-0.791599	-0.168867
C	-2.016649	-0.066647	-0.054156
H	-0.780939	1.432476	-0.811185
H	-1.137406	1.547375	0.904805

Molecule# 0293

E-5-azido-1-chloro-1-penten-3-yne

PointGroup: C1

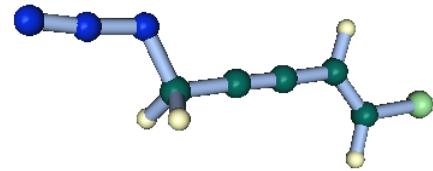
E= -817.405174439 au

ZPE= 0.084162 au

LUMO_eps= -0.05677 au

HOMO_eps= -0.25173 au

Dipole= 1.765 debye



13

C1	4.447941	-0.116167	0.000012
N	-3.025270	-0.496796	-0.000055
N	-4.225241	-0.238014	-0.000076
N	-5.349023	-0.121568	-0.000107
C	-2.135877	0.693862	0.000077
C	-0.744389	0.279137	0.000046
C	0.418235	-0.030637	0.000023
C	1.770768	-0.449000	-0.000006
C	2.794415	0.405041	0.000048
H	-2.339149	1.308733	-0.883213
H	-2.339163	1.308547	0.883494
H	1.960606	-1.516013	-0.000076
H	2.680539	1.477792	0.000117

Molecule# 0294

E-azodioxymethane

PointGroup: C2h

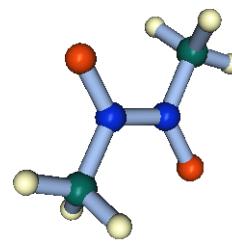
E= -339.768029926 au

ZPE= 0.093761 au

LUMO_eps= -0.06299 au

HOMO_eps= -0.22309 au

Dipole= 0.000 debye



12

N	-0.059500	0.647189	0.000000
N	0.059500	-0.647189	0.000000
O	-1.192188	1.211304	0.000000
O	1.192188	-1.211304	0.000000
C	1.192188	1.415406	0.000000
C	-1.192188	-1.415406	0.000000
H	0.895007	2.456379	0.000000
H	1.774488	1.156491	0.882046
H	1.774488	1.156491	-0.882046
H	-0.895007	-2.456379	0.000000
H	-1.774488	-1.156491	0.882046
H	-1.774488	-1.156491	-0.882046

Molecule# 0295

E-dimethyldiazine

PointGroup: Ci

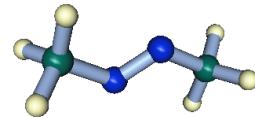
E= -189.351798445 au

ZPE= 0.084023 au

LUMO_eps= -0.04384 au

HOMO_eps= -0.23454 au

Dipole= 0.000 debye



10

C	-1.792925	0.132342	-0.066839
N	-0.414567	-0.229123	-0.392738
N	0.414567	0.229123	0.392738
C	1.792925	-0.132342	0.066839
H	-2.215579	0.652316	-0.927812
H	-1.855580	0.753706	0.827894
H	-2.359533	-0.790722	0.064186
H	2.215579	-0.652316	0.927812
H	1.855580	-0.753706	-0.827894
H	2.359533	0.790722	-0.064186

Molecule# 0296

E-E-2,4-hexadiene

PointGroup: C2h

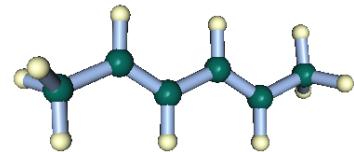
E= -234.724472470 au

ZPE= 0.140800 au

LUMO_eps= -0.02259 au

HOMO_eps= -0.21952 au

Dipole= 0.000 debye



16

C	-0.321563	-3.165600	0.000000
C	0.321563	3.165600	0.000000
C	0.321563	0.650169	0.000000
C	-0.321563	-0.650169	0.000000
C	-0.327188	1.819192	0.000000
C	0.327188	-1.819192	0.000000
H	-1.408837	-3.086565	0.000000
H	1.408837	3.086565	0.000000
H	-0.023595	-3.749001	0.875844
H	-0.023595	-3.749001	-0.875844
H	0.023595	3.749001	0.875844
H	0.023595	3.749001	-0.875844
H	1.408805	0.652661	0.000000
H	-1.408805	-0.652661	0.000000
H	-1.414062	1.807646	0.000000
H	1.414062	-1.807646	0.000000

Molecule# 0297

E-hept-2-ene

PointGroup: C1

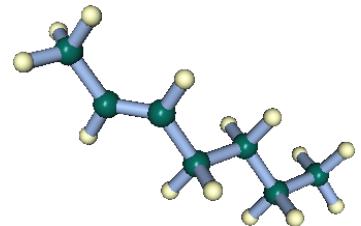
E= -275.274816727 au

ZPE= 0.192644 au

LUMO_eps= -0.00835 au

HOMO_eps= -0.24593 au

Dipole= 0.051 debye



21

C	2.441663	0.162598	-0.365182
C	1.385172	0.126631	0.440416
C	3.766263	-0.479321	-0.089056
C	-3.620200	-0.583267	-0.136932
C	0.056507	0.764266	0.164386
C	-2.466044	0.416907	-0.102935
C	-1.104645	-0.239625	0.126643
H	2.358643	0.700966	-1.306573
H	1.466900	-0.412762	1.382304
H	4.569757	0.262058	-0.075544
H	4.024236	-1.204082	-0.865896
H	3.767683	-0.996869	0.870489
H	-3.485464	-1.314681	-0.936498
H	-3.692335	-1.134107	0.803175
H	-4.576083	-0.084249	-0.302393
H	-0.155903	1.508409	0.940995
H	0.100952	1.309497	-0.782195
H	-2.646373	1.155223	0.684348
H	-2.441268	0.977092	-1.042548
H	-1.127620	-0.800201	1.066921
H	-0.915420	-0.975427	-0.660622

Molecule# 0298

E-hex-2-en-4-yne

PointGroup: C1

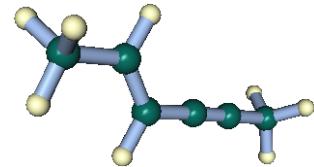
E= -233.473083643 au

ZPE= 0.117123 au

LUMO_eps= -0.02338 au

HOMO_eps= -0.22840 au

Dipole= 0.263 debye



14

C	-0.679556	0.246701	0.000059
C	-1.868935	0.053330	-0.000014
C	0.712990	0.524010	0.000070
C	1.678405	-0.401807	0.000097
C	-3.302324	-0.193398	-0.000060
C	3.141388	-0.102342	-0.000083
H	0.991810	1.574332	0.000000
H	1.392525	-1.448439	0.000167
H	-3.608764	-0.738322	0.895198
H	-3.862184	0.743039	-0.028117
H	-3.600383	-0.786260	-0.867207
H	3.630920	-0.536953	-0.875960
H	3.631186	-0.536992	0.875622
H	3.333073	0.970625	-0.000115

Molecule# 0299

E-hex-2-enal

PointGroup: C1

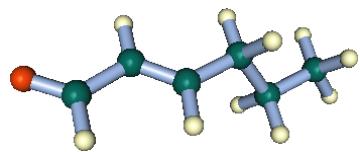
E= -309.984889874 au

ZPE= 0.146185 au

LUMO_eps= -0.06803 au

HOMO_eps= -0.26164 au

Dipole= 4.454 debye



17

C	1.353737	-0.368467	0.037834
C	0.245113	0.262988	0.434823
C	2.645333	0.319343	-0.004122
C	-3.556610	-0.151254	-0.231842
C	-1.123680	-0.325197	0.512772
C	-2.146913	0.421382	-0.360045
O	3.687325	-0.191449	-0.351651
H	1.345138	-1.409243	-0.265925
H	0.332449	1.309202	0.722433
H	2.616706	1.382207	0.314022
H	-3.585524	-1.200760	-0.530463
H	-3.915768	-0.089864	0.797239
H	-4.260573	0.392160	-0.862658
H	-1.094232	-1.380186	0.232496
H	-1.463655	-0.283003	1.554077
H	-2.152324	1.478782	-0.082114
H	-1.822698	0.379526	-1.402423

Molecule# 0300

E-hex-2-ene

PointGroup: C1

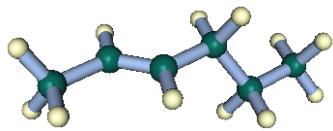
E= -235.946792268 au

ZPE= 0.164333 au

LUMO_eps= -0.00766 au

HOMO_eps= -0.24637 au

Dipole= 0.065 debye



18

C	3.184312	0.214662	-0.156388
C	1.804466	-0.364204	-0.216238
C	0.743151	0.105154	0.431736
C	-0.640500	-0.468565	0.368176
C	-1.685118	0.519417	-0.171606
C	-3.099443	-0.056883	-0.186480
H	3.223229	1.089985	0.492451
H	3.904316	-0.517661	0.218689
H	3.531684	0.512657	-1.149293
H	1.681810	-1.243047	-0.845147
H	0.864249	0.985574	1.060220
H	-0.950299	-0.782190	1.372044
H	-0.636597	-1.370501	-0.250054
H	-1.397617	0.823029	-1.181416
H	-1.666289	1.428500	0.436494
H	-3.819163	0.665084	-0.574592
H	-3.155216	-0.949735	-0.812711
H	-3.421316	-0.339183	0.818118

Molecule# 0301

E-hexa-1,5-diyne-3-ene

PointGroup: C2h

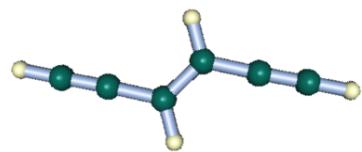
E= -230.975985516 au

ZPE= 0.070414 au

LUMO_eps= -0.07356 au

HOMO_eps= -0.24605 au

Dipole= 0.000 debye



10

C	-0.324304	0.589828	0.000000
C	0.324304	-0.589828	0.000000
C	0.324304	1.845570	0.000000
C	-0.324304	-1.845570	0.000000
H	-1.408272	0.599713	0.000000
H	1.408272	-0.599713	0.000000
C	0.841122	2.932151	0.000000
C	-0.841122	-2.932151	0.000000
H	1.305614	3.886246	0.000000
H	-1.305614	-3.886246	0.000000

Molecule# 0302

E-oct-2-enal

PointGroup: C1

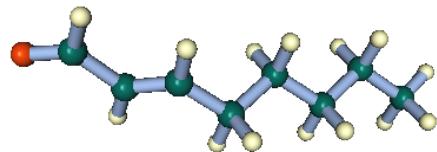
E= -388.641108346 au

ZPE= 0.202990 au

LUMO_eps= -0.06739 au

HOMO_eps= -0.26108 au

Dipole= 4.564 debye



23

C	2.611997	0.223827	-0.300825
C	1.549505	0.338129	0.501487
C	3.878275	-0.323343	0.188620
C	-4.786972	-0.124165	-0.302575
C	0.207729	0.863036	0.114332
C	-3.411591	-0.666545	0.081940
C	-0.908819	-0.183212	0.275038
C	-2.290909	0.359831	-0.087143
O	4.877910	-0.455105	-0.482993
H	2.582459	0.530856	-1.340266
H	1.654351	0.007675	1.533289
H	3.872769	-0.625229	1.256593
H	-5.051986	0.745375	0.302406
H	-5.564751	-0.875434	-0.160722
H	-4.810822	0.183879	-1.349781
H	-0.030363	1.722364	0.751305
H	0.231964	1.227423	-0.914648
H	-3.185367	-1.549033	-0.523759
H	-3.431941	-1.009179	1.120746
H	-0.917566	-0.545349	1.307622
H	-0.678207	-1.048957	-0.351592
H	-2.280124	0.713817	-1.123199
H	-2.508987	1.237280	0.530712

Molecule# 0303

E-pent-3-en-2-one

PointGroup: Cs

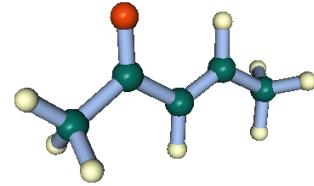
E= -270.664909185 au

ZPE= 0.116903 au

LUMO_eps= -0.06172 au

HOMO_eps= -0.25440 au

Dipole= 3.154 debye



14

C	0.000000	0.531086	0.000000
C	-1.331860	0.464679	0.000000
C	0.850788	-0.688356	0.000000
C	-2.260297	1.629509	0.000000
C	2.345543	-0.454617	0.000000
O	0.383363	-1.811009	0.000000
H	0.503575	1.491936	0.000000
H	-1.777905	-0.525425	0.000000
H	-1.728950	2.580430	0.000000
H	-2.916004	1.597195	0.874296
H	-2.916004	1.597195	-0.874296
H	2.872893	-1.404393	0.000000
H	2.635225	0.128660	0.877308
H	2.635225	0.128660	-0.877308

Molecule# 0304

ethane

PointGroup: D3d

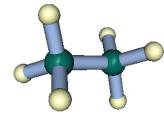
E= -79.864711301 au

ZPE= 0.074306 au

LUMO_eps= -0.00836 au

HOMO_eps= -0.34581 au

Dipole= 0.000 debye



8

C 0.000000 0.000000 0.763540

C 0.000000 0.000000 -0.763540

H 0.000000 1.016074 1.160929

H 0.000000 -1.016074 -1.160929

H -0.879946 -0.508037 1.160929

H 0.879946 0.508037 -1.160929

H 0.879946 -0.508037 1.160929

H -0.879946 0.508037 -1.160929

Molecule# 0305

ethanedial

PointGroup: C2h

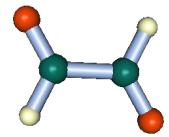
E= -227.914322042 au

ZPE= 0.036836 au

LUMO_eps= -0.12818 au

HOMO_eps= -0.28344 au

Dipole= 0.000 debye



6

C	-0.327410	0.688228	0.000000
C	0.327410	-0.688228	0.000000
H	-1.432549	0.678671	0.000000
H	1.432549	-0.678671	0.000000
O	0.327410	1.696141	0.000000
O	-0.327410	-1.696141	0.000000

Molecule# 0306

ethanethioamide

PointGroup: C1

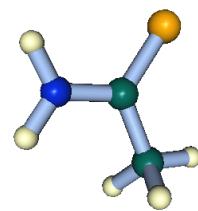
E= -532.263189177 au

ZPE= 0.071360 au

LUMO_eps= -0.04614 au

HOMO_eps= -0.21623 au

Dipole= 4.513 debye



9

C	-1.237894	-1.104197	-0.000349
C	-0.280575	0.059414	-0.004593
N	-0.872923	1.267541	0.000200
S	1.365722	-0.118344	0.000090
H	-1.971419	-1.006290	-0.804504
H	-0.698836	-2.036611	-0.119837
H	-1.784470	-1.132530	0.945767
H	-1.873504	1.369103	-0.005404
H	-0.302047	2.095742	0.010785

Molecule# 0307

ethanethiol

PointGroup: Cs

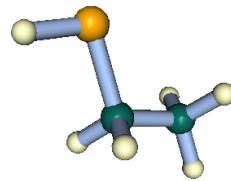
E= -478.085968371 au

ZPE= 0.074468 au

LUMO_eps= -0.01878 au

HOMO_eps= -0.24119 au

Dipole= 1.678 debye



9

C	1.516650	0.705578	0.000000
C	0.000000	0.834467	0.000000
S	-0.755427	-0.847361	0.000000
H	1.868133	0.170753	0.882762
H	1.868133	0.170753	-0.882762
H	1.975965	1.695046	0.000000
H	-0.341365	1.368763	-0.884290
H	-0.341365	1.368763	0.884290
H	-2.042577	-0.456566	0.000000

Molecule# 0308

ethanimine

PointGroup: Cs

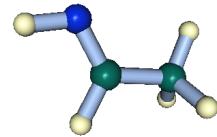
E= -134.011964309 au

ZPE= 0.068231 au

LUMO_eps= -0.01624 au

HOMO_eps= -0.27166 au

Dipole= 2.074 debye



8

C	-1.030686	-0.636526	0.000000
C	0.000000	0.445344	0.000000
N	1.241167	0.190751	0.000000
H	-0.556818	-1.615743	0.000000
H	-1.676866	-0.544559	0.876683
H	-1.676866	-0.544559	-0.876683
H	-0.389088	1.470939	0.000000
H	1.795584	1.045760	0.000000

Molecule# 0309

ethanol

PointGroup: C1

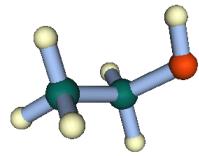
E= -155.110038792 au

ZPE= 0.079549 au

LUMO_eps= -0.01491 au

HOMO_eps= -0.28221 au

Dipole= 1.708 debye



9

C	-1.215127	-0.241882	-0.021159
C	0.077656	0.555024	0.046899
O	1.241995	-0.256233	-0.108913
H	-2.078754	0.421353	0.059053
H	-1.283191	-0.786082	-0.963270
H	-1.275073	-0.964301	0.796308
H	0.129488	1.119523	0.984758
H	0.123133	1.276394	-0.768848
H	1.273257	-0.895870	0.608864

Molecule# 0310

ethenamine

PointGroup: C1

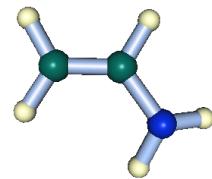
E= -134.008993238 au

ZPE= 0.068660 au

LUMO_eps= -0.01500 au

HOMO_eps= -0.21559 au

Dipole= 1.562 debye



8

C	1.249205	-0.196057	0.013814
C	0.069711	0.426754	-0.000397
N	-1.181689	-0.169404	-0.079242
H	1.330242	-1.275684	0.016682
H	2.164905	0.373573	0.006405
H	0.029960	1.509834	-0.008170
H	-1.221005	-1.153102	0.136560
H	-1.945772	0.347030	0.322711

Molecule# 0311

ethene

PointGroup: D2h

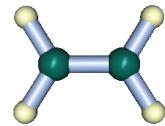
E= -78.624065047 au

ZPE= 0.050889 au

LUMO_eps= -0.01097 au

HOMO_eps= -0.28228 au

Dipole= 0.000 debye



6

C 0.000000 0.000000 0.662415

C 0.000000 0.000000 -0.662415

H 0.000000 0.920717 1.231649

H 0.000000 -0.920717 1.231649

H 0.000000 -0.920717 -1.231649

H 0.000000 0.920717 -1.231649

Molecule# 0312

ethenethione

PointGroup: Cs

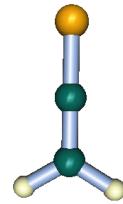
E= -475.621771990 au

ZPE= 0.029285 au

LUMO_eps= -0.08926 au

HOMO_eps= -0.23718 au

Dipole= 1.119 debye



5

S -0.000127 -1.112931 0.000000

C 0.000196 1.751740 0.000000

C 0.000000 0.447878 0.000000

H 0.000427 2.304594 0.929946

H 0.000427 2.304594 -0.929946

Molecule# 0313

ethenol

PointGroup: Cs

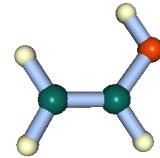
E= -153.881376928 au

ZPE= 0.056402 au

LUMO_eps= -0.01423 au

HOMO_eps= -0.24625 au

Dipole= 0.971 debye



7

C	1.211962	-0.100418	0.000000
C	0.000000	0.441434	0.000000
O	-1.190822	-0.218573	0.000000
H	1.366451	-1.172202	0.000000
H	2.084447	0.533775	0.000000
H	-0.160334	1.511121	0.000000
H	-1.035759	-1.170209	0.000000

Molecule# 0314

ethenylcyclopropane

PointGroup: Cs

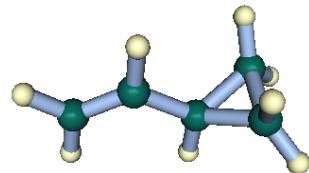
E= -195.369658854 au

ZPE= 0.114163 au

LUMO_eps= -0.00558 au

HOMO_eps= -0.24481 au

Dipole= 0.627 debye

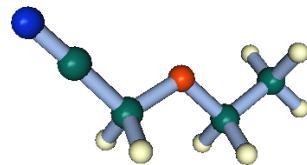


13

C	-0.252597	1.434985	0.748313
C	-0.252597	1.434985	-0.748313
C	0.389449	0.284544	0.000000
C	-0.252597	-1.039865	0.000000
C	0.387394	-2.205488	0.000000
H	0.401712	2.122298	1.265403
H	-1.185014	1.236819	1.258413
H	-1.185014	1.236819	-1.258413
H	0.401712	2.122298	-1.265403
H	1.471951	0.266496	0.000000
H	-1.339751	-1.036337	0.000000
H	1.469284	-2.259461	0.000000
H	-0.149199	-3.143904	0.000000

Molecule# 0315
ethoxyacetonitrile
PointGroup: Cs

E= -286.692980114 au
ZPE= 0.106542 au
LUMO_eps= -0.02425 au
HOMO_eps= -0.29560 au
Dipole= 4.898 debye



13

O	0.000000	0.357505	0.000000
H	0.720823	-1.378199	0.885457
H	0.720823	-1.378199	-0.885457
C	0.166852	-1.039701	0.000000
H	1.824588	0.770257	0.885970
H	1.824588	0.770257	-0.885970
C	1.244020	1.056932	0.000000
H	0.387071	2.824218	-0.883974
H	1.894071	3.101369	0.000000
H	0.387071	2.824218	0.883974
C	0.957977	2.542132	0.000000
N	-2.157411	-2.231286	0.000000
C	-1.145041	-1.688522	0.000000

Molecule# 0316

ethoxybenzene

PointGroup: Cs

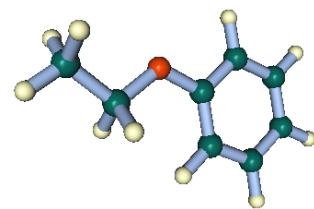
E= -386.236852570 au

ZPE= 0.160769 au

LUMO_eps= -0.01536 au

HOMO_eps= -0.22724 au

Dipole= 1.407 debye



19

C	2.782896	0.485045	0.000000
C	2.194136	-0.770352	0.000000
C	1.968374	1.616338	0.000000
C	0.807719	-0.912627	0.000000
C	0.589648	1.491986	0.000000
C	0.000000	0.224518	0.000000
C	-3.525326	-0.782670	0.000000
C	-2.036225	-1.053818	0.000000
O	-1.362668	0.203627	0.000000
H	3.859197	0.585368	0.000000
H	2.812468	-1.658314	0.000000
H	2.412071	2.603099	0.000000
H	0.376293	-1.901643	0.000000
H	-0.052598	2.361690	0.000000
H	-4.074153	-1.725007	0.000000
H	-3.814766	-0.215005	0.883932
H	-3.814766	-0.215005	-0.883932
H	-1.744865	-1.627360	-0.885629
H	-1.744865	-1.627360	0.885629

Molecule# 0317

ethoxyethane

PointGroup: C2v

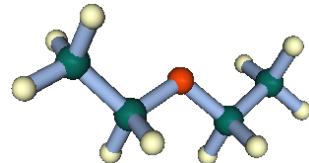
E= -233.759774105 au

ZPE= 0.135855 au

LUMO_eps= -0.00958 au

HOMO_eps= -0.26115 au

Dipole= 1.102 debye



15

C	0.000000	2.382161	0.411002
C	0.000000	-2.382161	0.411002
C	0.000000	1.185118	-0.517097
C	0.000000	-1.185118	-0.517097
O	0.000000	0.000000	0.260427
H	0.000000	3.307756	-0.166158
H	-0.883458	2.373885	1.049360
H	0.883458	2.373885	1.049360
H	0.000000	-3.307756	-0.166158
H	0.883458	-2.373885	1.049360
H	-0.883458	-2.373885	1.049360
H	0.884361	1.201870	-1.168850
H	-0.884361	1.201870	-1.168850
H	-0.884361	-1.201870	-1.168850
H	0.884361	-1.201870	-1.168850

Molecule# 0318

ethoxyethene

PointGroup: C1

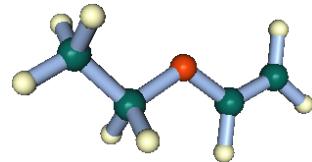
E= -232.527729505 au

ZPE= 0.112302 au

LUMO_eps= -0.01073 au

HOMO_eps= -0.23150 au

Dipole= 1.784 debye



13

C	2.445855	-0.294356	-0.000008
H	2.499430	-1.373583	0.000358
H	3.364930	0.269880	-0.000226
C	1.282938	0.346338	-0.000141
H	1.226582	1.430931	-0.000503
O	0.088531	-0.298764	0.000118
C	-1.073605	0.536374	0.000222
H	-1.057562	1.179175	-0.885919
H	-1.057825	1.178653	0.886755
C	-2.298114	-0.351311	-0.000172
H	-2.312414	-0.988238	-0.884210
H	-2.312552	-0.988828	0.883437
H	-3.201281	0.259848	-0.000035

Molecule# 0319

ethyl butanoate

PointGroup: C1

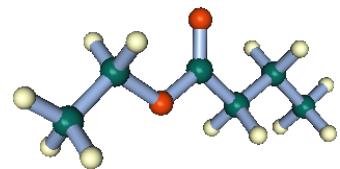
E= -386.489373213 au

ZPE= 0.174367 au

LUMO_eps= -0.01344 au

HOMO_eps= -0.27983 au

Dipole= 1.835 debye



20

C	0.075104	0.359100	0.000098
C	-3.701789	-0.602670	-0.000001
C	3.556061	-0.733886	-0.000152
C	-1.168900	-0.499935	0.000212
C	-2.468473	0.298186	-0.000293
C	2.452426	0.299222	0.000029
O	0.097456	1.565027	0.000074
O	1.188412	-0.404077	0.000059
H	-4.618593	-0.012460	-0.000388
H	-3.723582	-1.248219	-0.880573
H	-3.723777	-1.247370	0.881188
H	4.525714	-0.234679	-0.000156
H	3.498825	-1.368972	0.883727
H	3.498716	-1.368774	-0.884166
H	-1.114011	-1.161253	-0.869006
H	-1.114289	-1.160543	0.869994
H	-2.485329	0.956406	0.869828
H	-2.485160	0.955591	-0.871038
H	2.493919	0.941368	-0.879840
H	2.494054	0.941198	0.880017

Molecule# 0320

ethyl hexanoate

PointGroup: C1

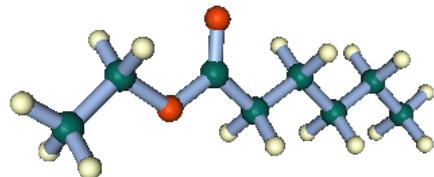
E= -465.145515195 au

ZPE= 0.231047 au

LUMO_eps= -0.01323 au

HOMO_eps= -0.27929 au

Dipole= 1.788 debye



26

C	0.023324	-0.446803	-0.001938
C	-1.248311	0.370867	-0.000992
O	-1.311122	1.575337	-0.000848
C	1.295426	0.393952	0.000986
H	-0.011251	-1.111297	0.865725
H	-0.010002	-1.106796	-0.873123
O	-2.335846	-0.428912	-0.000518
C	-3.622317	0.232251	-0.000074
H	-3.685904	0.871725	-0.880589
H	-3.684388	0.873508	0.879239
C	-4.691361	-0.836651	0.001907
H	-5.676911	-0.369592	0.002210
H	-4.612492	-1.468437	0.886478
H	-4.613940	-1.470332	-0.881440
H	1.291757	1.055257	-0.868109
C	2.564097	-0.458735	-0.000991
H	1.291137	1.050182	0.873940
H	2.560871	-1.120937	0.871655
C	3.850414	0.368061	0.002127
H	2.561668	-1.115615	-0.877655
H	3.854143	1.028939	-0.869607
C	5.116582	-0.486575	-0.000026
H	3.853418	1.023461	0.877993
H	5.157271	-1.133612	0.878700
H	6.015118	0.131837	0.002416
H	5.158130	-1.127901	-0.882890

Molecule# 0321

ethyl pentanoate

PointGroup: Cs

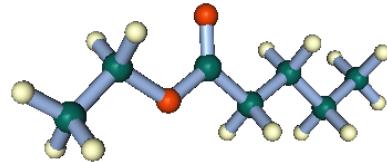
E= -425.817463076 au

ZPE= 0.202788 au

LUMO_eps= -0.01323 au

HOMO_eps= -0.27951 au

Dipole= 1.890 debye



23

C	0.000000	0.729498	0.000000
C	-2.141505	-3.891402	0.000000
C	2.549320	3.339800	0.000000
C	0.207382	-0.768043	0.000000
C	-0.847268	-3.079942	0.000000
C	-1.088975	-1.570401	0.000000
C	1.128138	2.824006	0.000000
O	-1.066056	1.293479	0.000000
O	1.183521	1.378692	0.000000
H	-2.746700	-3.667220	0.880566
H	-2.746700	-3.667220	-0.880566
H	-1.939443	-4.963233	0.000000
H	2.543948	4.430393	0.000000
H	3.089196	3.000657	0.883914
H	3.089196	3.000657	-0.883914
H	0.822926	-1.014904	-0.869453
H	0.822926	-1.014904	0.869453
H	-0.247536	-3.351756	0.874139
H	-0.247536	-3.351756	-0.874139
H	-1.685980	-1.291579	0.871119
H	-1.685980	-1.291579	-0.871119
H	0.574702	3.151987	-0.879985
H	0.574702	3.151987	0.879985

Molecule# 0322

ethyl propanoate

PointGroup: Cs

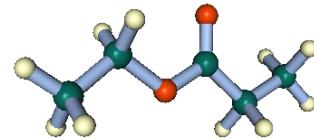
E= -347.161485988 au

ZPE= 0.146020 au

LUMO_eps= -0.01340 au

HOMO_eps= -0.28045 au

Dipole= 1.950 debye



17

C	0.000000	0.540816	0.000000
C	1.243175	2.751600	0.000000
C	-0.679664	-3.043361	0.000000
C	1.345131	1.232352	0.000000
C	-1.070032	-1.582821	0.000000
O	-1.072742	1.091993	0.000000
O	0.146706	-0.800498	0.000000
H	0.706894	3.109292	0.877772
H	2.237781	3.197410	0.000000
H	0.706894	3.109292	-0.877772
H	-1.577230	-3.662892	0.000000
H	-0.092760	-3.292082	-0.884003
H	-0.092760	-3.292082	0.884003
H	1.899563	0.870429	0.869102
H	1.899563	0.870429	-0.869102
H	-1.655657	-1.316641	0.880006
H	-1.655657	-1.316641	-0.880006

Molecule# 0323

ethylacetate

PointGroup: Cs

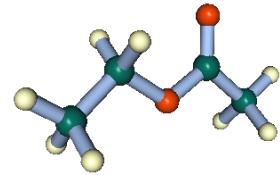
E= -307.833257244 au

ZPE= 0.117500 au

LUMO_eps= -0.01325 au

HOMO_eps= -0.28153 au

Dipole= 2.107 debye



14

C	0.909826	-0.524796	0.000000
C	2.312486	0.022275	0.000000
C	-2.229581	1.332555	0.000000
C	-1.391432	0.074275	0.000000
O	0.616627	-1.694503	0.000000
O	0.000000	0.471377	0.000000
H	2.468339	0.648836	0.878091
H	2.468339	0.648836	-0.878091
H	3.022001	-0.799004	0.000000
H	-3.287649	1.068275	0.000000
H	-2.028233	1.937197	0.884062
H	-2.028233	1.937197	-0.884062
H	-1.577685	-0.541093	-0.880090
H	-1.577685	-0.541093	0.880090

Molecule# 0324

ethylamine

PointGroup: Cs

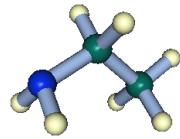
E= -135.234599111 au

ZPE= 0.092262 au

LUMO_eps= -0.01358 au

HOMO_eps= -0.24394 au

Dipole= 1.276 debye



10

C	1.217924	-0.353536	0.000000
C	0.000000	0.571510	0.000000
N	-1.306888	-0.088652	0.000000
H	1.220384	-0.996853	0.882589
H	1.220384	-0.996853	-0.882589
H	2.148415	0.218943	0.000000
H	0.037134	1.227011	-0.872854
H	0.037134	1.227011	0.872854
H	-1.411390	-0.683272	0.813701
H	-1.411390	-0.683272	-0.813701

Molecule# 0325

ethylbenzene

PointGroup: Cs

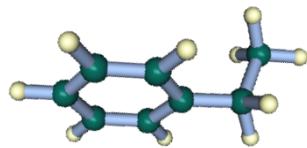
E= -310.994514418 au

ZPE= 0.156305 au

LUMO_eps= -0.01672 au

HOMO_eps= -0.24835 au

Dipole= 0.414 debye



18

C	0.232915	-2.318566	0.000000
C	0.234056	-1.617939	1.200385
C	0.234056	-1.617939	-1.200385
C	0.234056	-0.228276	1.197195
C	0.234056	-0.228276	-1.197195
C	0.231803	0.488886	0.000000
C	-1.235575	2.562053	0.000000
C	0.192517	1.998175	0.000000
H	0.236268	-3.400335	0.000000
H	0.239777	-2.153732	2.140626
H	0.239777	-2.153732	-2.140626
H	0.241085	0.308775	2.138169
H	0.241085	0.308775	-2.138169
H	-1.787127	2.229520	-0.880348
H	-1.223850	3.653141	0.000000
H	-1.787127	2.229520	0.880348
H	0.726399	2.374684	0.875281
H	0.726399	2.374684	-0.875281

Molecule# 0326

ethylcyclobutane

PointGroup: C1

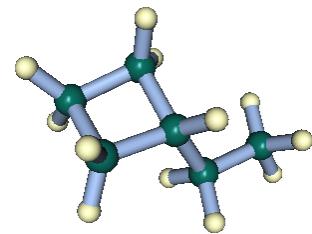
E= -235.929806715 au

ZPE= 0.166505 au

LUMO_eps= -0.00948 au

HOMO_eps= -0.29407 au

Dipole= 0.072 debye



18

C	2.426570	0.268454	-0.038318
H	2.760369	0.116017	0.990136
H	3.253108	0.001930	-0.698500
H	2.233139	1.334903	-0.166770
C	1.182111	-0.565869	-0.339346
H	1.417681	-1.627286	-0.214177
H	0.901208	-0.440117	-1.390298
C	-1.860514	0.318742	-0.486059
H	-2.881941	0.608681	-0.244065
H	-1.761084	0.301163	-1.570736
C	-0.724980	1.118216	0.203651
H	-1.069190	1.647720	1.091661
H	-0.170207	1.821261	-0.418230
C	-0.010079	-0.222816	0.548294
H	0.287769	-0.318234	1.594712
C	-1.322720	-0.972916	0.181963
H	-1.213766	-1.850521	-0.456380
H	-1.899417	-1.258384	1.061532

Molecule# 0327

ethylene diacetate

PointGroup: C2

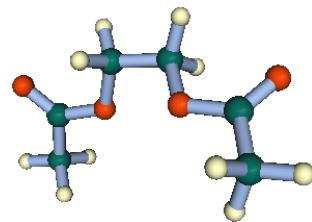
E= -535.798297294 au

ZPE= 0.160053 au

LUMO_eps= -0.01687 au

HOMO_eps= -0.28868 au

Dipole= 1.774 debye



20

C	-0.035271	2.693968	0.165692
C	0.035271	-2.693968	0.165692
C	-0.708324	3.282365	1.375353
C	0.708324	-3.282365	1.375353
C	0.235431	0.714142	-1.108083
C	-0.235431	-0.714142	-1.108083
O	0.708324	3.280261	-0.579645
O	-0.708324	-3.280261	-0.579645
O	-0.367648	1.393029	0.009128
O	0.367648	-1.393029	0.009128
H	-0.362315	2.770947	2.273853
H	-1.786580	3.138698	1.314018
H	-0.474667	4.340124	1.441134
H	0.362315	-2.770947	2.273853
H	1.786580	-3.138698	1.314018
H	0.474667	-4.340124	1.441134
H	-0.066747	1.203955	-2.034470
H	1.320178	0.776496	-1.028180
H	0.066747	-1.203955	-2.034470
H	-1.320178	-0.776496	-1.028180

Molecule# 0328

ethylenediamine

PointGroup: C2h

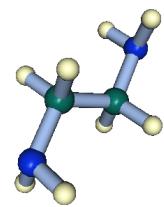
E= -190.604249690 au

ZPE= 0.110004 au

LUMO_eps= -0.01502 au

HOMO_eps= -0.23014 au

Dipole= 0.000 debye

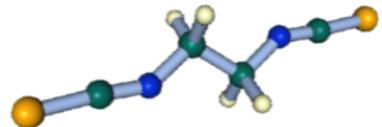


12

C	0.397467	0.657442	0.000000
C	-0.397467	-0.657442	0.000000
N	-0.397467	1.884333	0.000000
N	0.397467	-1.884333	0.000000
H	0.996875	-1.932923	0.815009
H	0.996875	-1.932923	-0.815009
H	-0.996875	1.932923	0.815009
H	-0.996875	1.932923	-0.815009
H	-1.053507	-0.679296	0.874859
H	-1.053507	-0.679296	-0.874859
H	1.053507	0.679296	0.874859
H	1.053507	0.679296	-0.874859

Molecule# 0329
ethylenediisothiocyanate
PointGroup: C1

E= -1060.866186550 au
ZPE= 0.078106 au
LUMO_eps= -0.05613 au
HOMO_eps= -0.26302 au
Dipole= 0.000 debye



12

S	-4.596838	-0.003107	-0.000137
S	4.596838	0.003103	-0.000056
N	-1.832054	-0.149686	0.000108
N	1.832054	0.149689	0.000098
C	-0.565103	0.514998	0.000097
C	0.565103	-0.514994	0.000093
C	-3.015809	-0.039311	-0.000005
C	3.015809	0.039311	0.000027
H	-0.483266	1.151721	0.883482
H	-0.483277	1.151723	-0.883288
H	0.483272	-1.151716	-0.883294
H	0.483270	-1.151720	0.883476

Molecule# 0330

ethylenedithiocyanate

PointGroup: C2

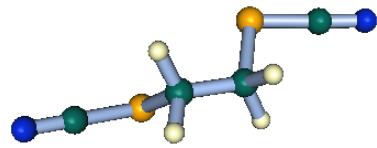
E= -1060.829809100 au

ZPE= 0.075437 au

LUMO_eps= -0.06818 au

HOMO_eps= -0.28632 au

Dipole= 1.609 debye



12

S	-0.485479	1.616939	-0.499622
S	0.485479	-1.616939	-0.499622
N	0.485479	4.238358	0.048550
N	-0.485479	-4.238358	0.048550
C	0.219813	0.726015	0.967138
C	-0.219813	-0.726015	0.967138
C	0.100064	3.168473	-0.157999
C	-0.100064	-3.168473	-0.157999
H	-0.158457	1.213127	1.862783
H	1.302444	0.822259	0.936478
H	-1.302444	-0.822259	0.936478
H	0.158457	-1.213127	1.862783

Molecule# 0331

ethylestercarbonochloridic acid

PointGroup: Cs

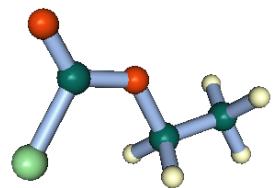
E= -728.126432175 au

ZPE= 0.080757 au

LUMO_eps= -0.02592 au

HOMO_eps= -0.31295 au

Dipole= 4.109 debye



11

O	0.000000	0.875253	0.000000
H	-1.597409	-0.112403	0.885605
H	-1.597409	-0.112403	-0.885605
C	-1.403897	0.489442	0.000000
H	-1.992692	2.365984	0.884747
H	-3.270428	1.523039	0.000000
H	-1.992692	2.365984	-0.884747
C	-2.208098	1.768537	0.000000
O	2.148853	0.326496	0.000000
Cl	0.523259	-1.724654	0.000000
C	1.006061	0.021175	0.000000

Molecule# 0332

ethylformate

PointGroup: Cs

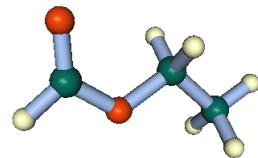
E= -268.493718312 au

ZPE= 0.089963 au

LUMO_eps= -0.01345 au

HOMO_eps= -0.29481 au

Dipole= 2.255 debye



11

C	1.335737	0.637655	0.000000
C	-2.183624	-0.287568	0.000000
C	-0.700940	-0.578325	0.000000
O	2.002533	-0.361066	0.000000
O	0.000000	0.693290	0.000000
H	1.739533	1.657904	0.000000
H	-2.739422	-1.225778	0.000000
H	-2.471547	0.280474	0.884202
H	-2.471547	0.280474	-0.884202
H	-0.392160	-1.140715	-0.880841
H	-0.392160	-1.140715	0.880841

Molecule# 0333

ethylhydroperoxide

PointGroup: C1

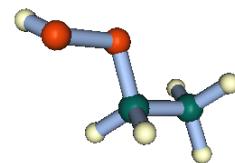
E= -230.272230565 au

ZPE= 0.082809 au

LUMO_eps= -0.01437 au

HOMO_eps= -0.27285 au

Dipole= 1.749 debye



10

C	0.459938	0.519040	0.021772
O	-0.510152	-0.525067	-0.027869
O	-1.815721	0.108175	-0.095134
C	1.818413	-0.154922	0.004015
H	0.327982	1.173442	-0.843321
H	0.318113	1.110577	0.931373
H	-2.200256	-0.182756	0.742877
H	1.942232	-0.811711	0.864757
H	2.600069	0.604443	0.037023
H	1.948740	-0.743562	-0.903410

Molecule# 0334

ethylidyneazane oxide

PointGroup: C1

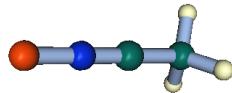
E= -207.985794678 au

ZPE= 0.049256 au

LUMO_eps= -0.02473 au

HOMO_eps= -0.26099 au

Dipole= 4.491 debye



7

O -0.000024 0.000054 1.941721

N 0.000008 -0.000047 0.729470

C -0.000025 0.000042 -1.881444

C 0.000075 -0.000109 -0.425458

H -0.063200 1.018651 -2.266021

H 0.913597 -0.454486 -2.266367

H -0.850557 -0.563861 -2.266253

Molecule# 0335

ethylmethylestersulfurous acid

PointGroup: C1

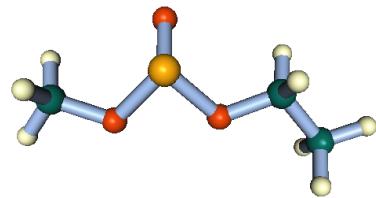
E= -743.130923998 au

ZPE= 0.117173 au

LUMO_eps= -0.02125 au

HOMO_eps= -0.27466 au

Dipole= 1.800 debye



15

C	3.202611	-0.606388	-0.196480
C	2.057940	0.309114	0.175790
O	0.826178	-0.417197	-0.065662
S	-0.533353	0.384629	0.403904
O	-0.730154	1.533535	-0.482721
O	-1.448610	-0.871512	-0.158233
C	-2.865846	-0.639006	-0.072695
H	3.194710	-1.508286	0.414470
H	3.137485	-0.896520	-1.244359
H	4.150175	-0.089481	-0.039400
H	2.057795	1.214467	-0.432283
H	2.110019	0.595329	1.230062
H	-3.159148	0.196081	-0.707639
H	-3.330310	-1.554113	-0.428240
H	-3.174611	-0.452460	0.958160

Molecule# 0336

ethylnitrate

PointGroup: Cs

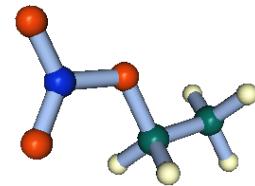
E= -359.658552381 au

ZPE= 0.082255 au

LUMO_eps= -0.07620 au

HOMO_eps= -0.32699 au

Dipole= 3.550 debye



11

N	-1.111550	-0.313232	0.000000
O	0.000000	0.559326	0.000000
O	-2.159770	0.267328	0.000000
O	-0.888584	-1.499078	0.000000
C	2.325207	0.990121	0.000000
C	1.286493	-0.110502	0.000000
H	3.318360	0.540496	0.000000
H	2.232623	1.618133	0.884918
H	2.232623	1.618133	-0.884918
H	1.356935	-0.741228	0.885089
H	1.356935	-0.741228	-0.885089

Molecule# 0337

ethylnitrite

PointGroup: C1

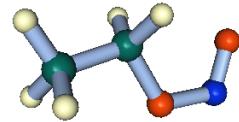
E= -284.442381870 au

ZPE= 0.076421 au

LUMO_eps= -0.08425 au

HOMO_eps= -0.28690 au

Dipole= 2.499 debye



10

C	-0.721786	0.465243	0.000043
O	0.102893	-0.724419	-0.000006
C	-2.163450	0.006048	0.000234
H	-0.479504	1.060827	0.881644
H	-0.479710	1.060747	-0.881667
N	1.487781	-0.524975	-0.000126
O	1.827924	0.603525	-0.000194
H	-2.384003	-0.591203	-0.883644
H	-2.822542	0.874902	0.000221
H	-2.383821	-0.591040	0.884268

Molecule# 0338

ethylpropylsulfide

PointGroup: Cs

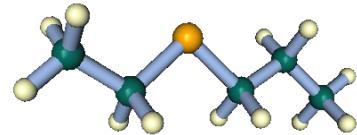
E= -596.069938082 au

ZPE= 0.160729 au

LUMO_eps= -0.01199 au

HOMO_eps= -0.21983 au

Dipole= 1.569 debye



18

C	2.375076	2.291871	0.000000
H	3.465991	2.277864	0.000000
H	2.044631	2.840367	0.882327
H	2.044631	2.840367	-0.882327
C	1.831458	0.869153	0.000000
H	2.172537	0.327306	-0.883073
H	2.172537	0.327306	0.883073
S	0.000000	0.889482	0.000000
C	-0.338622	-0.909728	0.000000
H	0.126062	-1.351508	-0.883539
H	0.126062	-1.351508	0.883539
C	-1.840977	-1.176175	0.000000
H	-2.290661	-0.701679	0.875094
H	-2.290661	-0.701679	-0.875094
C	-2.164305	-2.670386	0.000000
H	-1.752397	-3.165193	-0.881569
H	-1.752397	-3.165193	0.881569
H	-3.242119	-2.836574	0.000000

Molecule# 0339

ethylurea

PointGroup: C1

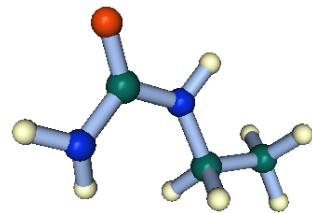
E= -304.018965179 au

ZPE= 0.119559 au

LUMO_eps= -0.02243 au

HOMO_eps= -0.25574 au

Dipole= 4.530 debye



14

C	-2.624091	-0.223414	0.002412
H	-2.704638	-0.964618	0.799272
H	-3.440588	0.487321	0.123953
H	-2.754705	-0.730974	-0.953978
C	-1.283867	0.494871	0.060801
H	-1.250407	1.248579	-0.732964
H	-1.188350	1.024473	1.014316
N	-0.191108	-0.449863	-0.112715
H	-0.395796	-1.431081	-0.024719
N	1.480161	1.166240	0.046537
H	2.460546	1.348304	-0.083400
H	0.852393	1.859667	-0.321530
C	1.149206	-0.174524	-0.013340
O	1.993836	-1.054739	0.042882

Molecule# 0340

ethyne

PointGroup: D(infinity)h

E= -77.364569612 au

ZPE= 0.027039 au

LUMO_eps= -0.00085 au

HOMO_eps= -0.30182 au

Dipole= 0.000 debye



4

C 0.000000 0.000000 0.598150

C 0.000000 0.000000 -0.598150

H 0.000000 0.000000 1.659779

H 0.000000 0.000000 -1.659779

Molecule# 0341

ethynoxyethyne

PointGroup: C1

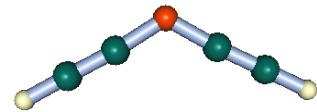
E= -228.737379020 au

ZPE= 0.041113 au

LUMO_eps= -0.01710 au

HOMO_eps= -0.26854 au

Dipole= 0.710 debye



7

O 0.000001 0.762059 -0.000003

C 1.132678 0.087612 -0.000010

C -1.132682 0.087622 0.000031

C 2.202434 -0.441297 0.000011

C -2.202430 -0.441306 -0.000042

H 3.145026 -0.926136 -0.000026

H -3.145031 -0.926124 0.000107

Molecule# 0342

ethynoxymethoxyacetylene

PointGroup: C1

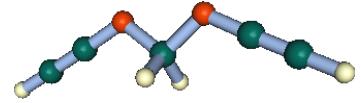
E= -343.314717048 au

ZPE= 0.073954 au

LUMO_eps= -0.01631 au

HOMO_eps= -0.27010 au

Dipole= 2.008 debye



11

O	1.114134	-0.637896	0.000386
O	-1.114134	-0.637904	-0.000379
C	-0.000004	0.243836	0.000033
C	2.273010	-0.042046	0.000077
C	-2.273014	-0.042063	-0.000138
C	3.353062	0.474479	-0.000141
C	-3.353053	0.474491	0.000162
H	-0.000326	0.856536	0.903526
H	0.000313	0.856601	-0.903415
H	4.314214	0.920528	-0.000423
H	-4.314202	0.920549	0.000292

Molecule# 0343

ethynyl hydrodisulfide

PointGroup: C1

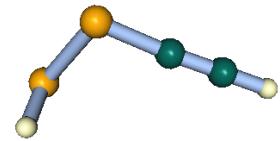
E= -873.821105389 au

ZPE= 0.029107 au

LUMO_eps= -0.07754 au

HOMO_eps= -0.25259 au

Dipole= 1.035 debye



6

S 0.004284 0.891567 0.012200

S -1.557225 -0.508946 -0.087104

C 1.406295 -0.051449 -0.001347

C 2.452012 -0.649297 -0.003520

H -1.672295 -0.734996 1.238559

H 3.369516 -1.182461 -0.010889

Molecule# 0344

ethynylformate

PointGroup: C1

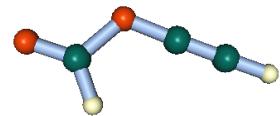
E= -265.975256046 au

ZPE= 0.041636 au

LUMO_eps= -0.05590 au

HOMO_eps= -0.28830 au

Dipole= 2.603 debye



7

O -0.029545 -0.591156 -0.000011

O -2.183481 0.034844 -0.000001

C -1.049749 0.363965 0.000007

C 1.205881 -0.154845 -0.000002

C 2.343204 0.213694 0.000005

H -0.647409 1.384949 0.000027

H 3.355602 0.528657 0.000011

Molecule# 0345

ethynylhydrazine

PointGroup: C1

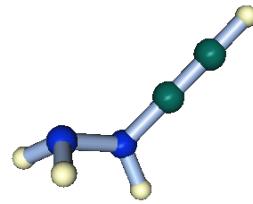
E= -188.078533437 au

ZPE= 0.061634 au

LUMO_eps= -0.02696 au

HOMO_eps= -0.22868 au

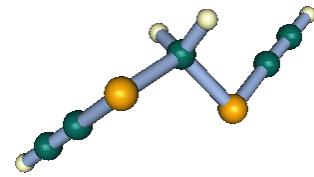
Dipole= 2.674 debye



8

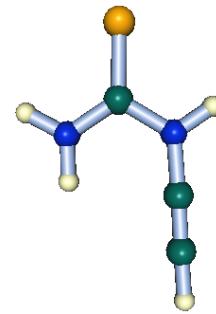
N	0.512308	0.546801	-0.071754
N	1.510698	-0.467956	-0.034828
C	-0.763301	0.125139	-0.013554
C	-1.913127	-0.223847	0.004210
H	0.705929	1.370690	0.481900
H	1.827585	-0.633181	0.915230
H	2.290894	-0.164761	-0.602259
H	-2.926878	-0.532418	0.007263

Molecule# 0346
ethynylsulfanylmethysulfanylethyne
PointGroup: C1
E= -989.302864872 au
ZPE= 0.067536 au
LUMO_eps= -0.04539 au
HOMO_eps= -0.24223 au
Dipole= 1.460 debye



11			
S	-1.085714	0.117394	0.777209
S	1.616055	-1.007193	0.004656
C	-0.092200	-0.704472	-0.547441
C	-2.551811	0.291449	-0.041856
C	2.295903	0.534104	-0.121587
C	-3.614199	0.432090	-0.592782
C	2.852247	1.598818	-0.193854
H	-0.096062	-0.091324	-1.442322
H	-0.512041	-1.685333	-0.754731
H	-4.551006	0.558816	-1.074999
H	3.334006	2.542688	-0.252663

Molecule# 0347
ethynylthiourea
PointGroup: C1
E= -624.482870944 au
ZPE= 0.069736 au
LUMO_eps= -0.03916 au
HOMO_eps= -0.22841 au
Dipole= 4.062 debye



10

S	-2.081317	-0.343098	0.000000
N	0.542113	-0.729566	0.000018
N	-0.127051	1.471695	-0.000093
C	-0.501303	0.182134	-0.000006
C	1.846197	-0.419257	-0.000003
C	3.006498	-0.108367	0.000000
H	0.254221	-1.695995	0.000037
H	0.842627	1.744288	0.000376
H	-0.845401	2.171629	0.000218
H	4.035849	0.147679	-0.000061

Molecule# 0348

fluoroacetonitrile

PointGroup: Cs

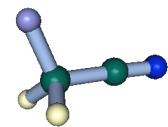
E= -232.067883830 au

ZPE= 0.038357 au

LUMO_eps= -0.04057 au

HOMO_eps= -0.35786 au

Dipole= 3.263 debye



6

F 0.332657 -1.506812 0.000000

N 0.468461 1.859310 0.000000

C -0.629654 -0.510772 0.000000

C 0.000000 0.810536 0.000000

H -1.247608 -0.626221 0.891185

H -1.247608 -0.626221 -0.891185

Molecule# 0349

fluoroacetylene

PointGroup: C(infinity)v

E= -176.616826761 au

ZPE= 0.020370 au

LUMO_eps= -0.01484 au

HOMO_eps= -0.29866 au

Dipole= 0.642 debye



4

C 0.000000 0.000000 -0.095596

C 0.000000 0.000000 -1.287136

F 0.000000 0.000000 1.182582

H 0.000000 0.000000 -2.346846

Molecule# 0350

fluorobenzene

PointGroup: C2v

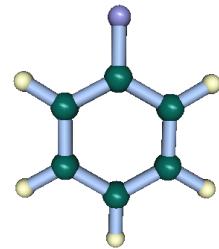
E= -331.613094888 au

ZPE= 0.092146 au

LUMO_eps= -0.02966 au

HOMO_eps= -0.25912 au

Dipole= 1.565 debye



12

C	0.000000	0.000000	-1.828651
C	0.000000	1.203661	-1.131682
C	0.000000	-1.203661	-1.131682
C	0.000000	1.212801	0.259047
C	0.000000	-1.212801	0.259047
C	0.000000	0.000000	0.924672
F	0.000000	0.000000	2.277491
H	0.000000	0.000000	-2.909624
H	0.000000	2.141917	-1.669399
H	0.000000	-2.141917	-1.669399
H	0.000000	2.134302	0.823249
H	0.000000	-2.134302	0.823249

Molecule# 0351

fluoroethane

PointGroup: Cs

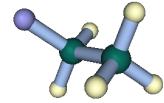
E= -179.139798664 au

ZPE= 0.067622 au

LUMO_eps= -0.01091 au

HOMO_eps= -0.33948 au

Dipole= 2.005 debye



8

C	0.000000	0.557702	0.000000
C	1.131396	-0.441623	0.000000
F	-1.231732	-0.112505	0.000000
H	0.016530	1.191540	0.888182
H	0.016530	1.191540	-0.888182
H	2.088160	0.083890	0.000000
H	1.087998	-1.075450	0.885435
H	1.087998	-1.075450	-0.885435

Molecule# 0352

fluoroethene

PointGroup: Cs

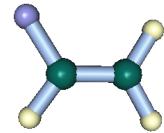
E= -177.901975578 au

ZPE= 0.043887 au

LUMO_eps= -0.00912 au

HOMO_eps= -0.27940 au

Dipole= 1.426 debye



6

C	0.000000	0.434774	0.000000
C	1.185792	-0.138856	0.000000
F	-1.143002	-0.282121	0.000000
H	-0.195129	1.498103	0.000000
H	1.296848	-1.213206	0.000000
H	2.070547	0.478682	0.000000

Molecule# 0353

fluoromethane

PointGroup: C3v

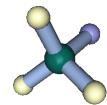
E= -139.804431026 au

ZPE= 0.039074 au

LUMO_eps= -0.00964 au

HOMO_eps= -0.35544 au

Dipole= 1.872 debye



5

C 0.000000 0.000000 -0.637684

F 0.000000 0.000000 0.754062

H 0.000000 1.032068 -0.986819

H 0.893797 -0.516034 -0.986819

H -0.893797 -0.516034 -0.986819

Molecule# 0354

formaldehyde

PointGroup: C2v

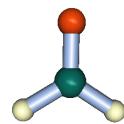
E= -114.552147494 au

ZPE= 0.026496 au

LUMO_eps= -0.06392 au

HOMO_eps= -0.28153 au

Dipole= 2.389 debye



4

C 0.000000 0.000000 -0.526958

O 0.000000 0.000000 0.673270

H 0.000000 0.938263 -1.112205

H 0.000000 -0.938263 -1.112205

Molecule# 0355

formamide

PointGroup: Cs

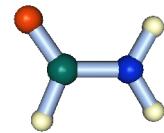
E= -169.970249123 au

ZPE= 0.045280 au

LUMO_eps= -0.02241 au

HOMO_eps= -0.27362 au

Dipole= 3.949 debye



6

C	0.000000	0.418868	0.000000
N	-0.937301	-0.562370	0.000000
O	1.196475	0.233417	0.000000
H	-0.446375	1.428379	0.000000
H	-0.646660	-1.526108	0.000000
H	-1.917653	-0.346222	0.000000

Molecule# 0356

formic acid

PointGroup: Cs

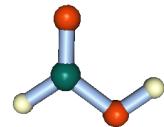
E= -189.845118856 au

ZPE= 0.033618 au

LUMO_eps= -0.02526 au

HOMO_eps= -0.30844 au

Dipole= 1.545 debye



5

C 0.000000 0.421048 0.000000

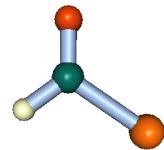
O -1.028183 -0.446144 0.000000

O 1.158545 0.117343 0.000000

H -0.383251 1.447877 0.000000

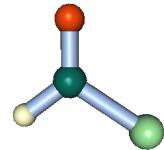
H -0.659642 -1.343762 0.000000

Molecule# 0357
formyl bromide
PointGroup: Cs
E= -2688.199847860 au
ZPE= 0.018399 au
LUMO_eps= -0.07619 au
HOMO_eps= -0.31251 au
Dipole= 1.784 debye



4
C 0.373819 -1.216214 0.000000
O -0.462526 -2.042953 0.000000
H 1.457289 -1.372735 0.000000
Br 0.000000 0.714675 0.000000

Molecule# 0358
formyl chloride
PointGroup: Cs
E= -574.206225974 au
ZPE= 0.018977 au
LUMO_eps= -0.07263 au
HOMO_eps= -0.32538 au
Dipole= 1.858 debye



4
C 0.000000 0.806204 0.000000
O 1.118460 1.175635 0.000000
Cl -0.473479 -0.921920 0.000000
H -0.898535 1.430335 0.000000

Molecule# 0359

formyl fluoride

PointGroup: Cs

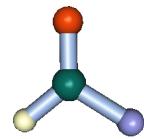
E= -213.859655866 au

ZPE= 0.020681 au

LUMO_eps= -0.05322 au

HOMO_eps= -0.34484 au

Dipole= 2.109 debye



4

C 0.000000 0.400163 0.000000

O 1.146373 0.135369 0.000000

F -0.967416 -0.541572 0.000000

H -0.464239 1.390219 0.000000

Molecule# 0360
fulminic acid
PointGroup: C(infinity)v
E= -168.645246056 au
ZPE= 0.019834 au
LUMO_eps= -0.01219 au
HOMO_eps= -0.28602 au
Dipole= 3.236 debye



4
O 0.000000 0.000000 1.179618
N 0.000000 0.000000 -0.020937
C 0.000000 0.000000 -1.175868
H 0.000000 0.000000 -2.235178

Molecule# 0361

fulvene

PointGroup: C2v

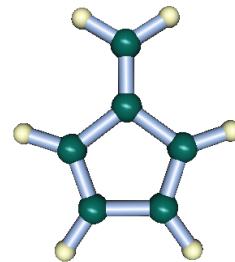
E= -232.279364992 au

ZPE= 0.097730 au

LUMO_eps= -0.07840 au

HOMO_eps= -0.22735 au

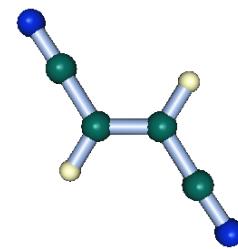
Dipole= 0.578 debye



12

C	0.000000	0.735787	-1.400081
C	0.000000	-0.735787	-1.400081
C	0.000000	1.175419	-0.125488
C	0.000000	-1.175419	-0.125488
C	0.000000	0.000000	0.758403
C	0.000000	0.000000	2.096421
H	0.000000	1.347657	-2.289398
H	0.000000	-1.347657	-2.289398
H	0.000000	2.197794	0.217520
H	0.000000	-2.197794	0.217520
H	0.000000	-0.923202	2.660823
H	0.000000	0.923202	2.660823

Molecule# 0362
fumaronitrile
PointGroup: C2h
E= -263.169035998 au
ZPE= 0.049618 au
LUMO_eps= -0.12513 au
HOMO_eps= -0.32069 au
Dipole= 0.000 debye



8

C	0.123949	-1.862885	0.000000
C	-0.123949	1.862885	0.000000
C	-0.463693	0.483335	0.000000
C	0.463693	-0.483335	0.000000
N	-0.123949	-2.988322	0.000000
N	0.123949	2.988322	0.000000
H	-1.519242	0.244524	0.000000
H	1.519242	-0.244524	0.000000

Molecule# 0363

furan-2-carbaldehyde

PointGroup: Cs

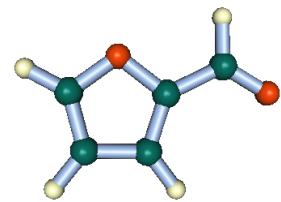
E= -343.481857363 au

ZPE= 0.079250 au

LUMO_eps= -0.07939 au

HOMO_eps= -0.26166 au

Dipole= 3.756 debye



11

C	-0.300615	-1.924790	0.000000
C	-0.970523	-0.674797	0.000000
C	1.032092	-1.640070	0.000000
C	0.000000	0.288032	0.000000
C	-0.029988	1.739577	0.000000
O	-1.049576	2.396115	0.000000
O	1.237658	-0.307636	0.000000
H	-0.741739	-2.906165	0.000000
H	-2.030305	-0.489429	0.000000
H	1.913637	-2.256025	0.000000
H	0.967952	2.216073	0.000000

Molecule# 0364

furan

PointGroup: C2v

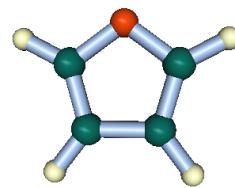
E= -230.111843411 au

ZPE= 0.069849 au

LUMO_eps= -0.00641 au

HOMO_eps= -0.23941 au

Dipole= 0.668 debye



9

C	0.000000	0.716076	-0.955449
C	0.000000	-0.716076	-0.955449
C	0.000000	1.093572	0.345603
C	0.000000	-1.093572	0.345603
O	0.000000	0.000000	1.157159
H	0.000000	1.369847	-1.810079
H	0.000000	-1.369847	-1.810079
H	0.000000	2.047381	0.840519
H	0.000000	-2.047381	0.840519

Molecule# 0365

gamma-butyrolactone

PointGroup: C1

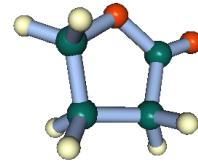
E= -306.614456705 au

ZPE= 0.098158 au

LUMO_eps= -0.02090 au

HOMO_eps= -0.28062 au

Dipole= 4.754 debye



12

H	-0.333392	2.025670	-0.458487
H	1.594629	0.802015	-1.272848
H	1.833366	-1.474020	-0.539014
H	-0.033157	1.529153	1.201325
C	0.022543	1.205712	0.159355
H	2.219734	1.139182	0.340551
C	1.405703	0.669564	-0.207531
H	1.546270	-1.040847	1.156693
C	1.270591	-0.821031	0.123306
O	-2.082550	-0.030351	-0.067109
C	-0.888795	-0.002092	0.002806
O	-0.128413	-1.131408	-0.044870

Molecule# 0366

glucose

PointGroup: C1

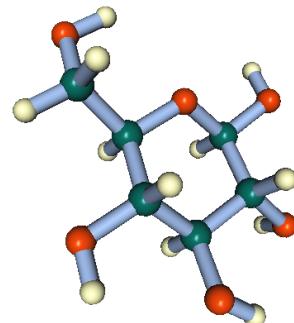
E= -687.458875629 au

ZPE= 0.195669 au

LUMO_eps= -0.02729 au

HOMO_eps= -0.28186 au

Dipole= 2.315 debye



24

C	1.115853	0.989979	0.201060
C	-0.314474	1.262685	-0.244860
C	1.590049	-0.399146	-0.223279
C	-1.222885	0.133264	0.240191
C	0.581955	-1.449023	0.245268
C	-2.647642	0.247392	-0.273872
O	-0.712544	-1.117915	-0.238783
O	1.938737	2.012668	-0.343122
O	-0.797977	2.486634	0.288000
O	2.916634	-0.629266	0.240675
O	0.944839	-2.686590	-0.268393
O	-3.477430	-0.790535	0.223836
H	1.140111	1.046893	1.299737
H	-0.336642	1.288486	-1.341217
H	1.646637	-0.454256	-1.310960
H	-1.241659	0.127736	1.337503
H	0.545143	-1.472520	1.349105
H	-2.633844	0.247751	-1.369821
H	-3.076579	1.187253	0.065541
H	2.858515	1.774040	-0.179127
H	-0.153038	3.172141	0.080576
H	2.899013	-0.846682	1.179337
H	0.327548	-3.352594	0.052774
H	-3.090410	-1.629125	-0.048206

Molecule# 0367

glutamic acid

PointGroup: C1

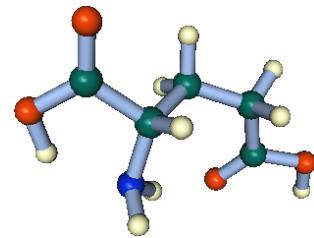
E= -551.862602445 au

ZPE= 0.152107 au

LUMO_eps= -0.03301 au

HOMO_eps= -0.26142 au

Dipole= 5.861 debye



19

N	0.630582	1.427132	0.497820
C	0.942174	-0.008642	0.479325
C	2.405547	-0.219182	0.025066
O	2.939125	-1.297716	0.031446
O	3.012778	0.899944	-0.375393
H	2.332608	1.605804	-0.257569
C	0.024429	-0.827843	-0.440883
C	-1.389805	-1.084945	0.084499
C	-2.385902	0.029375	-0.119800
O	-2.158654	1.123873	-0.578738
O	-3.623769	-0.339435	0.271599
H	0.891335	-0.439220	1.483407
H	-0.025257	-0.346028	-1.419975
H	0.508995	-1.791744	-0.586679
H	-1.813631	-1.966586	-0.401442
H	-1.380996	-1.327411	1.150793
H	-0.248077	1.634248	0.037933
H	0.602211	1.803939	1.434644
H	-4.215760	0.411176	0.113596

Molecule# 0368

glutamine

PointGroup: C1

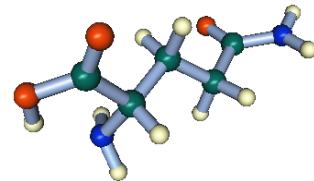
E= -531.982901426 au

ZPE= 0.163624 au

LUMO_eps= -0.03474 au

HOMO_eps= -0.26576 au

Dipole= 6.120 debye



20

N	-1.424042	1.687954	-0.315662
C	-1.175219	0.248620	-0.494595
C	-2.365563	-0.567051	0.058790
O	-2.366240	-1.768365	0.103385
O	-3.404107	0.178411	0.450947
H	-3.124488	1.108651	0.299481
C	0.140646	-0.242894	0.117615
C	1.376852	0.225616	-0.655543
C	2.649673	0.036162	0.158499
O	2.767995	0.503567	1.276755
N	3.647934	-0.665145	-0.444780
H	-1.174045	0.033000	-1.566491
H	0.210972	0.115142	1.147316
H	0.114142	-1.330876	0.160468
H	1.436071	-0.283556	-1.619729
H	1.310231	1.297639	-0.858898
H	3.536523	-1.093206	-1.344786
H	4.500031	-0.822115	0.066469
H	-0.866188	2.078023	0.433662
H	-1.250015	2.226005	-1.151686

Molecule# 0369

glycerine

PointGroup: C1

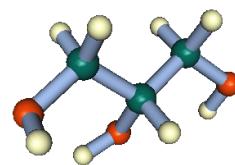
E= -344.935643959 au

ZPE= 0.118241 au

LUMO_eps= -0.02523 au

HOMO_eps= -0.28021 au

Dipole= 2.310 debye



14

O	-2.417963	0.047987	-0.123897
H	-1.254547	-0.774720	1.304580
H	-1.302489	-1.718686	-0.195314
C	-1.251091	-0.706463	0.216624
O	0.061919	1.328254	0.263126
H	0.015456	0.038391	-1.353421
C	0.012297	0.000165	-0.254588
H	1.281639	-0.756010	1.300499
H	1.324011	-1.707294	-0.195753
C	1.283432	-0.694142	0.205599
H	2.364208	0.899324	-0.013832
O	2.446879	-0.029282	-0.258813
H	-0.816557	1.714063	0.164460
H	-2.606229	-0.068088	-1.060358

Molecule# 0370

glycine

PointGroup: Cs

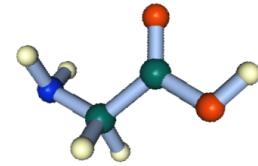
E= -284.555369060 au

ZPE= 0.079377 au

LUMO_eps= -0.01915 au

HOMO_eps= -0.26429 au

Dipole= 1.155 debye



10

C	0.000000	0.554399	0.000000
O	1.166268	0.850486	0.000000
O	-0.993246	1.475442	0.000000
C	-0.558650	-0.860872	0.000000
N	0.418261	-1.927134	0.000000
H	-0.577661	2.350468	0.000000
H	-1.213149	-0.954876	0.869365
H	-1.213149	-0.954876	-0.869365
H	1.021928	-1.859686	0.809956
H	1.021928	-1.859686	-0.809956

Molecule# 0371

glycolic acid

PointGroup: C1

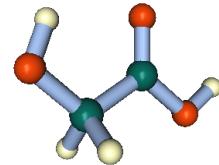
E= -304.429855728 au

ZPE= 0.066742 au

LUMO_eps= -0.02434 au

HOMO_eps= -0.29711 au

Dipole= 2.300 debye



9

C	-0.738863	-0.744609	0.000092
C	0.514163	0.098603	0.000027
O	1.636178	-0.642444	-0.000068
O	0.505630	1.304270	0.000046
O	-1.893095	0.053802	-0.000097
H	-0.715437	-1.394908	-0.880519
H	-0.715499	-1.394600	0.880937
H	-1.602727	0.976904	-0.000086
H	2.392158	-0.036383	-0.000096

Molecule# 0372

glyoxime

PointGroup: C2h

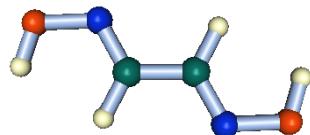
E= -338.571870481 au

ZPE= 0.070032 au

LUMO_eps= -0.07393 au

HOMO_eps= -0.26586 au

Dipole= 0.000 debye



10

O	1.166590	2.672477	0.000000
O	-1.166590	-2.672477	0.000000
N	1.166590	1.298532	0.000000
N	-1.166590	-1.298532	0.000000
C	0.027863	0.723227	0.000000
C	-0.027863	-0.723227	0.000000
H	0.248784	2.997834	0.000000
H	-0.248784	-2.997834	0.000000
H	-0.917383	1.269774	0.000000
H	0.917383	-1.269774	0.000000

Molecule# 0373

guanidine

PointGroup: C1

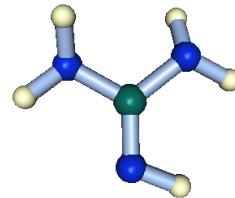
E= -205.466224899 au

ZPE= 0.075685 au

LUMO_eps= -0.02429 au

HOMO_eps= -0.24421 au

Dipole= 2.879 debye



9

C	-0.017919	0.121480	0.000209
N	-0.222845	1.381237	0.009408
N	-0.973006	-0.891055	0.074673
N	1.277018	-0.374139	-0.080092
H	-1.210366	1.609782	-0.043242
H	-1.924501	-0.586118	-0.046428
H	-0.761135	-1.727618	-0.447294
H	1.968806	0.351343	0.024724
H	1.466538	-1.188574	0.483063

Molecule# 0374

heptalene

PointGroup: C2

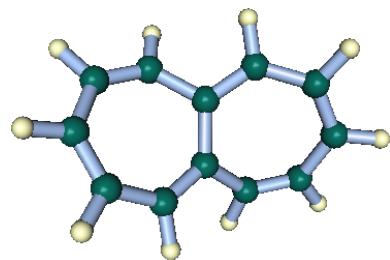
E= -463.377123941 au

ZPE= 0.179505 au

LUMO_eps= -0.08109 au

HOMO_eps= -0.18694 au

Dipole= 0.212 debye



22

C	1.510583	1.057959	-0.207635
C	1.131202	2.378179	-0.627087
C	-0.031282	3.021695	-0.376287
C	-1.131202	2.495684	0.390765
C	-1.415623	1.207590	0.659413
C	-0.736352	0.000021	0.155956
C	0.736352	-0.000021	0.155956
C	1.415623	-1.207590	0.659413
C	1.131202	-2.495684	0.390765
C	0.031282	-3.021695	-0.376287
C	-1.131202	-2.378179	-0.627087
C	-1.510583	-1.057959	-0.207635
H	2.580111	0.874669	-0.203910
H	1.905624	2.939917	-1.136925
H	-0.119386	4.051335	-0.699854
H	-1.817588	3.233906	0.791454
H	-2.284527	1.012644	1.278492
H	2.284527	-1.012644	1.278492
H	1.817588	-3.233906	0.791454
H	0.119386	-4.051335	-0.699854
H	-1.905624	-2.939917	-1.136925
H	-2.580111	-0.874669	-0.203910

Molecule# 0375

heptan-2-one

PointGroup: C1

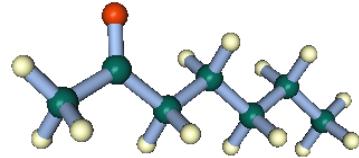
E= -350.548528280 au

ZPE= 0.196856 au

LUMO_eps= -0.02495 au

HOMO_eps= -0.25494 au

Dipole= 2.792 debye



22

C	2.331625	0.140596	-0.002766
C	3.562671	-0.742228	0.006967
C	-4.097798	-0.269419	-0.001780
C	0.990909	-0.574254	-0.007194
C	-2.775391	0.495292	0.007306
C	-0.224164	0.345462	0.004932
C	-1.548821	-0.417709	-0.003855
O	2.419096	1.348033	-0.005792
H	3.571661	-1.365777	0.903608
H	3.553384	-1.419544	-0.849424
H	4.460036	-0.129875	-0.019314
H	-4.183730	-0.919977	0.871115
H	-4.951146	0.409944	0.006808
H	-4.184176	-0.898252	-0.890409
H	0.972256	-1.232580	-0.883480
H	0.975011	-1.253830	0.852590
H	-2.733388	1.141611	0.888893
H	-2.733543	1.162627	-0.858464
H	-0.175148	1.014310	-0.856999
H	-0.174496	0.992679	0.883335
H	-1.591964	-1.065480	-0.886410
H	-1.591700	-1.086565	0.862830

Molecule# 0376

heptanal

PointGroup: Cs

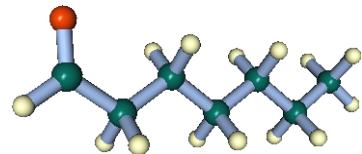
E= -350.537193868 au

ZPE= 0.197426 au

LUMO_eps= -0.03514 au

HOMO_eps= -0.26375 au

Dipole= 2.798 debye



22

C	2.934907	-1.847531	0.000000
C	-3.741441	1.922109	0.000000
C	2.204069	-0.532137	0.000000
C	-2.216713	2.017532	0.000000
C	0.683613	-0.629266	0.000000
C	-1.526489	0.653370	0.000000
C	0.000000	0.738127	0.000000
O	2.412916	-2.933644	0.000000
H	4.042127	-1.761298	0.000000
H	-4.203476	2.910263	0.000000
H	-4.102888	1.387142	0.880650
H	-4.102888	1.387142	-0.880650
H	2.570407	0.032064	0.867377
H	2.570407	0.032064	-0.867377
H	-1.887390	2.587509	0.874110
H	-1.887390	2.587509	-0.874110
H	0.362464	-1.205426	-0.870679
H	0.362464	-1.205426	0.870679
H	-1.856331	0.082600	0.874379
H	-1.856331	0.082600	-0.874379
H	0.328909	1.309595	-0.874725
H	0.328909	1.309595	0.874725

Molecule# 0377

heptane

PointGroup: C2v

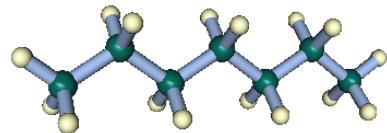
E= -276.505216234 au

ZPE= 0.216515 au

LUMO_eps= -0.00973 au

HOMO_eps= -0.30809 au

Dipole= 0.094 debye



23

C	0.000000	3.833474	-0.352624
C	0.000000	-3.833474	-0.352624
C	0.000000	2.560916	0.492939
C	0.000000	-2.560916	0.492939
C	0.000000	1.279918	-0.342345
C	0.000000	-1.279918	-0.342345
C	0.000000	0.000000	0.494121
H	0.000000	4.728440	0.271238
H	-0.880595	3.878602	-0.996848
H	0.880595	3.878602	-0.996848
H	-0.880595	-3.878602	-0.996848
H	0.880595	-3.878602	-0.996848
H	0.000000	-4.728440	0.271238
H	-0.873897	2.560727	1.151361
H	0.873897	2.560727	1.151361
H	0.873897	-2.560727	1.151361
H	-0.873897	-2.560727	1.151361
H	-0.874400	1.280845	-1.001938
H	0.874400	1.280845	-1.001938
H	0.874400	-1.280845	-1.001938
H	-0.874400	-1.280845	-1.001938
H	0.874450	0.000000	1.153429
H	-0.874450	0.000000	1.153429

Molecule# 0378

hexa-1,3-diene-5-yne

PointGroup: C1

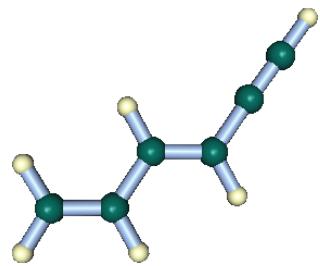
E= -232.234796027 au

ZPE= 0.094482 au

LUMO_eps= -0.06661 au

HOMO_eps= -0.23444 au

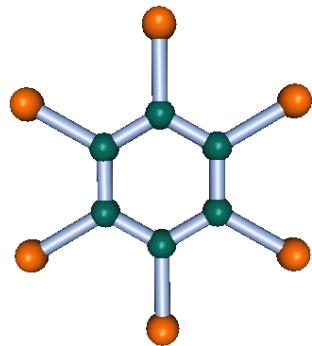
Dipole= 0.650 debye



12

C	3.128267	-0.342469	-0.000004
C	1.993557	0.059429	-0.000007
C	0.675269	0.570452	-0.000011
C	-0.435926	-0.189337	0.000004
C	-1.776186	0.350545	0.000000
C	-2.884737	-0.395944	0.000015
H	4.125512	-0.705141	-0.000001
H	0.578120	1.651724	-0.000027
H	-0.335274	-1.269130	0.000020
H	-1.864320	1.432522	-0.000016
H	-2.837239	-1.477747	0.000031
H	-3.868261	0.051719	0.000011

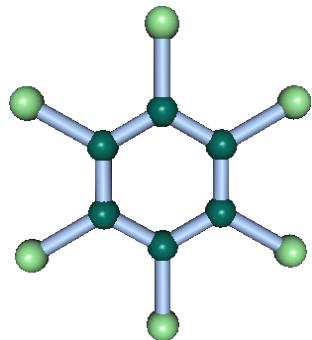
Molecule# 0379
hexabromobenzene
PointGroup: D6h
E= -15674.044476300 au
ZPE= 0.038056 au
LUMO_eps= -0.09578 au
HOMO_eps= -0.26557 au
Dipole= 0.000 debye



12

C	0.000000	1.399813	0.000000
C	1.212273	0.699906	0.000000
C	-1.212273	0.699906	0.000000
C	1.212273	-0.699906	0.000000
C	-1.212273	-0.699906	0.000000
C	0.000000	-1.399813	0.000000
Br	0.000000	3.295658	0.000000
Br	2.854123	1.647829	0.000000
Br	-2.854123	1.647829	0.000000
Br	2.854123	-1.647829	0.000000
Br	-2.854123	-1.647829	0.000000
Br	0.000000	-3.295658	0.000000

Molecule# 0380
hexachlorobenzene
PointGroup: D6h
E= -2990.089901190 au
ZPE= 0.042399 au
LUMO_eps= -0.06988 au
HOMO_eps= -0.27205 au
Dipole= 0.000 debye



12

C	0.000000	1.397768	0.000000
C	1.210502	0.698884	0.000000
C	-1.210502	0.698884	0.000000
C	1.210502	-0.698884	0.000000
C	-1.210502	-0.698884	0.000000
C	0.000000	-1.397768	0.000000
Cl	0.000000	3.126245	0.000000
Cl	2.707407	1.563122	0.000000
Cl	-2.707407	1.563122	0.000000
Cl	2.707407	-1.563122	0.000000
Cl	-2.707407	-1.563122	0.000000
Cl	0.000000	-3.126245	0.000000

Molecule# 0381

hexachloroethane

PointGroup: D3d

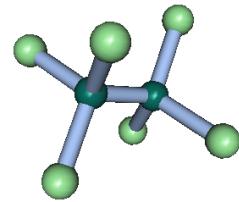
E= -2837.597001780 au

ZPE= 0.017705 au

LUMO_eps= -0.06124 au

HOMO_eps= -0.31643 au

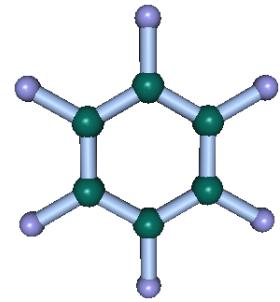
Dipole= 0.000 debye



8

C	0.000000	0.000000	0.792268
C	0.000000	0.000000	-0.792268
Cl	0.000000	1.679244	1.403393
Cl	-1.454268	-0.839622	1.403393
Cl	1.454268	-0.839622	1.403393
Cl	0.000000	-1.679244	-1.403393
Cl	-1.454268	0.839622	-1.403393
Cl	1.454268	0.839622	-1.403393

Molecule# 0382
hexafluorobenzene
PointGroup: D6h
E= -827.947035914 au
ZPE= 0.051743 au
LUMO_eps= -0.05985 au
HOMO_eps= -0.28788 au
Dipole= 0.000 debye



12

C	0.000000	1.388365	0.000000
C	1.202359	0.694182	0.000000
C	-1.202359	0.694182	0.000000
C	1.202359	-0.694182	0.000000
C	-1.202359	-0.694182	0.000000
C	0.000000	-1.388365	0.000000
F	0.000000	2.719949	0.000000
F	2.355545	1.359975	0.000000
F	-2.355545	1.359975	0.000000
F	2.355545	-1.359975	0.000000
F	-2.355545	-1.359975	0.000000
F	0.000000	-2.719949	0.000000

Molecule# 0383

hexafluoroethane

PointGroup: S6

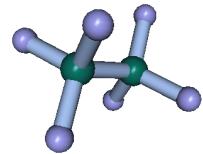
E= -675.548496733 au

ZPE= 0.028854 au

LUMO_eps= 0.00275 au

HOMO_eps= -0.41373 au

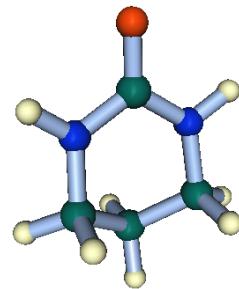
Dipole= 0.000 debye



8

C	0.000000	0.000000	0.778102
C	0.000000	0.000000	-0.778102
F	0.000000	1.254581	1.232191
F	-1.086499	-0.627290	1.232191
F	1.086499	-0.627291	1.232191
F	0.000000	-1.254581	-1.232191
F	-1.086499	0.627291	-1.232191
F	1.086499	0.627290	-1.232191

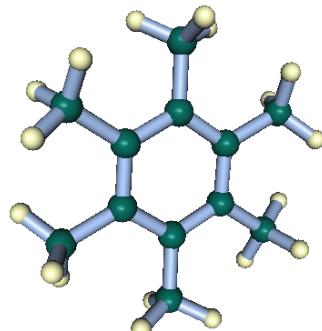
Molecule# 0384
hexahydropyrimidin-2-one
PointGroup: Cs
E= -342.131097581 au
ZPE= 0.128611 au
LUMO_eps= -0.02141 au
HOMO_eps= -0.25198 au
Dipole= 4.811 debye



15

C	-0.164367	1.106122	0.000000
C	0.630174	-1.644396	0.000000
C	-0.028352	-1.065946	1.246291
C	-0.028352	-1.065946	-1.246291
N	-0.028352	0.386872	1.163911
N	-0.028352	0.386872	-1.163911
O	-0.348128	2.315601	0.000000
H	1.692401	-1.394346	0.000000
H	0.538186	-2.730567	0.000000
H	-1.047815	-1.460098	1.343027
H	0.519860	-1.364705	2.140522
H	0.519860	-1.364705	-2.140522
H	-1.047815	-1.460098	-1.343027
H	-0.223673	0.927248	1.988963
H	-0.223673	0.927248	-1.988963

Molecule# 0385
 hexamethylbenzene
 PointGroup: C2h
 E= -468.302358982 au
 ZPE= 0.265490 au
 LUMO_eps= -0.01442 au
 HOMO_eps= -0.22013 au
 Dipole= 0.000 debye



30

C	0.000000	1.402717	0.011190
C	1.214788	0.701358	-0.011190
C	-1.214788	0.701358	-0.011190
C	1.214788	-0.701358	0.011190
C	-1.214788	-0.701358	0.011190
C	0.000000	-1.402717	-0.011190
C	0.000000	2.914685	0.082337
C	2.524191	1.457342	-0.082337
C	-2.524191	1.457342	-0.082337
C	2.524191	-1.457342	0.082337
C	-2.524191	-1.457342	0.082337
C	0.000000	-2.914685	-0.082337
H	-0.873575	3.289820	0.610244
H	0.873575	3.289820	0.610244
H	0.000000	3.376329	-0.910531
H	2.923987	1.688164	0.910531
H	3.285855	0.888372	-0.610244
H	2.412280	2.401448	-0.610244
H	-3.285855	0.888372	-0.610244
H	-2.923987	1.688164	0.910531
H	-2.412280	2.401448	-0.610244
H	2.412280	-2.401448	0.610244
H	2.923987	-1.688164	-0.910531
H	3.285855	-0.888372	0.610244
H	-2.923987	-1.688164	-0.910531
H	-2.412280	-2.401448	0.610244
H	-3.285855	-0.888372	0.610244
H	-0.873575	-3.289820	-0.610244
H	0.873575	-3.289820	-0.610244
H	0.000000	-3.376329	0.910531

Molecule# 0386

hexanal

PointGroup: Cs

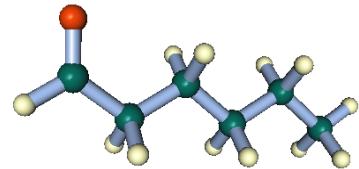
E= -311.209142771 au

ZPE= 0.168958 au

LUMO_eps= -0.03526 au

HOMO_eps= -0.26395 au

Dipole= 2.713 debye



19

C	1.730475	2.260799	0.000000
C	-1.877092	-3.067542	0.000000
C	1.469179	0.778822	0.000000
C	-1.675526	-1.553237	0.000000
C	0.000000	0.375846	0.000000
C	-0.203783	-1.139524	0.000000
O	0.882361	3.116832	0.000000
H	2.805089	2.541058	0.000000
H	-2.936193	-3.328318	0.000000
H	-1.423356	-3.526632	0.880821
H	-1.423356	-3.526632	-0.880821
H	1.999279	0.364970	0.867425
H	1.999279	0.364970	-0.867425
H	-2.170087	-1.119104	0.873840
H	-2.170087	-1.119104	-0.873840
H	-0.491084	0.816415	0.870631
H	-0.491084	0.816415	-0.870631
H	0.291599	-1.574837	-0.874744
H	0.291599	-1.574837	0.874744

Molecule# 0387

hexanamide

PointGroup: C1

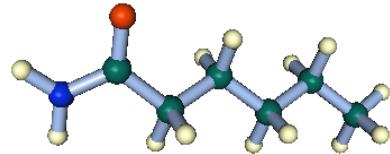
E= -366.619938728 au

ZPE= 0.186750 au

LUMO_eps= -0.02169 au

HOMO_eps= -0.25997 au

Dipole= 3.571 debye



21

C	-2.341682	0.111370	0.062323
C	4.074930	-0.182147	0.064954
C	-1.005389	-0.584989	0.280499
C	2.730567	0.451968	-0.287379
C	0.185855	0.257397	-0.174608
C	1.531563	-0.380318	0.168545
N	-3.379576	-0.706845	-0.277643
O	-2.490867	1.311718	0.200335
H	4.179038	-0.312677	1.144121
H	4.907792	0.434652	-0.275258
H	4.181268	-1.165989	-0.397058
H	-0.928223	-0.779637	1.355244
H	-0.998311	-1.560235	-0.212711
H	2.671429	0.604297	-1.369128
H	2.667243	1.447267	0.161800
H	0.120409	0.418511	-1.254432
H	0.107976	1.243573	0.284716
H	1.592586	-0.535216	1.251266
H	1.594355	-1.376608	-0.283106
H	-4.296353	-0.304735	-0.373362
H	-3.270304	-1.698720	-0.377277

Molecule# 0388

hexane

PointGroup: C1

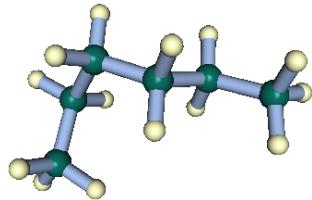
E= -237.174361846 au

ZPE= 0.188591 au

LUMO_eps= -0.01058 au

HOMO_eps= -0.31134 au

Dipole= 0.117 debye



20

C	1.752978	0.132983	0.595759
C	2.270241	-1.006545	-0.282683
C	0.797724	1.099291	-0.117681
C	-0.524607	0.497784	-0.611141
C	-1.447868	-0.017439	0.494787
C	-2.787022	-0.527764	-0.035684
H	-2.645338	-1.354700	-0.734820
H	2.766819	-0.619752	-1.175521
H	-3.427267	-0.884472	0.772434
H	2.992417	-1.620604	0.257299
H	1.465980	-1.665190	-0.613039
H	-3.327819	0.259908	-0.564432
H	1.267957	-0.282455	1.482703
H	-0.954091	-0.819080	1.049556
H	2.605211	0.708606	0.966413
H	-1.624471	0.786112	1.216882
H	0.573150	1.931568	0.556617
H	1.322016	1.537463	-0.972764
H	-0.325283	-0.311677	-1.319828
H	-1.057960	1.264417	-1.181643

Molecule# 0389

hexanoic acid

PointGroup: Cs

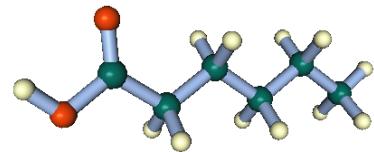
E= -386.498320281 au

ZPE= 0.175095 au

LUMO_eps= -0.01549 au

HOMO_eps= -0.28927 au

Dipole= 1.571 debye



20

C	-2.062686	-1.102443	0.000000
C	3.632108	1.858226	0.000000
C	-0.556479	-1.037078	0.000000
C	2.104874	1.829660	0.000000
C	0.000000	0.382472	0.000000
C	1.528055	0.413443	0.000000
O	-2.819045	-0.165656	0.000000
O	-2.503459	-2.387142	0.000000
H	4.011459	2.880818	0.000000
H	4.036027	1.354785	0.880787
H	4.036027	1.354785	-0.880787
H	-0.205394	-1.600622	0.869012
H	-0.205394	-1.600622	-0.869012
H	1.729349	2.370062	0.873830
H	1.729349	2.370062	-0.873830
H	-0.381981	0.918569	0.871350
H	-0.381981	0.918569	-0.871350
H	1.904359	-0.128002	-0.874719
H	1.904359	-0.128002	0.874719
H	-3.471375	-2.353691	0.000000

Molecule# 0390

hexatriyne

PointGroup: Cs

E= -229.732393706 au

ZPE= 0.047244 au

LUMO_eps= -0.07213 au

HOMO_eps= -0.26070 au

Dipole= 0.031 debye



8

C	0.000000	0.607495	0.000000
C	-0.022300	-0.607096	0.000000
C	0.032288	1.961729	0.000000
C	-0.037787	-1.961626	0.000000
C	0.067261	3.167962	0.000000
C	-0.047216	-3.168328	0.000000
H	0.098665	4.228824	0.000000
H	-0.052142	-4.229643	0.000000

Molecule# 0391

histidine

PointGroup: C1

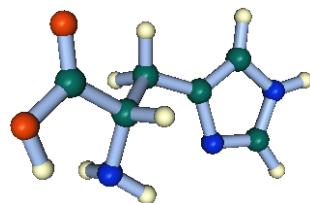
E= -548.990693414 au

ZPE= 0.160689 au

LUMO_eps= -0.02774 au

HOMO_eps= -0.24696 au

Dipole= 7.162 debye



20

N	-1.201957	1.645890	0.152460
C	-1.122137	0.221629	-0.199424
C	-2.533221	-0.393283	-0.152217
O	-2.748314	-1.574901	-0.095497
O	-3.514020	0.517294	-0.229519
H	-3.060866	1.389226	-0.232101
C	-0.112058	-0.609453	0.605562
C	1.310812	-0.315666	0.248158
N	1.798228	0.972889	0.135796
C	3.064823	0.857017	-0.182550
N	3.431444	-0.446678	-0.283277
C	2.315898	-1.207793	-0.013417
H	-0.839634	0.175548	-1.255509
H	-0.281816	-0.417857	1.670751
H	-0.320702	-1.665837	0.443593
H	3.752508	1.668827	-0.350821
H	4.345579	-0.792723	-0.516050
H	2.335670	-2.282388	-0.032339
H	-1.210332	1.750849	1.162273
H	-0.360429	2.115801	-0.161192

Molecule# 0392

hydrogen cyanide

PointGroup: C(infinity)v

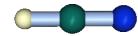
E= -93.462749635 au

ZPE= 0.016318 au

LUMO_eps= -0.01106 au

HOMO_eps= -0.37438 au

Dipole= 3.041 debye



3

C 0.000000 0.000000 -0.496902

N 0.000000 0.000000 0.649125

H 0.000000 0.000000 -1.562463

Molecule# 0393

hydroperoxyacetylene

PointGroup: C1

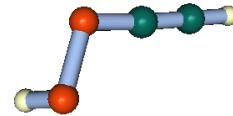
E= -227.761892153 au

ZPE= 0.034575 au

LUMO_eps= -0.08072 au

HOMO_eps= -0.26905 au

Dipole= 1.446 debye



6

O	0.500202	0.649433	-0.012191
O	1.498887	-0.464552	-0.099113
C	-0.689930	0.150600	0.001728
C	-1.824334	-0.241903	0.015562
H	1.923095	-0.355188	0.766050
H	-2.830223	-0.576039	0.020646

Molecule# 0394

hydroquinone

PointGroup: C2h

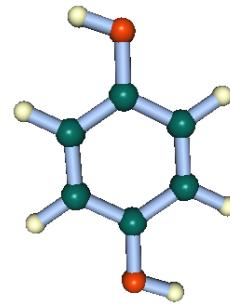
E= -382.841955867 au

ZPE= 0.108362 au

LUMO_eps= -0.02479 au

HOMO_eps= -0.21520 au

Dipole= 0.000 debye



14

O	-0.055278	2.766941	0.000000
C	0.001661	1.395041	0.000000
C	1.201394	0.689669	0.000000
C	1.201394	-0.699360	0.000000
C	-0.001661	-1.395041	0.000000
O	0.055278	-2.766941	0.000000
C	-1.201394	-0.689669	0.000000
C	-1.201394	0.699360	0.000000
H	0.835947	3.128399	0.000000
H	2.144114	1.223949	0.000000
H	2.130783	-1.251030	0.000000
H	-0.835947	-3.128399	0.000000
H	-2.144114	-1.223949	0.000000
H	-2.130783	1.251030	0.000000

Molecule# 0395

hydroxyacetaldehyde

PointGroup: Cs

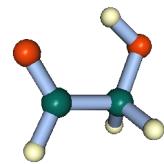
E= -229.142290973 au

ZPE= 0.060827 au

LUMO_eps= -0.05602 au

HOMO_eps= -0.29278 au

Dipole= 2.479 debye



8

C	0.000000	0.928126	0.000000
C	0.925344	-0.256408	0.000000
O	-1.349713	0.557465	0.000000
O	0.516462	-1.391513	0.000000
H	-1.374140	-0.411223	0.000000
H	0.240237	1.542269	0.879378
H	0.240237	1.542269	-0.879378
H	2.007614	-0.031238	0.000000

Molecule# 0396

hydroxyacetylene

PointGroup: C1

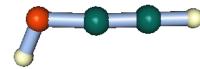
E= -152.607779721 au

ZPE= 0.031648 au

LUMO_eps= -0.02989 au

HOMO_eps= -0.26191 au

Dipole= 1.646 debye



5

O 1.180945 -0.108391 -0.000024

C -0.123542 -0.002551 0.000003

C -1.320286 0.013531 0.000025

H 1.594854 0.763873 -0.000012

H -2.379443 0.037377 0.000043

Molecule# 0397

hydroxymethyldisulfanylmethanol

PointGroup: C1

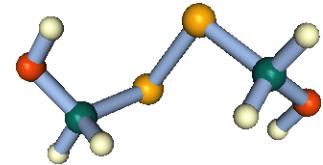
E= -1026.812549420 au

ZPE= 0.087717 au

LUMO_eps= -0.04481 au

HOMO_eps= -0.25969 au

Dipole= 2.163 debye



12

S	-0.588948	-0.854750	-0.597619
S	0.588932	0.854989	-0.597326
O	-2.696710	0.623868	0.346427
O	2.696697	-0.624032	0.346082
C	-1.855232	-0.435708	0.688286
C	1.855275	0.435453	0.688361
H	-1.332873	-0.262522	1.630730
H	-2.466770	-1.333392	0.769900
H	1.332960	0.261952	1.630771
H	2.466846	1.333087	0.770258
H	-2.164171	1.423911	0.259063
H	2.164119	-1.424019	0.258442

Molecule# 0398

hydroxymethylimine

PointGroup: Cs

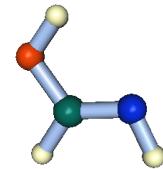
E= -169.950625964 au

ZPE= 0.045929 au

LUMO_eps= -0.01161 au

HOMO_eps= -0.29605 au

Dipole= 1.009 debye



6

C	0.000000	0.416584	0.000000
O	-1.110472	-0.343382	0.000000
N	1.156625	-0.083800	0.000000
H	-0.263473	1.473242	0.000000
H	-0.825628	-1.270023	0.000000
H	1.876503	0.630934	0.000000

Molecule# 0399

hydroxymethylperoxide

PointGroup: C1

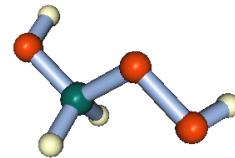
E= -266.191707581 au

ZPE= 0.059828 au

LUMO_eps= -0.02178 au

HOMO_eps= -0.28169 au

Dipole= 2.719 debye



8

C	-0.521080	0.491811	0.031617
O	-1.757960	-0.126244	-0.064518
O	0.469147	-0.535551	-0.126038
O	1.752362	0.137407	-0.041874
H	-1.897823	-0.685361	0.707197
H	2.117970	-0.266792	0.756685
H	-0.442357	1.205959	-0.787605
H	-0.359703	0.990434	0.993457

Molecule# 0400

hydroxysulfanylethyne

PointGroup: C1

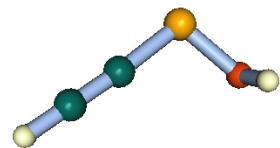
E= -550.825868630 au

ZPE= 0.033262 au

LUMO_eps= -0.07027 au

HOMO_eps= -0.24408 au

Dipole= 1.567 debye



6

S -0.560952 -0.610114 0.012357

O -1.476085 0.795532 -0.118724

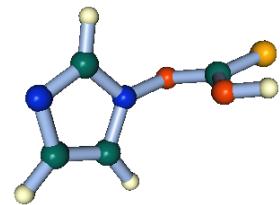
C 1.020613 -0.035441 0.000928

C 2.177382 0.307670 -0.001983

H -1.598128 1.151695 0.770681

H 3.194069 0.612498 -0.012273

Molecule# 0401
 imidazol-1-ylloxymethanethioic O-acid
 PointGroup: C1
 E= -813.083152317 au
 ZPE= 0.086371 au
 LUMO_eps= -0.06894 au
 HOMO_eps= -0.25848 au
 Dipole= 2.210 debye



13

S	2.996748	0.021824	-0.268596
O	0.456110	0.082338	-0.793882
O	0.927761	-0.148682	1.382040
N	-0.867057	0.036647	-0.354945
N	-2.862943	0.732728	0.190086
C	1.424260	-0.020504	0.159117
C	-1.640834	1.120155	-0.072639
C	-1.634472	-1.100967	-0.292195
C	-2.871350	-0.637105	0.057407
H	1.677808	-0.212492	1.990373
H	-1.254127	2.124562	-0.078045
H	-1.230660	-2.075076	-0.495225
H	-3.767578	-1.210522	0.219041

Molecule# 0402

indane

PointGroup: Cs

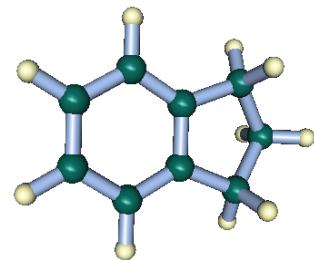
E= -349.111526844 au

ZPE= 0.164061 au

LUMO_eps= -0.01814 au

HOMO_eps= -0.23888 au

Dipole= 0.691 debye



19

C	-0.045568	-2.249090	0.696137
C	-0.045568	-2.249090	-0.696137
C	0.004095	-1.048325	1.400520
C	0.004095	-1.048325	-1.400520
C	0.049674	0.148504	0.698241
C	0.049674	0.148504	-0.698241
C	0.125739	1.561338	1.227438
C	0.125739	1.561338	-1.227438
C	-0.258685	2.418849	0.000000
H	-0.089794	-3.187131	1.233424
H	-0.089794	-3.187131	-1.233424
H	0.001095	-1.053757	2.483428
H	0.001095	-1.053757	-2.483428
H	-0.526446	1.733848	2.084324
H	1.145985	1.785770	1.556006
H	1.145985	1.785770	-1.556006
H	-0.526446	1.733848	-2.084324
H	-1.337645	2.583506	0.000000
H	0.220799	3.396809	0.000000

Molecule# 0403

inositol

PointGroup: Ci

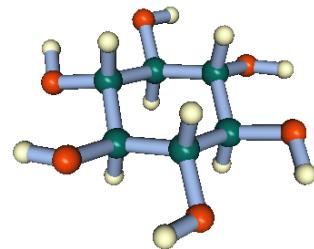
E= -687.475238091 au

ZPE= 0.196264 au

LUMO_eps= -0.01770 au

HOMO_eps= -0.29267 au

Dipole= 0.000 debye



24

C	-1.325775	0.584643	0.237990
C	0.155142	-1.441860	0.227032
C	1.169971	0.852886	0.241238
C	-0.155142	1.441860	-0.227032
C	-1.169971	-0.852886	-0.241238
C	1.325775	-0.584643	-0.237990
O	-2.565352	1.060854	-0.274243
O	0.365045	-2.749548	-0.293829
O	2.199913	1.693855	-0.266419
O	-0.365045	2.749548	0.293829
O	-2.199913	-1.693855	0.266419
O	2.565352	-1.060854	0.274243
H	-1.353744	0.594834	1.334200
H	0.153684	-1.479157	1.323029
H	1.196484	0.861338	1.337560
H	-0.153684	1.479157	-1.323029
H	-1.196484	-0.861338	-1.337560
H	1.353744	-0.594834	-1.334200
H	-2.646403	1.991559	-0.037548
H	-0.403701	-3.285449	-0.068670
H	3.047455	1.296990	-0.036282
H	0.403701	3.285449	0.068670
H	-3.047455	-1.296990	0.036282
H	2.646403	-1.991559	0.037548

Molecule# 0404

isatin

PointGroup: C1

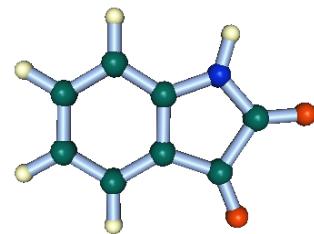
E= -513.255791402 au

ZPE= 0.115001 au

LUMO_eps= -0.11331 au

HOMO_eps= -0.25491 au

Dipole= 6.279 debye



16

O	-1.742007	1.965021	-0.000021
C	-1.177229	0.903277	-0.000010
C	0.255043	0.578698	-0.000007
C	0.379731	-0.819241	0.000009
C	1.623314	-1.425094	0.000016
C	2.745582	-0.595433	0.000007
C	2.634874	0.794760	-0.000010
C	1.378592	1.391778	-0.000017
N	-0.883171	-1.422253	0.000016
C	-1.904802	-0.492965	0.000006
O	-3.086643	-0.710872	0.000008
H	1.729179	-2.501176	0.000029
H	3.728266	-1.047628	0.000012
H	3.527112	1.404141	-0.000017
H	1.265488	2.467328	-0.000029
H	-1.049284	-2.414768	0.000030

Molecule# 0405

isobutane

PointGroup: C3v

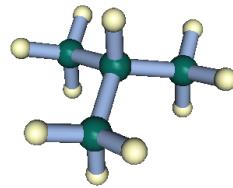
E= -158.521946475 au

ZPE= 0.130900 au

LUMO_eps= -0.01096 au

HOMO_eps= -0.32389 au

Dipole= 0.142 debye



14

C	0.000000	0.000000	0.371001
C	0.000000	1.458065	-0.095429
C	-1.262722	-0.729033	-0.095429
C	1.262722	-0.729033	-0.095429
H	-1.282986	-1.759266	0.264412
H	1.282986	-1.759266	0.264412
H	-0.882076	1.990731	0.264412
H	0.882076	1.990731	0.264412
H	-2.165062	-0.231466	0.264412
H	-1.313214	-0.758184	-1.187000
H	2.165062	-0.231466	0.264412
H	0.000000	1.516369	-1.187000
H	1.313214	-0.758184	-1.187000
H	0.000000	0.000000	1.466243

Molecule# 0406

isobutyl acetate

PointGroup: C1

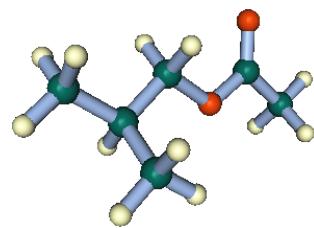
E= -386.489606072 au

ZPE= 0.173742 au

LUMO_eps= -0.01410 au

HOMO_eps= -0.28108 au

Dipole= 2.230 debye



20

C	-1.888132	-0.186303	0.038084
C	-2.956955	0.824440	-0.283481
C	1.958051	1.395183	0.513927
C	2.923162	-0.824646	-0.220717
C	0.456498	-0.579654	0.020652
C	1.743964	0.144881	-0.342302
O	-2.082486	-1.286641	0.491535
O	-0.661558	0.297410	-0.245338
H	-2.889982	1.121863	-1.329676
H	-2.812725	1.721105	0.319523
H	-3.933425	0.396820	-0.079568
H	2.870252	1.915116	0.218046
H	2.055108	1.129449	1.569732
H	1.126417	2.091889	0.417111
H	3.854481	-0.335170	-0.506854
H	2.793952	-1.698388	-0.861379
H	3.038067	-1.176866	0.807098
H	0.330891	-1.489124	-0.567547
H	0.440158	-0.859686	1.075856
H	1.659630	0.453440	-1.388885

Molecule# 0407

isobutyl formate

PointGroup: C1

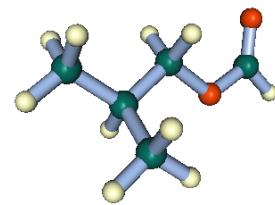
E= -347.150148471 au

ZPE= 0.146277 au

LUMO_eps= -0.01387 au

HOMO_eps= -0.29404 au

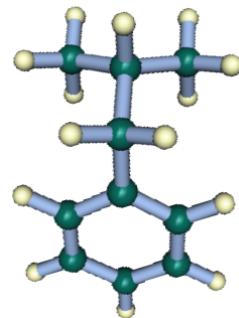
Dipole= 2.394 debye



17

C	-2.290734	0.312473	-0.152529
C	1.730575	1.318317	0.376938
C	2.349480	-1.102336	-0.024284
C	-0.050404	-0.444296	0.035206
C	1.350871	0.017165	-0.333148
O	-2.730830	-0.652419	0.410787
O	-1.002022	0.556886	-0.408491
H	-2.898837	1.139165	-0.541138
H	2.726140	1.646204	0.075225
H	1.741116	1.179254	1.460987
H	1.028303	2.118260	0.146337
H	3.358716	-0.805723	-0.310746
H	2.105762	-2.020077	-0.561819
H	2.364512	-1.333019	1.043503
H	-0.300747	-1.390490	-0.444761
H	-0.160689	-0.574017	1.113477
H	1.359807	0.196764	-1.412535

Molecule# 0408
 isobutylbenzene
 PointGroup: Cs
 E= -389.648652386 au
 ZPE= 0.212990 au
 LUMO_eps= -0.01894 au
 HOMO_eps= -0.24748 au
 Dipole= 0.462 debye



24

C	1.333873	2.598690	0.000000
C	0.875686	2.067268	1.199941
C	0.875686	2.067268	-1.199941
C	-0.026619	1.009896	1.196493
C	-0.026619	1.009896	-1.196493
C	-0.488807	0.456180	0.000000
C	-0.026619	-2.412117	-1.261997
C	-0.026619	-2.412117	1.261997
C	-1.461521	-0.699761	0.000000
C	-0.842543	-2.122471	0.000000
H	2.032977	3.424064	0.000000
H	1.216030	2.479956	2.140563
H	1.216030	2.479956	-2.140563
H	-0.383900	0.613202	2.138360
H	-0.383900	0.613202	-2.138360
H	0.854188	-1.771177	-1.323883
H	-0.618707	-2.255130	-2.165763
H	0.317444	-3.447758	-1.266811
H	0.317444	-3.447758	1.266811
H	0.854188	-1.771177	1.323883
H	-0.618707	-2.255130	2.165763
H	-2.110211	-0.616300	0.875339
H	-2.110211	-0.616300	-0.875339
H	-1.698056	-2.806051	0.000000

Molecule# 0409

isocyanato[(isocyanatomethyl)sulfanyl]methane

PointGroup: C1

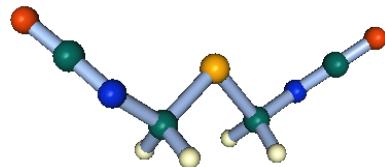
E= -813.154915156 au

ZPE= 0.084199 au

LUMO_eps= -0.04123 au

HOMO_eps= -0.25867 au

Dipole= 3.914 debye



13

S	0.000005	0.180949	-0.000031
O	4.161913	1.053413	0.440220
O	-4.161949	1.053366	-0.440227
N	2.574769	-0.356348	-0.604807
N	-2.574743	-0.356296	0.604841
C	1.346924	-1.035946	-0.351650
C	-1.346915	-1.035919	0.351674
C	3.340117	0.359645	-0.014871
C	-3.340125	0.359642	0.014882
H	1.444429	-1.712184	0.498745
H	1.081666	-1.610562	-1.235849
H	-1.081634	-1.610502	1.235889
H	-1.444453	-1.712191	-0.498690

Molecule# 0410

isocyanatomethanethiol

PointGroup: C1

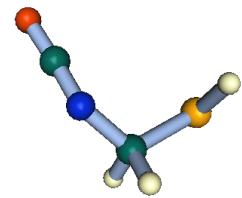
E= -606.296166194 au

ZPE= 0.050548 au

LUMO_eps= -0.03736 au

HOMO_eps= -0.26848 au

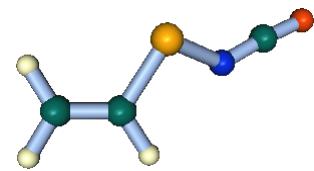
Dipole= 2.327 debye



8

S	-1.706782	-0.543256	-0.058637
O	2.540354	-0.659034	-0.086094
N	0.706588	0.801429	0.239004
C	-0.664935	0.969752	-0.139339
C	1.599379	0.023801	0.031598
H	-1.726078	-0.641935	1.283273
H	-1.104325	1.734549	0.492248
H	-0.736693	1.300429	-1.175164

Molecule# 0411
isocyanatosulfanylethene
PointGroup: C1
E= -644.377866219 au
ZPE= 0.056158 au
LUMO_eps= -0.05835 au
HOMO_eps= -0.23681 au
Dipole= 2.531 debye



9
S 0.457966 0.685420 -0.130775
O -3.222564 -0.127058 0.122495
N -0.866252 -0.384315 0.004694
C -2.057415 -0.194178 0.059640
C 1.757292 -0.498441 -0.193213
C 2.970929 -0.238236 0.278239
H 1.512657 -1.411103 -0.721146
H 3.781289 -0.934480 0.113673
H 3.198043 0.670651 0.819051

Molecule# 0412

isocyanic acid

PointGroup: Cs

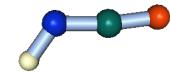
E= -168.754790049 au

ZPE= 0.021292 au

LUMO_eps= -0.02314 au

HOMO_eps= -0.31798 au

Dipole= 2.107 debye



4

H 1.358380 -1.380419 0.000000

N 0.395111 -1.094787 0.000000

C 0.000000 0.049280 0.000000

O -0.515520 1.093531 0.000000

Molecule# 0413

isoflurane

PointGroup: C1

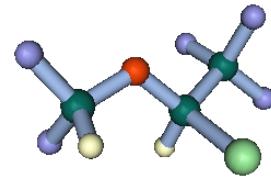
E= -1150.473961900 au

ZPE= 0.060832 au

LUMO_eps= -0.03432 au

HOMO_eps= -0.34383 au

Dipole= 1.818 debye



12

C	-0.218615	0.231720	-0.334249
C	2.099372	0.063633	0.050519
C	-1.485571	-0.576666	-0.009374
O	0.817838	-0.322832	0.399628
F	2.373326	-0.321108	-1.226533
F	2.924768	-0.591330	0.873399
F	-1.301155	-1.854169	-0.377515
F	-2.528100	-0.095040	-0.699597
F	-1.784593	-0.552251	1.290062
Cl	-0.487352	1.980503	0.064712
H	-0.042858	0.187772	-1.406517
H	2.255795	1.139294	0.129683

Molecule# 0414

isoleucine

PointGroup: C1

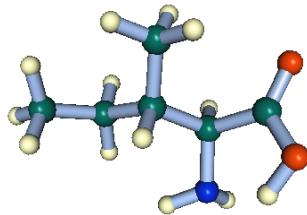
E= -441.863730380 au

ZPE= 0.192804 au

LUMO_eps= -0.02609 au

HOMO_eps= -0.26758 au

Dipole= 5.270 debye

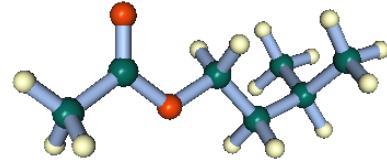


22

N	-0.597265	1.880669	-0.121090
C	-0.495562	0.459188	-0.493741
C	-1.805491	-0.236189	-0.085662
O	-2.217442	-1.236297	-0.608791
O	-2.449652	0.365789	0.927683
H	-1.968150	1.206422	1.080701
C	0.740774	-0.181501	0.194975
C	2.036361	0.322896	-0.473170
C	0.692385	-1.712042	0.209785
C	3.305554	0.081041	0.344256
H	-0.402470	0.308887	-1.572904
H	0.731995	0.170577	1.233213
H	2.129419	-0.159520	-1.450886
H	1.964888	1.394467	-0.677881
H	1.596770	-2.114151	0.664101
H	-0.156498	-2.089792	0.775213
H	0.613261	-2.111699	-0.802100
H	4.176666	0.493046	-0.166281
H	3.239861	0.558480	1.324121
H	3.494746	-0.979801	0.504685
H	0.309205	2.294943	0.044674
H	-1.056201	2.427172	-0.838822

Molecule# 0415
isopentyl acetate
PointGroup: C1

E= -425.814560157 au
ZPE= 0.202276 au
LUMO_eps= -0.01491 au
HOMO_eps= -0.27989 au
Dipole= 2.270 debye

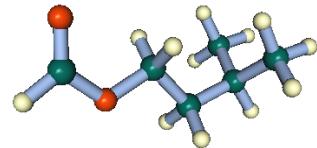


23

C	2.403276	0.235094	0.003580
C	3.664247	-0.587957	-0.004238
C	-2.836541	0.358121	1.268379
C	-2.835699	0.381755	-1.261372
C	-1.045343	-0.950015	-0.008083
C	0.028571	0.122851	-0.001652
C	-2.494529	-0.425752	-0.003810
O	2.357473	1.440315	0.011576
O	1.309148	-0.552959	-0.002627
H	3.706070	-1.193141	-0.909987
H	3.671524	-1.271694	0.844196
H	4.526585	0.069656	0.039536
H	-3.900505	0.597961	1.298851
H	-2.290462	1.301687	1.321379
H	-2.599340	-0.216217	2.165809
H	-2.290329	1.326588	-1.295750
H	-3.899825	0.621256	-1.288528
H	-2.596999	-0.175253	-2.169285
H	-0.897174	-1.580633	-0.888276
H	-0.896159	-1.591756	0.863846
H	-0.019806	0.767018	-0.878748
H	-0.022517	0.759280	0.880916
H	-3.127922	-1.318173	-0.012356

Molecule# 0416
isopentyl formate
PointGroup: Cs

E= -386.475105863 au
ZPE= 0.174846 au
LUMO_eps= -0.01576 au
HOMO_eps= -0.29269 au
Dipole= 2.509 debye



20

C	-0.221060	2.864428	0.000000
C	-0.221060	-2.371524	1.265102
C	-0.221060	-2.371524	-1.265102
C	1.048508	-0.544433	0.000000
C	-0.053651	0.498440	0.000000
C	0.564195	-2.007414	0.000000
O	-1.421923	2.840809	0.000000
O	0.588857	1.801614	0.000000
H	0.384539	3.779558	0.000000
H	-0.428507	-3.442220	1.294360
H	-1.181810	-1.855200	1.308497
H	0.337007	-2.116386	2.167817
H	-1.181810	-1.855200	-1.308497
H	-0.428507	-3.442220	-1.294360
H	0.337007	-2.116386	-2.167817
H	1.679808	-0.377477	-0.876121
H	1.679808	-0.377477	0.876121
H	-0.691293	0.435316	-0.880677
H	-0.691293	0.435316	0.880677
H	1.474353	-2.614843	0.000000

Molecule# 0417

isopropenylbenzene

PointGroup: C1

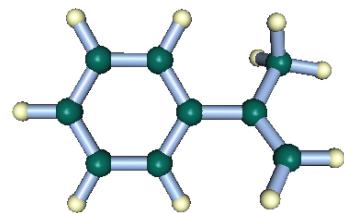
E= -349.092755324 au

ZPE= 0.161225 au

LUMO_eps= -0.04046 au

HOMO_eps= -0.23453 au

Dipole= 0.343 debye



19

C	-2.607951	-0.070177	-0.002533
C	-1.956385	1.138080	0.223390
C	-1.855508	-1.217102	-0.220271
C	-0.570564	1.197284	0.222786
C	-0.467158	-1.156536	-0.216683
C	0.205539	0.053889	-0.010474
C	2.337269	1.223085	-0.419484
C	1.689055	0.121675	-0.030681
C	2.453037	-1.107640	0.391878
H	-3.688478	-0.117438	0.001289
H	-2.529999	2.035788	0.412585
H	-2.348629	-2.164590	-0.392684
H	-0.080152	2.138271	0.429309
H	0.095144	-2.062538	-0.391815
H	3.417985	1.266340	-0.413429
H	1.818583	2.103555	-0.771554
H	2.308302	-1.930951	-0.311139
H	2.122756	-1.463201	1.369923
H	3.520478	-0.900594	0.439945

Molecule# 0418

isopropyl acetate

PointGroup: C1

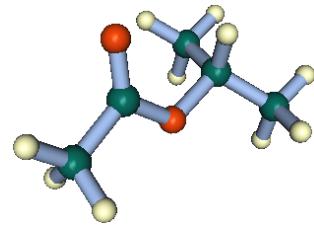
E= -347.165234095 au

ZPE= 0.145190 au

LUMO_eps= -0.01331 au

HOMO_eps= -0.27994 au

Dipole= 2.014 debye



17

C	1.268727	0.080167	-0.135548
C	2.457391	-0.631709	0.455479
C	-2.121048	-1.091773	-0.335245
C	-1.578136	1.165030	0.695009
C	-1.134427	0.057348	-0.246875
O	1.327987	1.053724	-0.845937
O	0.117817	-0.516965	0.234551
H	2.448277	-1.682083	0.165657
H	2.406702	-0.594627	1.543829
H	3.371738	-0.157764	0.112852
H	-3.078523	-0.731193	-0.712382
H	-1.756978	-1.866034	-1.009806
H	-2.285710	-1.538625	0.646050
H	-2.518095	1.595146	0.346575
H	-0.836390	1.960880	0.734621
H	-1.733027	0.773621	1.701565
H	-0.939471	0.472232	-1.234796

Molecule# 0419

isopropyl formate

PointGroup: C1

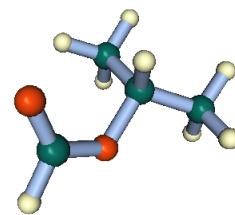
E= -307.825862884 au

ZPE= 0.117858 au

LUMO_eps= -0.01329 au

HOMO_eps= -0.29234 au

Dipole= 2.229 debye



14

C	1.617743	-0.394675	0.283252
C	-1.893251	-0.863530	-0.252957
C	-0.944016	1.436162	0.264110
C	-0.675794	0.040279	-0.273129
O	2.051181	0.295615	-0.599753
O	0.330551	-0.615131	0.565758
H	2.240430	-0.955104	0.992486
H	-2.678480	-0.440562	-0.880088
H	-1.648581	-1.854994	-0.632319
H	-2.282128	-0.967445	0.760564
H	-1.698111	1.930159	-0.349869
H	-0.039874	2.042006	0.242524
H	-1.314363	1.388173	1.289063
H	-0.260844	0.104471	-1.278058

Molecule# 0420

isopropyl nitrate

PointGroup: C1

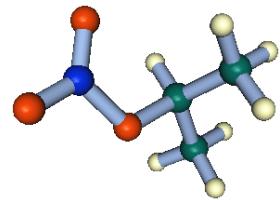
E= -398.990405450 au

ZPE= 0.110036 au

LUMO_eps= -0.07471 au

HOMO_eps= -0.32358 au

Dipole= 3.658 debye



14

N	1.373307	-0.063009	0.041264
O	1.396548	0.879733	0.795043
O	2.285464	-0.632107	-0.489189
O	0.119309	-0.621395	-0.286499
C	-1.052332	0.063916	0.267361
C	-1.394970	1.283353	-0.571030
C	-2.136583	-0.999878	0.268157
H	-0.806612	0.356435	1.286240
H	-0.581577	2.006220	-0.570003
H	-1.610830	0.992297	-1.599382
H	-2.278986	1.772046	-0.159761
H	-1.843059	-1.856641	0.872465
H	-3.052372	-0.580247	0.684532
H	-2.346969	-1.343252	-0.744705

Molecule# 0421

isopropyl nitrite

PointGroup: Cs

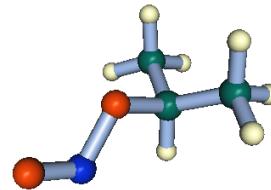
E= -323.775393691 au

ZPE= 0.103929 au

LUMO_eps= -0.08457 au

HOMO_eps= -0.28074 au

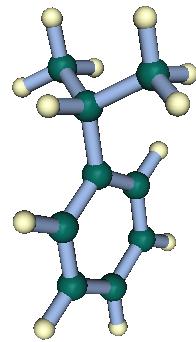
Dipole= 2.871 debye



13

H	1.230807	-0.798909	0.000000
C	0.140652	-0.856817	0.000000
H	0.007049	-2.562492	1.308766
H	-1.436380	-1.541527	1.309424
H	0.023820	-1.009617	2.153756
C	-0.346546	-1.531370	1.272020
H	0.007049	-2.562492	-1.308766
H	0.023820	-1.009617	-2.153756
H	-1.436380	-1.541527	-1.309424
C	-0.346546	-1.531370	-1.272020
O	-0.346546	0.512894	0.000000
O	0.328520	2.544021	0.000000
N	0.719868	1.441172	0.000000

Molecule# 0422
 isopropylbenzene
 PointGroup: Cs
 E= -350.321660948 au
 ZPE= 0.184384 au
 LUMO_eps= -0.01505 au
 HOMO_eps= -0.24827 au
 Dipole= 0.404 debye



21

C	-0.601226	-2.584627	0.000000
C	0.748982	-2.260917	0.000000
C	-1.547135	-1.565096	0.000000
C	1.146365	-0.928060	0.000000
C	-1.144028	-0.236286	0.000000
C	0.210818	0.106161	0.000000
C	0.210818	2.299507	1.265971
C	0.210818	2.299507	-1.265971
C	0.662737	1.556271	0.000000
H	-0.915190	-3.619865	0.000000
H	1.495397	-3.044499	0.000000
H	-2.602280	-1.805893	0.000000
H	2.202394	-0.686488	0.000000
H	-1.896202	0.542418	0.000000
H	-0.877383	2.362280	1.320609
H	0.602440	3.318326	1.273546
H	0.560437	1.794019	2.166585
H	0.560437	1.794019	-2.166585
H	0.602440	3.318326	-1.273546
H	-0.877383	2.362280	-1.320609
H	1.755995	1.546317	0.000000

Molecule# 0423

isopropylcyclopropane

PointGroup: Cs

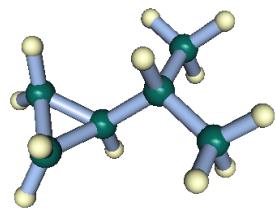
E= -235.931061364 au

ZPE= 0.165258 au

LUMO_eps= -0.00806 au

HOMO_eps= -0.28210 au

Dipole= 0.029 debye



18

C	0.467629	0.583634	0.000000
C	-0.031191	1.784928	0.753865
C	-0.031191	1.784928	-0.753865
C	-0.315789	-0.714728	0.000000
C	-0.031191	-1.532744	1.263884
C	-0.031191	-1.532744	-1.263884
H	1.544280	0.445861	0.000000
H	-0.986654	1.703209	-1.255077
H	0.685059	2.411395	1.266643
H	0.685059	2.411395	-1.266643
H	-0.986654	1.703209	1.255077
H	-0.623644	-2.449214	1.283788
H	-0.623644	-2.449214	-1.283788
H	-0.260425	-0.962286	-2.164879
H	-0.260425	-0.962286	2.164879
H	1.022414	-1.819061	-1.310538
H	1.022414	-1.819061	1.310538
H	-1.380233	-0.453598	0.000000

Molecule# 0424

isoquinoline

PointGroup: Cs

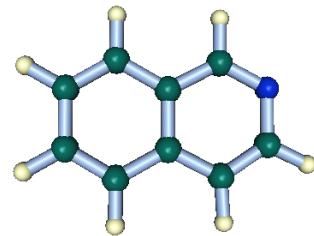
E= -402.070040786 au

ZPE= 0.135496 au

LUMO_eps= -0.06499 au

HOMO_eps= -0.24077 au

Dipole= 2.612 debye



17

N	-2.411694	0.770500	0.000000
C	-1.247199	1.371403	0.000000
C	0.000000	0.696957	0.000000
C	-0.018996	-0.725328	0.000000
C	-1.285073	-1.354625	0.000000
C	-2.419419	-0.587737	0.000000
C	1.211455	-1.424550	0.000000
C	2.397856	-0.737303	0.000000
C	2.414486	0.675356	0.000000
C	1.238322	1.379037	0.000000
H	-1.255568	2.457887	0.000000
H	-1.354484	-2.434581	0.000000
H	-3.398779	-1.049786	0.000000
H	1.202991	-2.506847	0.000000
H	3.334572	-1.278500	0.000000
H	3.361605	1.197408	0.000000
H	1.242936	2.461653	0.000000

Molecule# 0425

isothiazole

PointGroup: Cs

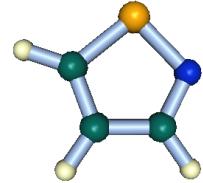
E= -569.145514737 au

ZPE= 0.054951 au

LUMO_eps= -0.04801 au

HOMO_eps= -0.27155 au

Dipole= 2.458 debye



8

C	0.654473	-1.275757	0.000000
C	-0.759568	-1.159013	0.000000
C	1.232534	-0.038075	0.000000
N	-1.256067	0.058336	0.000000
S	0.000000	1.151175	0.000000
H	1.194557	-2.209548	0.000000
H	-1.446653	-1.995169	0.000000
H	2.279932	0.214642	0.000000

Molecule# 0426

isothiocyanatoacetonitrile

PointGroup: C1

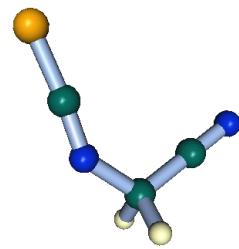
E= -623.295531210 au

ZPE= 0.047118 au

LUMO_eps= -0.06544 au

HOMO_eps= -0.27412 au

Dipole= 3.442 debye



8

S	2.278497	-0.427178	-0.000076
N	-0.046708	1.072004	-0.000069
N	-2.433025	-1.423286	-0.000046
C	-1.477822	1.012116	0.000203
C	-2.013110	-0.354003	0.000063
C	0.927544	0.377873	-0.000052
H	-1.858915	1.539109	-0.876755
H	-1.858578	1.538797	0.877498

Molecule# 0427

isothiocyanatomethanol

PointGroup: C1

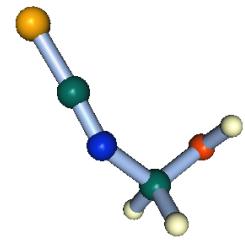
E= -606.284600079 au

ZPE= 0.053383 au

LUMO_eps= -0.04131 au

HOMO_eps= -0.25914 au

Dipole= 2.686 debye



8

S	2.147620	0.209811	0.031553
O	-2.177251	0.884502	0.079532
N	-0.449502	-0.736185	-0.147699
C	0.650412	-0.289749	-0.045393
C	-1.845506	-0.478904	0.091503
H	-2.115777	1.223264	-0.819967
H	-2.414295	-1.043253	-0.649351
H	-2.096761	-0.847779	1.085447

Molecule# 0428

isoxazole

PointGroup: Cs

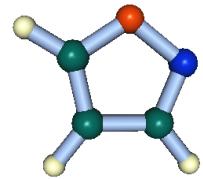
E= -246.129693617 au

ZPE= 0.057789 au

LUMO_eps= -0.03467 au

HOMO_eps= -0.28133 au

Dipole= 3.027 debye



8

C	1.121838	0.366816	0.000000
C	0.615592	-0.959856	0.000000
C	0.000000	1.124633	0.000000
N	-0.689000	-0.992693	0.000000
O	-1.091411	0.346235	0.000000
H	2.145312	0.693430	0.000000
H	1.160098	-1.890521	0.000000
H	-0.175703	2.186501	0.000000

Molecule# 0429

ketene

PointGroup: C2v

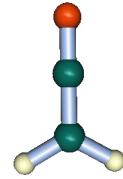
E= -152.666125086 au

ZPE= 0.031493 au

LUMO_eps= -0.04733 au

HOMO_eps= -0.25535 au

Dipole= 1.516 debye



5

C 0.000000 0.000000 -1.205838

C 0.000000 0.000000 0.102176

O 0.000000 0.000000 1.262386

H 0.000000 0.937241 -1.738559

H 0.000000 -0.937241 -1.738559

Molecule# 0430

leucine

PointGroup: C1

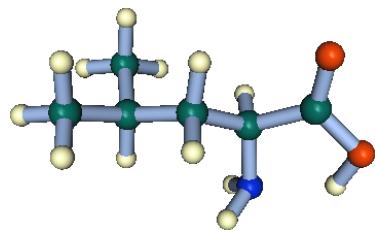
E= -441.868122984 au

ZPE= 0.192619 au

LUMO_eps= -0.03135 au

HOMO_eps= -0.26393 au

Dipole= 5.577 debye



22

N	0.889792	1.733167	-0.084168
C	0.653062	0.324866	0.279326
C	1.942908	-0.495104	0.057054
O	1.987940	-1.690661	0.174653
O	3.015494	0.245946	-0.248211
H	2.687089	1.172239	-0.274368
C	-0.530559	-0.332551	-0.440004
C	-1.916908	0.221973	-0.078321
C	-2.973038	-0.350115	-1.029174
C	-2.296085	-0.059131	1.378824
H	0.489109	0.281675	1.357974
H	-0.369734	-0.225663	-1.518607
H	-0.496406	-1.403150	-0.233024
H	-1.902453	1.308771	-0.219438
H	-3.962107	0.053227	-0.807413
H	-2.741372	-0.116292	-2.069654
H	-3.029551	-1.437289	-0.938398
H	-3.288045	0.335699	1.602720
H	-2.313437	-1.133743	1.574081
H	-1.600962	0.393952	2.087128
H	0.485395	1.959508	-0.984328
H	0.510182	2.376995	0.594739

Molecule# 0431

lysine

PointGroup: C1

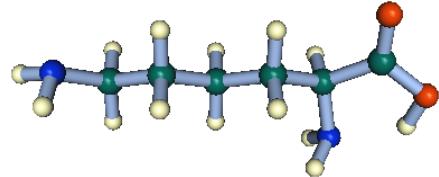
E= -497.237987117 au

ZPE= 0.210678 au

LUMO_eps= -0.03073 au

HOMO_eps= -0.25107 au

Dipole= 6.464 debye



24

N	1.748606	1.711717	-0.110623
C	1.505536	0.334496	0.352601
C	2.743343	-0.539294	0.053037
O	2.755177	-1.732408	0.197432
O	3.816383	0.153863	-0.349539
H	3.520520	1.090385	-0.381692
C	0.229447	-0.318859	-0.188199
C	-1.059289	0.316065	0.333331
C	-2.318639	-0.348453	-0.223242
C	-3.608418	0.279792	0.294578
N	-4.779870	-0.416009	-0.243436
H	1.447816	0.361100	1.444428
H	0.251892	-0.273372	-1.283075
H	0.258775	-1.376399	0.073343
H	-1.070260	0.251414	1.426664
H	-1.077545	1.383378	0.090243
H	-2.306561	-0.289099	-1.317231
H	-2.322972	-1.411934	0.025905
H	-3.642216	0.188063	1.382961
H	-3.599403	1.356577	0.069884
H	-5.636961	-0.050753	0.151625
H	-4.841888	-0.299571	-1.247876
H	1.314168	1.882851	-1.009374
H	1.399106	2.403285	0.536824

Molecule# 0432

m-cresol

PointGroup: C1

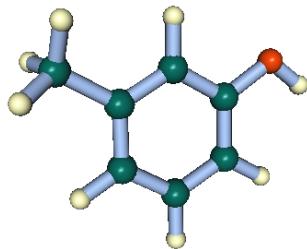
E= -346.921843235 au

ZPE= 0.131644 au

LUMO_eps= -0.01679 au

HOMO_eps= -0.23021 au

Dipole= 0.946 debye



16

C	0.151273	1.784647	0.002216
C	-1.096568	1.176867	-0.008450
C	1.312680	1.021029	0.007796
C	-0.038671	-0.979205	-0.009708
C	-1.203017	-0.216446	-0.011775
C	1.211066	-0.366488	0.000942
C	-2.552960	-0.884863	0.009391
O	2.309364	-1.184166	0.000798
H	0.225667	2.863983	0.002825
H	-1.992065	1.784194	-0.016938
H	2.285648	1.497705	0.012651
H	-0.084931	-2.060188	-0.018605
H	-2.509721	-1.885386	-0.419767
H	-2.922457	-0.982907	1.033294
H	-3.290088	-0.306426	-0.547493
H	3.110211	-0.650896	0.005175

Molecule# 0433

m-dibromobenzene

PointGroup: C2v

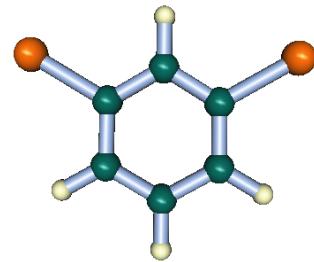
E= -5379.586060700 au

ZPE= 0.080089 au

LUMO_eps= -0.04454 au

HOMO_eps= -0.25935 au

Dipole= 1.658 debye



12

C	0.000000	0.000000	2.410928
C	0.000000	1.209040	1.726086
C	0.000000	-1.209040	1.726086
C	0.000000	0.000000	-0.375043
C	0.000000	1.191157	0.338567
C	0.000000	-1.191157	0.338567
Br	0.000000	2.842433	-0.622159
Br	0.000000	-2.842433	-0.622159
H	0.000000	0.000000	3.492446
H	0.000000	2.146877	2.260530
H	0.000000	-2.146877	2.260530
H	0.000000	0.000000	-1.453512

Molecule# 0434

m-dichlorobenzene

PointGroup: C2v

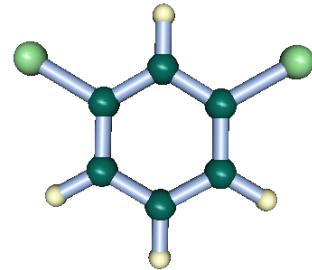
E= -1151.598763520 au

ZPE= 0.081227 au

LUMO_eps= -0.04326 au

HOMO_eps= -0.26277 au

Dipole= 1.676 debye



12

C	0.000000	0.000000	2.071388
C	0.000000	1.208808	1.386957
C	0.000000	-1.208808	1.386957
C	0.000000	0.000000	-0.713068
C	0.000000	1.191420	-0.000840
C	0.000000	-1.191420	-0.000840
Cl	0.000000	2.703797	-0.881717
Cl	0.000000	-2.703797	-0.881717
H	0.000000	0.000000	3.152761
H	0.000000	2.149253	1.916981
H	0.000000	-2.149253	1.916981
H	0.000000	0.000000	-1.791679

Molecule# 0435

m-difluorobenzene

PointGroup: C2v

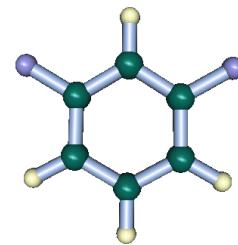
E= -430.889455566 au

ZPE= 0.083991 au

LUMO_eps= -0.03582 au

HOMO_eps= -0.26522 au

Dipole= 1.544 debye



12

C	0.000000	0.000000	1.764506
C	0.000000	1.210426	1.080320
C	0.000000	-1.210426	1.080320
C	0.000000	0.000000	-1.026563
C	0.000000	1.180185	-0.303243
C	0.000000	-1.180185	-0.303243
F	0.000000	2.345713	-0.982604
F	0.000000	-2.345713	-0.982604
H	0.000000	0.000000	2.845406
H	0.000000	2.158300	1.597384
H	0.000000	-2.158300	1.597384
H	0.000000	0.000000	-2.105879

Molecule# 0436

m-nitrophenol

PointGroup: Cs

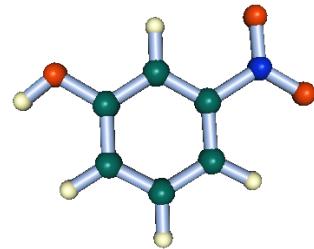
E= -512.171649369 au

ZPE= 0.106906 au

LUMO_eps= -0.10373 au

HOMO_eps= -0.26318 au

Dipole= 5.850 debye



15

C	2.017694	-0.664820	0.000000
C	1.387653	0.571113	0.000000
C	1.276764	-1.840590	0.000000
C	-0.768595	-0.561020	0.000000
C	0.000000	0.590564	0.000000
C	-0.116519	-1.789441	0.000000
N	-0.695089	1.896684	0.000000
O	-0.004530	2.904797	0.000000
O	-1.916677	1.890568	0.000000
O	-0.896581	-2.906357	0.000000
H	3.097332	-0.716014	0.000000
H	1.940706	1.495858	0.000000
H	1.780940	-2.799344	0.000000
H	-1.845347	-0.507182	0.000000
H	-0.347696	-3.696993	0.000000

Molecule# 0437

m-xylene

PointGroup: C1

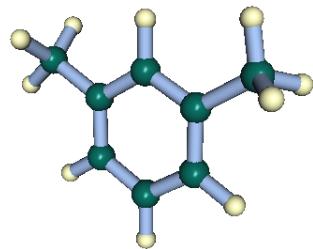
E= -310.998213968 au

ZPE= 0.154767 au

LUMO_eps= -0.01486 au

HOMO_eps= -0.24134 au

Dipole= 0.379 debye



18

C	-0.006539	1.816315	0.000770
C	-1.206885	1.122732	0.003227
C	1.203615	1.128282	-0.003363
C	0.003201	-0.944349	-0.003037
C	-1.217101	-0.275020	0.000767
C	1.224038	-0.263414	-0.004087
C	-2.520205	-1.031510	-0.000034
C	2.523101	-1.026861	0.003313
H	-0.009355	2.898503	0.000809
H	-2.143779	1.666030	0.005352
H	2.135935	1.678679	-0.006919
H	0.006865	-2.028704	-0.006327
H	-2.355320	-2.108183	0.003671
H	-3.122522	-0.782103	0.875925
H	-3.118135	-0.787666	-0.880617
H	2.555129	-1.763345	-0.801592
H	3.375896	-0.360048	-0.117283
H	2.655935	-1.570209	0.941651

Molecule# 0438

maleic anydride

PointGroup: C2v

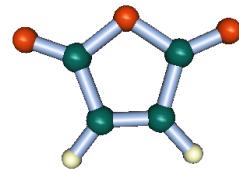
E= -379.440257243 au

ZPE= 0.055628 au

LUMO_eps= -0.12899 au

HOMO_eps= -0.31388 au

Dipole= 4.225 debye



9

O	0.000000	2.236047	0.597444
C	0.000000	1.129930	0.158173
O	0.000000	0.000000	0.969792
C	0.000000	-1.129930	0.158173
O	0.000000	-2.236047	0.597444
C	0.000000	-0.664242	-1.254113
C	0.000000	0.664242	-1.254113
H	0.000000	-1.352815	-2.083086
H	0.000000	1.352815	-2.083086

Molecule# 0439

mercapto (Z)-3-mercaptopoacrylate

PointGroup: C1

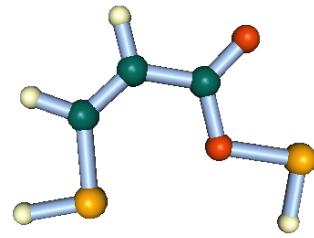
E= -1063.692835460 au

ZPE= 0.065804 au

LUMO_eps= -0.06883 au

HOMO_eps= -0.25114 au

Dipole= 3.930 debye



11

S	-2.265968	-0.918361	-0.000001
S	2.145504	-0.995460	0.000002
O	-0.634755	-0.362504	0.000000
O	-1.517867	1.704175	-0.000002
C	-0.541512	0.991131	-0.000001
C	0.843271	1.467699	0.000000
C	1.974268	0.747540	0.000000
H	-1.833773	-2.193713	0.000000
H	3.490805	-0.983923	0.000003
H	0.921463	2.545287	-0.000001
H	2.913753	1.281908	0.000000

Molecule# 0440

mesitylene

PointGroup: C3

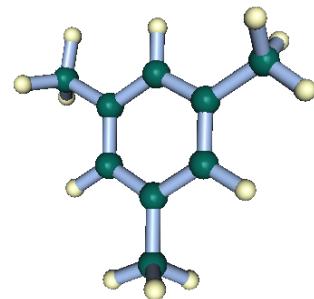
E= -350.329470595 au

ZPE= 0.181891 au

LUMO_eps= -0.01080 au

HOMO_eps= -0.23871 au

Dipole= 0.001 debye



21

C	1.195072	0.696188	-0.000003
C	-1.200452	0.686869	-0.000003
C	0.005380	-1.383057	-0.000003
C	0.000000	1.404022	-0.000002
C	1.215919	-0.702011	-0.000002
C	-1.215919	-0.702011	-0.000002
C	-0.014264	2.911190	0.000003
C	2.528296	-1.443242	0.000003
C	-2.514032	-1.467948	0.000003
H	2.133281	1.239569	-0.000006
H	-2.140139	1.227691	-0.000006
H	0.006857	-2.467260	-0.000006
H	-0.532837	3.302058	-0.878113
H	-0.532703	3.302052	0.878201
H	0.996060	3.318393	-0.000072
H	2.375782	-2.521810	-0.000072
H	3.126084	-1.189578	-0.878113
H	3.126012	-1.189692	0.878201
H	-2.593309	-2.112360	0.878201
H	-3.371843	-0.796583	-0.000072
H	-2.593247	-2.112479	-0.878113

Molecule# 0441

methacrylamide

PointGroup: C1

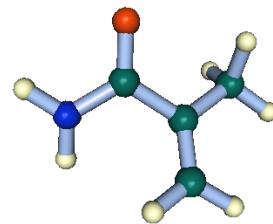
E= -286.732208163 au

ZPE= 0.106814 au

LUMO_eps= -0.04590 au

HOMO_eps= -0.26527 au

Dipole= 3.449 debye



13

N	-1.672206	0.735432	0.281233
H	-2.635471	0.448331	0.316740
H	-1.408035	1.582616	0.748896
C	1.669363	-0.902956	0.274192
H	1.491299	-1.339113	1.259311
H	1.537891	-1.708491	-0.448267
H	2.695543	-0.542835	0.230507
C	1.067908	1.453999	-0.283116
H	0.354906	2.225169	-0.540582
H	2.112388	1.736805	-0.297815
C	-0.747453	-0.216273	-0.042278
O	-1.070845	-1.348227	-0.361502
C	0.697462	0.204449	-0.006366

Molecule# 0442

methane

PointGroup: Td

E= -40.538430986 au

ZPE= 0.044550 au

LUMO_eps= -0.00813 au

HOMO_eps= -0.39560 au

Dipole= 0.000 debye



5

C 0.000000 0.000000 0.000000

H 0.628317 0.628317 0.628317

H -0.628317 -0.628317 0.628317

H -0.628317 0.628317 -0.628317

H 0.628317 -0.628317 -0.628317

Molecule# 0443

methanediol

PointGroup: C2

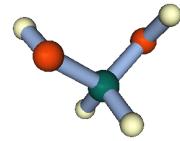
E= -191.037783504 au

ZPE= 0.056942 au

LUMO_eps= -0.01620 au

HOMO_eps= -0.30032 au

Dipole= 0.055 debye



7

C 0.000000 0.000000 0.529544

O 0.000000 1.174198 -0.247524

O 0.000000 -1.174198 -0.247524

H -0.891011 -0.071326 1.155757

H 0.891011 0.071326 1.155757

H -0.812903 1.199741 -0.764202

H 0.812903 -1.199741 -0.764202

Molecule# 0444

methanedithioicacid

PointGroup: Cs

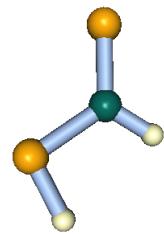
E= -835.755752249 au

ZPE= 0.025698 au

LUMO_eps= -0.09431 au

HOMO_eps= -0.24133 au

Dipole= 2.826 debye



5

S -1.379699 -0.462768 0.000000

S 1.542184 0.101951 0.000000

C 0.000000 0.604111 0.000000

H -0.264368 1.658591 0.000000

H -2.335387 0.489817 0.000000

Molecule# 0445

methanesulfonyl chloride

PointGroup: Cs

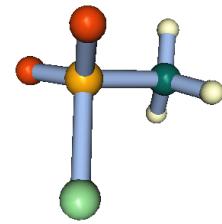
E= -1048.866412060 au

ZPE= 0.048310 au

LUMO_eps= -0.08763 au

HOMO_eps= -0.32938 au

Dipole= 3.910 debye



8

C	0.838039	1.595359	0.000000
O	0.838039	-0.743500	1.259473
O	0.838039	-0.743500	-1.259473
S	0.445322	-0.156189	0.000000
Cl	-1.666500	-0.052456	0.000000
H	0.421587	2.033909	0.900953
H	1.925327	1.646800	0.000000
H	0.421587	2.033909	-0.900953

Molecule# 0446

methanethiol

PointGroup: Cs

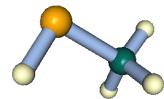
E= -438.757045585 au

ZPE= 0.045824 au

LUMO_eps= -0.01990 au

HOMO_eps= -0.24356 au

Dipole= 1.557 debye



6

C	0.048051	1.161675	0.000000
S	0.048051	-0.668872	0.000000
H	-0.431921	1.553804	0.892468
H	-0.431921	1.553804	-0.892468
H	1.092879	1.462961	0.000000
H	-1.286160	-0.838674	0.000000

Molecule# 0447

methanimidamide

PointGroup: C1

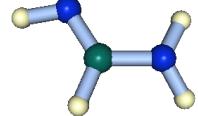
E= -150.074749506 au

ZPE= 0.057813 au

LUMO_eps= -0.01779 au

HOMO_eps= -0.25179 au

Dipole= 2.735 debye



7

C -0.122869 0.390343 -0.000727

N 1.132778 -0.147911 -0.053004

N -1.171312 -0.329822 0.010738

H -0.118022 1.483848 -0.004688

H 1.919698 0.417616 0.206986

H 1.214009 -1.140910 0.095135

H -2.008734 0.241521 0.002787

Molecule# 0448

methanimine

PointGroup: Cs

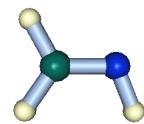
E= -94.671996175 au

ZPE= 0.039761 au

LUMO_eps= -0.03427 au

HOMO_eps= -0.27959 au

Dipole= 2.013 debye



5

C 0.056004 0.583317 0.000000

N 0.056004 -0.680483 0.000000

H -0.843040 1.205928 0.000000

H 1.009028 1.110493 0.000000

H -0.894042 -1.052940 0.000000

Molecule# 0449

methanol

PointGroup: Cs

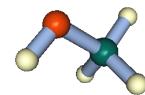
E= -115.776759424 au

ZPE= 0.051023 au

LUMO_eps= -0.01532 au

HOMO_eps= -0.28503 au

Dipole= 1.656 debye



6

C 0.046493 0.666056 0.000000

O 0.046493 -0.757300 0.000000

H -0.438632 1.076138 0.890767

H -0.438632 1.076138 -0.890767

H 1.088355 0.979641 0.000000

H -0.861989 -1.069858 0.000000

Molecule# 0450

methionine

PointGroup: C1

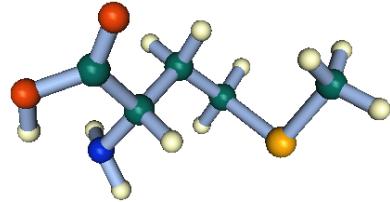
E= -800.761554297 au

ZPE= 0.165699 au

LUMO_eps= -0.02975 au

HOMO_eps= -0.23870 au

Dipole= 4.435 debye



20

N	1.383360	-1.709403	-0.280672
C	0.902676	-0.326707	-0.137165
C	2.097848	0.644277	-0.084187
O	1.986464	1.809740	0.191438
O	3.270321	0.085065	-0.408810
H	3.067922	-0.861838	-0.574079
C	-0.045437	-0.081707	1.039348
C	-1.394296	-0.791390	0.929264
S	-2.401897	-0.377571	-0.542342
C	-2.782880	1.376943	-0.230855
H	0.370857	-0.069835	-1.056761
H	0.441708	-0.411029	1.964287
H	-0.185549	0.993103	1.140986
H	-1.266805	-1.872991	0.865831
H	-1.989980	-0.594509	1.821028
H	-3.454759	1.689893	-1.027050
H	-3.289548	1.495435	0.725679
H	-1.889992	1.996927	-0.261114
H	1.404146	-2.198452	0.605725
H	0.817076	-2.246682	-0.921820

Molecule# 0451

methoxyacetonitrile

PointGroup: Cs

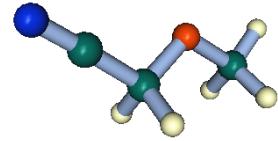
E= -247.359203206 au

ZPE= 0.078349 au

LUMO_eps= -0.02579 au

HOMO_eps= -0.29929 au

Dipole= 4.819 debye



10

H	2.599637	-1.376904	0.000000
H	2.446132	0.154878	0.891870
H	2.446132	0.154878	-0.891870
C	2.130026	-0.397042	0.000000
O	0.728282	-0.616731	0.000000
H	0.230030	1.194926	-0.885833
H	0.230030	1.194926	0.885833
C	0.000000	0.588434	0.000000
N	-2.565567	0.100471	0.000000
C	-1.433235	0.293249	0.000000

Molecule# 0452

methoxyethane

PointGroup: Cs

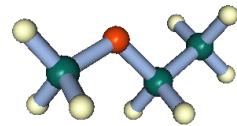
E= -194.426525456 au

ZPE= 0.107578 au

LUMO_eps= -0.00963 au

HOMO_eps= -0.26331 au

Dipole= 1.181 debye



12

C	1.436557	1.185794	0.000000
C	-1.314175	-1.253686	0.000000
C	0.000000	0.706828	0.000000
O	-0.011621	-0.711204	0.000000
H	1.471309	2.276007	0.000000
H	1.962303	0.823929	0.883530
H	1.962303	0.823929	-0.883530
H	-1.877412	-0.946607	0.889974
H	-1.215654	-2.337382	0.000000
H	-1.877412	-0.946607	-0.889974
H	-0.533380	1.081375	-0.884588
H	-0.533380	1.081375	0.884588

Molecule# 0453

methoxyflurane

PointGroup: C1

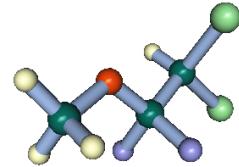
E= -1312.253906740 au

ZPE= 0.073880 au

LUMO_eps= -0.02908 au

HOMO_eps= -0.31711 au

Dipole= 2.546 debye



12

C	-2.942068	0.313165	-0.088641
C	0.735707	0.108753	-0.508616
C	-0.654620	-0.311306	0.007121
O	-1.574078	0.542788	-0.481566
F	-0.678682	-0.369389	1.367117
F	-0.901211	-1.593523	-0.415518
Cl	1.144790	1.756836	0.037582
Cl	1.979103	-1.067794	-0.011846
H	-3.270321	-0.674881	-0.406191
H	-3.516616	1.078339	-0.599716
H	-3.051412	0.421676	0.988511
H	0.709733	0.121384	-1.591166

Molecule# 0454

methyl-2-chloroacetate

PointGroup: Cs

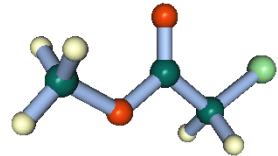
E= -728.122915049 au

ZPE= 0.080733 au

LUMO_eps= -0.01829 au

HOMO_eps= -0.30177 au

Dipole= 3.415 debye



11

C	0.000000	0.466246	0.000000
C	-0.565797	2.760319	0.000000
C	-0.633002	-0.915121	0.000000
O	1.170077	0.724321	0.000000
O	-0.987371	1.382600	0.000000
Cl	0.569257	-2.233268	0.000000
H	0.026696	2.973494	0.887304
H	-1.480710	3.343662	0.000000
H	0.026696	2.973494	-0.887304
H	-1.259449	-1.024561	-0.881342
H	-1.259449	-1.024561	0.881342

Molecule# 0455

methyl-2-cyanoacetate

PointGroup: Cs

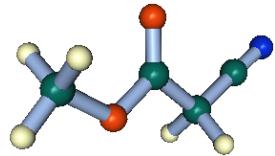
E= -360.762982773 au

ZPE= 0.088423 au

LUMO_eps= -0.02756 au

HOMO_eps= -0.31285 au

Dipole= 5.585 debye



12

C	-0.309415	-2.118342	0.000000
C	0.000000	0.358652	0.000000
C	0.510898	2.662545	0.000000
C	0.648261	-1.022919	0.000000
N	-1.032584	-3.010339	0.000000
O	-1.177335	0.583267	0.000000
O	0.963844	1.293027	0.000000
H	1.413063	3.264948	0.000000
H	-0.085786	2.861008	0.887616
H	-0.085786	2.861008	-0.887616
H	1.298037	-1.102284	0.873564
H	1.298037	-1.102284	-0.873564

Molecule# 0456

methyl-2,2-dimethylpropanoate

PointGroup: Cs

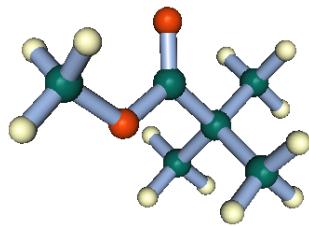
E= -386.482545525 au

ZPE= 0.173554 au

LUMO_eps= -0.01323 au

HOMO_eps= -0.27717 au

Dipole= 1.864 debye



20

C	-0.018703	0.623324	0.000000
C	-0.018703	-1.537398	1.260653
C	-2.067621	-0.796408	0.000000
C	-0.018703	-1.537398	-1.260653
C	1.913511	1.985730	0.000000
C	-0.535531	-0.817672	0.000000
O	-0.704653	1.615360	0.000000
O	1.331529	0.672656	0.000000
H	-0.353319	-1.032473	2.168179
H	-0.406978	-2.556799	1.283172
H	1.068644	-1.583922	1.275217
H	-2.456671	-0.283818	0.878679
H	-2.447056	-1.819081	0.000000
H	-2.456671	-0.283818	-0.878679
H	1.068644	-1.583922	-1.275217
H	-0.406978	-2.556799	-1.283172
H	-0.353319	-1.032473	-2.168179
H	1.607640	2.539254	0.885978
H	1.607640	2.539254	-0.885978
H	2.987917	1.829400	0.000000

Molecule# 0457

methyl-3-furancarboxylate

PointGroup: Cs

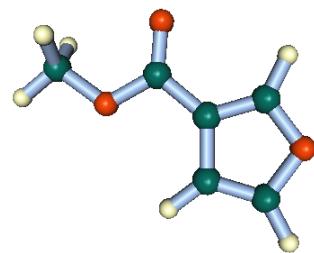
E= -458.080320278 au

ZPE= 0.112737 au

LUMO_eps= -0.04437 au

HOMO_eps= -0.25426 au

Dipole= 2.148 debye



15

C	-1.374452	0.901229	0.000000
C	-1.354402	2.251618	0.000000
C	0.741286	1.626446	0.000000
C	0.000000	0.483904	0.000000
C	0.566044	-0.870351	0.000000
C	0.057679	-3.174642	0.000000
O	1.747782	-1.126769	0.000000
O	-0.063377	2.708616	0.000000
O	-0.400911	-1.813271	0.000000
H	-2.241521	0.265834	0.000000
H	-2.117954	3.007351	0.000000
H	1.801169	1.802830	0.000000
H	0.656818	-3.374632	0.886389
H	0.656818	-3.374632	-0.886389
H	-0.840215	-3.784584	0.000000

Molecule# 0458

methyl-4-methoxybenzoate

PointGroup: Cs

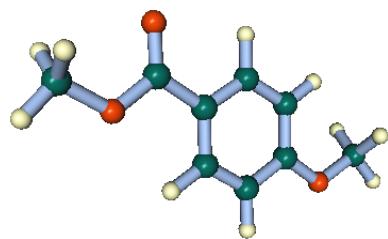
E= -574.873225434 au

ZPE= 0.175436 au

LUMO_eps= -0.04739 au

HOMO_eps= -0.24057 au

Dipole= 2.113 debye



22

C	1.212750	-0.008767	0.000000
C	-1.191217	-0.059999	0.000000
C	1.253899	-1.395528	0.000000
C	-1.163891	-1.439772	0.000000
C	0.000000	0.676566	0.000000
C	0.059380	-2.119086	0.000000
C	0.029615	2.157734	0.000000
C	1.187057	-4.229322	0.000000
C	-1.258011	4.136065	0.000000
O	1.037630	2.827599	0.000000
O	-0.016913	-3.473560	0.000000
O	-1.208484	2.702078	0.000000
H	2.130570	0.561741	0.000000
H	-2.138564	0.457542	0.000000
H	2.208636	-1.897967	0.000000
H	-2.077198	-2.017737	0.000000
H	1.783547	-4.025408	0.892035
H	1.783547	-4.025408	-0.892035
H	0.883035	-5.272089	0.000000
H	-2.313254	4.391701	0.000000
H	-0.767834	4.535668	-0.886018
H	-0.767834	4.535668	0.886018

Molecule# 0459

methyl-4-nitrobenzoate

PointGroup: Cs

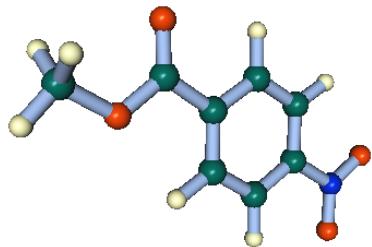
E= -664.883058192 au

ZPE= 0.145383 au

LUMO_eps= -0.11772 au

HOMO_eps= -0.29765 au

Dipole= 4.499 debye



20

C	-1.286273	0.390991	0.000000
C	1.112125	0.088865	0.000000
C	-1.467836	-0.981974	0.000000
C	0.942643	-1.286930	0.000000
C	0.000000	0.932795	0.000000
C	-0.346334	-1.799458	0.000000
C	0.128280	2.421778	0.000000
C	1.617644	4.250574	0.000000
N	-0.530904	-3.266994	0.000000
O	-0.811383	3.179716	0.000000
O	-1.675584	-3.692985	0.000000
O	0.472906	-3.963304	0.000000
O	1.410358	2.826665	0.000000
H	-2.134031	1.060043	0.000000
H	2.105499	0.509823	0.000000
H	-2.451989	-1.422851	0.000000
H	1.785123	-1.960132	0.000000
H	2.694123	4.387094	0.000000
H	1.172868	4.697195	0.886917
H	1.172868	4.697195	-0.886917

Molecule# 0460

methyl-N-cyanocarbamodithioate

PointGroup: C1

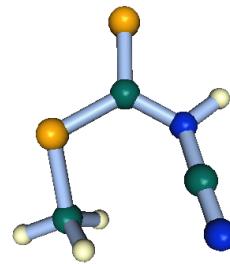
E= -1022.728914440 au

ZPE= 0.071048 au

LUMO_eps= -0.09133 au

HOMO_eps= -0.24939 au

Dipole= 1.955 debye



11

S	-0.076909	1.429668	-0.296124
S	-2.320711	-0.430992	0.003087
N	0.165442	-1.221447	0.348448
N	2.533503	-1.512399	-0.373747
C	-0.698146	-0.166640	0.047913
C	1.601582	1.576805	0.424261
C	1.436783	-1.360875	-0.047466
H	2.364171	1.136291	-0.207540
H	1.754503	2.651749	0.498792
H	1.630211	1.146821	1.421550
H	-0.320892	-2.072484	0.604643

Molecule# 0461

methyl-N-methylcarbamate

PointGroup: C1

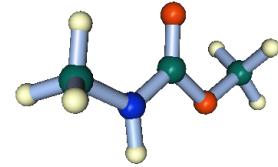
E= -323.884524057 au

ZPE= 0.106898 au

LUMO_eps= -0.01490 au

HOMO_eps= -0.26462 au

Dipole= 2.403 debye



13

C	0.017458	0.114976	-0.000014
C	-2.442157	-0.010060	0.000035
C	2.370388	-0.058037	0.000016
N	-1.126195	-0.614338	-0.000060
O	0.091274	1.325205	-0.000014
O	1.096157	-0.714172	0.000010
H	-2.316092	1.068892	-0.000449
H	-3.008671	-0.296928	0.887756
H	-3.009081	-0.297691	-0.887170
H	2.483823	0.563324	0.886629
H	2.483850	0.563286	-0.886620
H	3.107408	-0.855675	0.000044
H	-1.031457	-1.614379	0.000035

Molecule# 0462

methyl 4-amino-1,2,5-oxadiazole-3-carboxylate

PointGroup: C1

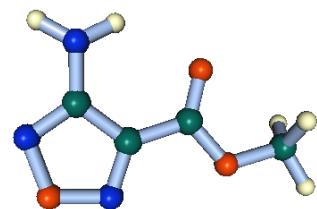
E= -545.497651221 au

ZPE= 0.105176 au

LUMO_eps= -0.08373 au

HOMO_eps= -0.26317 au

Dipole= 3.504 debye



15

O	2.016475	-1.532303	0.023208
O	-1.977891	-0.721593	-0.043326
O	-1.306736	1.428753	0.077244
N	0.673411	-1.516062	0.017123
N	2.549934	-0.243148	0.003763
N	1.568662	1.902573	-0.089651
C	0.322741	-0.259915	-0.006268
C	1.509470	0.550011	-0.017954
C	-1.061961	0.241317	0.012304
C	-3.352842	-0.290458	-0.016320
H	0.715764	2.400412	0.105126
H	2.442779	2.350901	0.120191
H	-3.562178	0.355303	-0.866446
H	-3.561230	0.246902	0.906438
H	-3.938417	-1.201652	-0.071525

Molecule# 0463

methyl acetate

PointGroup: Cs

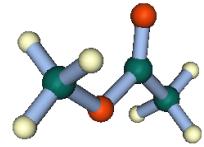
E= -268.500285466 au

ZPE= 0.089213 au

LUMO_eps= -0.01244 au

HOMO_eps= -0.28501 au

Dipole= 1.921 debye



11

C	0.000000	0.495796	0.000000
C	-1.126166	1.493825	0.000000
C	0.518397	-1.810474	0.000000
O	1.175144	0.763556	0.000000
O	-0.472599	-0.769316	0.000000
H	-1.754646	1.346302	0.878098
H	-1.754646	1.346302	-0.878098
H	-0.719073	2.499833	0.000000
H	1.146150	-1.739249	-0.886325
H	-0.037679	-2.742743	0.000000
H	1.146150	-1.739249	0.886325

Molecule# 0464

methyl azide

PointGroup: Cs

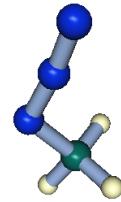
E= -204.175253550 au

ZPE= 0.050227 au

LUMO_eps= -0.04134 au

HOMO_eps= -0.26628 au

Dipole= 2.327 debye



7

N 0.000000 0.723823 0.000000

N -0.513023 1.731413 0.000000

N 0.675733 -0.298488 0.000000

C -0.069885 -1.567760 0.000000

H 0.668896 -2.362474 0.000000

H -0.694278 -1.664099 0.890793

H -0.694278 -1.664099 -0.890793

Molecule# 0465

methyl benzoate

PointGroup: Cs

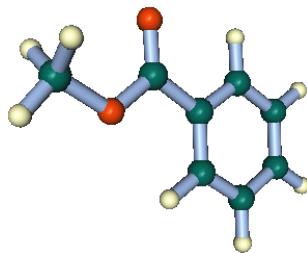
E= -460.303103265 au

ZPE= 0.143054 au

LUMO_eps= -0.05931 au

HOMO_eps= -0.27025 au

Dipole= 1.986 debye



18

C	-1.629703	2.519691	0.000000
C	-0.245437	2.661629	0.000000
C	-2.199329	1.250750	0.000000
C	0.567055	1.537570	0.000000
C	-1.389364	0.123082	0.000000
C	0.000000	0.261893	0.000000
C	0.918942	-0.909822	0.000000
C	1.082579	-3.263273	0.000000
O	2.125324	-0.833326	0.000000
O	0.258943	-2.087035	0.000000
H	-2.263404	3.396510	0.000000
H	0.198432	3.647794	0.000000
H	-3.275165	1.139998	0.000000
H	1.643793	1.627324	0.000000
H	-1.827393	-0.863439	0.000000
H	1.713986	-3.286294	0.886283
H	1.713986	-3.286294	-0.886283
H	0.393171	-4.101840	0.000000

Molecule# 0466

methyl cyclopropanecarboxylate

PointGroup: Cs

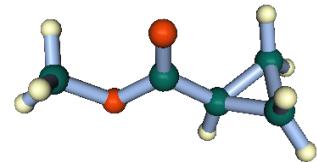
E= -345.913305738 au

ZPE= 0.124398 au

LUMO_eps= -0.00940 au

HOMO_eps= -0.28447 au

Dipole= 1.701 debye



15

C	0.042677	0.344157	0.000000
C	-0.973754	-1.889957	0.743851
C	-0.973754	-1.889957	-0.743851
C	0.111176	-1.135227	0.000000
C	1.324994	2.327509	0.000000
O	-0.973754	0.998522	0.000000
O	1.277432	0.891383	0.000000
H	-1.716618	-1.286124	1.243595
H	-0.669468	-2.784850	1.266689
H	-0.669468	-2.784850	-1.266689
H	-1.716618	-1.286124	-1.243595
H	1.106406	-1.551725	0.000000
H	2.379774	2.584262	0.000000
H	0.834268	2.725508	0.886305
H	0.834268	2.725508	-0.886305

Molecule# 0467

methyl formate

PointGroup: Cs

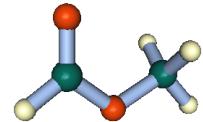
E= -229.160579914 au

ZPE= 0.061716 au

LUMO_eps= -0.01617 au

HOMO_eps= -0.29914 au

Dipole= 1.965 debye



8

C	0.932507	-0.092918	0.000000
C	-1.369372	0.416095	0.000000
O	0.725872	-1.275132	0.000000
O	0.000000	0.866990	0.000000
H	1.926421	0.370591	0.000000
H	-1.972732	1.317760	0.000000
H	-1.569738	-0.181136	0.887236
H	-1.569738	-0.181136	-0.887236

Molecule# 0468

methyl hexanoate

PointGroup: Cs

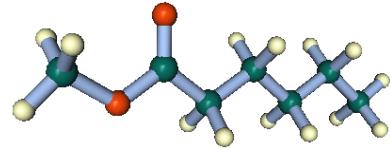
E= -425.812570389 au

ZPE= 0.202734 au

LUMO_eps= -0.01280 au

HOMO_eps= -0.28262 au

Dipole= 1.619 debye



23

C	1.488939	1.017839	0.000000
C	-3.766271	-2.671937	0.000000
C	3.138511	2.711319	0.000000
C	0.000000	0.760101	0.000000
C	-2.256886	-2.436231	0.000000
C	-0.365395	-0.720041	0.000000
C	-1.876026	-0.955711	0.000000
O	2.352499	0.176679	0.000000
O	1.749338	2.343823	0.000000
H	-4.235468	-2.228565	0.880789
H	-4.235468	-2.228565	-0.880789
H	-4.003230	-3.736674	0.000000
H	3.153724	3.796785	0.000000
H	3.636516	2.322018	-0.886207
H	3.636516	2.322018	0.886207
H	-0.422849	1.270771	-0.869472
H	-0.422849	1.270771	0.869472
H	-1.811861	-2.921057	-0.873831
H	-1.811861	-2.921057	0.873831
H	0.084585	-1.201251	0.871034
H	0.084585	-1.201251	-0.871034
H	-2.322130	-0.469995	-0.874710
H	-2.322130	-0.469995	0.874710

Molecule# 0469

methyl hydroperoxide

PointGroup: C1

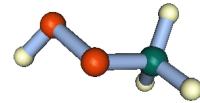
E= -190.938909679 au

ZPE= 0.054417 au

LUMO_eps= -0.01728 au

HOMO_eps= -0.27525 au

Dipole= 1.630 debye



7

C 1.130346 -0.225128 0.025065

O -0.015267 0.606026 -0.027255

O -1.167167 -0.278825 -0.095051

H 1.971335 0.468788 0.022108

H 1.147766 -0.826787 0.937012

H 1.184789 -0.873635 -0.851239

H -1.626495 -0.035207 0.720173

Molecule# 0470

methyl hypochlorite

PointGroup: Cs

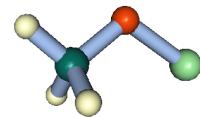
E= -575.348123870 au

ZPE= 0.041661 au

LUMO_eps= -0.08214 au

HOMO_eps= -0.28031 au

Dipole= 1.835 debye



6

O 0.000000 0.802908 0.000000

Cl -0.811552 -0.704077 0.000000

C 1.415082 0.620626 0.000000

H 1.809715 1.636753 0.000000

H 1.748086 0.092767 0.894890

H 1.748086 0.092767 -0.894890

Molecule# 0471

methyl nitrate

PointGroup: Cs

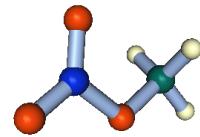
E= -320.325240829 au

ZPE= 0.054036 au

LUMO_eps= -0.07982 au

HOMO_eps= -0.33201 au

Dipole= 3.163 debye



8

N	0.000000	0.625382	0.000000
O	-1.204276	0.568235	0.000000
O	0.724269	1.578295	0.000000
O	0.708849	-0.603160	0.000000
C	-0.143421	-1.760352	0.000000
H	0.559744	-2.588769	0.000000
H	-0.764976	-1.786875	0.892235
H	-0.764976	-1.786875	-0.892235

Molecule# 0472

methyl octanoate

PointGroup: C1

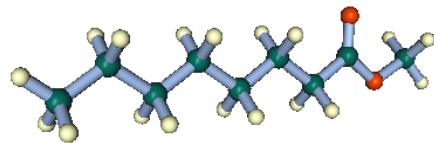
E= -504.468703858 au

ZPE= 0.259625 au

LUMO_eps= -0.01287 au

HOMO_eps= -0.28239 au

Dipole= 1.610 debye



29

C	-3.009194	0.132720	0.000067
C	5.949220	-0.256907	0.000078
C	-5.358960	-0.130980	-0.000089
C	-1.695422	-0.613559	0.000091
C	4.637910	0.526987	-0.000135
C	-0.471203	0.295500	-0.000112
C	3.398027	-0.367925	0.000074
C	0.841821	-0.487584	0.000072
C	2.080878	0.408235	-0.000139
O	-3.143099	1.330753	0.000219
O	-4.051638	-0.727268	-0.000120
H	6.025429	-0.898227	-0.880487
H	6.025395	-0.897805	0.880953
H	6.812866	0.409515	-0.000065
H	-6.058778	-0.960891	-0.000238
H	-5.497418	0.485846	-0.886256
H	-5.497491	0.485592	0.886244
H	-1.693478	-1.276884	-0.869154
H	-1.693380	-1.276583	0.869569
H	4.606452	1.184753	0.873644
H	4.606474	1.184314	-0.874245
H	-0.510948	0.953181	0.870826
H	-0.510932	0.952783	-0.871354
H	3.430023	-1.026718	-0.874390
H	3.430000	-1.026275	0.874873
H	0.873319	-1.146380	-0.874384
H	0.873315	-1.145960	0.874844
H	2.049304	1.066245	-0.874663
H	2.049281	1.066686	0.874053

Molecule# 0473

methyl pentanoate

PointGroup: Cs

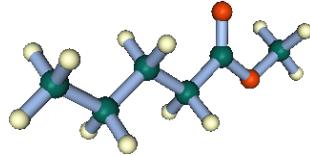
E= -386.484517460 au

ZPE= 0.174505 au

LUMO_eps= -0.01280 au

HOMO_eps= -0.28285 au

Dipole= 1.718 debye



20

C	-1.162065	-0.316600	0.000000
C	3.891987	0.293233	0.000000
C	-3.521231	-0.471592	0.000000
C	0.000000	0.649193	0.000000
C	2.521478	0.967777	0.000000
C	1.364398	-0.031139	0.000000
O	-1.082593	-1.519471	0.000000
O	-2.339681	0.346164	0.000000
H	4.019803	-0.339306	0.880577
H	4.019803	-0.339306	-0.880577
H	4.697325	1.028826	0.000000
H	-3.548612	-1.103036	0.886262
H	-3.548612	-1.103036	-0.886262
H	-4.356547	0.221758	0.000000
H	-0.114752	1.302305	-0.869458
H	-0.114752	1.302305	0.869458
H	2.437814	1.621046	0.874090
H	2.437814	1.621046	-0.874090
H	1.440757	-0.685686	0.871083
H	1.440757	-0.685686	-0.871083

Molecule# 0474

methyl peroxycyanate

PointGroup: C1

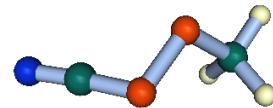
E= -283.182386109 au

ZPE= 0.052743 au

LUMO_eps= -0.09953 au

HOMO_eps= -0.31278 au

Dipole= 4.525 debye



8

O	0.168175	0.731979	-0.169936
O	-0.875385	0.011600	0.633516
N	2.292619	-0.465281	-0.025231
C	1.271007	0.074684	-0.071494
C	-1.910219	-0.317169	-0.281016
H	-2.328484	0.577593	-0.741855
H	-1.568489	-1.027299	-1.034576
H	-2.658412	-0.787050	0.359468

Molecule# 0475

methyl propanoate

PointGroup: Cs

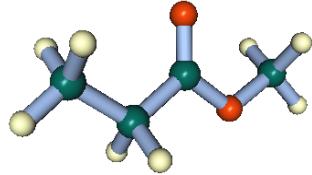
E= -307.828548319 au

ZPE= 0.117869 au

LUMO_eps= -0.01301 au

HOMO_eps= -0.28382 au

Dipole= 1.771 debye



14

C	0.000000	0.105348	0.000000
C	2.229810	-1.101248	0.000000
C	-2.125328	1.140307	0.000000
C	0.712415	-1.227832	0.000000
O	0.529639	1.188224	0.000000
O	-1.340167	-0.063276	0.000000
H	2.578825	-0.559466	0.877868
H	2.691306	-2.088610	0.000000
H	2.578825	-0.559466	-0.877868
H	-3.160662	0.813935	0.000000
H	-1.911948	1.735162	-0.886287
H	-1.911948	1.735162	0.886287
H	0.359222	-1.787875	0.869073
H	0.359222	-1.787875	-0.869073

Molecule# 0476

methylamine

PointGroup: Cs

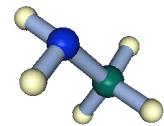
E= -95.903413589 au

ZPE= 0.063752 au

LUMO_eps= -0.01360 au

HOMO_eps= -0.24426 au

Dipole= 1.288 debye



7

C -0.048962 0.706625 0.000000

N -0.048962 -0.757428 0.000000

H 0.945026 1.171177 0.000000

H -0.587216 1.065175 0.877567

H -0.587216 1.065175 -0.877567

H 0.432957 -1.119643 0.812861

H 0.432957 -1.119643 -0.812861

Molecule# 0477

methylbenzoquinone

PointGroup: Cs

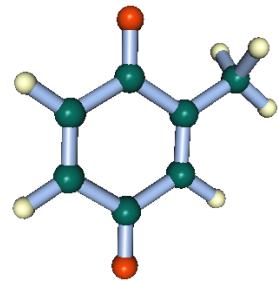
E= -420.933824360 au

ZPE= 0.112612 au

LUMO_eps= -0.13687 au

HOMO_eps= -0.27937 au

Dipole= 0.841 debye



15

C	0.157346	2.550685	0.000000
C	0.000000	1.065125	0.000000
C	1.254968	0.250008	0.000000
C	-1.184685	0.435491	0.000000
O	2.350763	0.783788	0.000000
C	1.133424	-1.225777	0.000000
C	-1.308516	-1.034538	0.000000
C	-0.057139	-1.827836	0.000000
O	-2.399405	-1.581506	0.000000
H	-0.810637	3.047202	0.000000
H	0.726761	2.875723	0.872072
H	0.726761	2.875723	-0.872072
H	-2.120792	0.980088	0.000000
H	2.067297	-1.772322	0.000000
H	-0.172634	-2.903622	0.000000

Molecule# 0478

methylcarbamodithioic acid

PointGroup: Cs

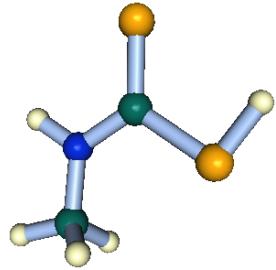
E= -930.478390686 au

ZPE= 0.071462 au

LUMO_eps= -0.04638 au

HOMO_eps= -0.22308 au

Dipole= 4.033 debye



10

C	1.860208	-1.388426	0.000000
N	1.300486	-0.046394	0.000000
C	0.000000	0.288733	0.000000
S	-0.535187	1.859700	0.000000
S	-1.092712	-1.125087	0.000000
H	1.555773	-1.946049	0.887371
H	1.555773	-1.946049	-0.887371
H	2.943735	-1.305923	0.000000
H	1.930390	0.739868	0.000000
H	-2.203937	-0.372747	0.000000

Molecule# 0479

methylcrotonate

PointGroup: C1

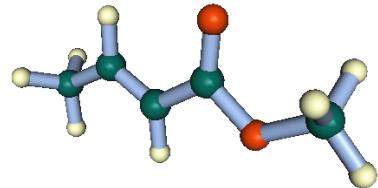
E= -345.928863879 au

ZPE= 0.122850 au

LUMO_eps= -0.05034 au

HOMO_eps= -0.27844 au

Dipole= 1.803 debye

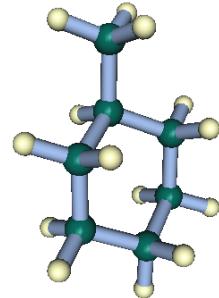


15

O	-0.793144	1.368201	-0.000236
C	-0.564751	0.180694	-0.000163
C	0.769320	-0.452538	-0.000259
C	1.881122	0.280508	0.000126
C	3.269891	-0.259619	0.000137
O	-1.538842	-0.759642	0.000060
C	-2.885236	-0.262814	0.000226
H	0.797736	-1.534345	-0.001112
H	1.768232	1.360075	0.000946
H	3.819852	0.096612	0.875095
H	3.287143	-1.348669	-0.000445
H	3.820235	0.097410	-0.874284
H	-3.068501	0.342864	0.886099
H	-3.068919	0.342320	-0.885935
H	-3.521975	-1.142120	0.000642

Molecule# 0480
methylcyclohexane
PointGroup: Cs

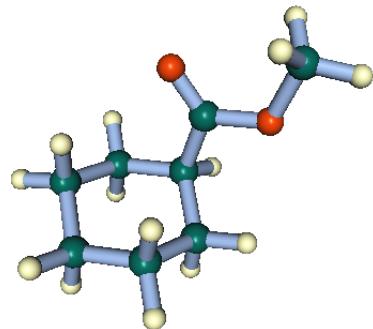
E= -275.296344908 au
ZPE= 0.197069 au
LUMO_eps= -0.00986 au
HOMO_eps= -0.29515 au
Dipole= 0.132 debye



21

C	-0.739782	-1.773761	0.000000
C	-0.089048	-1.206811	1.264899
C	-0.089048	-1.206811	-1.264899
C	-0.089048	0.324852	1.260545
C	-0.089048	0.324852	-1.260545
C	0.566508	0.906527	0.000000
C	0.533702	2.434333	0.000000
H	-0.680166	-2.864513	0.000000
H	-1.805477	-1.520961	0.000000
H	-0.602476	-1.579676	2.154131
H	0.943314	-1.566555	1.330389
H	0.943314	-1.566555	-1.330389
H	-0.602476	-1.579676	-2.154131
H	-1.122408	0.686328	1.318579
H	0.419978	0.704095	2.150588
H	0.419978	0.704095	-2.150588
H	-1.122408	0.686328	-1.318579
H	1.617471	0.591208	0.000000
H	1.030791	2.842574	0.882126
H	1.030791	2.842574	-0.882126
H	-0.495635	2.801645	0.000000

Molecule# 0481
 methylcyclohexanoate
 PointGroup: C1
 E= -463.928130126 au
 ZPE= 0.212491 au
 LUMO_eps= -0.01548 au
 HOMO_eps= -0.27703 au
 Dipole= 1.716 debye

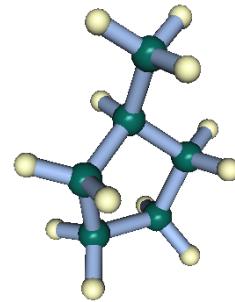


24

C	-1.111854	-0.407602	0.125096
C	2.519955	0.359470	-0.688408
C	1.969676	-1.052974	-0.470654
C	1.411901	1.411583	-0.589259
C	1.194356	-1.168658	0.847170
C	0.666104	1.312877	0.744533
C	0.099900	-0.101797	0.994429
C	-3.281670	0.319162	-0.471198
O	-1.250170	-1.370670	-0.588255
O	-2.072170	0.532062	0.273850
H	3.284420	0.574297	0.066511
H	3.016327	0.424143	-1.659020
H	1.308119	-1.318004	-1.297782
H	2.784895	-1.779646	-0.477318
H	1.828011	2.414978	-0.702103
H	0.706946	1.275720	-1.416225
H	0.756983	-2.162764	0.937526
H	1.888488	-1.047022	1.684150
H	1.361886	1.538168	1.557947
H	-0.133635	2.050051	0.799485
H	-0.284837	-0.125874	2.018897
H	-3.073608	0.295602	-1.539403
H	-3.927090	1.157271	-0.226901
H	-3.748380	-0.620419	-0.180785

Molecule# 0482
methylcyclopentane
PointGroup: C1

E= -235.960116455 au
ZPE= 0.167871 au
LUMO_eps= -0.01070 au
HOMO_eps= -0.31253 au
Dipole= 0.102 debye



18

C	-1.527992	-0.778219	-0.025802
C	-1.527998	0.778215	-0.025762
C	-0.054746	-1.195602	0.153522
C	-0.054742	1.195610	0.153491
C	0.759977	-0.000005	-0.361654
C	2.225909	-0.000001	0.053568
H	-2.163452	-1.189245	0.758393
H	-1.917173	-1.155891	-0.972214
H	-1.917255	1.155933	-0.972124
H	-2.163406	1.189187	0.758504
H	0.170715	-1.346139	1.213831
H	0.187200	-2.127106	-0.360157
H	0.187182	2.127090	-0.360241
H	0.170755	1.346201	1.213784
H	0.706863	-0.000021	-1.457058
H	2.748064	0.880936	-0.324665
H	2.320004	0.000014	1.142416
H	2.748063	-0.880949	-0.324642

Molecule# 0483

methylcyclopropylketone

PointGroup: Cs

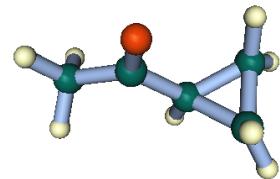
E= -270.650260837 au

ZPE= 0.118529 au

LUMO_eps= -0.02565 au

HOMO_eps= -0.25659 au

Dipole= 2.989 debye



14

C	0.284009	-0.759507	0.000000
C	-0.302823	1.638533	0.742121
C	-0.302823	1.638533	-0.742121
C	-0.688018	0.369102	0.000000
C	-0.302823	-2.152697	0.000000
O	1.484030	-0.570889	0.000000
H	0.655236	1.614399	1.240617
H	-1.093428	2.156153	1.265732
H	-1.093428	2.156153	-1.265732
H	0.655236	1.614399	-1.240617
H	-1.734635	0.099083	0.000000
H	-0.938808	-2.291274	0.877339
H	-0.938808	-2.291274	-0.877339
H	0.491252	-2.894317	0.000000

Molecule# 0484

methyldisulfanylethane

PointGroup: C1

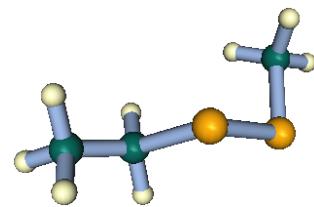
E= -915.647077981 au

ZPE= 0.105426 au

LUMO_eps= -0.02751 au

HOMO_eps= -0.23944 au

Dipole= 2.139 debye



13

C	-2.888226	0.352672	0.043352
C	2.230326	1.007436	0.361276
C	-1.472280	0.450501	-0.510263
S	1.475203	-0.449173	-0.449721
S	-0.358677	-0.632636	0.485898
H	-3.263170	-0.670018	-0.003336
H	-2.934951	0.684419	1.080970
H	-3.559094	0.983985	-0.541222
H	1.664668	1.911244	0.149935
H	3.229499	1.100849	-0.064440
H	2.305148	0.847335	1.433383
H	-1.100520	1.472025	-0.456081
H	-1.424923	0.115456	-1.544229

Molecule# 0485

methylene cyclobutane

PointGroup: Cs

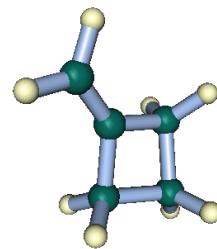
E= -195.369390971 au

ZPE= 0.114353 au

LUMO_eps= -0.01138 au

HOMO_eps= -0.25108 au

Dipole= 0.592 debye



13

C	0.233750	-0.388334	1.091648
C	0.233750	-0.388334	-1.091648
C	-0.103047	0.613325	0.000000
C	0.233750	-1.499323	0.000000
C	-0.627950	1.827559	0.000000
H	-0.477778	-0.485850	1.911239
H	-0.477778	-0.485850	-1.911239
H	1.227026	-0.224070	1.515020
H	1.227026	-0.224070	-1.515020
H	-0.853925	2.345913	0.923515
H	-0.853925	2.345913	-0.923515
H	1.077726	-2.185964	0.000000
H	-0.689886	-2.075382	0.000000

Molecule# 0486

methylenecyclopropane

PointGroup: C2v

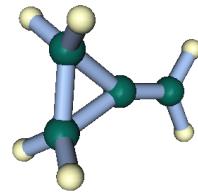
E= -156.024906640 au

ZPE= 0.084817 au

LUMO_eps= -0.01296 au

HOMO_eps= -0.26509 au

Dipole= 0.460 debye



10

C	0.000000	0.000000	1.631581
C	0.000000	0.000000	0.315547
H	0.000000	0.924656	2.195166
H	0.000000	-0.924656	2.195166
C	0.000000	0.769087	-0.928764
C	0.000000	-0.769087	-0.928764
H	0.910119	1.272300	-1.231981
H	-0.910119	1.272300	-1.231981
H	-0.910119	-1.272300	-1.231981
H	0.910119	-1.272300	-1.231981

Molecule# 0487

methylester-2-propenoicacid

PointGroup: Cs

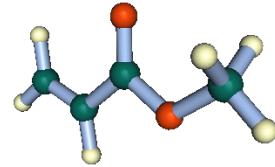
E= -306.593088014 au

ZPE= 0.094958 au

LUMO_eps= -0.06172 au

HOMO_eps= -0.28867 au

Dipole= 1.613 debye



12

H	2.527150	-1.893203	0.000000
H	2.462309	-0.342027	0.886291
H	2.462309	-0.342027	-0.886291
C	2.133452	-0.881675	0.000000
O	0.704179	-1.022573	0.000000
O	0.512478	1.224123	0.000000
C	0.000000	0.130493	0.000000
H	-1.752520	-1.187537	0.000000
C	-1.456302	-0.147598	0.000000
H	-3.407145	0.640284	0.000000
H	-2.020476	1.871183	0.000000
C	-2.344631	0.838935	0.000000

Molecule# 0488

methylethylsulfone

PointGroup: C1

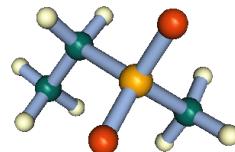
E= -667.888483473 au

ZPE= 0.113167 au

LUMO_eps= -0.02387 au

HOMO_eps= -0.29513 au

Dipole= 4.860 debye



14

C	2.288662	0.176351	0.057230
C	1.130294	-0.527360	-0.632556
C	-0.786688	1.583975	-0.306161
S	-0.501180	-0.154526	0.071483
O	-0.417269	-0.287283	1.523670
O	-1.483277	-0.935076	-0.675425
H	2.280785	-0.024085	1.126808
H	3.231448	-0.185743	-0.353456
H	2.258771	1.255472	-0.093143
H	1.185809	-1.610963	-0.523095
H	1.058079	-0.300708	-1.695857
H	-0.772893	1.722266	-1.384003
H	-1.774988	1.803771	0.091152
H	-0.037380	2.193478	0.190821

Molecule# 0489

methylethylsulfoxide

PointGroup: C1

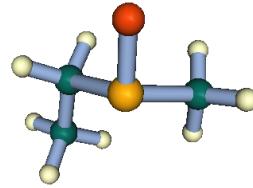
E= -592.634046960 au

ZPE= 0.107552 au

LUMO_eps= -0.01892 au

HOMO_eps= -0.23527 au

Dipole= 4.349 debye



13

C	-2.236697	0.080677	-0.129130
H	-2.322637	-0.067127	-1.206237
H	-3.133658	-0.332836	0.333139
H	-2.233285	1.152436	0.067774
C	-1.000479	-0.609481	0.429352
H	-1.046983	-1.689171	0.288441
H	-0.841528	-0.414738	1.490353
C	0.730937	1.540292	0.218013
H	-0.093206	2.158259	-0.133594
S	0.566260	-0.160011	-0.432652
O	1.651899	-0.967089	0.229435
H	1.671903	1.924648	-0.167830
H	0.761473	1.496490	1.305499

Molecule# 0490

methylhydrazine

PointGroup: C1

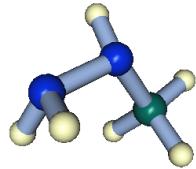
E= -151.243951847 au

ZPE= 0.081189 au

LUMO_eps= -0.01517 au

HOMO_eps= -0.24247 au

Dipole= 1.690 debye



9

C	-1.176124	-0.240930	-0.001430
N	0.026647	0.569467	-0.122671
N	1.244597	-0.148622	0.053689
H	1.130779	-0.914669	0.717137
H	1.508519	-0.549814	-0.837623
H	-1.242751	-0.927801	-0.846695
H	-1.212149	-0.834846	0.925321
H	-2.049950	0.411665	-0.026287
H	0.023585	1.315124	0.559605

Molecule# 0491

methylketene

PointGroup: Cs

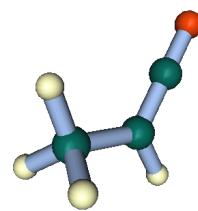
E= -191.993875313 au

ZPE= 0.060763 au

LUMO_eps= -0.04458 au

HOMO_eps= -0.23659 au

Dipole= 1.951 debye



8

C	-0.671285	-0.386770	0.000000
C	0.000000	0.736156	0.000000
C	1.508464	0.811358	0.000000
O	-1.266323	-1.387836	0.000000
H	-0.595082	1.639797	0.000000
H	1.954606	-0.181706	0.000000
H	1.873994	1.340067	0.882008
H	1.873994	1.340067	-0.882008

Molecule# 0492

methylnitrite

PointGroup: Cs

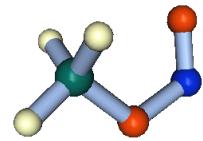
E= -245.109769485 au

ZPE= 0.048120 au

LUMO_eps= -0.08799 au

HOMO_eps= -0.29308 au

Dipole= 2.221 debye



7

C 1.328264 0.334723 0.000000

O 0.000000 0.884876 0.000000

H 1.983497 1.199685 0.000000

H 1.493655 -0.273528 0.888518

H 1.493655 -0.273528 -0.888518

N -1.045924 -0.048758 0.000000

O -0.702365 -1.174834 0.000000

Molecule# 0493

methylperoxyacetylene

PointGroup: C1

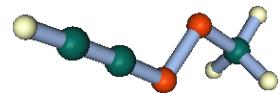
E= -267.085085961 au

ZPE= 0.062454 au

LUMO_eps= -0.07853 au

HOMO_eps= -0.25483 au

Dipole= 1.408 debye



9

O	0.113175	0.611906	-0.000481
O	-0.850519	-0.571912	-0.000730
C	1.313138	0.157342	-0.000011
C	-2.131835	0.020694	0.000616
C	2.457104	-0.211516	0.000417
H	-2.297771	0.619401	-0.896754
H	-2.296639	0.617800	0.899259
H	-2.808117	-0.835719	0.000264
H	3.470842	-0.520554	0.000796

Molecule# 0494

methylphenylsulfone

PointGroup: Cs

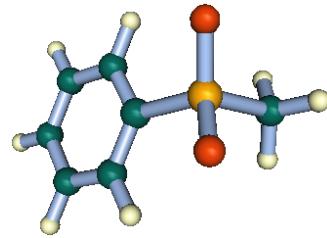
E= -820.356728721 au

ZPE= 0.138029 au

LUMO_eps= -0.05743 au

HOMO_eps= -0.28537 au

Dipole= 5.137 debye



18

C	0.091342	3.082579	0.000000
C	0.094844	2.390597	1.206836
C	0.094844	2.390597	-1.206836
C	0.094844	1.001048	1.213029
C	0.094844	1.001048	-1.213029
C	0.088331	0.322160	0.000000
C	-1.655962	-1.917459	0.000000
O	0.656057	-1.929130	-1.266976
O	0.656057	-1.929130	1.266976
S	0.091079	-1.476746	0.000000
H	0.094921	4.164148	0.000000
H	0.106394	2.931653	2.142942
H	0.106394	2.931653	-2.142942
H	0.122551	0.445707	2.139560
H	0.122551	0.445707	-2.139560
H	-2.120878	-1.521537	-0.898564
H	-1.683749	-3.005188	0.000000
H	-2.120878	-1.521537	0.898564

Molecule# 0495

methylsulfanyl thiocyanate

PointGroup: C1

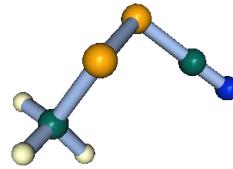
E= -929.250239279 au

ZPE= 0.048034 au

LUMO_eps= -0.08600 au

HOMO_eps= -0.27745 au

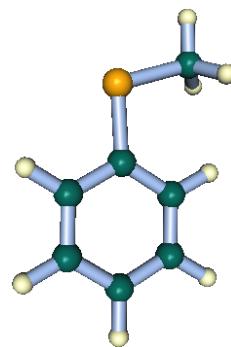
Dipole= 3.996 debye



8

S	-1.181973	-0.258533	-0.605061
S	0.526277	-0.912219	0.396167
N	2.499926	1.048130	-0.266984
C	-1.850452	1.006228	0.528769
C	1.684030	0.266004	-0.023640
H	-2.789196	1.324506	0.074977
H	-1.175486	1.854944	0.595860
H	-2.045134	0.582281	1.509582

Molecule# 0496
 methylsulfanylbenzene
 PointGroup: C1
 E= -669.886370975 au
 ZPE= 0.128909 au
 LUMO_eps= -0.02083 au
 HOMO_eps= -0.21623 au
 Dipole= 1.321 debye



16

C	2.631509	0.344451	0.000050
C	1.698472	1.371404	-0.000121
C	2.188597	-0.975522	0.000179
C	0.334547	1.093914	-0.000188
C	0.832934	-1.262341	0.000136
C	-0.109855	-0.227934	-0.000068
C	-2.721440	0.856894	0.000405
S	-1.818130	-0.717138	-0.000261
H	3.689808	0.566132	0.000100
H	2.026789	2.402640	-0.000214
H	2.903178	-1.788083	0.000345
H	-0.367984	1.913568	-0.000322
H	0.498331	-2.291718	0.000281
H	-2.506706	1.440121	0.893802
H	-3.774965	0.585558	0.000442
H	-2.506952	1.440801	-0.892611

Molecule# 0497

methylsulfonylmethylbenzene

PointGroup: Cs

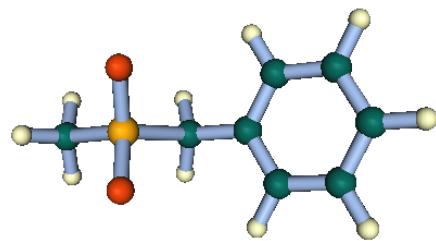
E= -859.688503879 au

ZPE= 0.166175 au

LUMO_eps= -0.03637 au

HOMO_eps= -0.26042 au

Dipole= 4.174 debye



21

C	1.247559	-0.078864	0.000000
S	0.450603	-1.735060	0.000000
C	0.228680	1.019883	0.000000
C	1.856507	-2.863468	0.000000
O	-0.258876	-1.906083	1.263753
O	-0.258876	-1.906083	-1.263753
C	-0.258876	1.531692	1.203024
C	-0.258876	1.531692	-1.203024
C	-1.209742	2.543679	1.202823
C	-1.209742	2.543679	-1.202823
C	-1.686443	3.052509	0.000000
H	1.873727	-0.060312	0.890609
H	1.873727	-0.060312	-0.890609
H	1.425456	-3.862087	0.000000
H	2.444385	-2.705370	-0.900271
H	2.444385	-2.705370	0.900271
H	0.101136	1.130017	2.140706
H	0.101136	1.130017	-2.140706
H	-1.579760	2.932792	2.141610
H	-1.579760	2.932792	-2.141610
H	-2.426453	3.841310	0.000000

Molecule# 0498

methylthiirane

PointGroup: C1

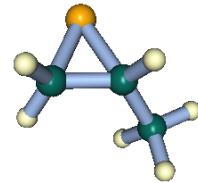
E= -516.184183602 au

ZPE= 0.082833 au

LUMO_eps= -0.01423 au

HOMO_eps= -0.23076 au

Dipole= 2.152 debye



10

C	-1.779558	-0.307747	-0.176939
C	-0.520387	0.167305	0.499192
C	0.364858	1.153255	-0.152316
S	1.096395	-0.525749	-0.053924
H	-1.640106	-0.377917	-1.255255
H	-2.077985	-1.288840	0.191938
H	-2.597663	0.389956	0.023094
H	-0.579906	0.234408	1.579077
H	0.109461	1.476866	-1.153106
H	0.854404	1.900623	0.457404

Molecule# 0499

methylthioethane

PointGroup: Cs

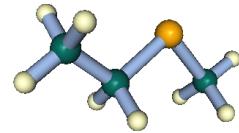
E= -517.413388575 au

ZPE= 0.103880 au

LUMO_eps= -0.01141 au

HOMO_eps= -0.22224 au

Dipole= 1.628 debye



12

C	-1.716415	-1.342580	0.000000
C	1.817500	0.896420	0.000000
C	-0.231871	-1.002452	0.000000
S	0.000000	0.813744	0.000000
H	-2.213283	-0.938659	0.882278
H	-2.213283	-0.938659	-0.882278
H	-1.855592	-2.424603	0.000000
H	2.231538	0.426391	0.891139
H	2.087879	1.950284	0.000000
H	2.231538	0.426391	-0.891139
H	0.257960	-1.414687	-0.883038
H	0.257960	-1.414687	0.883038

Molecule# 0500

methyltrifluoroacetate

PointGroup: Cs

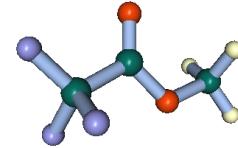
E= -566.331737377 au

ZPE= 0.066461 au

LUMO_eps= -0.04798 au

HOMO_eps= -0.32376 au

Dipole= 3.074 debye



11

C	0.050669	0.624607	0.000000
C	-1.855094	2.001586	0.000000
C	0.511832	-0.857791	0.000000
O	0.811982	1.547940	0.000000
O	-1.275222	0.677957	0.000000
F	0.050669	-1.497770	1.087625
F	0.050669	-1.497770	-1.087625
F	1.840087	-0.932253	0.000000
H	-1.541783	2.544186	0.888968
H	-2.927775	1.844167	0.000000
H	-1.541783	2.544186	-0.888968

Molecule# 0501

methylurea

PointGroup: C1

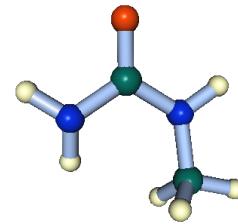
E= -264.688323054 au

ZPE= 0.091172 au

LUMO_eps= -0.02386 au

HOMO_eps= -0.25802 au

Dipole= 4.365 debye



11

C	-1.883880	0.052683	0.051156
H	-2.056506	0.749901	-0.773592
H	-2.696495	-0.669693	0.034127
H	-1.939587	0.605039	0.992852
H	-0.628998	-1.659843	-0.030177
N	-0.629825	-0.657566	-0.098325
C	0.625516	-0.112385	-0.011604
H	-0.085368	1.818229	-0.316218
H	1.594033	1.648111	-0.085107
N	0.672759	1.267776	0.047964
O	1.632821	-0.800625	0.036666

Molecule# 0502

morpholine

PointGroup: Cs

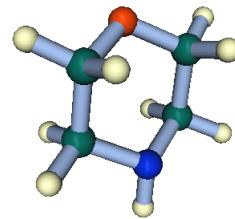
E= -287.909584726 au

ZPE= 0.134574 au

LUMO_eps= -0.01273 au

HOMO_eps= -0.23460 au

Dipole= 1.556 debye



15

C	-0.005439	0.742948	1.206807
C	-0.005439	0.742948	-1.206807
C	-0.005439	-0.778359	1.177882
C	-0.005439	-0.778359	-1.177882
N	0.657361	1.234334	0.000000
O	-0.635671	-1.270842	0.000000
H	-1.046564	1.092682	1.289352
H	0.540160	1.092900	2.084922
H	0.540160	1.092900	-2.084922
H	-1.046564	1.092682	-1.289352
H	1.027148	-1.146672	1.227425
H	-0.566071	-1.185206	2.018469
H	-0.566071	-1.185206	-2.018469
H	1.027148	-1.146672	-1.227425
H	0.705027	2.243917	0.000000

Molecule# 0503

N'-ethynoxymethanimidamide

PointGroup: C1

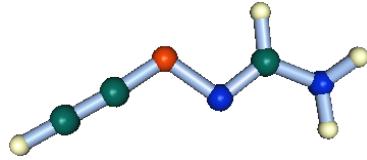
E= -301.419751070 au

ZPE= 0.069765 au

LUMO_eps= -0.03013 au

HOMO_eps= -0.23091 au

Dipole= 4.274 debye



10

O	-0.689613	0.644791	-0.033712
N	0.397947	-0.341322	-0.020979
N	2.699526	-0.326539	-0.051220
C	1.495578	0.309910	0.018594
C	-1.853711	0.076390	-0.000732
C	-2.964471	-0.373779	0.028776
H	3.498737	0.148468	0.328845
H	2.698373	-1.329150	0.048330
H	1.518689	1.394723	0.066269
H	-3.945580	-0.772460	0.051811

Molecule# 0504

N'-methylformic hydrazide

PointGroup: C1

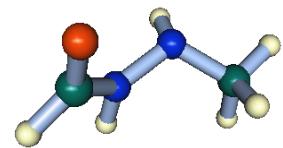
E= -264.624791144 au

ZPE= 0.090538 au

LUMO_eps= -0.02564 au

HOMO_eps= -0.26533 au

Dipole= 4.860 debye



11

C	-1.389634	0.299814	-0.198766
C	1.952053	-0.334792	-0.368307
N	-0.126016	0.752446	0.062428
N	0.873407	-0.070871	0.575294
O	-1.831251	-0.798313	0.032910
H	-1.989676	1.107143	-0.659469
H	2.420897	0.574948	-0.769208
H	1.565322	-0.922739	-1.199271
H	2.715072	-0.922090	0.141351
H	0.119098	1.672856	-0.284035
H	1.213038	0.315233	1.445736

Molecule# 0505

N-(4-pyridinyl)acetamide

PointGroup: Cs

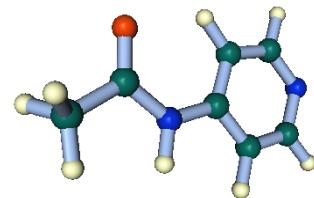
E= -456.477411080 au

ZPE= 0.143109 au

LUMO_eps= -0.04664 au

HOMO_eps= -0.25983 au

Dipole= 4.744 debye



18

C	1.276347	-0.143704	0.000000
C	-0.094534	1.815947	0.000000
C	2.368941	0.714696	0.000000
C	1.065879	2.570549	0.000000
C	0.000000	0.420948	0.000000
C	-1.364098	-1.686589	0.000000
C	-2.811083	-2.138228	0.000000
N	2.292696	2.045547	0.000000
N	-1.189731	-0.317431	0.000000
O	-0.446472	-2.481401	0.000000
H	1.408310	-1.211468	0.000000
H	-1.059712	2.307235	0.000000
H	3.368384	0.294912	0.000000
H	1.004291	3.652813	0.000000
H	-2.977485	-2.760972	0.878119
H	-2.977485	-2.760972	-0.878119
H	-3.532976	-1.322843	0.000000
H	-2.031016	0.233980	0.000000

Molecule# 0506

N-(formyloxy)imidoformamide

PointGroup: C1

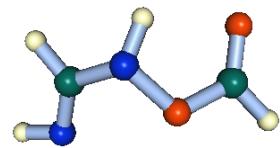
E= -338.639579031 au

ZPE= 0.072120 au

LUMO_eps= -0.03408 au

HOMO_eps= -0.27314 au

Dipole= 1.331 debye



10

O	0.398686	-0.658181	0.432310
O	2.110858	0.540150	-0.435213
N	-0.324934	0.558558	0.529684
N	-2.184383	-0.564932	-0.359925
C	1.635791	-0.499882	-0.069258
C	-1.596806	0.501735	-0.024181
H	0.269573	1.312628	0.194878
H	-3.129950	-0.371180	-0.673543
H	2.131567	-1.475260	-0.070979
H	-2.016233	1.511565	-0.054807

Molecule# 0507

N-(oxomethylene)-beta-alanyl chloride

PointGroup: C1

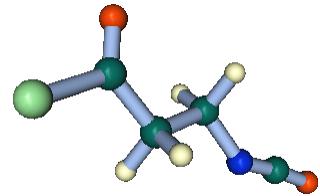
E= -820.415454453 au

ZPE= 0.079836 au

LUMO_eps= -0.06309 au

HOMO_eps= -0.30448 au

Dipole= 0.491 debye



12

C1	-3.060401	-0.655123	-0.000036
O	-1.695936	1.586291	0.000019
O	4.467584	-0.178785	-0.000057
N	2.105957	-0.328874	0.000063
C	-0.315239	-0.391161	0.000014
C	0.924008	0.501299	0.000045
C	-1.585387	0.409377	0.000004
C	3.297525	-0.188848	-0.000003
H	-0.325259	-1.048562	0.871003
H	-0.325232	-1.048540	-0.870992
H	0.918478	1.146124	0.879487
H	0.918511	1.146144	-0.879383

Molecule# 0508

N-[(1E)-1-propen-1-yl]acetamide

PointGroup: Cs

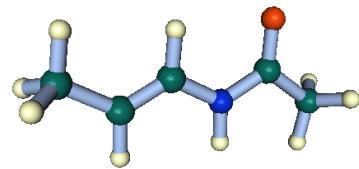
E= -326.062198015 au

ZPE= 0.134656 au

LUMO_eps= -0.02023 au

HOMO_eps= -0.22896 au

Dipole= 3.654 debye



16

C	-1.936874	-0.817158	0.000000
C	-0.619074	-0.628886	0.000000
C	1.363850	0.795633	0.000000
C	-2.590379	-2.163352	0.000000
C	1.836552	2.234079	0.000000
N	0.000000	0.623665	0.000000
O	2.140869	-0.141131	0.000000
H	-2.595791	0.047327	0.000000
H	0.088707	-1.445676	0.000000
H	-3.229378	-2.296210	0.877032
H	-3.229378	-2.296210	-0.877032
H	-1.850635	-2.963831	0.000000
H	2.460883	2.395108	-0.878171
H	2.460883	2.395108	0.878171
H	1.027080	2.963093	0.000000
H	-0.583780	1.442786	0.000000

Molecule# 0509

N-acetylacetamide

PointGroup: C2v

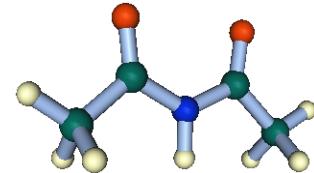
E= -362.008623008 au

ZPE= 0.110570 au

LUMO_eps= -0.03765 au

HOMO_eps= -0.25842 au

Dipole= 6.261 debye



14

C	0.000000	1.265036	-0.119107
C	0.000000	-1.265036	-0.119107
C	0.000000	2.401004	0.887119
C	0.000000	-2.401004	0.887119
N	0.000000	0.000000	0.490686
O	0.000000	1.434626	-1.309734
O	0.000000	-1.434626	-1.309734
H	0.000000	3.342860	0.347946
H	-0.882484	2.352586	1.527823
H	0.882484	2.352586	1.527823
H	-0.882484	-2.352586	1.527823
H	0.882484	-2.352586	1.527823
H	0.000000	-3.342860	0.347946
H	0.000000	0.000000	1.497619

Molecule# 0510

N-azido-2,3-dihydro-1,2-thiazole

PointGroup: C1

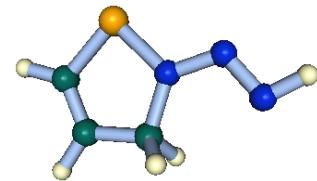
E= -679.805750972 au

ZPE= 0.086927 au

LUMO_eps= -0.03815 au

HOMO_eps= -0.21003 au

Dipole= 2.456 debye



12

S	0.865517	-1.220324	0.000033
N	-0.472803	-0.109850	0.001005
N	-1.693397	-0.595410	-0.000089
N	-2.596092	0.285481	-0.000471
C	-0.129116	1.320148	0.000374
C	1.958652	0.149745	-0.000464
C	1.366917	1.340992	-0.000208
H	-3.475838	-0.230299	-0.001183
H	-0.574130	1.802666	-0.877164
H	-0.573436	1.803341	0.877870
H	3.018570	-0.049442	-0.000901
H	1.913895	2.272063	-0.000472

Molecule# 0511

N-butyl-1-butanamine

PointGroup: Cs

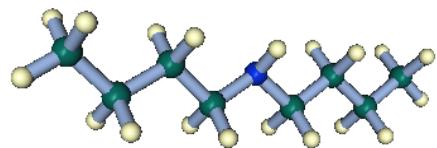
E= -371.196274449 au

ZPE= 0.262067 au

LUMO_eps= -0.01121 au

HOMO_eps= -0.22515 au

Dipole= 0.850 debye



28

C	-0.455055	0.007781	5.014090
C	-0.455055	0.007781	-5.014090
C	0.435676	-0.020717	3.773122
C	0.435676	-0.020717	-3.773122
C	-0.355461	0.027942	2.465843
C	-0.355461	0.027942	-2.465843
C	0.527885	-0.001819	1.223683
C	0.527885	-0.001819	-1.223683
N	-0.261779	0.067908	0.000000
H	0.135970	-0.027454	5.930256
H	-1.060071	0.916136	5.043881
H	-1.138956	-0.843381	5.027731
H	0.135970	-0.027454	-5.930256
H	-1.138956	-0.843381	-5.027731
H	-1.060071	0.916136	-5.043881
H	1.130138	0.824101	3.804951
H	1.054579	-0.922676	3.790225
H	1.054579	-0.922676	-3.790225
H	1.130138	0.824101	-3.804951
H	-1.049164	-0.820022	2.434262
H	-0.971786	0.930230	2.437138
H	-0.971786	0.930230	-2.437138
H	-1.049164	-0.820022	-2.434262
H	1.201869	0.860165	1.235204
H	1.172318	-0.897454	1.253831
H	1.172318	-0.897454	-1.253831
H	1.201869	0.860165	-1.235204
H	-0.953883	-0.672892	0.000000

Molecule# 0512

N-chloro-N-(cyanomethyl)formamide

PointGroup: C1

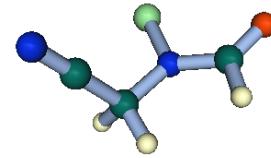
E= -761.135294973 au

ZPE= 0.062674 au

LUMO_eps= -0.07248 au

HOMO_eps= -0.29286 au

Dipole= 4.018 debye



10

C1	-0.701864	1.462003	-0.034783
O	-2.283438	-0.979375	-0.549331
N	-0.344081	-0.165493	0.372382
N	2.914608	-0.191919	-0.838450
C	0.978044	-0.423781	0.908893
C	-1.224862	-1.151741	-0.010019
C	2.060093	-0.287664	-0.076810
H	1.172647	0.247397	1.745782
H	0.982654	-1.443332	1.297214
H	-0.829457	-2.142106	0.273049

Molecule# 0513

N-chloro-N-cyano-N'-methylimidoformamide

PointGroup: C1

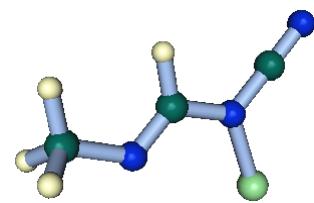
E= -741.228337391 au

ZPE= 0.073732 au

LUMO_eps= -0.09214 au

HOMO_eps= -0.27237 au

Dipole= 3.546 debye



11

C1	-0.857697	1.572767	0.000268
N	-0.570057	-0.129205	-0.000081
N	1.743589	0.140834	0.000082
N	-2.544730	-1.638675	-0.000357
C	0.749729	-0.615993	-0.000106
C	-1.632177	-0.928384	-0.000224
C	3.070199	-0.442365	0.000029
H	0.755182	-1.709286	-0.000314
H	3.613291	-0.089928	0.877506
H	3.613351	-0.089629	-0.877292
H	3.070905	-1.538419	-0.000158

Molecule# 0514

N-chlorocysteine

PointGroup: C1

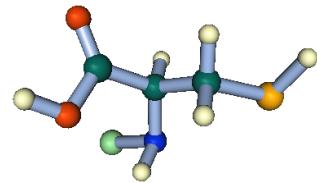
E= -1181.691689220 au

ZPE= 0.097429 au

LUMO_eps= -0.05572 au

HOMO_eps= -0.25501 au

Dipole= 2.914 debye



14

C1	1.560711	1.893407	-0.220108
S	-2.790812	0.329751	-0.047708
O	1.341983	-2.035398	-1.015709
O	1.598920	-1.268082	1.083308
N	0.161310	1.041443	0.439465
C	-0.069935	-0.213443	-0.269978
C	1.035385	-1.265596	-0.146657
C	-1.382089	-0.820778	0.246351
H	-3.701568	-0.633058	-0.277035
H	2.276249	-1.960533	1.095104
H	0.436799	0.846291	1.397865
H	-0.173273	0.009303	-1.329322
H	-1.303752	-1.040723	1.310335
H	-1.570111	-1.748572	-0.287123

Molecule# 0515

N-chlorosuccinimide

PointGroup: Cs

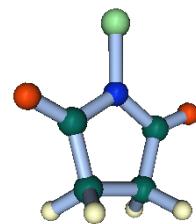
E= -820.393254487 au

ZPE= 0.081323 au

LUMO_eps= -0.05725 au

HOMO_eps= -0.28908 au

Dipole= 3.323 debye



12

C	-0.000029	-1.883915	0.767287
N	0.000023	0.323654	0.000000
C	0.000000	-0.423893	-1.187980
C	-0.000029	-1.883915	-0.767287
C	0.000000	-0.423893	1.187980
Cl	0.000020	2.020882	0.000000
H	0.876572	-2.363854	-1.200021
H	-0.876661	-2.363803	-1.200016
H	0.876572	-2.363854	1.200021
H	-0.876661	-2.363803	1.200016
O	0.000000	0.033027	-2.295994
O	0.000000	0.033027	2.295994

Molecule# 0516

N-cyanoimidoformamide

PointGroup: C1

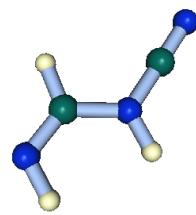
E= -242.325968979 au

ZPE= 0.056348 au

LUMO_eps= -0.03631 au

HOMO_eps= -0.28913 au

Dipole= 3.107 debye



8

N	-0.047335	0.494707	0.000095
N	-2.426020	-0.243839	-0.000088
N	2.256899	-0.124368	0.000008
C	-1.325935	0.106762	-0.000003
C	1.029441	-0.407626	-0.000048
H	0.145193	1.485628	0.000247
H	2.449675	0.876936	0.000174
H	0.699288	-1.442885	-0.000220

Molecule# 0517

N-disulfanylacetamide

PointGroup: C1

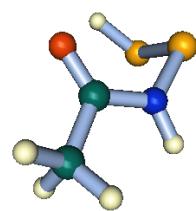
E= -1005.747358130 au

ZPE= 0.074266 au

LUMO_eps= -0.05378 au

HOMO_eps= -0.26390 au

Dipole= 3.228 debye



11

S	-0.977841	0.897750	0.426091
S	-2.081995	-0.635586	-0.451951
O	1.307860	-0.949315	1.030107
N	0.582338	0.797816	-0.241341
C	1.521372	-0.149599	0.148699
C	2.812887	-0.107552	-0.640961
H	-1.741791	-1.618901	0.408674
H	0.761070	1.334091	-1.076406
H	2.715102	-0.758963	-1.511499
H	3.614677	-0.492310	-0.016893
H	3.063516	0.894181	-0.987999

Molecule# 0518

N-ethylaniline

PointGroup: C1

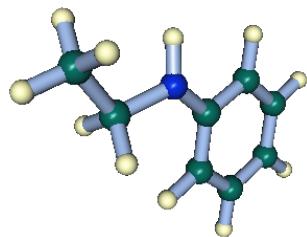
E= -366.366146171 au

ZPE= 0.173179 au

LUMO_eps= -0.01455 au

HOMO_eps= -0.20218 au

Dipole= 1.990 debye



20

C	2.855440	0.252651	0.039517
C	1.955251	1.308154	-0.006830
C	2.360141	-1.050018	0.041527
C	0.583533	1.082280	-0.050241
C	0.997959	-1.289253	-0.005941
C	0.080290	-0.226157	-0.056360
C	-3.683656	-0.105023	0.019100
C	-2.294319	0.511126	0.087695
N	-1.276349	-0.497538	-0.143162
H	3.919858	0.436494	0.075585
H	2.318186	2.327791	-0.005576
H	3.043134	-1.888633	0.080058
H	-0.090520	1.925367	-0.082058
H	0.628256	-2.307784	-0.011219
H	-3.861554	-0.559934	-0.955872
H	-3.812010	-0.873971	0.784186
H	-4.445779	0.655703	0.185234
H	-2.153505	1.006369	1.058333
H	-2.204125	1.287273	-0.676443
H	-1.535324	-1.428467	0.139104

Molecule# 0519

N-ethynylacetylenamine

PointGroup: C1

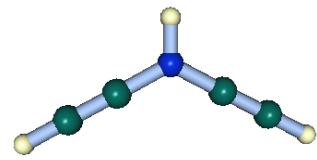
E= -208.896075117 au

ZPE= 0.053167 au

LUMO_eps= -0.02283 au

HOMO_eps= -0.23140 au

Dipole= 1.107 debye



8

N	0.000000	0.712570	-0.000004
C	1.187127	0.077814	-0.000007
C	-1.187127	0.077815	-0.000007
C	2.251031	-0.475403	0.000008
C	-2.251031	-0.475403	0.000009
H	0.000000	1.720650	0.000024
H	3.189310	-0.968793	-0.000008
H	-3.189310	-0.968793	-0.000007

Molecule# 0520

N-ethynylcarbamoyl chloride

PointGroup: C1

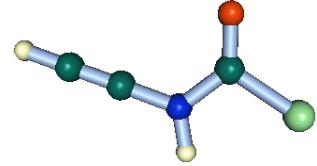
E= -705.763212996 au

ZPE= 0.045767 au

LUMO_eps= -0.03886 au

HOMO_eps= -0.27636 au

Dipole= 3.048 debye



8

C1	2.020286	-0.360915	0.000049
O	0.203450	1.555974	-0.000169
N	-0.574181	-0.605015	0.000072
C	0.376440	0.384407	-0.000039
C	-1.897702	-0.346943	0.000026
C	-3.075438	-0.133700	-0.000002
H	-0.254865	-1.560965	0.000162
H	-4.118136	0.061245	-0.000060

Molecule# 0521

N-fluoroglycine

PointGroup: C1

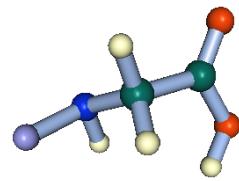
E= -383.744655093 au

ZPE= 0.070688 au

LUMO_eps= -0.05365 au

HOMO_eps= -0.29923 au

Dipole= 3.694 debye



10

F	2.523812	-0.000530	0.037332
O	-1.881341	-1.007854	-0.239265
O	-1.539739	1.170779	0.004238
N	1.215026	-0.004014	-0.555021
C	-1.136839	-0.128298	0.067470
C	0.302592	-0.347682	0.537573
H	-0.888066	1.766285	0.392635
H	1.117050	0.980700	-0.797020
H	0.422906	-1.402721	0.762868
H	0.502739	0.241088	1.440632

Molecule# 0522

N-hydroxy-2-propynamide

PointGroup: C1

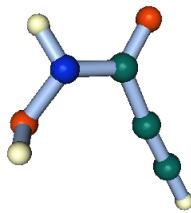
E= -321.324155695 au

ZPE= 0.059133 au

LUMO_eps= -0.06348 au

HOMO_eps= -0.28493 au

Dipole= 3.362 debye



9

O	0.003809	1.878896	-0.058549
O	-1.325094	-1.341270	-0.193926
N	-1.242362	0.008952	0.182819
C	-0.039394	0.667675	0.014547
C	1.144130	-0.169619	0.016092
C	2.171402	-0.787529	0.007182
H	-1.418256	-1.824659	0.635941
H	-2.054044	0.531652	-0.119875
H	3.082283	-1.333824	-0.002916

Molecule# 0523

N-hydroxy-3-pyridinecarboximidic acid

PointGroup: C1

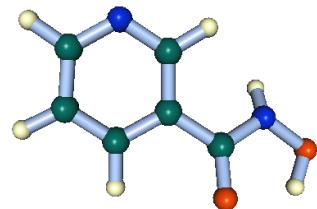
E= -492.340518735 au

ZPE= 0.119453 au

LUMO_eps= -0.07446 au

HOMO_eps= -0.26285 au

Dipole= 2.376 debye



16

C	-2.434690	1.007305	0.195988
C	-1.066080	1.206618	0.141234
C	-2.925749	-0.286900	0.055755
C	-0.831663	-1.149867	-0.199198
C	-0.234965	0.103590	-0.047113
C	1.234805	0.320466	-0.099690
N	-2.146220	-1.349895	-0.145302
N	2.025184	-0.770786	0.116502
O	1.753325	1.403823	-0.352026
O	3.394425	-0.509645	0.206692
H	-3.113977	1.834745	0.344733
H	-0.627372	2.189562	0.238840
H	-3.991491	-0.478121	0.101031
H	-0.227759	-2.027390	-0.401000
H	1.753487	-1.488411	0.769860
H	3.422406	0.453688	0.028951

Molecule# 0524

N-hydroxy-N-methylacetamide

PointGroup: C1

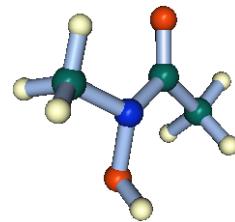
E= -323.820428202 au

ZPE= 0.105134 au

LUMO_eps= -0.02847 au

HOMO_eps= -0.25796 au

Dipole= 3.310 debye



13

C	0.691531	-0.351810	-0.035843
C	1.785942	0.685648	0.044153
C	-1.753536	-0.709923	0.070079
N	-0.596467	0.122694	-0.200791
O	0.907289	-1.549850	-0.004258
O	-0.805591	1.479569	0.133264
H	2.738393	0.164728	0.040895
H	1.688929	1.273709	0.956539
H	1.741301	1.381719	-0.792856
H	-2.070590	-0.610444	1.110769
H	-1.471281	-1.739112	-0.127674
H	-2.574605	-0.421529	-0.584996
H	-1.034080	1.910829	-0.699522

Molecule# 0525

N-hydroxyformamide

PointGroup: C1

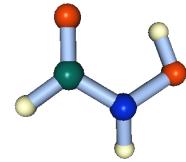
E= -245.159955039 au

ZPE= 0.049695 au

LUMO_eps= -0.02113 au

HOMO_eps= -0.26570 au

Dipole= 2.956 debye



7

C	-0.776157	0.482170	0.010862
N	0.561163	0.638019	-0.078048
O	-1.303837	-0.617381	0.001319
O	1.345896	-0.512290	0.011708
H	-1.318051	1.436615	0.052353
H	1.043410	1.455182	0.258679
H	0.666967	-1.213576	0.065911

Molecule# 0526

N-hydroxyheptan-2-imine

PointGroup: C1

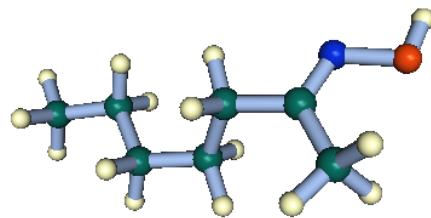
E= -405.870263828 au

ZPE= 0.214009 au

LUMO_eps= -0.01232 au

HOMO_eps= -0.25451 au

Dipole= 1.020 debye



24

O	3.657272	-0.908486	0.267264
N	2.280419	-1.049466	-0.034086
C	1.723395	0.078313	-0.240657
C	0.252045	0.045182	-0.552072
C	-0.612702	0.655783	0.563633
C	2.452308	1.390511	-0.181512
C	-2.104484	0.739914	0.222819
C	-2.812872	-0.610021	0.085967
C	-4.311099	-0.469861	-0.179030
H	3.935602	-1.821933	0.382506
H	0.079088	0.601638	-1.480057
H	-0.033680	-0.989673	-0.733020
H	-0.477778	0.065952	1.474702
H	-0.249404	1.660864	0.792252
H	1.801297	2.215730	-0.461660
H	3.314651	1.372956	-0.848863
H	2.840303	1.572750	0.821967
H	-2.605873	1.318775	1.004289
H	-2.232338	1.310663	-0.703449
H	-2.358845	-1.189949	-0.720907
H	-2.656457	-1.188678	1.001435
H	-4.805958	0.071843	0.629774
H	-4.498308	0.078583	-1.104556
H	-4.792947	-1.444298	-0.268812

Molecule# 0527

N-methyl-2-propanimine

PointGroup: Cs

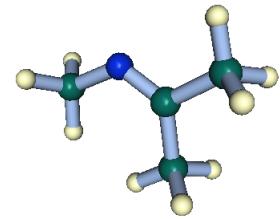
E= -212.665898916 au

ZPE= 0.123378 au

LUMO_eps= -0.01368 au

HOMO_eps= -0.24171 au

Dipole= 1.849 debye



14

C	0.000000	0.400135	0.000000
C	-0.559646	1.800763	0.000000
C	1.512118	0.333612	0.000000
C	-0.421806	-1.955288	0.000000
N	-0.823365	-0.565462	0.000000
H	-0.214550	2.354611	0.877083
H	-0.214550	2.354611	-0.877083
H	-1.645869	1.770131	0.000000
H	1.903128	0.856799	0.875493
H	1.903128	0.856799	-0.875493
H	1.909280	-0.676287	0.000000
H	-0.857799	-2.442000	-0.874888
H	-0.857799	-2.442000	0.874888
H	0.654591	-2.149764	0.000000

Molecule# 0528

N-methyl-N-2,2,2-trifluoroethylaniline

PointGroup: C1

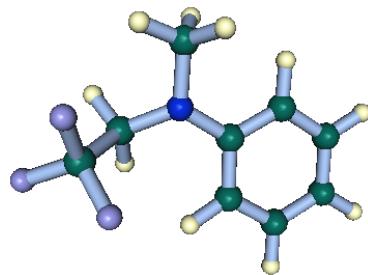
E= -703.532517886 au

ZPE= 0.178536 au

LUMO_eps= -0.01822 au

HOMO_eps= -0.21384 au

Dipole= 2.237 debye



23

C	-3.674067	-0.853951	-0.083418
C	-2.544884	-1.650937	0.067775
C	-3.509148	0.522321	-0.154373
C	-1.279010	-1.090719	0.146626
C	-2.248330	1.098967	-0.065846
C	-1.102333	0.302544	0.091353
C	0.314133	2.318038	0.012392
C	1.235426	0.205711	0.866884
C	2.316851	-0.367967	-0.044102
N	0.170829	0.879498	0.166684
F	3.284492	-0.950410	0.698778
F	1.843375	-1.300588	-0.890331
F	2.908950	0.584737	-0.794752
H	-4.657463	-1.297035	-0.151204
H	-2.643137	-2.727701	0.109315
H	-4.370757	1.166188	-0.272823
H	-0.425739	-1.747886	0.213334
H	-2.166729	2.173555	-0.110469
H	-0.155118	2.650083	-0.912697
H	1.369780	2.566254	-0.050624
H	-0.127388	2.879150	0.846120
H	1.743693	0.891876	1.548447
H	0.853873	-0.618659	1.466816

Molecule# 0529

N-methylacetamide

PointGroup: C1

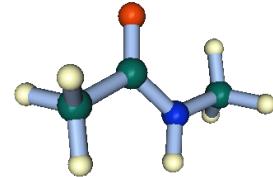
E= -248.628962591 au

ZPE= 0.101487 au

LUMO_eps= -0.02121 au

HOMO_eps= -0.25854 au

Dipole= 3.838 debye



12

C	0.484528	0.165592	0.000016
C	1.812482	-0.565934	-0.000009
C	-1.975116	-0.101915	-0.000016
N	-0.623641	-0.629072	0.000038
O	0.425955	1.384169	0.000000
H	2.378559	-0.258444	-0.878404
H	2.378838	-0.257978	0.878038
H	1.716856	-1.651294	0.000288
H	-2.523186	-0.423664	-0.887098
H	-1.906742	0.982265	-0.000850
H	-2.522801	-0.422285	0.887811
H	-0.495040	-1.624899	0.000005

Molecule# 0530

N-methylacetamidine

PointGroup: C1

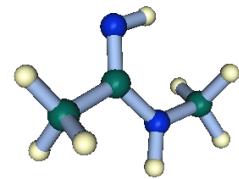
E= -228.728258480 au

ZPE= 0.113377 au

LUMO_eps= -0.02045 au

HOMO_eps= -0.23667 au

Dipole= 3.717 debye



13

C	0.504007	0.162021	-0.000522
C	1.815083	-0.581550	0.000816
C	-1.959986	-0.145515	0.001321
N	0.504425	1.442302	0.000085
N	-0.605061	-0.647080	-0.003604
H	1.900600	-1.219398	0.883090
H	1.902657	-1.218859	-0.881594
H	2.630056	0.134963	0.002108
H	-2.164863	0.459162	0.889530
H	-2.648126	-0.987714	-0.000986
H	-2.167537	0.465376	-0.881811
H	-0.436074	1.830537	-0.000616
H	-0.466885	-1.640362	0.005221

Molecule# 0531

N-methylaniline

PointGroup: C1

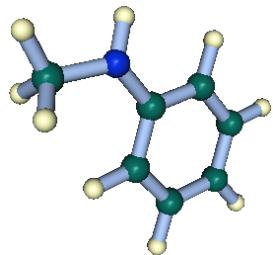
E= -327.035498393 au

ZPE= 0.144950 au

LUMO_eps= -0.01466 au

HOMO_eps= -0.20281 au

Dipole= 1.876 debye



17

C	2.308280	0.333913	0.032715
C	1.874791	-0.990670	0.036977
C	1.359701	1.346306	-0.009499
C	0.525138	-1.293489	-0.004025
C	-0.000206	1.056554	-0.046565
C	-0.440752	-0.273922	-0.049701
C	-2.835641	0.363095	0.089889
N	-1.783597	-0.606016	-0.128315
H	3.363058	0.567419	0.063881
H	2.596525	-1.796291	0.072123
H	1.674892	2.381687	-0.010024
H	0.202937	-2.328068	-0.007472
H	-0.713687	1.866797	-0.075478
H	-2.839553	1.117185	-0.699380
H	-2.751251	0.880801	1.053410
H	-3.794605	-0.149894	0.057667
H	-2.001002	-1.548246	0.144734

Molecule# 0532

N-methylethanesulfinamide

PointGroup: C1

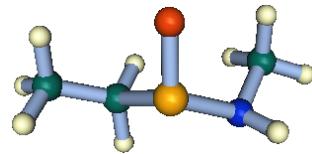
E= -648.005152875 au

ZPE= 0.125131 au

LUMO_eps= -0.01484 au

HOMO_eps= -0.23982 au

Dipole= 2.959 debye



15

C	-2.139834	-0.710922	0.596826
C	1.068695	-0.883406	-0.030439
N	-1.459776	-0.309985	-0.644054
O	0.011483	1.442982	0.707174
S	0.021665	0.552366	-0.498920
H	-1.644773	-1.577025	1.031747
H	-3.157132	-1.003061	0.342196
H	-2.170598	0.089547	1.338748
C	2.503165	-0.427132	0.192491
H	0.977363	-1.601303	-0.844626
H	0.639979	-1.306459	0.877147
H	-2.062842	0.266509	-1.218062
H	2.551572	0.320870	0.982347
H	2.931112	0.002810	-0.714236
H	3.123098	-1.274945	0.485174

Molecule# 0533

N-methylmethanesulfinamide

PointGroup: C1

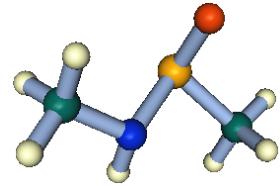
E= -608.670060188 au

ZPE= 0.096059 au

LUMO_eps= -0.02078 au

HOMO_eps= -0.23631 au

Dipole= 4.041 debye



12

C	-2.176225	-0.108634	0.025106
C	1.750470	-0.864926	0.195527
N	-0.860662	-0.714324	0.273353
O	0.496434	1.481896	0.368384
S	0.435590	0.228882	-0.434302
H	-2.186081	0.887800	0.460796
H	-2.927918	-0.708978	0.535442
H	-2.441606	-0.034928	-1.035315
H	1.646109	-0.917873	1.276493
H	2.694683	-0.403665	-0.084828
H	1.666868	-1.848965	-0.264591
H	-0.813806	-1.649042	-0.123504

Molecule# 0534

N-methylmethanesulfonamide

PointGroup: C1

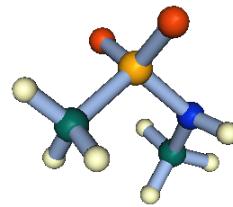
E= -683.929753681 au

ZPE= 0.102064 au

LUMO_eps= -0.02628 au

HOMO_eps= -0.29161 au

Dipole= 5.233 debye



13

C	2.232485	0.157278	-0.013976
C	-0.853827	1.545278	-0.325744
N	1.037219	-0.489380	-0.546136
O	-0.349336	-0.241094	1.524633
O	-1.388574	-1.007152	-0.660628
S	-0.465777	-0.166383	0.079766
H	3.102438	-0.419525	-0.323302
H	2.182272	0.139563	1.071682
H	2.358894	1.190382	-0.351993
H	-0.896516	1.650085	-1.406514
H	-1.825831	1.753159	0.115159
H	-0.099484	2.195057	0.110415
H	1.001456	-0.650307	-1.542474

Molecule# 0535

N-methylmethanimine

PointGroup: Cs

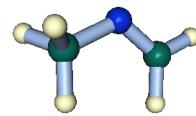
E= -133.997326154 au

ZPE= 0.067819 au

LUMO_eps= -0.02703 au

HOMO_eps= -0.26285 au

Dipole= 1.515 debye



8

C	-1.074952	-0.423350	0.000000
N	0.000000	0.548631	0.000000
C	1.187443	0.128587	0.000000
H	-0.726044	-1.464229	0.000000
H	-1.702940	-0.256326	0.876539
H	-1.702940	-0.256326	-0.876539
H	1.449451	-0.937256	0.000000
H	2.007530	0.842294	0.000000

Molecule# 0536

N-methylpyrimidine-2-carboxamide

PointGroup: C1

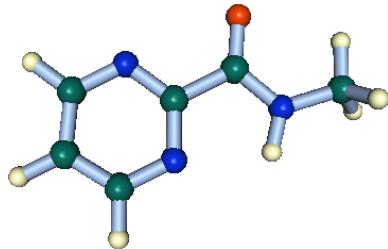
E= -472.514510670 au

ZPE= 0.131494 au

LUMO_eps= -0.07155 au

HOMO_eps= -0.25854 au

Dipole= 5.005 debye



17

C	-2.911807	-0.353161	0.000000
C	-1.970075	-1.370420	0.000028
C	-2.420063	0.945020	-0.000029
C	-0.295388	0.168403	-0.000001
C	1.202333	0.467839	0.000009
C	3.415957	-0.609641	-0.000010
N	-0.663500	-1.117055	0.000026
N	-1.117120	1.213429	-0.000028
N	1.969122	-0.648818	-0.000052
O	1.629250	1.606620	0.000055
H	-3.971769	-0.560591	0.000002
H	-2.264814	-2.413448	0.000052
H	-3.089232	1.798175	-0.000054
H	3.820894	-1.101243	-0.886355
H	3.820882	-1.099999	0.887039
H	3.726013	0.431675	-0.000714
H	1.478770	-1.528660	-0.000016

Molecule# 0537

N-methylpyrimidine-5-sulfinamide

PointGroup: C1

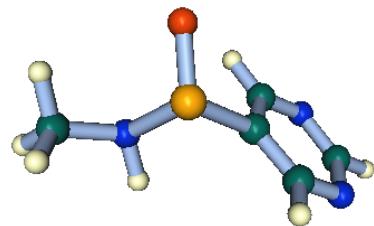
E= -832.547906678 au

ZPE= 0.125947 au

LUMO_eps= -0.07468 au

HOMO_eps= -0.25289 au

Dipole= 3.754 debye



17

C	-1.066927	0.993447	0.503517
C	-1.369945	-1.059353	-0.651102
C	-3.086115	-0.027909	0.398756
C	-0.518719	-0.048949	-0.236276
C	3.264554	-0.589277	0.915395
N	-2.356726	1.004528	0.828796
N	-2.664799	-1.059267	-0.329369
N	1.810425	-0.382266	0.877742
O	1.609131	1.384777	-0.978583
S	1.227894	-0.030720	-0.731013
H	-0.454317	1.827531	0.822442
H	-1.012893	-1.886063	-1.256520
H	-4.135818	-0.021604	0.667155
H	3.754433	0.313715	0.557523
H	3.609015	-1.442093	0.321297
H	3.556910	-0.741479	1.953119
H	1.303932	-1.185425	1.237919

Molecule# 0538

N-methylpyrimidine-5-sulfonamide

PointGroup: C1

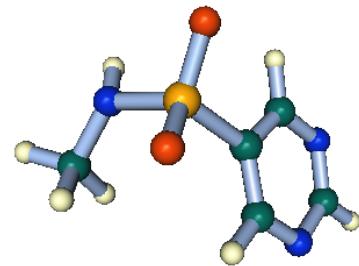
E= -907.806710016 au

ZPE= 0.131918 au

LUMO_eps= -0.07918 au

HOMO_eps= -0.28550 au

Dipole= 4.250 debye



18

C	-1.325488	-1.023014	-0.620671
C	-1.153772	0.908207	0.754322
C	-3.123935	0.272789	-0.162363
C	-0.530909	-0.169977	0.137241
C	1.986994	1.737827	-1.056432
N	-2.628272	-0.802402	-0.775809
N	-2.457181	1.136617	0.601107
N	1.994174	0.281587	-0.935689
O	1.635439	0.218540	1.535945
O	1.440056	-1.889346	0.122330
S	1.229691	-0.470095	0.327322
H	-0.905378	-1.902771	-1.092500
H	-0.596738	1.583105	1.391696
H	-4.183013	0.459324	-0.293879
H	1.020179	2.141933	-1.369626
H	2.740545	2.019831	-1.789059
H	2.264660	2.168978	-0.098408
H	1.902340	-0.248049	-1.791428

Molecule# 0539

N-methylsulfinamoylmethanamine

PointGroup: C1

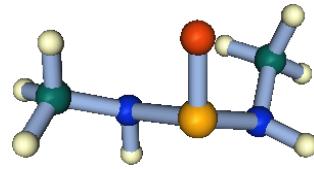
E= -664.044972415 au

ZPE= 0.114114 au

LUMO_eps= -0.01569 au

HOMO_eps= -0.23994 au

Dipole= 2.943 debye



14

C	2.348792	-0.536780	0.248659
C	-2.054949	-0.747002	0.633612
N	0.953152	-0.827439	-0.095931
N	-1.433378	-0.277244	-0.614256
O	0.101328	1.411281	0.730744
S	0.030842	0.587441	-0.500901
H	2.820782	-1.466819	0.562554
H	2.364292	0.153252	1.088342
H	2.932278	-0.107281	-0.573544
H	-2.298120	0.067754	1.317861
H	-1.373670	-1.430882	1.131354
H	-2.964289	-1.286453	0.373636
H	0.877511	-1.467415	-0.879936
H	-2.064357	0.284026	-1.174130

Molecule# 0540

N-oxocysteine

PointGroup: C1

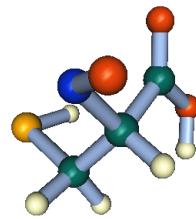
E= -796.042648284 au

ZPE= 0.085524 au

LUMO_eps= -0.11612 au

HOMO_eps= -0.25178 au

Dipole= 5.312 debye



13

S	2.138126	-0.471424	-0.497762
O	-1.262728	1.239322	-1.123753
O	-0.184106	2.173393	0.574489
O	-2.195916	-1.611940	0.020091
N	-1.071021	-1.335428	-0.264211
C	-0.489680	-0.243773	0.615987
C	-0.694454	1.099412	-0.085165
C	0.973673	-0.594469	0.910781
H	2.200865	0.872262	-0.543734
H	0.192088	1.925376	1.427496
H	-1.071763	-0.233746	1.544268
H	1.349553	-0.008418	1.748575
H	1.021152	-1.637918	1.220832

Molecule# 0541

n-pentanoic acid

PointGroup: Cs

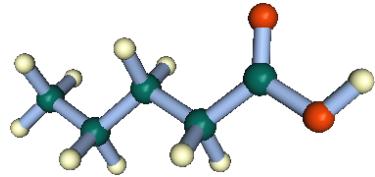
E= -347.170240449 au

ZPE= 0.146777 au

LUMO_eps= -0.01543 au

HOMO_eps= -0.28956 au

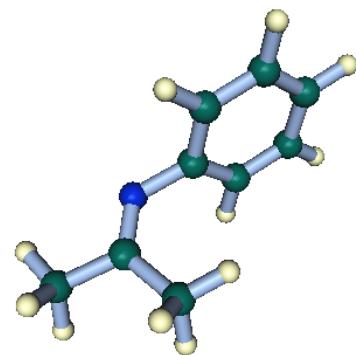
Dipole= 1.653 debye



17

C	-1.505345	0.854261	0.000000
C	2.618558	-2.127663	0.000000
C	0.000000	0.771586	0.000000
C	2.068350	-0.702640	0.000000
C	0.540531	-0.653982	0.000000
O	-2.272406	-0.073756	0.000000
O	-1.931154	2.143966	0.000000
H	3.709158	-2.132876	0.000000
H	2.283560	-2.679277	0.880542
H	2.283560	-2.679277	-0.880542
H	0.357515	1.331075	-0.869047
H	0.357515	1.331075	0.869047
H	2.448656	-0.165278	-0.874152
H	2.448656	-0.165278	0.874152
H	0.153343	-1.186524	-0.871351
H	0.153343	-1.186524	0.871351
H	-2.899395	2.121831	0.000000

Molecule# 0542
 N-phenylpropan-2-imine
 PointGroup: C1
 E= -404.475719032 au
 ZPE= 0.176429 au
 LUMO_eps= -0.02253 au
 HOMO_eps= -0.22172 au
 Dipole= 2.278 debye



21

C	2.998166	-0.117026	0.186742
C	2.250260	-1.206555	-0.245165
C	2.377431	1.120060	0.328290
C	0.896545	-1.067455	-0.525584
C	1.027004	1.269555	0.042344
C	0.267676	0.172124	-0.374549
C	-2.052493	0.014676	0.007335
C	-3.450793	0.232807	-0.503277
C	-1.944865	-0.582860	1.389174
N	-1.078820	0.350050	-0.736188
H	4.051545	-0.228318	0.403476
H	2.721570	-2.173091	-0.366506
H	2.949124	1.977574	0.658099
H	0.319634	-1.913528	-0.874264
H	0.548756	2.235247	0.134308
H	-4.006387	0.889434	0.170715
H	-3.995891	-0.713622	-0.539447
H	-3.427654	0.672409	-1.496672
H	-2.429938	-1.561221	1.412890
H	-2.478210	0.046473	2.105055
H	-0.914394	-0.693657	1.713800

Molecule# 0543

n-propyl acetate

PointGroup: C1

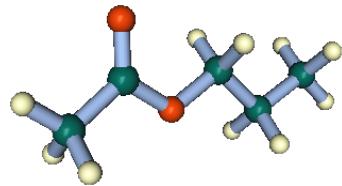
E= -347.161082634 au

ZPE= 0.145846 au

LUMO_eps= -0.01307 au

HOMO_eps= -0.28094 au

Dipole= 2.201 debye



17

C	-1.603643	0.174878	-0.000006
C	-2.767397	-0.780438	0.000006
C	3.283501	0.155432	0.000008
C	1.963727	-0.615105	-0.000005
C	0.769150	0.317432	-0.000001
O	-1.688090	1.377808	-0.000001
O	-0.429939	-0.489876	-0.000012
H	-2.721291	-1.424419	0.878141
H	-2.721158	-1.424638	-0.877958
H	-3.696732	-0.219858	-0.000125
H	3.372308	0.793346	0.881230
H	4.132141	-0.528255	0.000005
H	3.372315	0.793363	-0.881202
H	1.908444	-1.264592	0.876224
H	1.908451	-1.264576	-0.876246
H	0.758862	0.961481	0.880478
H	0.758869	0.961496	-0.880469

Molecule# 0544

n-propyl formate

PointGroup: Cs

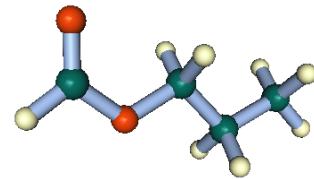
E= -307.821578657 au

ZPE= 0.118380 au

LUMO_eps= -0.01354 au

HOMO_eps= -0.29405 au

Dipole= 2.378 debye



14

C	-1.071395	-1.776836	0.000000
C	1.414442	2.421868	0.000000
C	1.409577	0.893657	0.000000
C	0.000000	0.338803	0.000000
O	-2.169335	-1.290400	0.000000
O	0.086608	-1.109139	0.000000
H	-0.866386	-2.854791	0.000000
H	0.909790	2.821701	0.881287
H	2.434143	2.805918	0.000000
H	0.909790	2.821701	-0.881287
H	1.940343	0.515991	0.876316
H	1.940343	0.515991	-0.876316
H	-0.560976	0.652422	0.881239
H	-0.560976	0.652422	-0.881239

Molecule# 0545

N-pyrazin-2-ylmethanesulfinamide

PointGroup: C1

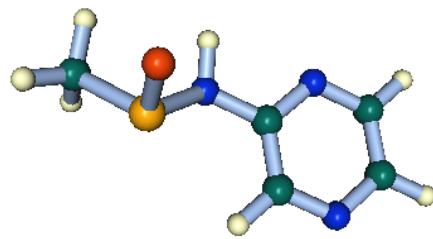
E= -832.568757440 au

ZPE= 0.125465 au

LUMO_eps= -0.06645 au

HOMO_eps= -0.25358 au

Dipole= 3.235 debye



17

C	3.276469	-0.292227	0.099087
C	2.790514	0.999064	0.229996
C	1.181024	-1.031756	-0.375895
C	0.688197	0.275288	-0.221938
C	-3.203955	0.336431	-0.890716
N	2.463709	-1.307293	-0.206599
N	1.497661	1.284923	0.078596
N	-0.655790	0.607184	-0.433652
O	-2.260256	-0.137191	1.534977
S	-1.909653	-0.449316	0.121673
H	4.326381	-0.516346	0.234552
H	3.449330	1.825368	0.467782
H	0.524349	-1.850733	-0.640400
H	-4.132247	-0.170891	-0.639919
H	-2.965474	0.215129	-1.944190
H	-3.270616	1.387654	-0.614934
H	-0.827771	1.581914	-0.201099

Molecule# 0546

N-pyrazin-2-ylmethanesulfonamide

PointGroup: C1

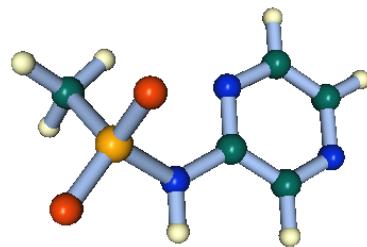
E= -907.820642912 au

ZPE= 0.131121 au

LUMO_eps= -0.07468 au

HOMO_eps= -0.26586 au

Dipole= 3.616 debye



18

C	3.364850	0.398763	0.150943
C	2.326412	1.312586	0.065958
C	1.891085	-1.300109	-0.147133
C	0.842900	-0.369826	-0.242482
C	-2.122614	1.334764	-0.896648
N	3.141045	-0.913697	0.037962
N	1.065571	0.934122	-0.143705
N	-0.461515	-0.797266	-0.495355
O	-2.884414	-1.071196	-0.072187
O	-1.587626	0.402262	1.509475
S	-1.856311	-0.074094	0.169128
H	4.385597	0.718852	0.312895
H	2.507994	2.376178	0.160123
H	1.700423	-2.365075	-0.225096
H	-3.002391	1.842073	-0.507181
H	-1.240827	1.965017	-0.832434
H	-2.293340	0.973464	-1.906154
H	-0.611669	-1.792707	-0.582644

Molecule# 0547

N-sulfanylguanidine

PointGroup: C1

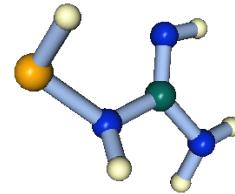
E= -603.665702934 au

ZPE= 0.074499 au

LUMO_eps= -0.03051 au

HOMO_eps= -0.24542 au

Dipole= 3.312 debye



10

S	-1.804112	-0.039089	-0.085409
N	-0.228364	-0.684420	0.016954
N	0.819790	1.392841	-0.011749
N	2.070170	-0.650194	0.057789
C	0.910802	0.124627	-0.000028
H	-1.789467	0.778881	0.993822
H	-0.146667	-1.513718	0.584188
H	1.724397	1.840201	-0.118314
H	2.927975	-0.134408	-0.049798
H	2.053559	-1.500893	-0.484146

Molecule# 0548

N,N'-dimethylsulfamide

PointGroup: C1

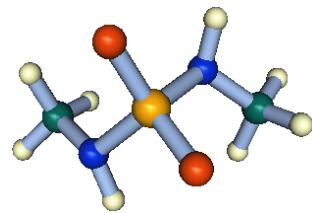
E= -739.300255960 au

ZPE= 0.119623 au

LUMO_eps= -0.02365 au

HOMO_eps= -0.27512 au

Dipole= 4.734 debye



15

C	-2.061141	1.167898	0.047427
C	2.042644	1.195619	-0.057100
N	-0.984023	0.568342	-0.743304
N	1.205917	0.297792	0.735190
O	-0.706460	-1.214268	1.093487
O	0.585495	-1.313495	-1.089732
S	0.003297	-0.568296	0.006116
H	-2.593209	1.870367	-0.591540
H	-1.635479	1.730384	0.877392
H	-2.760962	0.433271	0.448081
H	1.506342	2.078498	-0.412353
H	2.430424	0.647758	-0.912276
H	2.883696	1.505789	0.560159
H	-1.279673	0.182618	-1.630608
H	0.921539	0.622114	1.648067

Molecule# 0549

N,N'-dimethylurea

PointGroup: C2

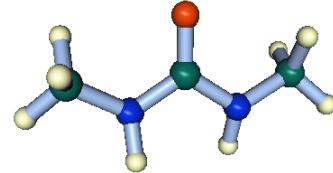
E= -304.008921183 au

ZPE= 0.119111 au

LUMO_eps= -0.02286 au

HOMO_eps= -0.25175 au

Dipole= 3.768 debye



14

C	0.000000	0.000000	0.096002
C	0.000000	2.447119	0.009890
C	0.000000	-2.447119	0.009890
N	0.094200	1.156237	-0.651588
N	-0.094200	-1.156237	-0.651588
O	0.000000	0.000000	1.316825
H	-1.012864	2.672349	0.355132
H	0.320580	3.222188	-0.683998
H	0.658299	2.453848	0.874307
H	1.012864	-2.672349	0.355132
H	-0.320580	-3.222188	-0.683998
H	-0.658299	-2.453848	0.874307
H	-0.241505	1.113406	-1.598970
H	0.241505	-1.113406	-1.598970

Molecule# 0550

N,N-dichloro-beta-alanine

PointGroup: C1

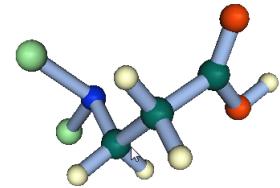
E= -1243.066114370 au

ZPE= 0.087955 au

LUMO_eps= -0.09071 au

HOMO_eps= -0.27678 au

Dipole= 2.771 debye



13

C1	-1.403966	1.580358	-0.186597
C1	-2.213265	-1.174993	-0.243708
O	2.873057	0.758059	-0.738556
O	2.277698	-1.354913	-0.264765
N	-0.804970	-0.095332	-0.210337
C	-0.056679	-0.361932	1.040612
C	1.277873	0.375527	1.029972
C	2.216236	-0.012637	-0.091722
H	2.900728	-1.522198	-0.987239
H	0.107577	-1.437333	1.044710
H	-0.639389	-0.090423	1.923058
H	1.143470	1.452829	0.989941
H	1.784708	0.142322	1.970482

Molecule# 0551

N,N-dichloroalanine

PointGroup: C1

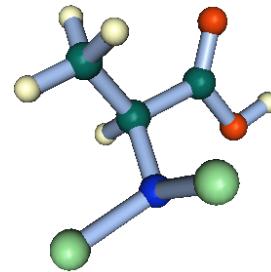
E= -1243.059887150 au

ZPE= 0.086902 au

LUMO_eps= -0.09600 au

HOMO_eps= -0.27341 au

Dipole= 1.273 debye



13

C1	0.728531	1.497292	0.772640
C1	2.223389	-0.562465	-0.591632
O	-2.668641	-0.240390	0.519523
O	-1.881708	0.532517	-1.435981
N	0.638389	0.232441	-0.474123
C	-0.389595	-0.778712	-0.100354
C	-1.770143	-0.126666	-0.269201
C	-0.253722	-1.474534	1.243293
H	-2.779254	0.895548	-1.477125
H	-0.305243	-1.508256	-0.910817
H	0.726260	-1.938756	1.327217
H	-0.395120	-0.777206	2.064971
H	-1.014466	-2.248024	1.326727

Molecule# 0552

N,N-difluoro-2-propen-1-amine

PointGroup: C1

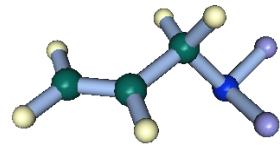
E= -371.758615727 au

ZPE= 0.079909 au

LUMO_eps= -0.03529 au

HOMO_eps= -0.29409 au

Dipole= 2.868 debye



11

F	-1.941746	-0.828965	-0.048656
F	-1.207342	1.234561	0.002398
N	-0.837230	-0.049645	-0.459202
C	0.253975	-0.468738	0.449582
C	1.490150	0.334470	0.186438
C	2.628245	-0.194799	-0.239489
H	0.410259	-1.522526	0.224676
H	-0.096603	-0.362385	1.478991
H	1.421730	1.396780	0.385841
H	2.723117	-1.253412	-0.447875
H	3.509677	0.413089	-0.390093

Molecule# 0553

N,N-difluorobut-2-yn-1-amine

PointGroup: C1

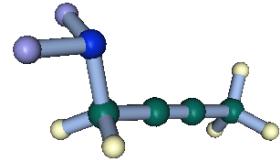
E= -409.840026586 au

ZPE= 0.084193 au

LUMO_eps= -0.01724 au

HOMO_eps= -0.28142 au

Dipole= 3.224 debye



12

F	2.662788	-0.389952	-0.184145
F	1.350478	1.307291	0.242723
N	1.365233	0.093381	-0.468109
C	0.486442	-0.814523	0.318269
C	-0.906899	-0.447656	0.149345
C	-3.460800	0.209456	-0.144708
C	-2.062686	-0.155069	0.017364
H	0.689215	-1.805176	-0.090461
H	0.800414	-0.789621	1.363966
H	-3.548554	1.185872	-0.623577
H	-3.988577	-0.517719	-0.763260
H	-3.964868	0.263674	0.821272

Molecule# 0554

N,N-difluoroethenamine

PointGroup: C1

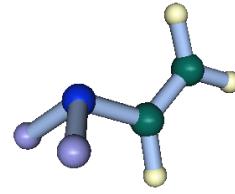
E= -332.427268956 au

ZPE= 0.051185 au

LUMO_eps= -0.06035 au

HOMO_eps= -0.31292 au

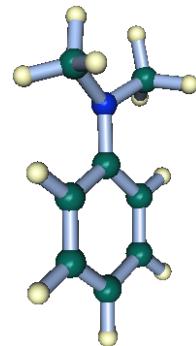
Dipole= 3.009 debye



8

F	1.116105	1.093260	0.040175
F	1.116118	-1.093252	0.040168
N	0.345864	0.000000	-0.426963
C	-0.813920	-0.000009	0.420336
C	-2.001377	0.000000	-0.157052
H	-0.622645	-0.000022	1.485320
H	-2.091523	0.000012	-1.234028
H	-2.905105	-0.000005	0.434659

Molecule# 0555
 N,N-dimethylaniline
 PointGroup: Cs
 E= -366.351335818 au
 ZPE= 0.172930 au
 LUMO_eps= -0.01539 au
 HOMO_eps= -0.19721 au
 Dipole= 2.010 debye



20

C	-0.060027	-2.648826	0.000000
C	-0.034335	-1.937551	1.193561
C	-0.034335	-1.937551	-1.193561
C	0.022378	-0.551433	1.203052
C	0.022378	-0.551433	-1.203052
C	0.066946	0.180520	0.000000
C	-0.034335	2.290729	1.239444
C	-0.034335	2.290729	-1.239444
N	0.163911	1.564753	0.000000
H	-0.106296	-3.728607	0.000000
H	-0.063515	-2.465030	2.138258
H	-0.063515	-2.465030	-2.138258
H	0.033546	-0.040931	2.153087
H	0.033546	-0.040931	-2.153087
H	-1.037990	2.148981	1.661823
H	0.110493	3.352219	1.055557
H	0.693922	1.986879	1.992824
H	0.110493	3.352219	-1.055557
H	-1.037990	2.148981	-1.661823
H	0.693922	1.986879	-1.992824

Molecule# 0556

N,N-dimethylformamide

PointGroup: Cs

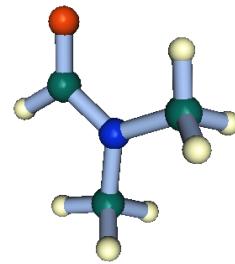
E= -248.613414042 au

ZPE= 0.101860 au

LUMO_eps= -0.01914 au

HOMO_eps= -0.25576 au

Dipole= 4.125 debye



12

C	-0.691463	-0.825035	0.000000
C	1.451045	0.342396	0.000000
C	-0.673160	1.625303	0.000000
N	0.000000	0.344183	0.000000
O	-0.204681	-1.939050	0.000000
H	-1.782485	-0.660464	0.000000
H	1.835600	0.852868	0.886378
H	1.835600	0.852868	-0.886378
H	1.793661	-0.687964	0.000000
H	-0.406192	2.208353	0.885441
H	-1.751076	1.473118	0.000000
H	-0.406192	2.208353	-0.885441

Molecule# 0557

N,N-dimethylthioformamide

PointGroup: Cs

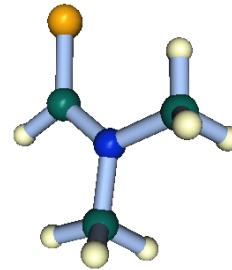
E= -571.571867760 au

ZPE= 0.099661 au

LUMO_eps= -0.03969 au

HOMO_eps= -0.21316 au

Dipole= 5.080 debye



12

C	0.000000	0.771893	0.000000
S	1.640420	0.979773	0.000000
N	-0.700922	-0.369480	0.000000
C	-0.070945	-1.678921	0.000000
C	-2.154440	-0.362728	0.000000
H	-0.648724	1.645722	0.000000
H	-0.374521	-2.239525	0.886803
H	-0.374521	-2.239525	-0.886803
H	1.006974	-1.550438	0.000000
H	-2.539090	-0.874548	-0.885289
H	-2.539090	-0.874548	0.885289
H	-2.518989	0.661390	0.000000

Molecule# 0558

N,N-dimethylurea

PointGroup: C1

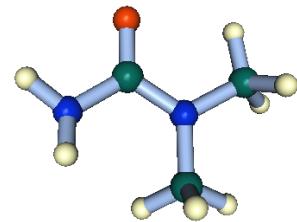
E= -304.007206397 au

ZPE= 0.119091 au

LUMO_eps= -0.02204 au

HOMO_eps= -0.24481 au

Dipole= 4.117 debye



14

H	2.546292	0.664510	0.165310
O	1.231997	-1.340449	-0.051260
C	0.759803	-0.212659	-0.016985
N	-0.589131	0.040718	-0.042504
H	1.276432	1.747193	0.451488
N	1.584512	0.906330	-0.005452
H	-2.218134	-1.068197	-0.768577
H	-2.090342	-1.011668	0.999406
H	-0.951852	-1.996650	0.058184
C	-1.517068	-1.071094	0.069328
H	-1.231220	1.809057	0.957610
H	-2.152797	1.337971	-0.470531
H	-0.559592	2.045476	-0.673917
C	-1.149808	1.378179	-0.047877

Molecule# 0559

N,N,4-trimethylbenzamide

PointGroup: C1

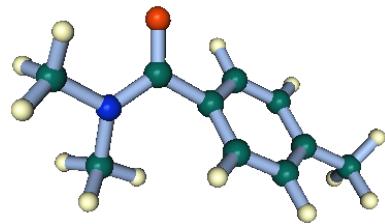
E= -519.075257693 au

ZPE= 0.210045 au

LUMO_eps= -0.03640 au

HOMO_eps= -0.24272 au

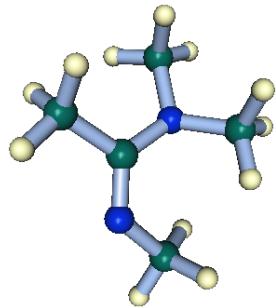
Dipole= 3.759 debye



25

C	-0.824709	1.228044	0.516573
C	-0.551689	-0.837659	-0.670034
C	-2.192547	1.016290	0.567183
C	-1.928178	-1.033187	-0.636809
C	0.016971	0.292751	-0.088553
C	-2.771189	-0.118200	-0.009775
C	1.480040	0.615826	-0.196992
C	-4.260063	-0.333800	0.047428
C	3.800000	-0.087883	-0.163135
C	2.129735	-1.553398	0.876092
N	2.392421	-0.372582	0.069758
O	1.827343	1.734039	-0.557225
H	-0.393860	2.126909	0.935086
H	0.076121	-1.560776	-1.173451
H	-2.825569	1.749761	1.051454
H	-2.351256	-1.910030	-1.110565
H	-4.560652	-1.194770	-0.547754
H	-4.593447	-0.504188	1.073579
H	-4.800270	0.538795	-0.323928
H	4.294841	-0.991603	-0.522094
H	4.298732	0.238192	0.755175
H	3.890077	0.701076	-0.901854
H	2.743352	-1.528530	1.781764
H	2.377510	-2.465691	0.327084
H	1.088513	-1.596087	1.173131

Molecule# 0560
 N,N,N'-trimethylethanimidamide
 PointGroup: C1
 E= -307.351566832 au
 ZPE= 0.169209 au
 LUMO_eps= -0.01663 au
 HOMO_eps= -0.22094 au
 Dipole= 2.648 debye



19

C	-0.187905	0.651224	0.062869
C	0.516351	1.963676	0.319752
C	-2.243533	-0.480238	-0.361032
C	0.408532	-1.679218	0.623345
C	2.013376	-0.300958	-0.547808
N	-1.463119	0.665717	0.054242
N	0.620090	-0.477546	-0.174016
H	-0.225648	2.696922	0.619317
H	1.012868	2.331307	-0.580297
H	1.278208	1.872960	1.096432
H	-3.133483	-0.114305	-0.874912
H	-2.599264	-1.057251	0.498552
H	-1.707657	-1.161888	-1.031043
H	1.084452	-1.699902	1.489156
H	0.600243	-2.572869	0.025300
H	-0.607803	-1.727617	0.994091
H	2.367240	-1.220180	-1.017111
H	2.668083	-0.091653	0.309584
H	2.123038	0.500365	-1.273403

Molecule# 0561

N^2-formylglycinamide

PointGroup: Cs

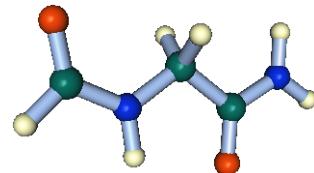
E= -378.066534601 au

ZPE= 0.101104 au

LUMO_eps= -0.02932 au

HOMO_eps= -0.26714 au

Dipole= 3.770 debye



13

C	2.188329	-0.578455	0.000000
C	-1.460704	0.073620	0.000000
C	0.000000	0.510660	0.000000
N	-2.360917	1.087263	0.000000
N	0.840666	-0.658435	0.000000
O	2.817916	0.462897	0.000000
O	-1.784599	-1.100738	0.000000
H	2.671946	-1.568981	0.000000
H	0.198935	1.134237	0.876265
H	0.198935	1.134237	-0.876265
H	-3.341011	0.863104	0.000000
H	-2.082734	2.051773	0.000000
H	0.363396	-1.548392	0.000000

Molecule# 0562

N^3,N^3-difluoro-3,4-pyridinediamine

PointGroup: C1

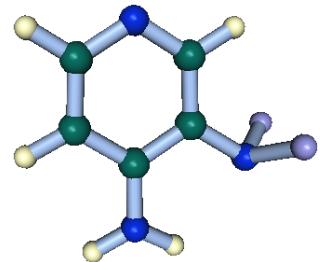
E= -557.561711414 au

ZPE= 0.103817 au

LUMO_eps= -0.06449 au

HOMO_eps= -0.25754 au

Dipole= 4.558 debye



15

F	-2.192510	-0.268440	1.108615
F	-2.196021	-0.431782	-1.071868
N	-1.580972	0.316470	-0.035136
N	1.505260	-1.737413	0.024215
N	0.347175	2.296354	0.002544
C	-0.202650	-0.061410	-0.009063
C	0.727919	0.992051	-0.013556
C	0.228543	-1.384447	0.013005
C	2.079236	0.604782	-0.004927
C	2.400219	-0.735610	0.013200
H	1.025447	3.014652	-0.169637
H	-0.622485	2.526037	-0.124140
H	-0.507894	-2.178420	0.017074
H	2.859819	1.353746	-0.007846
H	3.442048	-1.034086	0.020506

Molecule# 0563

naphthalen-1-amine

PointGroup: C1

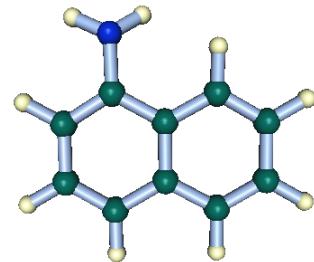
E= -441.409274084 au

ZPE= 0.163956 au

LUMO_eps= -0.04465 au

HOMO_eps= -0.20136 au

Dipole= 1.492 debye



20

C	-2.745482	-0.250488	0.015139
C	-2.350376	1.101274	-0.020876
C	1.894620	-1.629753	-0.016536
C	-1.798435	-1.240778	0.025645
C	-1.018277	1.430836	-0.033362
C	0.565283	-1.959620	0.002317
C	2.304363	-0.285408	-0.011578
C	-0.414684	-0.938347	0.010052
C	-0.013885	0.433355	-0.006243
C	1.383991	0.743412	-0.000677
N	1.805666	2.071855	-0.042792
H	-3.797274	-0.503107	0.026539
H	-3.099801	1.880731	-0.046991
H	2.647310	-2.406938	-0.024601
H	-2.097908	-2.281072	0.043095
H	-0.742879	2.474995	-0.088131
H	0.249676	-2.994190	0.010295
H	3.361776	-0.050767	-0.011365
H	2.778199	2.210429	0.179331
H	1.218530	2.740032	0.428091

Molecule# 0564

naphthalen-1-ol

PointGroup: C1

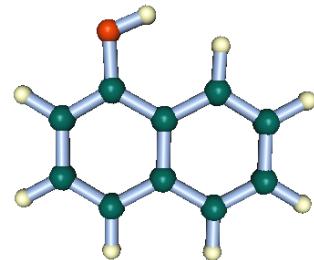
E= -461.281607980 au

ZPE= 0.151209 au

LUMO_eps= -0.05193 au

HOMO_eps= -0.21532 au

Dipole= 1.346 debye



19

C	-2.727109	-0.326483	0.000000
C	-2.375260	1.038390	0.000000
C	1.957686	-1.557474	0.000000
C	-1.750278	-1.286970	0.000000
C	-1.055155	1.409855	0.000000
C	0.638110	-1.927342	0.000000
C	2.326734	-0.200714	0.000000
C	-0.376443	-0.941789	0.000000
C	-0.019952	0.443553	0.000000
C	1.365002	0.779883	0.000000
O	1.794772	2.076411	0.000000
H	-3.770509	-0.611247	0.000000
H	-3.148862	1.793966	0.000000
H	2.733146	-2.311550	0.000000
H	-2.017573	-2.335991	0.000000
H	-0.825143	2.468776	0.000000
H	0.356325	-2.971639	0.000000
H	3.367436	0.091086	0.000000
H	1.046996	2.679866	0.000001

Molecule# 0565

naphthalen-2-amine

PointGroup: C1

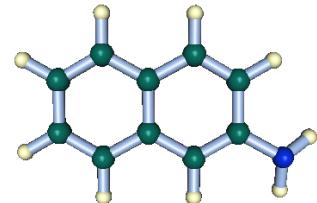
E= -441.411112449 au

ZPE= 0.163652 au

LUMO_eps= -0.04299 au

HOMO_eps= -0.20374 au

Dipole= 1.878 debye



20

C	2.934750	0.367685	0.004894
C	2.687481	-1.021705	0.002229
C	1.883651	1.248979	0.004210
C	1.403115	-1.502176	-0.001292
C	-0.563413	1.664514	-0.000104
C	-1.844909	1.189940	-0.005795
C	-1.040095	-1.082969	-0.003076
C	0.547644	0.786363	0.000560
C	0.294326	-0.618925	-0.002537
C	-2.104204	-0.206518	-0.005473
N	-3.423722	-0.650874	-0.067870
H	3.952870	0.732442	0.007200
H	3.520954	-1.711733	0.002509
H	2.064878	2.316734	0.006029
H	1.220915	-2.569562	-0.003920
H	-0.385911	2.732646	0.001922
H	-2.680007	1.879584	-0.016198
H	-1.221281	-2.151525	-0.006138
H	-4.116285	-0.020662	0.301917
H	-3.580151	-1.602931	0.220075

Molecule# 0566

naphthalen-2-ol

PointGroup: Cs

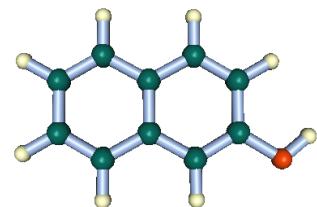
E= -461.283306020 au

ZPE= 0.151191 au

LUMO_eps= -0.04992 au

HOMO_eps= -0.21707 au

Dipole= 1.489 debye



19

C	-2.810255	0.874015	0.000000
C	-2.014183	2.040128	0.000000
C	-2.216594	-0.361309	0.000000
C	-0.646606	1.950634	0.000000
C	-0.160779	-1.748178	0.000000
C	1.205234	-1.842363	0.000000
C	1.407649	0.566607	0.000000
C	-0.807166	-0.489734	0.000000
C	0.000000	0.689037	0.000000
C	1.997415	-0.671969	0.000000
O	3.364255	-0.741235	0.000000
H	-3.888286	0.960491	0.000000
H	-2.491116	3.011227	0.000000
H	-2.821658	-1.259354	0.000000
H	-0.040456	2.847562	0.000000
H	-0.762742	-2.647866	0.000000
H	1.687194	-2.813217	0.000000
H	2.030075	1.451183	0.000000
H	3.644668	-1.661357	0.000000

Molecule# 0567

naphthalene

PointGroup: D2h

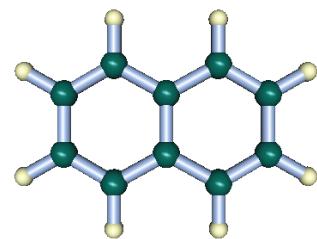
E= -386.029027609 au

ZPE= 0.147230 au

LUMO_eps= -0.05096 au

HOMO_eps= -0.22592 au

Dipole= 0.000 debye



18

C	0.000000	0.000000	0.713923
C	0.000000	1.240542	1.396864
C	0.000000	-1.240542	1.396864
C	0.000000	2.423616	0.705779
C	0.000000	2.423616	-0.705779
C	0.000000	1.240542	-1.396864
C	0.000000	-2.423616	0.705779
C	0.000000	-2.423616	-0.705779
C	0.000000	-1.240542	-1.396864
C	0.000000	0.000000	-0.713923
H	0.000000	-3.364265	1.240162
H	0.000000	-3.364265	-1.240162
H	0.000000	3.364265	-1.240162
H	0.000000	3.364265	1.240162
H	0.000000	1.239118	-2.479712
H	0.000000	-1.239118	2.479712
H	0.000000	-1.239118	-2.479712
H	0.000000	1.239118	2.479712

Molecule# 0568

nitrobenzene

PointGroup: C2v

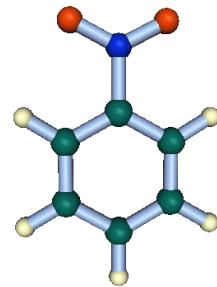
E= -436.917931019 au

ZPE= 0.102880 au

LUMO_eps= -0.10437 au

HOMO_eps= -0.29125 au

Dipole= 4.706 debye



14

C	0.000000	0.000000	-2.509568
C	0.000000	1.206952	-1.817042
C	0.000000	-1.206952	-1.817042
C	0.000000	1.215022	-0.429244
C	0.000000	-1.215022	-0.429244
C	0.000000	0.000000	0.241376
N	0.000000	0.000000	1.718131
O	0.000000	1.082390	2.285939
O	0.000000	-1.082390	2.285939
H	0.000000	0.000000	-3.590995
H	0.000000	2.143267	-2.357131
H	0.000000	-2.143267	-2.357131
H	0.000000	2.134833	0.133951
H	0.000000	-2.134833	0.133951

Molecule# 0569

nitroethane

PointGroup: Cs

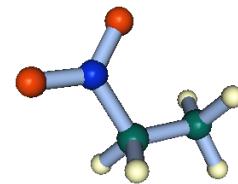
E= -284.447027889 au

ZPE= 0.078161 au

LUMO_eps= -0.08099 au

HOMO_eps= -0.30882 au

Dipole= 3.800 debye



10

C	-0.252099	-1.864578	0.000000
C	0.698505	-0.690619	0.000000
N	0.000000	0.657769	0.000000
O	0.728213	1.635752	0.000000
O	-1.217324	0.683616	0.000000
H	-0.889475	-1.861633	0.881474
H	-0.889475	-1.861633	-0.881474
H	0.333046	-2.784908	0.000000
H	1.340180	-0.659983	-0.878434
H	1.340180	-0.659983	0.878434

Molecule# 0570

nitromethane

PointGroup: Cs

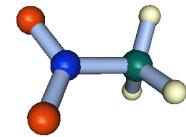
E= -245.115210191 au

ZPE= 0.049605 au

LUMO_eps= -0.08667 au

HOMO_eps= -0.31295 au

Dipole= 3.599 debye



7

C 0.000229 -1.324841 0.000000

N -0.009436 0.173920 0.000000

O 0.000229 0.730465 1.084390

O 0.000229 0.730465 -1.084390

H -0.491970 -1.664331 -0.903741

H -0.491970 -1.664331 0.903741

H 1.044943 -1.627166 0.000000

Molecule# 0571

non-1-ene

PointGroup: C1

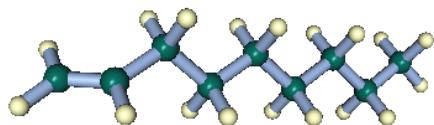
E= -353.926159215 au

ZPE= 0.249801 au

LUMO_eps= -0.01028 au

HOMO_eps= -0.26122 au

Dipole= 0.496 debye



27

C	4.970457	-0.129620	0.573340
C	3.980470	-0.194879	-0.308575
C	-3.651956	-0.553136	0.088042
C	2.695911	0.573157	-0.232484
C	-2.411683	0.337221	0.003428
C	1.456682	-0.330273	-0.147562
C	-1.096612	-0.441957	-0.031602
C	0.142340	0.449970	-0.118069
C	-4.960299	0.234816	0.126740
H	5.870978	-0.718575	0.461701
H	4.915733	0.519817	1.439288
H	4.082499	-0.862497	-1.160575
H	-3.662992	-1.236357	-0.766511
H	-3.581017	-1.184624	0.978831
H	2.603275	1.205727	-1.122753
H	2.721293	1.246627	0.628130
H	-2.482102	0.968002	-0.889247
H	-2.402836	1.023095	0.857279
H	1.452629	-1.017103	-0.999926
H	1.532776	-0.955399	0.746703
H	-1.106759	-1.128904	-0.884359
H	-1.026517	-1.070974	0.862031
H	0.074720	1.076852	-1.013503
H	0.150888	1.138809	0.733091
H	-5.824377	-0.428184	0.188857
H	-5.077618	0.848983	-0.768541
H	-4.992428	0.902909	0.989943

Molecule# 0572

nonan-1-ol

PointGroup: C1

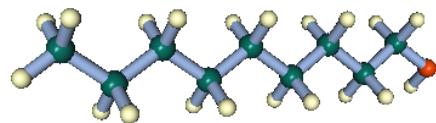
E= -430.406179803 au

ZPE= 0.278281 au

LUMO_eps= -0.01416 au

HOMO_eps= -0.27660 au

Dipole= 1.829 debye



30

C	5.737654	0.300711	0.011156
C	4.448192	-0.518362	-0.011562
C	3.184431	0.342309	0.009963
C	1.888085	-0.468013	-0.011393
C	0.625303	0.394075	0.008474
C	-0.671025	-0.416506	-0.012685
C	-1.932920	0.447391	0.006322
C	-3.228540	-0.365266	-0.019608
C	-4.476648	0.508022	0.005687
O	-5.690067	-0.238804	-0.075332
H	6.619389	-0.341382	-0.006380
H	5.796144	0.967682	-0.851502
H	5.795907	0.919276	0.909188
H	4.433983	-1.199317	0.844790
H	4.435354	-1.153265	-0.902627
H	3.198187	0.979052	0.901047
H	3.198984	1.023585	-0.847491
H	1.874006	-1.148349	0.846661
H	1.875740	-1.105201	-0.901950
H	0.637718	1.031678	0.898752
H	0.639314	1.073915	-0.849865
H	-0.686189	-1.095875	0.845940
H	-0.684331	-1.053895	-0.902720
H	-1.919452	1.084161	0.897002
H	-1.916317	1.126849	-0.852022
H	-3.259860	-0.993407	-0.913658
H	-3.249682	-1.044442	0.840338
H	-4.476569	1.142168	0.900551
H	-4.490512	1.170814	-0.860513
H	-5.748466	-0.819778	0.688990

Molecule# 0573

nonane

PointGroup: C2v

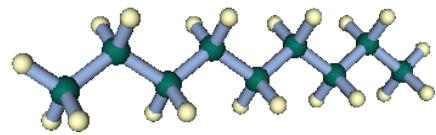
E= -355.161306222 au

ZPE= 0.273232 au

LUMO_eps= -0.01009 au

HOMO_eps= -0.30150 au

Dipole= 0.094 debye



29

C	0.000000	5.113451	0.369764
C	0.000000	-5.113451	0.369764
C	0.000000	3.841175	-0.476207
C	0.000000	-3.841175	-0.476207
C	0.000000	2.559853	0.358568
C	0.000000	-2.559853	0.358568
C	0.000000	1.280240	-0.478345
C	0.000000	-1.280240	-0.478345
C	0.000000	0.000000	0.358018
H	0.880614	5.158370	1.014023
H	0.000000	6.008632	-0.253795
H	-0.880614	5.158370	1.014023
H	0.000000	-6.008632	-0.253795
H	-0.880614	-5.158370	1.014023
H	0.880614	-5.158370	1.014023
H	-0.873886	3.841226	-1.134700
H	0.873886	3.841226	-1.134700
H	-0.873886	-3.841226	-1.134700
H	0.873886	-3.841226	-1.134700
H	0.874404	2.560551	1.018190
H	-0.874404	2.560551	1.018190
H	-0.874404	-2.560551	1.018190
H	0.874404	-2.560551	1.018190
H	0.874440	1.280475	-1.137677
H	-0.874440	1.280475	-1.137677
H	-0.874440	-1.280475	-1.137677
H	0.874440	-1.280475	-1.137677
H	0.874372	0.000000	1.017387
H	-0.874372	0.000000	1.017387

Molecule# 0574

norborane

PointGroup: C2v

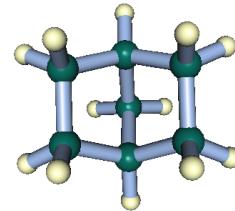
E= -274.065634522 au

ZPE= 0.176431 au

LUMO_eps= -0.01245 au

HOMO_eps= -0.29142 au

Dipole= 0.095 debye



19

C	0.000000	0.000000	1.385266
C	0.000000	1.130265	0.339297
C	0.000000	-1.130265	0.339297
C	1.252143	0.780951	-0.492266
C	-1.252143	0.780951	-0.492266
C	-1.252143	-0.780951	-0.492266
C	1.252143	-0.780951	-0.492266
H	-0.887352	0.000000	2.020515
H	0.887352	0.000000	2.020515
H	0.000000	2.146851	0.729171
H	0.000000	-2.146851	0.729171
H	2.153759	1.172887	-0.019845
H	-2.153759	-1.172887	-0.019845
H	2.153759	-1.172887	-0.019845
H	-2.153759	1.172887	-0.019845
H	1.204295	-1.201509	-1.497189
H	-1.204295	1.201509	-1.497189
H	1.204295	1.201509	-1.497189
H	-1.204295	-1.201509	-1.497189

Molecule# 0575

norbornadiene

PointGroup: C2v

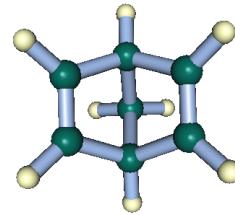
E= -271.575782683 au

ZPE= 0.128074 au

LUMO_eps= -0.02290 au

HOMO_eps= -0.23098 au

Dipole= 0.086 debye



15

C	0.000000	0.000000	1.353978
C	0.000000	1.120429	0.272438
C	0.000000	-1.120429	0.272438
C	1.240122	0.664758	-0.520057
C	1.240122	-0.664758	-0.520057
C	-1.240122	0.664758	-0.520057
C	-1.240122	-0.664758	-0.520057
H	-0.896605	0.000000	1.972745
H	0.896605	0.000000	1.972745
H	0.000000	2.152954	0.608976
H	0.000000	-2.152954	0.608976
H	1.927551	1.330663	-1.018798
H	1.927551	-1.330663	-1.018798
H	-1.927551	1.330663	-1.018798
H	-1.927551	-1.330663	-1.018798

Molecule# 0576

norcarane

PointGroup: C1

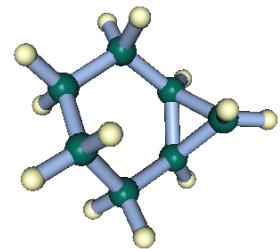
E= -274.045202050 au

ZPE= 0.175099 au

LUMO_eps= -0.01066 au

HOMO_eps= -0.26749 au

Dipole= 0.188 debye



19

C	0.975299	0.827111	-0.352809
C	1.037330	-0.681581	-0.465009
C	1.707835	0.013482	0.686561
C	-0.339639	1.518890	0.000186
C	-0.218086	-1.511099	-0.270848
C	-1.568408	0.613209	-0.153427
C	-1.336768	-0.765176	0.466692
H	1.606840	1.375880	-1.039268
H	1.707047	-1.069245	-1.223026
H	2.788502	0.048694	0.705499
H	1.251515	-0.062096	1.665475
H	-0.295481	1.889223	1.028594
H	-0.460026	2.400340	-0.631932
H	-0.593963	-1.797410	-1.258217
H	0.025275	-2.442322	0.248361
H	-2.438162	1.095924	0.297128
H	-1.797265	0.485618	-1.216378
H	-2.251524	-1.359759	0.428994
H	-1.088138	-0.653867	1.526702

Molecule# 0577

o-cresol

PointGroup: Cs

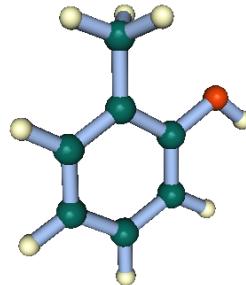
E= -346.922075284 au

ZPE= 0.132112 au

LUMO_eps= -0.01596 au

HOMO_eps= -0.22880 au

Dipole= 0.976 debye



16

C	1.183630	-1.657236	0.000000
C	1.978197	-0.519415	0.000000
C	-0.201692	-1.524488	0.000000
C	1.385481	0.737927	0.000000
C	-0.822901	-0.278622	0.000000
C	0.000000	0.854617	0.000000
C	-2.318300	-0.130060	0.000000
O	-0.625320	2.075643	0.000000
H	1.634666	-2.639701	0.000000
H	3.056498	-0.602769	0.000000
H	-0.822640	-2.411682	0.000000
H	1.999453	1.631427	0.000000
H	-2.661652	0.425255	0.874779
H	-2.661652	0.425255	-0.874779
H	-2.803146	-1.104999	0.000000
H	0.034538	2.775735	0.000000

Molecule# 0578

o-dichlorobenzene

PointGroup: C2v

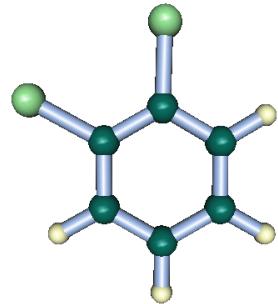
E= -1151.595076190 au

ZPE= 0.081275 au

LUMO_eps= -0.04130 au

HOMO_eps= -0.26020 au

Dipole= 2.540 debye



12

C	0.000000	0.694844	2.382562
C	0.000000	-0.694844	2.382562
C	0.000000	1.388047	1.181404
C	0.000000	-1.388047	1.181404
C	0.000000	0.697332	-0.025757
C	0.000000	-0.697332	-0.025757
Cl	0.000000	1.605090	-1.512263
Cl	0.000000	-1.605090	-1.512263
H	0.000000	1.242555	3.314599
H	0.000000	-1.242555	3.314599
H	0.000000	2.468014	1.164618
H	0.000000	-2.468014	1.164618

Molecule# 0579

o-difluorobenzene

PointGroup: C2v

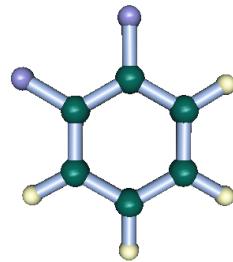
E= -430.883452910 au

ZPE= 0.084122 au

LUMO_eps= -0.03508 au

HOMO_eps= -0.26344 au

Dipole= 2.592 debye



12

C	0.000000	0.694295	-0.532279
C	0.000000	1.395728	0.658951
C	0.000000	0.694955	1.860549
C	0.000000	-0.694955	1.860549
C	0.000000	-1.395728	0.658951
C	0.000000	-0.694295	-0.532279
F	0.000000	-1.349838	-1.705237
F	0.000000	1.349838	-1.705237
H	0.000000	2.476041	0.629411
H	0.000000	1.238774	2.794390
H	0.000000	-1.238774	2.794390
H	0.000000	-2.476041	0.629411

Molecule# 0580

O-ethynylhydroxylamine

PointGroup: C1

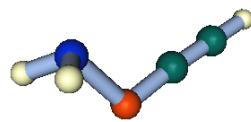
E= -207.921434817 au

ZPE= 0.048421 au

LUMO_eps= -0.02769 au

HOMO_eps= -0.25428 au

Dipole= 1.982 debye



7

O -0.485466 0.609325 0.000033

N -1.490658 -0.472251 -0.000012

C 0.723672 0.132472 0.000000

C 1.867234 -0.225589 -0.000026

H -2.052385 -0.232984 -0.814329

H -2.052359 -0.233078 0.814350

H 2.877638 -0.544080 -0.000049

Molecule# 0581

o-toluidine

PointGroup: C1

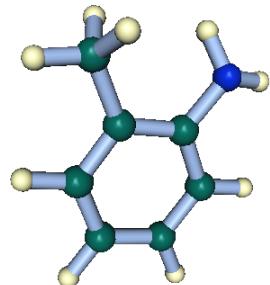
E= -327.048539142 au

ZPE= 0.144563 au

LUMO_eps= -0.01684 au

HOMO_eps= -0.20925 au

Dipole= 1.659 debye



17

C	-1.885447	-0.818106	0.007501
C	-1.975051	0.568350	-0.000697
C	-0.628773	-1.412605	0.008802
C	-0.822932	1.340246	-0.004708
C	0.543272	-0.661462	0.000704
C	0.440882	0.742403	-0.003804
C	1.892340	-1.326342	-0.010307
N	1.590034	1.533681	-0.069114
H	-2.777856	-1.428093	0.012258
H	-2.942118	1.053384	-0.001815
H	-0.550201	-2.492945	0.013468
H	-0.896228	2.421222	-0.012731
H	2.483420	-1.022758	-0.878512
H	2.479480	-1.078545	0.880504
H	1.791171	-2.409860	-0.037583
H	2.429428	1.133051	0.315391
H	1.466926	2.493869	0.207873

Molecule# 0582

o-xylene

PointGroup: C2v

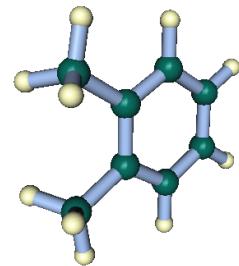
E= -310.997610014 au

ZPE= 0.155421 au

LUMO_eps= -0.01131 au

HOMO_eps= -0.24142 au

Dipole= 0.680 debye



18

C	0.000000	0.693498	1.952555
C	0.000000	-0.693498	1.952555
C	0.000000	1.377876	0.743109
C	0.000000	-1.377876	0.743109
C	0.000000	0.703110	-0.476273
C	0.000000	-0.703110	-0.476273
C	0.000000	1.477433	-1.768050
C	0.000000	-1.477433	-1.768050
H	0.000000	1.241957	2.885153
H	0.000000	-1.241957	2.885153
H	0.000000	2.461031	0.743277
H	0.000000	-2.461031	0.743277
H	0.876446	1.245249	-2.378000
H	-0.876446	1.245249	-2.378000
H	0.000000	2.550074	-1.580471
H	0.876446	-1.245249	-2.378000
H	0.000000	-2.550074	-1.580471
H	-0.876446	-1.245249	-2.378000

Molecule# 0583

octahydropentalene

PointGroup: Cs

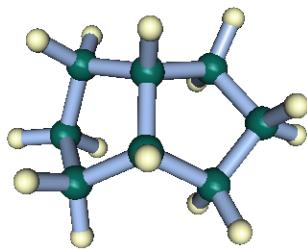
E= -313.401924709 au

ZPE= 0.204927 au

LUMO_eps= -0.01134 au

HOMO_eps= -0.30753 au

Dipole= 0.117 debye



22

C	0.107535	-2.168802	0.000000
C	-0.072713	-1.229601	1.197282
C	-0.072713	-1.229601	-1.197282
C	0.643552	0.075590	0.785834
C	-0.072713	1.375568	1.203592
C	-0.955423	1.735879	0.000000
C	-0.072713	1.375568	-1.203592
C	0.643552	0.075590	-0.785834
H	-0.591384	-3.006411	0.000000
H	-0.635977	1.262705	-2.131346
H	-0.635977	1.262705	2.131346
H	0.312527	-1.639812	-2.131505
H	-1.275571	2.778231	0.000000
H	0.312527	-1.639812	2.131505
H	1.117840	-2.587719	0.000000
H	-1.860267	1.122424	0.000000
H	1.664077	0.059193	-1.169844
H	0.658197	2.171586	-1.366919
H	1.664077	0.059193	1.169844
H	-1.139228	-1.037507	1.348434
H	0.658197	2.171586	1.366919
H	-1.139228	-1.037507	-1.348434

Molecule# 0584

octan-2-one

PointGroup: C1

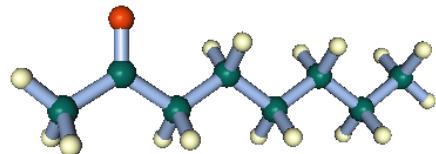
E= -389.876567131 au

ZPE= 0.225228 au

LUMO_eps= -0.02485 au

HOMO_eps= -0.25480 au

Dipole= 2.875 debye



25

C	2.934682	0.194779	-0.004319
C	4.206745	-0.627668	0.015541
C	-4.735634	0.345804	0.007764
C	1.629987	-0.583788	-0.011871
C	-3.474297	-0.516071	-0.008273
C	0.371967	0.276168	0.007321
C	-2.183074	0.302813	0.008272
C	-0.914399	-0.550257	-0.008442
O	2.963972	1.405012	-0.011805
H	5.073473	0.025936	-0.034823
H	4.252724	-1.223691	0.929740
H	4.223317	-1.329172	-0.820869
H	-4.771299	1.007919	-0.859773
H	-4.773151	0.972598	0.901088
H	-5.638271	-0.266633	-0.005463
H	1.647676	-1.270090	0.842461
H	1.642249	-1.235279	-0.893437
H	-3.483287	-1.191182	0.852863
H	-3.482233	-1.157183	-0.895044
H	0.388911	0.953592	-0.849010
H	0.390148	0.917782	0.891046
H	-2.174223	0.979058	-0.852885
H	-2.174641	0.944692	0.895375
H	-0.924559	-1.192399	-0.895918
H	-0.924462	-1.226723	0.853135

Molecule# 0585

octanal

PointGroup: Cs

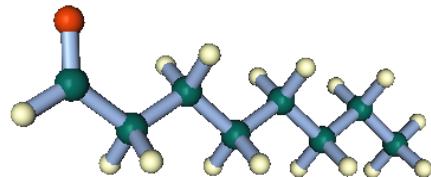
E= -389.865318732 au

ZPE= 0.225891 au

LUMO_eps= -0.03506 au

HOMO_eps= -0.26364 au

Dipole= 2.716 debye



25

C	3.802531	1.530625	0.000000
C	-4.637584	-1.541445	0.000000
C	2.306092	1.687856	0.000000
C	-3.126767	-1.767415	0.000000
C	1.512129	0.387412	0.000000
C	-2.319569	-0.468725	0.000000
C	0.000000	0.612534	0.000000
C	-0.806536	-0.686509	0.000000
O	4.392118	0.479692	0.000000
H	4.367576	2.486731	0.000000
H	-4.952565	-0.978042	0.880795
H	-5.181814	-2.486837	0.000000
H	-4.952565	-0.978042	-0.880795
H	2.054742	2.311831	-0.867367
H	2.054742	2.311831	0.867367
H	-2.848014	-2.363887	-0.873950
H	-2.848014	-2.363887	0.873950
H	1.799348	-0.206318	0.870716
H	1.799348	-0.206318	-0.870716
H	-2.599270	0.128270	-0.874711
H	-2.599270	0.128270	0.874711
H	-0.279114	1.209821	0.874730
H	-0.279114	1.209821	-0.874730
H	-0.527370	-1.283394	-0.874398
H	-0.527370	-1.283394	0.874398

Molecule# 0586

octanamine

PointGroup: C1

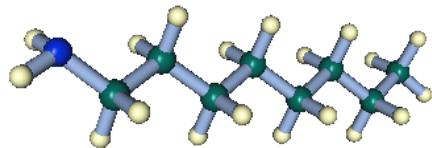
E= -371.202678447 au

ZPE= 0.262575 au

LUMO_eps= -0.01268 au

HOMO_eps= -0.24255 au

Dipole= 1.222 debye



28

C	5.101251	-0.357927	-0.007494
C	3.825718	0.482347	0.025964
C	2.547647	-0.356251	-0.014566
C	1.264914	0.475125	0.016833
C	-0.011971	-0.365198	-0.021296
C	-1.294964	0.466445	0.009286
C	-2.568842	-0.377394	-0.031588
C	-3.845971	0.454973	0.002143
N	-5.033409	-0.402959	-0.068536
H	5.152333	-0.960610	-0.916686
H	5.145033	-1.041786	0.842745
H	5.993780	0.268535	0.025090
H	3.820683	1.101568	0.928131
H	3.825838	1.178470	-0.818216
H	2.553701	-0.977563	-0.916520
H	2.547940	-1.052494	0.830938
H	1.260595	1.097575	0.917951
H	1.264843	1.169787	-0.829777
H	-0.007756	-0.987992	-0.921778
H	-0.012300	-1.059295	0.825700
H	-1.298111	1.089499	0.909813
H	-1.294044	1.159823	-0.838338
H	-2.580405	-0.997246	-0.931668
H	-2.571992	-1.069529	0.818063
H	-3.867157	1.118505	-0.865912
H	-3.829717	1.101269	0.891642
H	-5.881430	0.149049	-0.095245
H	-5.094663	-0.999577	0.748129

Molecule# 0587

octane

PointGroup: C1

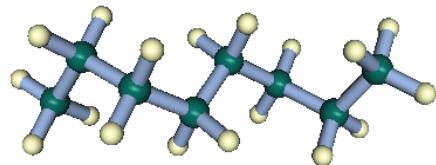
E= -315.827558627 au

ZPE= 0.245568 au

LUMO_eps= -0.01152 au

HOMO_eps= -0.30405 au

Dipole= 0.000 debye



26

C	2.743376	0.386487	0.533004
C	3.403443	-0.769047	-0.220309
C	1.628643	1.096455	-0.247194
C	0.402478	0.244625	-0.603456
C	-0.402478	-0.244624	0.603457
C	-1.628643	-1.096455	0.247194
C	-2.743376	-0.386487	-0.533004
C	-3.403443	0.769047	0.220308
H	3.803237	-0.434641	-1.180362
H	4.230374	-1.189255	0.353881
H	-3.507182	-1.127157	-0.783972
H	-4.230374	1.189255	-0.353882
H	-2.701500	1.579527	0.420693
H	-3.803238	0.434642	1.180362
H	2.701500	-1.579527	-0.420694
H	-0.242366	0.842416	-1.252097
H	2.055029	1.496389	-1.172579
H	3.507182	1.127157	0.783972
H	2.356936	0.024239	1.488923
H	-1.295689	-1.964325	-0.330509
H	-2.356936	-0.024240	-1.488923
H	0.709119	-0.617126	-1.204218
H	1.295689	1.964325	0.330509
H	0.242366	-0.842416	1.252098
H	-0.709119	0.617127	1.204218
H	-2.055029	-1.496389	1.172580

Molecule# 0588

octene

PointGroup: C1

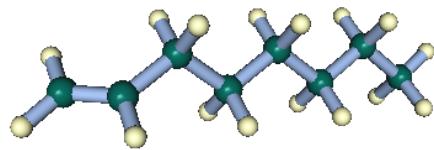
E= -314.598114127 au

ZPE= 0.221450 au

LUMO_eps= -0.01001 au

HOMO_eps= -0.26133 au

Dipole= 0.506 debye



24

C	4.339193	-0.239943	0.516430
C	3.327634	-0.231568	-0.343062
C	-4.298854	-0.403949	0.124866
C	2.068612	0.568357	-0.199112
C	-3.042666	0.464354	0.079878
C	0.803711	-0.301438	-0.153528
C	-1.749886	-0.346967	-0.014527
C	-0.486737	0.513029	-0.061371
H	5.218634	-0.848262	0.352660
H	4.324601	0.365016	1.415596
H	3.390219	-0.857805	-1.229651
H	-4.383423	-1.021698	-0.771594
H	-4.283461	-1.075093	0.986132
H	-5.202181	0.203631	0.194727
H	1.984175	1.258703	-1.046285
H	2.125947	1.184941	0.701645
H	-3.101914	1.147047	-0.773197
H	-3.005278	1.097541	0.971468
H	0.770340	-0.934721	-1.045813
H	0.870178	-0.981984	0.700136
H	-1.788071	-0.982079	-0.905996
H	-1.691063	-1.029675	0.839789
H	-0.544961	1.194564	-0.916651
H	-0.449783	1.148628	0.829586

Molecule# 0589

octyne

PointGroup: Cs

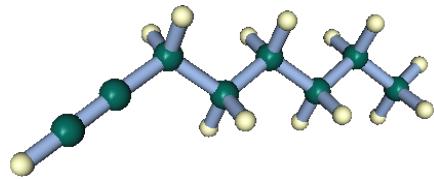
E= -313.345275045 au

ZPE= 0.197820 au

LUMO_eps= -0.01206 au

HOMO_eps= -0.27215 au

Dipole= 1.035 debye

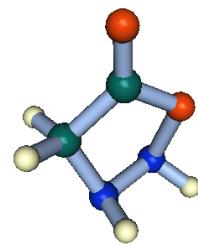


22

C	-3.346877	-3.031775	0.000000
C	-2.834619	-1.946702	0.000000
C	3.714400	1.932692	0.000000
C	-2.190041	-0.639220	0.000000
C	2.187929	1.995002	0.000000
C	-0.653223	-0.713523	0.000000
C	1.528109	0.615773	0.000000
C	0.000000	0.667374	0.000000
H	-3.805160	-3.988782	0.000000
H	4.087265	1.405598	0.880672
H	4.155073	2.930520	0.000000
H	4.087265	1.405598	-0.880672
H	-2.527896	-0.075379	-0.874546
H	-2.527896	-0.075379	0.874546
H	1.845994	2.557334	0.874089
H	1.845994	2.557334	-0.874089
H	-0.326053	-1.280282	-0.874781
H	-0.326053	-1.280282	0.874781
H	1.870789	0.052846	0.874570
H	1.870789	0.052846	-0.874570
H	-0.342088	1.230153	-0.875038
H	-0.342088	1.230153	0.875038

Molecule# 0590
oxadiazolidin-5-one
PointGroup: C1

E= -338.619279739 au
ZPE= 0.074527 au
LUMO_eps= -0.03081 au
HOMO_eps= -0.26952 au
Dipole= 3.747 debye



10

O	-0.105885	-1.140297	-0.063377
O	-2.056550	-0.017889	-0.074554
N	1.295288	-0.679344	0.308891
N	1.383531	0.622036	-0.219008
C	-0.862295	-0.019042	0.010796
C	0.089800	1.168812	0.183518
H	1.867042	-1.302225	-0.257604
H	1.412350	0.590975	-1.239324
H	-0.209208	2.014166	-0.427950
H	0.112541	1.465110	1.233260

Molecule# 0591

oxadithiolane

PointGroup: C1

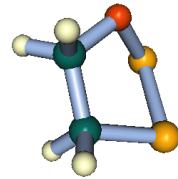
E= -950.322408246 au

ZPE= 0.062256 au

LUMO_eps= -0.05242 au

HOMO_eps= -0.22507 au

Dipole= 2.596 debye



9

S	0.050457	-1.283028	0.254896
S	1.318484	0.295909	-0.230152
O	-1.268667	-0.524946	-0.458383
C	0.011024	1.451390	0.341037
C	-1.372949	0.839488	-0.008592
H	0.172355	2.395956	-0.175996
H	0.109777	1.603307	1.412522
H	-1.847822	1.369365	-0.831999
H	-2.016479	0.879572	0.871964

Molecule# 0592

oxalamide

PointGroup: C2

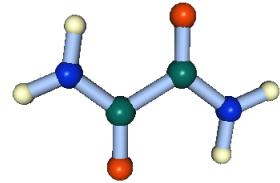
E= -338.752967802 au

ZPE= 0.073371 au

LUMO_eps= -0.05641 au

HOMO_eps= -0.26290 au

Dipole= 0.002 debye



10

C	0.331694	0.699305	-0.000060
C	-0.331694	-0.699305	-0.000060
O	-0.331694	1.722137	-0.000002
O	0.331694	-1.722137	-0.000002
N	1.672475	0.623238	-0.000051
N	-1.672475	-0.623238	-0.000051
H	2.224941	1.462119	0.000258
H	2.104637	-0.286302	0.000475
H	-2.224941	-1.462119	0.000258
H	-2.104637	0.286302	0.000475

Molecule# 0593

oxalic acid

PointGroup: C2h

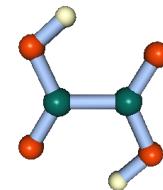
E= -378.490128561 au

ZPE= 0.049396 au

LUMO_eps= -0.10059 au

HOMO_eps= -0.31251 au

Dipole= 0.000 debye



8

C	-0.054169	0.770269	0.000000
C	0.054169	-0.770269	0.000000
O	-1.121261	1.323096	0.000000
O	1.121261	-1.323096	0.000000
O	1.121261	1.380321	0.000000
O	-1.121261	-1.380321	0.000000
H	1.811137	0.691631	0.000000
H	-1.811137	-0.691631	0.000000

Molecule# 0594

oxamic acid

PointGroup: C1

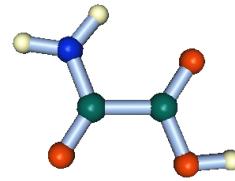
E= -358.616712065 au

ZPE= 0.060975 au

LUMO_eps= -0.07427 au

HOMO_eps= -0.27744 au

Dipole= 2.233 debye



9

N	-1.545214	0.875722	0.000075
H	-2.543731	0.764446	0.000029
H	-1.130576	1.791761	0.000310
O	1.533181	-0.905280	0.000099
H	2.449443	-0.589400	0.000108
O	-1.138031	-1.371045	-0.000085
O	1.125097	1.307223	-0.000114
C	0.739014	0.164691	-0.000013
C	-0.759117	-0.222031	-0.000015

Molecule# 0595

oxathiazin-4-one

PointGroup: C1

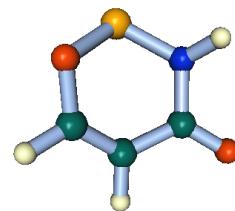
E= -719.624323258 au

ZPE= 0.063808 au

LUMO_eps= -0.08259 au

HOMO_eps= -0.25814 au

Dipole= 2.344 debye



10

S	1.225174	-0.898935	-0.254228
O	1.535098	0.658588	0.407850
O	-2.480973	-0.262291	0.091047
N	-0.366881	-1.120825	0.191149
C	-1.293951	-0.078457	-0.057482
C	-0.684163	1.233340	-0.309598
C	0.572566	1.541966	0.062753
H	-1.361545	2.031989	-0.568230
H	-0.591464	-1.718951	0.976121
H	0.918677	2.564229	0.156502

Molecule# 0596

oxazole

PointGroup: Cs

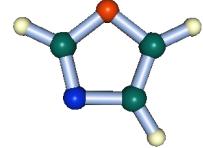
E= -246.165802476 au

ZPE= 0.058423 au

LUMO_eps= -0.02165 au

HOMO_eps= -0.26524 au

Dipole= 1.538 debye



8

C	0.752140	-0.876732	0.000000
C	-0.594330	-0.964738	0.000000
C	0.000000	1.101527	0.000000
N	1.118628	0.463667	0.000000
O	-1.098400	0.308078	0.000000
H	1.482368	-1.666223	0.000000
H	-1.305329	-1.768953	0.000000
H	-0.167090	2.164537	0.000000

Molecule# 0597

oxazolidin-2-one

PointGroup: C1

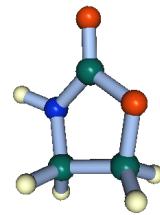
E= -322.669551343 au

ZPE= 0.087244 au

LUMO_eps= -0.02285 au

HOMO_eps= -0.27841 au

Dipole= 5.350 debye



11

C	0.863078	-0.004934	-0.012038
C	-1.345484	0.742595	0.139382
C	-1.296433	-0.772693	-0.105039
N	0.032123	1.081398	-0.166734
O	2.061521	-0.022202	0.030559
O	0.084494	-1.127510	0.081246
H	-2.049443	1.241627	-0.524845
H	-1.609416	0.978619	1.174750
H	-1.897195	-1.346525	0.595247
H	-1.584158	-1.025162	-1.126673
H	0.420261	1.989541	0.020394

Molecule# 0598

oxetane

PointGroup: Cs

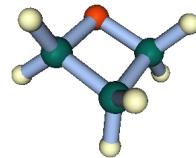
E= -193.183324192 au

ZPE= 0.086487 au

LUMO_eps= -0.01093 au

HOMO_eps= -0.25594 au

Dipole= 1.989 debye



10

C	-0.000362	-0.062016	1.039066
C	-0.000362	-0.062016	-1.039066
H	-0.886662	1.703368	0.000000
H	0.886384	1.702690	0.000000
C	-0.000362	1.073690	0.000000
H	-0.890999	-0.134448	1.666799
H	0.889472	-0.133116	1.668112
H	-0.890999	-0.134448	-1.666799
H	0.889472	-0.133116	-1.668112
O	0.001231	-1.071110	0.000000

Molecule# 0599

oxirane

PointGroup: C2v

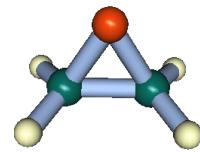
E= -153.852563254 au

ZPE= 0.057247 au

LUMO_eps= -0.00823 au

HOMO_eps= -0.28319 au

Dipole= 1.918 debye



7

O 0.000000 0.000000 0.854896

C 0.000000 0.731605 -0.373327

C 0.000000 -0.731605 -0.373327

H 0.917863 1.266951 -0.589809

H -0.917863 1.266951 -0.589809

H -0.917863 -1.266951 -0.589809

H 0.917863 -1.266951 -0.589809

Molecule# 0600

oxirene

PointGroup: Cs

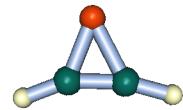
E= -152.537032589 au

ZPE= 0.029070 au

LUMO_eps= -0.03037 au

HOMO_eps= -0.21367 au

Dipole= 2.395 debye



5

O -0.749026 -0.493037 0.000000

C 0.778446 -0.240644 0.000000

C 0.000000 0.750804 0.000000

H 1.619799 -0.896149 0.000000

H -0.298263 1.779489 0.000000

Molecule# 0601

oxoacetic acid

PointGroup: Cs

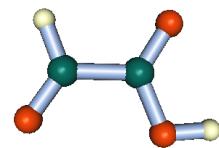
E= -303.199462846 au

ZPE= 0.042900 au

LUMO_eps= -0.11244 au

HOMO_eps= -0.29235 au

Dipole= 1.197 debye



7

C -0.718651 -0.816155 0.000000

C 0.000000 0.539124 0.000000

O 1.331696 0.432025 0.000000

O -0.618671 1.571383 0.000000

O -0.159963 -1.873970 0.000000

H -1.815745 -0.700767 0.000000

H 1.703152 1.327452 0.000000

Molecule# 0602

p-aminobenzoic acid

PointGroup: C1

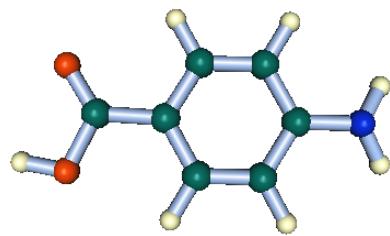
E= -476.374502867 au

ZPE= 0.131825 au

LUMO_eps= -0.04759 au

HOMO_eps= -0.22818 au

Dipole= 4.187 debye



17

O	2.762394	-1.105018	0.003022
C	2.156561	0.114744	0.002536
O	2.803915	1.137760	0.005269
C	0.686414	0.034495	-0.001330
C	-0.049953	1.223608	-0.002784
C	-1.429416	1.203832	-0.004972
C	-2.123979	-0.016126	-0.004799
N	-3.503279	-0.040515	-0.054095
C	-1.386039	-1.209122	-0.004321
C	-0.004739	-1.181360	-0.002372
H	3.714017	-0.931351	0.005078
H	0.483823	2.163304	-0.001130
H	-1.984440	2.133422	-0.009930
H	-3.992208	0.795011	0.217353
H	-3.962914	-0.892079	0.218605
H	-1.907089	-2.158183	-0.008827
H	0.548189	-2.108876	-0.000570

Molecule# 0603

p-bromotoluene

PointGroup: C1

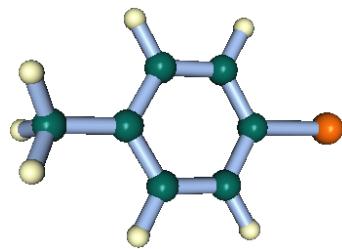
E= -2845.292972020 au

ZPE= 0.117395 au

LUMO_eps= -0.03039 au

HOMO_eps= -0.24479 au

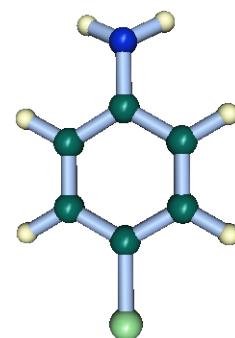
Dipole= 2.340 debye



15

C	1.737843	1.195180	-0.010347
C	1.737853	-1.194962	-0.010341
C	0.347810	1.206239	-0.004724
C	0.347993	-1.206083	-0.004728
C	2.457404	0.000211	-0.010323
C	-0.336699	0.000119	-0.000585
C	3.963093	-0.000145	0.015748
Br	-2.250263	-0.000066	0.003253
H	2.268493	2.138997	-0.017455
H	2.268547	-2.138775	-0.017460
H	-0.192595	2.141409	-0.006935
H	-0.192414	-2.141254	-0.006960
H	4.369539	-0.873408	-0.494005
H	4.369331	0.891017	-0.461955
H	4.336524	-0.019036	1.042713

Molecule# 0604
 p-chloroaniline
 PointGroup: Cs
 E= -747.349244273 au
 ZPE= 0.107262 au
 LUMO_eps= -0.02740 au
 HOMO_eps= -0.21652 au
 Dipole= 3.406 debye



14

C	0.002824	1.104180	1.201145
C	0.002824	1.104180	-1.201145
C	0.002824	-0.282935	1.203368
C	0.002824	-0.282935	-1.203368
C	0.001749	1.821531	0.000000
C	0.002775	-0.973267	0.000000
N	0.059244	3.213615	0.000000
Cl	0.000656	-2.729245	0.000000
H	0.008179	1.636737	2.143798
H	0.008179	1.636737	-2.143798
H	0.002153	-0.824965	2.137851
H	0.002153	-0.824965	-2.137851
H	-0.270719	3.666897	0.836100
H	-0.270719	3.666897	-0.836100

Molecule# 0605

p-cresol

PointGroup: C1

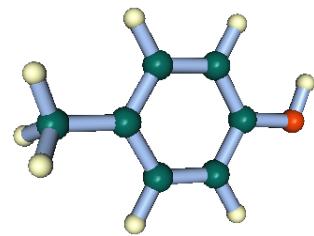
E= -346.920843445 au

ZPE= 0.131636 au

LUMO_eps= -0.01962 au

HOMO_eps= -0.22515 au

Dipole= 1.295 debye



16

C	0.644121	1.194052	-0.006494
C	0.662041	-1.191017	-0.006314
C	-0.747351	1.189109	-0.001233
C	-0.724096	-1.215100	-0.001196
C	1.376677	0.009928	-0.007134
C	-1.435402	-0.018408	0.002343
C	2.883482	0.016860	0.008658
O	-2.803606	-0.093184	0.005561
H	1.164240	2.143785	-0.011774
H	1.201078	-2.130513	-0.011627
H	-1.293225	2.125496	-0.002769
H	-1.266997	-2.150003	-0.002681
H	3.293415	-0.687622	-0.716746
H	3.277225	1.005159	-0.226732
H	3.273067	-0.266943	0.989489
H	-3.176785	0.793560	0.006570

Molecule# 0606

p-cyanonitrobenzene

PointGroup: C2v

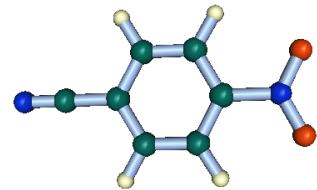
E= -529.187753761 au

ZPE= 0.101295 au

LUMO_eps= -0.12986 au

HOMO_eps= -0.30986 au

Dipole= 0.086 debye



15

O	0.000000	1.083262	-3.015657
N	0.000000	0.000000	-2.452829
O	0.000000	-1.083262	-3.015657
C	0.000000	0.000000	-0.973083
C	0.000000	-1.215143	-0.304010
C	0.000000	-1.213700	1.080544
C	0.000000	0.000000	1.777046
C	0.000000	0.000000	3.207339
N	0.000000	0.000000	4.359138
C	0.000000	1.213700	1.080544
C	0.000000	1.215143	-0.304010
H	0.000000	-2.135421	-0.866311
H	0.000000	-2.145531	1.626371
H	0.000000	2.145531	1.626371
H	0.000000	2.135421	-0.866311

Molecule# 0607
p-dichlorobenzene

PointGroup: D2h

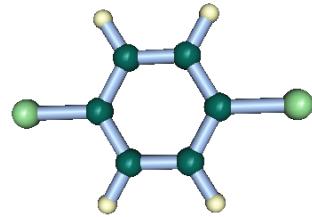
E= -1151.598770460 au

ZPE= 0.081204 au

LUMO_eps= -0.04437 au

HOMO_eps= -0.25578 au

Dipole= 0.000 debye



12

C	0.000000	1.207774	0.694419
C	0.000000	1.207774	-0.694419
C	0.000000	-1.207774	0.694419
C	0.000000	-1.207774	-0.694419
C	0.000000	0.000000	1.378331
C	0.000000	0.000000	-1.378331
Cl	0.000000	0.000000	3.128670
Cl	0.000000	0.000000	-3.128670
H	0.000000	2.139873	1.239951
H	0.000000	2.139873	-1.239951
H	0.000000	-2.139873	1.239951
H	0.000000	-2.139873	-1.239951

Molecule# 0608

p-difluorobenzene

PointGroup: D2h

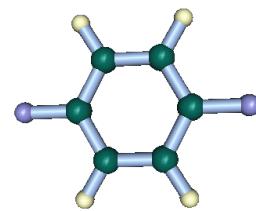
E= -430.888404323 au

ZPE= 0.083905 au

LUMO_eps= -0.04188 au

HOMO_eps= -0.25817 au

Dipole= 0.000 debye



12

C	0.000000	0.000000	1.363040
C	0.000000	0.000000	-1.363040
C	0.000000	1.211776	0.695210
C	0.000000	-1.211776	0.695210
C	0.000000	-1.211776	-0.695210
C	0.000000	1.211776	-0.695210
F	0.000000	0.000000	2.715276
F	0.000000	0.000000	-2.715276
H	0.000000	2.134857	1.256229
H	0.000000	-2.134857	1.256229
H	0.000000	-2.134857	-1.256229
H	0.000000	2.134857	-1.256229

Molecule# 0609

p-formylphenol

PointGroup: Cs

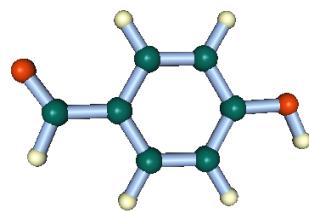
E= -420.960030701 au

ZPE= 0.113822 au

LUMO_eps= -0.06961 au

HOMO_eps= -0.25403 au

Dipole= 4.638 debye



15

C	1.264505	0.437243	0.000000
C	-1.134314	0.204052	0.000000
C	1.405404	-0.941236	0.000000
C	-1.007552	-1.169144	0.000000
C	0.000000	1.026568	0.000000
C	0.266706	-1.745847	0.000000
C	-0.123034	2.491555	0.000000
O	-1.167015	3.105905	0.000000
O	0.332247	-3.103791	0.000000
H	2.146215	1.066352	0.000000
H	-2.110754	0.668386	0.000000
H	2.389487	-1.394063	0.000000
H	-1.872992	-1.816544	0.000000
H	0.845206	3.032775	0.000000
H	1.250697	-3.392963	0.000000

Molecule# 0610

p-methoxyaniline

PointGroup: C1

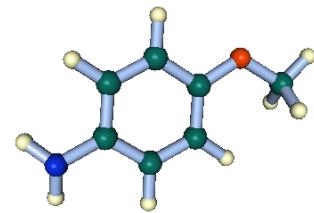
E= -402.281983509 au

ZPE= 0.149005 au

LUMO_eps= -0.01500 au

HOMO_eps= -0.19542 au

Dipole= 1.607 debye



18

C	0.968305	-1.191866	-0.005659
C	1.297498	1.177941	-0.005925
C	-0.412677	-1.004932	-0.001215
C	-0.072135	1.370804	-0.000176
C	1.845461	-0.110566	-0.007083
C	-0.943492	0.281050	0.001739
C	-3.203619	-0.496341	0.002648
N	3.234655	-0.299516	-0.075261
O	-2.281512	0.577362	0.007741
H	1.361714	-2.200914	-0.013324
H	1.955088	2.038508	-0.014741
H	-1.054456	-1.872710	0.000780
H	-0.487426	2.369078	0.002544
H	-3.093299	-1.125308	0.890843
H	-3.093184	-1.116539	-0.891616
H	-4.192458	-0.045145	0.004971
H	3.556642	-1.185853	0.280103
H	3.780840	0.460055	0.299362

Molecule# 0611

p-methoxybenzaldehyde

PointGroup: Cs

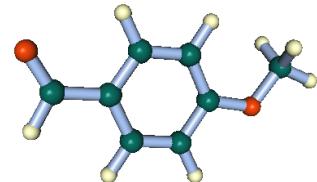
E= -460.273658032 au

ZPE= 0.141957 au

LUMO_eps= -0.06739 au

HOMO_eps= -0.24703 au

Dipole= 4.294 debye



18

C	2.356270	-1.777173	0.000000
O	3.482232	-1.329055	0.000000
C	1.122819	-0.978189	0.000000
C	-0.122816	-1.616318	0.000000
C	-1.293641	-0.885835	0.000000
C	-1.239473	0.512535	0.000000
C	0.000000	1.164562	0.000000
C	1.165300	0.417042	0.000000
O	-2.435229	1.147852	0.000000
C	-2.463378	2.570550	0.000000
H	2.191197	-2.874062	0.000000
H	-0.165916	-2.698728	0.000000
H	-2.261088	-1.367425	0.000000
H	0.057823	2.241984	0.000000
H	2.129488	0.906789	0.000000
H	-1.981978	2.976345	0.892234
H	-1.981978	2.976345	-0.892234
H	-3.514049	2.845335	0.000000

Molecule# 0612

p-nitroaniline

PointGroup: Cs

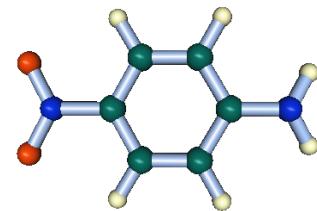
E= -492.304770432 au

ZPE= 0.119334 au

LUMO_eps= -0.08791 au

HOMO_eps= -0.24281 au

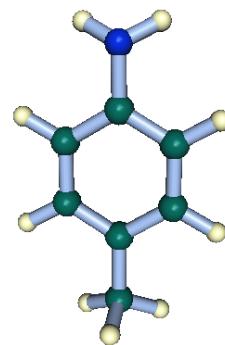
Dipole= 7.282 debye



16

C	-0.002527	-1.360148	1.209015
C	-0.002527	-1.360148	-1.209015
C	-0.002527	0.019496	1.209747
C	-0.002527	0.019496	-1.209747
C	-0.001512	-2.076412	0.000000
C	-0.002390	0.706727	0.000000
N	-0.043718	-3.450313	0.000000
N	-0.000096	2.164119	0.000000
O	0.000905	2.738949	1.083563
O	0.000905	2.738949	-1.083563
H	-0.005983	-1.897716	2.148203
H	-0.005983	-1.897716	-2.148203
H	-0.001593	0.575824	2.134036
H	-0.001593	0.575824	-2.134036
H	0.195712	-3.935056	0.846913
H	0.195712	-3.935056	-0.846913

Molecule# 0613
 p-toluidine
 PointGroup: C1
 E= -327.047684890 au
 ZPE= 0.143930 au
 LUMO_eps= -0.01475 au
 HOMO_eps= -0.20544 au
 Dipole= 1.266 debye



17

C	0.669588	1.190338	-0.009937
C	0.669666	-1.190178	-0.009924
C	-0.718186	1.198300	0.003054
C	-0.717909	-1.198256	0.003081
C	1.396835	0.000223	-0.013482
C	-1.437175	0.000049	0.010600
C	2.903547	-0.000073	0.006732
N	-2.833422	-0.000219	0.080437
H	1.197270	2.136416	-0.020466
H	1.197417	-2.136238	-0.020449
H	-1.250749	2.141644	0.007895
H	-1.250429	-2.141628	0.007947
H	3.308495	-0.870548	-0.510365
H	3.307829	0.891793	-0.472804
H	3.289746	-0.021962	1.029503
H	-3.281770	-0.834223	-0.262806
H	-3.282044	0.833864	-0.262259

Molecule# 0614

p-xylene

PointGroup: C2

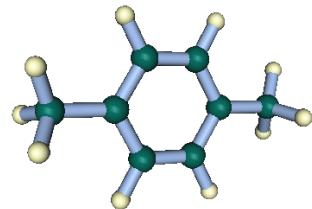
E= -310.998038631 au

ZPE= 0.154659 au

LUMO_eps= -0.01476 au

HOMO_eps= -0.23713 au

Dipole= 0.042 debye

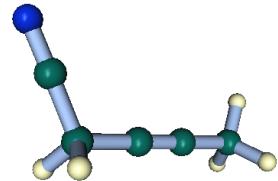


18

C	-0.006126	0.695514	1.193928
C	0.006126	-0.695514	1.193928
C	-0.005956	0.693932	-1.191741
C	0.005956	-0.693932	-1.191741
C	-0.010665	1.417282	0.002438
C	0.010665	-1.417282	0.002438
C	0.005956	2.923660	-0.002240
C	-0.005956	-2.923660	-0.002240
H	-0.011287	1.226083	2.138293
H	0.011287	-1.226083	2.138293
H	-0.010880	1.224834	-2.136140
H	0.010880	-1.224834	-2.136140
H	-0.642816	3.326662	-0.780885
H	-0.324391	3.327444	0.954402
H	1.012311	3.306699	-0.189982
H	0.642816	-3.326662	-0.780885
H	0.324391	-3.327444	0.954402
H	-1.012311	-3.306699	-0.189982

Molecule# 0615
pent-3-yenenitrile
PointGroup: Cs

E= -248.306978480 au
ZPE= 0.083377 au
LUMO_eps= -0.02232 au
HOMO_eps= -0.28256 au
Dipole= 4.254 debye



11

C	1.101422	1.086436	0.000000
C	0.000000	0.612760	0.000000
C	-1.353510	-1.424068	0.000000
C	2.441080	1.653556	0.000000
C	-1.345349	0.043042	0.000000
N	-1.379143	-2.572655	0.000000
H	2.603677	2.273574	0.882742
H	3.194285	0.864356	0.000000
H	2.603677	2.273574	-0.882742
H	-1.904748	0.383361	-0.875875
H	-1.904748	0.383361	0.875875

Molecule# 0616

penta-1,4-diyn-3-one

PointGroup: C1

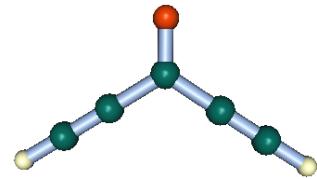
E= -266.896432062 au

ZPE= 0.046757 au

LUMO_eps= -0.10737 au

HOMO_eps= -0.29579 au

Dipole= 3.311 debye



8

O	-0.000002	1.727755	0.000063
C	0.000000	0.513409	-0.000056
C	-1.221816	-0.263144	-0.000092
C	1.221818	-0.263140	-0.000093
C	-2.237923	-0.902147	0.000052
C	2.237924	-0.902146	0.000041
H	-3.142391	-1.459515	0.000203
H	3.142392	-1.459515	0.000184

Molecule# 0617

penta-2,4-diynal

PointGroup: C1

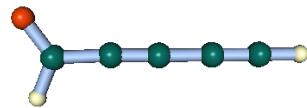
E= -266.910007105 au

ZPE= 0.047165 au

LUMO_eps= -0.10831 au

HOMO_eps= -0.28967 au

Dipole= 3.466 debye



8

O	-2.769216	-0.536264	0.000215
C	-0.546543	0.198083	-0.000698
C	-1.974175	0.375575	0.000309
C	0.660285	0.101518	-0.000632
C	2.012661	-0.024555	-0.000207
C	3.212576	-0.134634	0.000498
H	-2.304988	1.428398	0.001460
H	4.269894	-0.234210	0.001198

Molecule# 0618
pentafluorobenzene

PointGroup: C2v

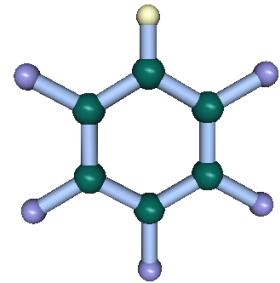
E= -728.687137922 au

ZPE= 0.059762 au

LUMO_eps= -0.05006 au

HOMO_eps= -0.27784 au

Dipole= 1.385 debye



12

C	0.000000	0.000000	1.114207
C	0.000000	1.205172	0.423331
C	0.000000	1.190132	-0.964430
C	0.000000	0.000000	-1.669598
C	0.000000	-1.190132	-0.964430
C	0.000000	-1.205172	0.423331
F	0.000000	0.000000	2.445370
F	0.000000	2.356848	1.095325
F	0.000000	2.356407	-1.619428
H	0.000000	0.000000	-2.748927
F	0.000000	-2.356407	-1.619428
F	0.000000	-2.356848	1.095325

Molecule# 0619

pentafluorochloroethane

PointGroup: Cs

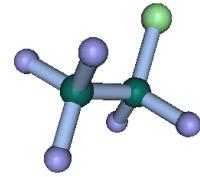
E= -1035.888296810 au

ZPE= 0.026940 au

LUMO_eps= -0.03296 au

HOMO_eps= -0.36393 au

Dipole= 0.493 debye



8

C	0.088227	-0.640097	0.000000
C	-0.628654	0.743753	0.000000
Cl	1.853861	-0.454917	0.000000
F	-0.297556	-1.321635	1.086547
F	-0.297556	-1.321635	-1.086547
F	-1.951228	0.550467	0.000000
F	-0.297556	1.441493	1.086607
F	-0.297556	1.441493	-1.086607

Molecule# 0620

pentalene

PointGroup: C2h

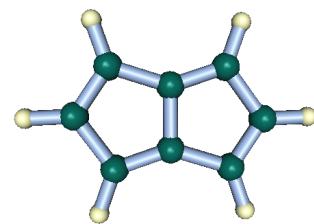
E= -308.479221171 au

ZPE= 0.109949 au

LUMO_eps= -0.10747 au

HOMO_eps= -0.20244 au

Dipole= 0.000 debye



14

C	1.340358	1.082599	0.000000
C	2.159435	-0.166489	0.000000
C	1.340358	-1.239684	0.000000
C	-1.340358	-1.082599	0.000000
C	-2.159435	0.166489	0.000000
C	-1.340358	1.239684	0.000000
C	0.038329	0.726381	0.000000
C	-0.038329	-0.726381	0.000000
H	1.756064	2.079976	0.000000
H	3.238150	-0.182744	0.000000
H	1.637830	-2.276002	0.000000
H	-1.756064	-2.079976	0.000000
H	-3.238150	0.182744	0.000000
H	-1.637830	2.276002	0.000000

Molecule# 0621

pentanal

PointGroup: Cs

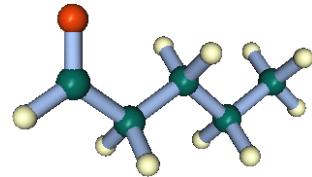
E= -271.881101445 au

ZPE= 0.140693 au

LUMO_eps= -0.03541 au

HOMO_eps= -0.26428 au

Dipole= 2.793 debye



16

C	-0.854017	-2.053209	0.000000
C	0.913211	2.739799	0.000000
C	0.331799	-1.126885	0.000000
C	1.244470	1.248574	0.000000
C	0.000000	0.360098	0.000000
O	-2.008076	-1.706587	0.000000
H	-0.596414	-3.133487	0.000000
H	1.818200	3.348531	0.000000
H	0.328751	3.013404	0.880532
H	0.328751	3.013404	-0.880532
H	0.945985	-1.401209	0.867354
H	0.945985	-1.401209	-0.867354
H	1.858867	1.012250	0.874251
H	1.858867	1.012250	-0.874251
H	-0.618581	0.589247	-0.870767
H	-0.618581	0.589247	0.870767

Molecule# 0622

pentanamide

PointGroup: C1

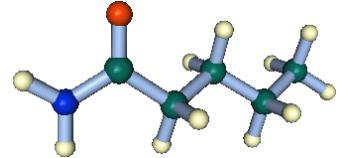
E= -327.291888756 au

ZPE= 0.158524 au

LUMO_eps= -0.02174 au

HOMO_eps= -0.26018 au

Dipole= 3.655 debye



18

C	-0.428305	-0.603318	0.292946
C	-1.730980	0.145991	0.048752
C	0.804689	0.186857	-0.143412
N	-2.798137	-0.632363	-0.294446
O	-1.831047	1.353253	0.169304
C	2.116704	-0.509009	0.218058
C	3.349645	0.278591	-0.221813
H	-0.378232	-0.797219	1.369502
H	-0.452804	-1.579947	-0.197097
H	0.763288	0.351634	-1.223970
H	0.764447	1.175441	0.315734
H	-3.696408	-0.193737	-0.404160
H	-2.730511	-1.629614	-0.375823
H	2.153180	-0.667921	1.300253
H	2.140943	-1.504976	-0.235220
H	4.270724	-0.237101	0.052854
H	3.359798	0.422536	-1.304049
H	3.370399	1.266751	0.241480

Molecule# 0623

pentanamine

PointGroup: C1

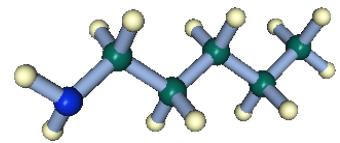
E= -253.218548621 au

ZPE= 0.177495 au

LUMO_eps= -0.01254 au

HOMO_eps= -0.24277 au

Dipole= 1.173 debye



19

C	-3.193395	0.219196	0.022962
C	-1.870687	-0.543222	-0.031096
C	-0.644306	0.369108	0.017163
C	0.681934	-0.388325	-0.039089
C	1.902025	0.524730	0.012238
N	3.142821	-0.252296	-0.075802
H	-4.046943	-0.459069	-0.014935
H	-3.274969	0.803363	0.942009
H	-3.283672	0.912302	-0.816050
H	-1.834066	-1.145994	-0.943292
H	-1.824205	-1.251686	0.801403
H	-0.682799	0.973279	0.929858
H	-0.692022	1.077721	-0.816618
H	0.733834	-0.987957	-0.951398
H	0.730562	-1.095733	0.796545
H	1.844936	1.150237	0.914816
H	1.879005	1.205826	-0.842025
H	3.244316	-0.859616	0.728902
H	3.952849	0.354475	-0.091672

Molecule# 0624

pentane

PointGroup: C2v

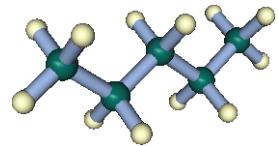
E= -197.849124461 au

ZPE= 0.159767 au

LUMO_eps= -0.00918 au

HOMO_eps= -0.31906 au

Dipole= 0.094 debye



17

C	0.000000	2.553552	0.323437
C	0.000000	-2.553552	0.323437
C	0.000000	1.280666	-0.521619
C	0.000000	-1.280666	-0.521619
C	0.000000	0.000000	0.313781
H	0.880619	2.598968	0.967590
H	-0.880619	2.598968	0.967590
H	0.000000	3.448219	-0.300839
H	0.880619	-2.598968	0.967590
H	0.000000	-3.448219	-0.300839
H	-0.880619	-2.598968	0.967590
H	-0.873927	1.280219	-1.180074
H	0.873927	1.280219	-1.180074
H	-0.873927	-1.280219	-1.180074
H	0.873927	-1.280219	-1.180074
H	-0.874435	0.000000	0.973556
H	0.874435	0.000000	0.973556

Molecule# 0625

pentanedinitrile

PointGroup: C2v

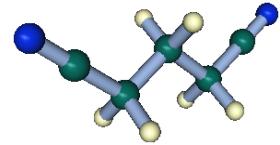
E= -303.732880756 au

ZPE= 0.101836 au

LUMO_eps= -0.03677 au

HOMO_eps= -0.34486 au

Dipole= 4.005 debye



13

C	0.000000	2.488837	0.088743
C	0.000000	-2.488837	0.088743
C	0.000000	1.264960	-0.705030
C	0.000000	-1.264960	-0.705030
C	0.000000	0.000000	0.168023
N	0.000000	3.444883	0.727024
N	0.000000	-3.444883	0.727024
H	-0.877475	1.279493	-1.355740
H	0.877475	1.279493	-1.355740
H	0.877475	-1.279493	-1.355740
H	-0.877475	-1.279493	-1.355740
H	-0.875721	0.000000	0.815966
H	0.875721	0.000000	0.815966

Molecule# 0626

pentanenitrile

PointGroup: Cs

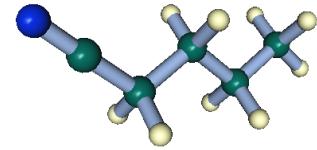
E= -250.793398002 au

ZPE= 0.130830 au

LUMO_eps= -0.02064 au

HOMO_eps= -0.32939 au

Dipole= 4.412 debye



15

C	-1.381391	-1.674027	0.000000
C	1.469740	2.485294	0.000000
C	-0.027455	-1.130038	0.000000
C	1.425482	0.958648	0.000000
C	0.000000	0.407830	0.000000
N	-2.455764	-2.084510	0.000000
H	0.971625	2.894129	0.880933
H	2.497069	2.850311	0.000000
H	0.971625	2.894129	-0.880933
H	0.496473	-1.517892	-0.876678
H	0.496473	-1.517892	0.876678
H	1.960400	0.577288	-0.874787
H	1.960400	0.577288	0.874787
H	-0.540986	0.773987	-0.875086
H	-0.540986	0.773987	0.875086

Molecule# 0627

pentazine

PointGroup: C2v

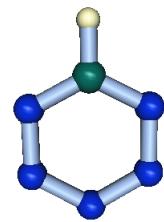
E= -312.417397515 au

ZPE= 0.037111 au

LUMO_eps= -0.14491 au

HOMO_eps= -0.28602 au

Dipole= 2.730 debye



7

N 0.000000 1.175961 -0.636160

N 0.000000 1.151724 0.677844

N 0.000000 0.000000 1.324042

N 0.000000 -1.151724 0.677844

N 0.000000 -1.175961 -0.636160

C 0.000000 0.000000 -1.252774

H 0.000000 0.000000 -2.335236

Molecule# 0628

pentyl acetate

PointGroup: Cs

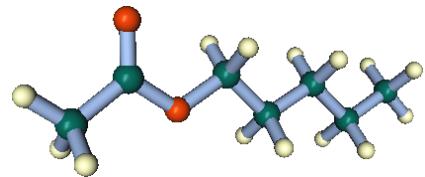
E= -425.817109451 au

ZPE= 0.202399 au

LUMO_eps= -0.01331 au

HOMO_eps= -0.28025 au

Dipole= 2.262 debye



23

C	-1.760775	2.179912	0.000000
C	-3.257433	2.344694	0.000000
C	3.309060	-3.268875	0.000000
C	1.838693	-2.855555	0.000000
C	1.639526	-1.339018	0.000000
C	0.167821	-0.923390	0.000000
C	0.000000	0.582801	0.000000
O	-0.959601	3.081295	0.000000
O	-1.416146	0.876019	0.000000
H	-3.685781	1.861519	0.878050
H	-3.685781	1.861519	-0.878050
H	-3.506083	3.401176	0.000000
H	3.827078	-2.884132	-0.880810
H	3.827078	-2.884132	0.880810
H	3.417166	-4.354194	0.000000
H	1.339037	-3.283396	0.874078
H	1.339037	-3.283396	-0.874078
H	2.140097	-0.911420	0.874802
H	2.140097	-0.911420	-0.874802
H	-0.335676	-1.338585	0.876781
H	-0.335676	-1.338585	-0.876781
H	0.452021	1.041556	-0.880361
H	0.452021	1.041556	0.880361

Molecule# 0629

pentylbenzene

PointGroup: Cs

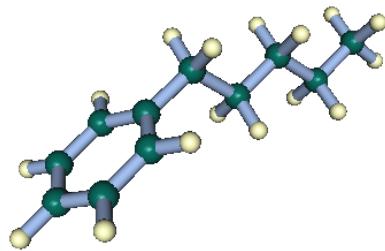
E= -428.978974171 au

ZPE= 0.241298 au

LUMO_eps= -0.01439 au

HOMO_eps= -0.24693 au

Dipole= 0.478 debye



27

C	0.900306	-3.825697	0.000000
C	0.901539	-3.124972	1.200332
C	0.901539	-3.124972	-1.200332
C	0.901539	-1.735317	1.197099
C	0.901539	-1.735317	-1.197099
C	0.899114	-1.017757	0.000000
C	-2.041142	4.699080	0.000000
C	0.860460	0.490669	0.000000
C	-2.015889	3.171462	0.000000
C	-0.566581	1.063132	0.000000
C	-0.600850	2.591122	0.000000
H	0.903787	-4.907472	0.000000
H	0.907522	-3.660707	2.140621
H	0.907522	-3.660707	-2.140621
H	0.909093	-1.198296	2.138067
H	0.909093	-1.198296	-2.138067
H	-1.536298	5.101628	-0.880619
H	-3.062669	5.081774	0.000000
H	-1.536298	5.101628	0.880619
H	1.394032	0.869083	0.875785
H	1.394032	0.869083	-0.875785
H	-2.557854	2.797729	0.873851
H	-2.557854	2.797729	-0.873851
H	-1.103777	0.683533	0.873971
H	-1.103777	0.683533	-0.873971
H	-0.058001	2.965583	0.874525
H	-0.058001	2.965583	-0.874525

Molecule# 0630

pentyne

PointGroup: Cs

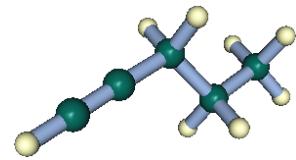
E= -195.361113984 au

ZPE= 0.112781 au

LUMO_eps= -0.01178 au

HOMO_eps= -0.27347 au

Dipole= 0.915 debye



13

C	-2.632692	0.270492	0.000000
C	-1.445615	0.445322	0.000000
C	2.298303	-0.462071	0.000000
C	0.000000	0.632435	0.000000
C	0.789039	-0.688491	0.000000
H	-3.683318	0.121999	0.000000
H	2.615695	0.098825	0.881392
H	2.836529	-1.410299	0.000000
H	2.615695	0.098825	-0.881392
H	0.283301	1.225765	-0.874581
H	0.283301	1.225765	0.874581
H	0.497294	-1.273503	-0.874226
H	0.497294	-1.273503	0.874226

Molecule# 0631

perfluorobutadiene

PointGroup: C2

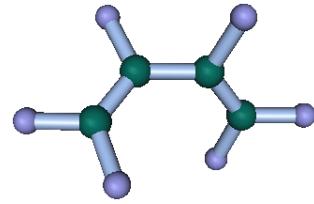
E= -751.685713694 au

ZPE= 0.038999 au

LUMO_eps= -0.05027 au

HOMO_eps= -0.27614 au

Dipole= 0.938 debye



10

C	-0.188443	1.576098	-0.366092
C	0.153555	0.706793	0.580006
C	-0.153555	-0.706793	0.580006
C	0.188443	-1.576098	-0.366092
F	0.153555	2.842567	-0.356772
F	-0.892260	1.266786	-1.433390
F	0.843111	1.168575	1.647552
F	-0.843111	-1.168575	1.647552
F	0.892260	-1.266786	-1.433390
F	-0.153555	-2.842567	-0.356772

Molecule# 0632

perfluorobutane

PointGroup: C1

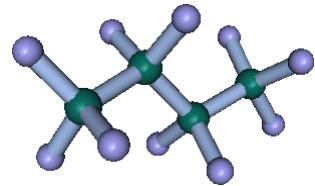
E= -1151.302559380 au

ZPE= 0.052939 au

LUMO_eps= -0.00714 au

HOMO_eps= -0.38325 au

Dipole= 0.036 debye



14

C	-0.588673	0.514586	-0.092762
C	0.588673	-0.514586	-0.092763
C	-2.009338	-0.118245	0.074227
C	2.009338	0.118245	0.074228
F	-0.415550	1.394344	0.915469
F	-0.572838	1.184057	-1.260942
F	0.415550	-1.394345	0.915467
F	0.572838	-1.184055	-1.260944
F	-2.925528	0.830845	-0.129852
F	2.925528	-0.830845	-0.129853
F	-2.197432	-1.096346	-0.814973
F	-2.171696	-0.609091	1.302656
F	2.197432	1.096347	-0.814971
F	2.171696	0.609089	1.302657

Molecule# 0633

perfluorooctane

PointGroup: C1

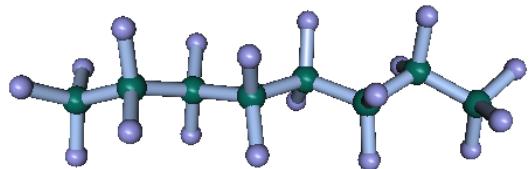
E= -2102.809569810 au

ZPE= 0.101040 au

LUMO_eps= -0.03753 au

HOMO_eps= -0.36261 au

Dipole= 0.089 debye



26

C	-0.643755	0.451811	-0.116063
C	0.643754	-0.451811	-0.116065
C	-1.971641	-0.359225	0.109674
C	1.971641	0.359224	0.109675
C	-3.260971	0.423128	-0.322117
C	3.260972	-0.423127	-0.322118
C	-4.593120	-0.161784	0.255224
C	4.593120	0.161783	0.255225
F	-0.717886	1.087551	-1.301534
F	-0.534691	1.367522	0.866508
F	0.717886	-1.087547	-1.301538
F	0.534691	-1.367525	0.866504
F	-2.067751	-0.666456	1.418445
F	-1.915832	-1.502658	-0.602171
F	2.067750	0.666452	1.418447
F	1.915832	1.502659	-0.602167
F	-3.354065	0.399093	-1.664116
F	-3.170091	1.704673	0.088792
F	3.170091	-1.704673	0.088788
F	3.354066	-0.399089	-1.664117
F	-5.619910	0.441189	-0.347993
F	-4.668993	-1.475221	0.024297
F	-4.683604	0.056486	1.566635
F	4.668993	1.475221	0.024300
F	5.619909	-0.441188	-0.347994
F	4.683603	-0.056489	1.566635

Molecule# 0634

perfluoropentane

PointGroup: C2

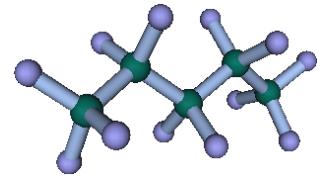
E= -1389.179271390 au

ZPE= 0.064971 au

LUMO_eps= -0.01844 au

HOMO_eps= -0.37511 au

Dipole= 0.103 debye



17

C	0.000000	0.000000	0.338951
C	-0.058312	1.310999	-0.518663
C	0.058312	-1.310999	-0.518663
C	0.291389	2.615577	0.272146
C	-0.291389	-2.615577	0.272146
F	1.094395	0.038571	1.125903
F	-1.094395	-0.038571	1.125903
F	0.809009	1.215438	-1.547143
F	-1.303708	1.452288	-1.008386
F	-0.809009	-1.215438	-1.547143
F	1.303708	-1.452288	-1.008386
F	0.000000	3.669670	-0.493082
F	0.000000	-3.669670	-0.493082
F	-0.424553	2.689340	1.397413
F	1.587918	2.657401	0.576655
F	0.424553	-2.689340	1.397413
F	-1.587918	-2.657401	0.576655

Molecule# 0635

perfluoropropane

PointGroup: C2v

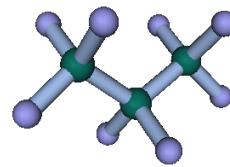
E= -913.425918596 au

ZPE= 0.040893 au

LUMO_eps= -0.00213 au

HOMO_eps= -0.39546 au

Dipole= 0.135 debye



11

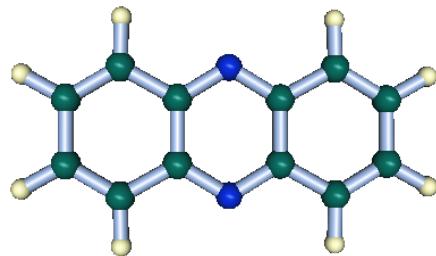
C	0.000000	0.000000	0.590836
C	0.000000	1.321706	-0.236848
C	0.000000	-1.321706	-0.236848
F	1.097195	0.000000	1.372804
F	-1.097195	0.000000	1.372804
F	0.000000	2.356688	0.605533
F	0.000000	-2.356688	0.605533
F	1.086235	1.396250	-1.008692
F	-1.086235	1.396250	-1.008692
F	-1.086235	-1.396250	-1.008692
F	1.086235	-1.396250	-1.008692

Molecule# 0636

phenazine

PointGroup: D2h

E= -571.802599718 au
ZPE= 0.169880 au
LUMO_eps= -0.10288 au
HOMO_eps= -0.23612 au
Dipole= 0.000 debye



22

C	0.000000	1.141350	0.720815
C	0.000000	1.141350	-0.720815
N	0.000000	0.000000	1.415067
C	0.000000	2.387462	1.410508
N	0.000000	0.000000	-1.415067
C	0.000000	2.387462	-1.410508
C	0.000000	-1.141350	0.720815
C	0.000000	3.557969	0.711879
C	0.000000	-1.141350	-0.720815
C	0.000000	3.557969	-0.711879
C	0.000000	-2.387462	1.410508
C	0.000000	-2.387462	-1.410508
C	0.000000	-3.557969	0.711879
C	0.000000	-3.557969	-0.711879
H	0.000000	2.364656	2.491337
H	0.000000	2.364656	-2.491337
H	0.000000	4.502732	1.238686
H	0.000000	4.502732	-1.238686
H	0.000000	-2.364656	2.491337
H	0.000000	-2.364656	-2.491337
H	0.000000	-4.502732	1.238686
H	0.000000	-4.502732	-1.238686

Molecule# 0637

phenol

PointGroup: Cs

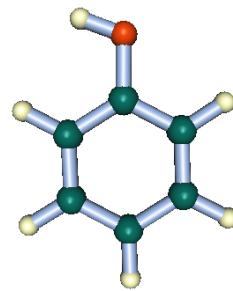
E= -307.590315378 au

ZPE= 0.104483 au

LUMO_eps= -0.02072 au

HOMO_eps= -0.23460 au

Dipole= 1.268 debye



13

C	0.021569	-1.850874	0.000000
C	-1.183942	-1.160029	0.000000
C	1.216077	-1.136120	0.000000
C	-1.200429	0.230252	0.000000
C	1.212740	0.251632	0.000000
C	0.000000	0.935940	0.000000
O	0.048212	2.303596	0.000000
H	0.031441	-2.931667	0.000000
H	-2.120454	-1.701426	0.000000
H	2.160924	-1.662963	0.000000
H	-2.142899	0.765406	0.000000
H	2.134448	0.816335	0.000000
H	-0.845249	2.660743	0.000000

Molecule# 0638

phenyl formate

PointGroup: C1

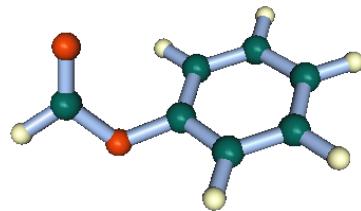
E= -420.961168929 au

ZPE= 0.114141 au

LUMO_eps= -0.03451 au

HOMO_eps= -0.26227 au

Dipole= 1.736 debye



15

C	2.487747	0.326580	0.218061
C	2.045807	-0.986436	0.330087
C	1.598711	1.325573	-0.163943
C	0.718272	-1.302587	0.064989
C	0.269988	1.021727	-0.434324
C	-0.152532	-0.293089	-0.311684
C	-2.512580	-0.121577	0.007190
O	-2.466293	0.684083	0.887913
O	-1.461326	-0.671192	-0.645444
H	3.520254	0.570857	0.425766
H	2.732232	-1.768633	0.623796
H	1.937995	2.348421	-0.253363
H	0.355162	-2.317509	0.142752
H	-0.426389	1.792073	-0.729422
H	-3.430787	-0.549489	-0.411541

Molecule# 0639

phenylacetylene

PointGroup: C2v

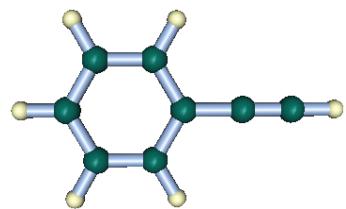
E= -308.509265759 au

ZPE= 0.109377 au

LUMO_eps= -0.04693 au

HOMO_eps= -0.24589 au

Dipole= 0.720 debye



14

C	0.000000	0.000000	0.592096
C	0.000000	0.000000	2.018067
C	0.000000	1.207433	-0.119647
C	0.000000	-1.207433	-0.119647
C	0.000000	1.203152	-1.506425
C	0.000000	-1.203152	-1.506425
C	0.000000	0.000000	-2.204188
C	0.000000	0.000000	3.219986
H	0.000000	0.000000	4.280998
H	0.000000	2.140945	0.425266
H	0.000000	-2.140945	0.425266
H	0.000000	2.141685	-2.044307
H	0.000000	-2.141685	-2.044307
H	0.000000	0.000000	-3.285824

Molecule# 0640

phenylalanine

PointGroup: C1

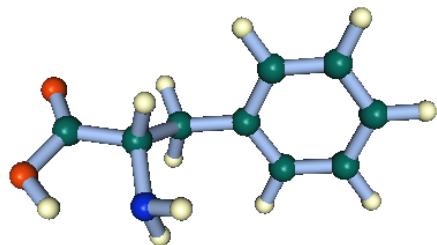
E= -555.014688221 au

ZPE= 0.189470 au

LUMO_eps= -0.03290 au

HOMO_eps= -0.25935 au

Dipole= 5.282 debye



23

N	-1.339042	1.450654	-0.784825
C	-1.389756	0.054525	-0.330039
C	-2.841838	-0.324033	0.031390
O	-3.133850	-1.336349	0.609477
O	-3.754709	0.560078	-0.391499
H	-3.240979	1.282550	-0.814313
C	-0.428785	-0.303489	0.819231
C	1.025254	-0.197841	0.432381
C	1.621881	-1.185950	-0.355385
C	2.953581	-1.088667	-0.737089
C	3.718469	0.001996	-0.335343
C	3.141002	0.988624	0.453392
C	1.805840	0.886727	0.832293
H	-1.147606	-0.573924	-1.190629
H	-0.639640	0.355030	1.665991
H	-0.667999	-1.315484	1.143917
H	1.040607	-2.046855	-0.662923
H	3.397501	-1.868361	-1.341580
H	4.756749	0.076482	-0.628637
H	3.729078	1.836137	0.779435
H	1.370663	1.654866	1.459995
H	-1.109294	2.078090	-0.023130
H	-0.641205	1.585711	-1.503173

Molecule# 0641

phenylhydrazine

PointGroup: C1

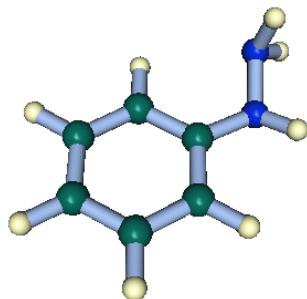
E= -343.053457374 au

ZPE= 0.134087 au

LUMO_eps= -0.02219 au

HOMO_eps= -0.20787 au

Dipole= 2.618 debye



16

C	-2.302046	0.304648	0.048681
C	-1.844743	-1.009740	0.055890
C	-1.374107	1.337593	-0.016270
C	-0.487064	-1.284841	-0.001073
C	-0.010704	1.076510	-0.076066
C	0.447055	-0.243648	-0.073095
N	2.746630	0.431456	0.133713
N	1.804819	-0.563693	-0.195804
H	-3.360760	0.517610	0.095676
H	-2.549315	-1.829261	0.110144
H	-1.711935	2.365825	-0.020205
H	-0.143401	-2.312664	0.003216
H	0.705591	1.881657	-0.126272
H	3.542157	0.355481	-0.484296
H	3.057771	0.357060	1.097408
H	2.029412	-1.493179	0.130559

Molecule# 0642

phenylsulfonylbenzene

PointGroup: C2

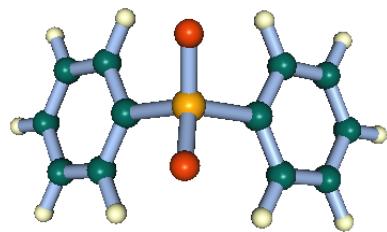
E= -1012.152893150 au

ZPE= 0.191328 au

LUMO_eps= -0.06667 au

HOMO_eps= -0.27352 au

Dipole= 5.359 debye



25

O	1.182952	0.463928	2.029051
S	0.000000	0.000000	1.311979
O	-1.182952	-0.463928	2.029051
C	-0.520392	1.327106	0.212950
C	0.409097	2.277935	-0.192069
C	0.000000	3.304743	-1.033775
C	-1.322848	3.373603	-1.458638
C	-2.245249	2.421077	-1.037808
C	-1.847361	1.389895	-0.196106
C	0.520392	-1.327106	0.212950
C	-0.409097	-2.277935	-0.192069
C	0.000000	-3.304743	-1.033775
C	1.322848	-3.373603	-1.458638
C	2.245249	-2.421077	-1.037808
C	1.847361	-1.389895	-0.196106
H	1.426580	2.222201	0.166269
H	0.711915	4.054300	-1.350886
H	-1.637459	4.175977	-2.112088
H	-3.276080	2.484727	-1.358041
H	-2.555114	0.655284	0.159175
H	-1.426580	-2.222201	0.166269
H	-0.711915	-4.054300	-1.350886
H	1.637459	-4.175977	-2.112088
H	3.276080	-2.484727	-1.358041
H	2.555114	-0.655284	0.159175

Molecule# 0643

phosgene

PointGroup: C2v

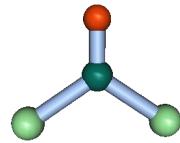
E= -1033.841345920 au

ZPE= 0.010353 au

LUMO_eps= -0.07524 au

HOMO_eps= -0.33247 au

Dipole= 1.202 debye



4

O 0.000000 0.000000 1.676657

C 0.000000 0.000000 0.503213

Cl 0.000000 1.457697 -0.483310

Cl 0.000000 -1.457697 -0.483310

Molecule# 0644

phthalazine

PointGroup: C2v

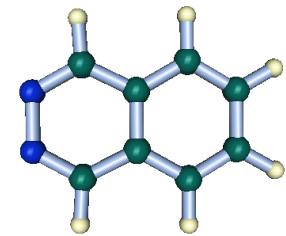
E= -418.080398341 au

ZPE= 0.123005 au

LUMO_eps= -0.07738 au

HOMO_eps= -0.24523 au

Dipole= 5.254 debye

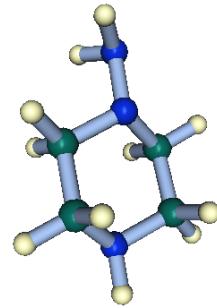


16

C	0.000000	0.705485	-0.012772
C	0.000000	1.324526	-1.289733
C	0.000000	-0.705485	-0.012772
N	0.000000	0.681794	-2.426927
C	0.000000	-1.324526	-1.289733
N	0.000000	-0.681794	-2.426927
C	0.000000	1.404939	1.211306
C	0.000000	0.705423	2.392790
C	0.000000	-0.705423	2.392790
C	0.000000	-1.404939	1.211306
H	0.000000	-2.407381	-1.364362
H	0.000000	2.407381	-1.364362
H	0.000000	-1.235415	3.335672
H	0.000000	1.235415	3.335672
H	0.000000	-2.487234	1.207629
H	0.000000	2.487234	1.207629

Molecule# 0645
piperazin-1-amine
PointGroup: C1

E= -323.381262469 au
ZPE= 0.163693 au
LUMO_eps= -0.01282 au
HOMO_eps= -0.22959 au
Dipole= 1.437 debye



18

C	1.133555	1.224172	-0.194407
C	1.181841	-1.187001	-0.202712
C	-0.343283	1.191042	0.180257
C	-0.292244	-1.224360	0.177403
N	1.789141	0.030617	0.328985
N	-0.969018	-0.030842	-0.322800
N	-2.357848	-0.114512	-0.018199
H	1.212514	1.304089	-1.289776
H	1.599464	2.108612	0.242171
H	1.688428	-2.052619	0.225623
H	1.262640	-1.252758	-1.298708
H	-0.442955	1.259930	1.277609
H	-0.857002	2.046876	-0.260956
H	-0.780392	-2.092624	-0.261687
H	-0.379815	-1.300473	1.273848
H	2.781405	0.052276	0.136985
H	-2.540805	0.215439	0.932435
H	-2.858621	0.491294	-0.656692

Molecule# 0646

piperazine

PointGroup: Ci

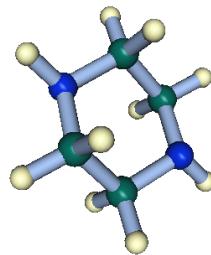
E= -268.036652479 au

ZPE= 0.147400 au

LUMO_eps= -0.01205 au

HOMO_eps= -0.22559 au

Dipole= 0.000 debye



16

C	-0.834927	0.310226	-1.120699
C	-0.863686	-1.052974	-0.441012
C	0.863686	1.052974	0.441012
C	0.834927	-0.310226	1.120699
N	-0.450116	1.325039	-0.140555
N	0.450116	-1.325039	0.140555
H	-0.136260	0.260567	-1.970344
H	-1.825522	0.552488	-1.508068
H	-1.664933	-1.048703	0.314250
H	-1.091286	-1.828069	-1.174163
H	1.091286	1.828069	1.174163
H	1.664933	1.048703	-0.314250
H	1.825522	-0.552488	1.508068
H	0.136260	-0.260567	1.970344
H	-0.474735	2.247690	-0.552801
H	0.474735	-2.247690	0.552801

Molecule# 0647

piperidine

PointGroup: Cs

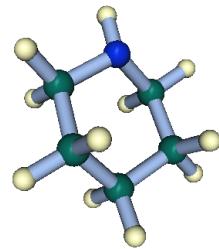
E= -252.002149816 au

ZPE= 0.158396 au

LUMO_eps= -0.01181 au

HOMO_eps= -0.22609 au

Dipole= 0.826 debye



17

C	0.627734	1.332116	0.000000
C	-0.015015	0.749126	1.262844
C	-0.015015	0.749126	-1.262844
C	-0.015015	-0.777813	1.216280
C	-0.015015	-0.777813	-1.216280
N	-0.683238	-1.236622	0.000000
H	0.550093	2.421274	0.000000
H	1.697146	1.095686	0.000000
H	0.514966	1.090753	2.154644
H	-1.048069	1.096853	1.343790
H	-1.048069	1.096853	-1.343790
H	0.514966	1.090753	-2.154644
H	1.028243	-1.134962	1.275130
H	-0.545722	-1.185262	2.078063
H	-0.545722	-1.185262	-2.078063
H	1.028243	-1.134962	-1.275130
H	-0.769444	-2.243821	0.000000

Molecule# 0648

proline

PointGroup: C1

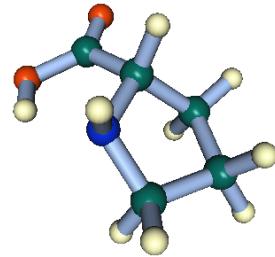
E= -401.319745934 au

ZPE= 0.144725 au

LUMO_eps= -0.02923 au

HOMO_eps= -0.25931 au

Dipole= 5.790 debye



17

N	0.636602	-1.058123	0.492208
C	-0.121601	0.212497	0.582235
C	-1.541645	0.060070	0.027611
O	-2.347827	0.951873	0.041962
O	-1.796324	-1.151121	-0.486153
C	0.698716	1.255847	-0.214727
C	2.124667	0.698806	-0.171428
C	1.890352	-0.811433	-0.258644
H	-0.226886	0.531260	1.620367
H	0.341413	1.305448	-1.244399
H	0.600663	2.251274	0.210253
H	2.751505	1.078563	-0.977576
H	2.605897	0.951778	0.776149
H	1.755051	-1.114676	-1.299508
H	2.701458	-1.409225	0.154057
H	0.836365	-1.421455	1.412453
H	-0.971410	-1.666847	-0.334004

Molecule# 0649

prop-1-ynylbenzene

PointGroup: C1

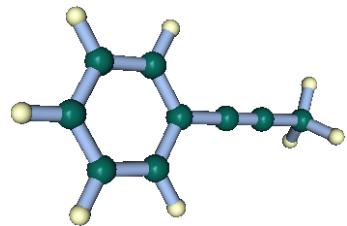
E= -347.848527965 au

ZPE= 0.137601 au

LUMO_eps= -0.03698 au

HOMO_eps= -0.23254 au

Dipole= 0.528 debye



17

C	-1.391545	0.000201	-0.000002
C	-2.595600	0.000392	-0.000004
C	2.836362	-0.000147	0.000002
C	2.137248	1.202242	0.000001
C	2.137077	-1.202403	0.000001
C	0.750328	1.206082	-0.000001
C	0.750116	-1.206050	-0.000001
C	0.034638	0.000067	-0.000002
C	-4.050167	-0.000024	0.000003
H	3.918041	-0.000216	0.000003
H	2.674572	2.141336	0.000001
H	2.674269	-2.141571	0.000002
H	0.206696	2.140516	-0.000001
H	0.206275	-2.140361	-0.000001
H	-4.443661	-0.509666	0.881896
H	-4.443259	1.018099	-0.000365
H	-4.443669	-0.510309	-0.881514

Molecule# 0650

prop-2-enenitrileoxide

PointGroup: C1

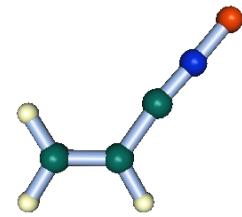
E= -246.081184497 au

ZPE= 0.054748 au

LUMO_eps= -0.06700 au

HOMO_eps= -0.25694 au

Dipole= 3.859 debye



8

O	-2.423172	-0.167625	0.000000
N	-1.229268	0.011793	-0.000004
C	-0.078874	0.155417	-0.000002
C	1.300610	0.480348	0.000003
C	2.286856	-0.419406	0.000002
H	1.529592	1.540379	0.000009
H	2.091078	-1.482044	-0.000004
H	3.318032	-0.098033	0.000007

Molecule# 0651

prop-2-yne-1,1-diol

PointGroup: C1

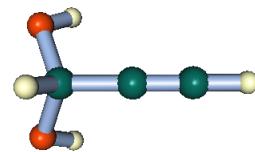
E= -267.200280041 au

ZPE= 0.065475 au

LUMO_eps= -0.02533 au

HOMO_eps= -0.29650 au

Dipole= 2.689 debye



9

O	-1.069401	-1.177081	-0.114653
O	-1.069399	1.177108	-0.114381
C	-0.471048	-0.000047	0.382369
C	0.979054	-0.000017	0.143241
C	2.155246	0.000008	-0.089537
H	-0.691133	-1.390931	-0.974818
H	-0.691105	1.391185	-0.974478
H	-0.685912	-0.000169	1.449763
H	3.199039	0.000030	-0.284622

Molecule# 0652

prop-2-ynethioic acid

PointGroup: C1

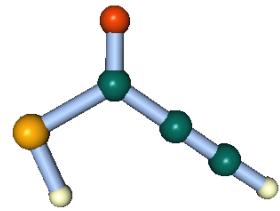
E= -588.966008441 au

ZPE= 0.037246 au

LUMO_eps= -0.08721 au

HOMO_eps= -0.29110 au

Dipole= 3.632 debye



7

S -1.415690 -0.626525 -0.000006

O -0.221616 1.707573 0.000000

C -0.028547 0.519090 0.000000

C 1.281666 -0.084082 0.000004

C 2.374298 -0.580157 0.000009

H -0.687542 -1.757741 -0.000004

H 3.347002 -1.007548 0.000013

Molecule# 0653

prop-2-ynoyl bromide

PointGroup: C1

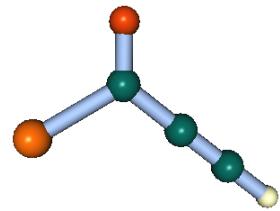
E= -2764.367176230 au

ZPE= 0.028047 au

LUMO_eps= -0.10512 au

HOMO_eps= -0.30091 au

Dipole= 3.029 debye



6

Br	1.106115	-0.290476	-0.000002
O	-0.655686	1.863976	0.000027
C	-0.618098	0.678982	-0.000012
C	-1.721581	-0.223075	-0.000091
C	-2.657273	-0.973771	0.000044
H	-3.486825	-1.637971	0.000197

Molecule# 0654

prop-2-ynoyl chloride

PointGroup: C1

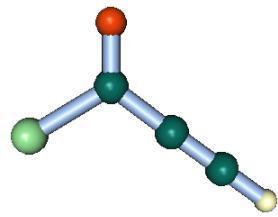
E= -650.373111087 au

ZPE= 0.028599 au

LUMO_eps= -0.10276 au

HOMO_eps= -0.31607 au

Dipole= 3.034 debye



6

Cl -1.342896 -0.692618 -0.000002

O -0.259567 1.696079 0.000019

C -0.024306 0.532850 -0.000069

C 1.265435 -0.081591 -0.000088

C 2.355970 -0.580206 0.000092

H 3.323175 -1.020441 0.000275

Molecule# 0655

prop-2-ynoyl fluoride

PointGroup: C1

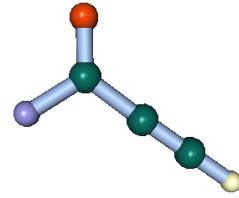
E= -290.026751909 au

ZPE= 0.030292 au

LUMO_eps= -0.09228 au

HOMO_eps= -0.32752 au

Dipole= 3.207 debye



6

F 1.053714 1.101216 0.000007

O 1.153455 -1.111284 0.000013

C 0.490920 -0.130271 -0.000038

C -0.939398 -0.040028 -0.000063

C -2.136840 -0.004245 0.000046

H -3.199160 0.026597 0.000161

Molecule# 0656

propa-1,2-dien-1-ol

PointGroup: Cs

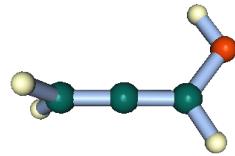
E= -191.955508424 au

ZPE= 0.060784 au

LUMO_eps= -0.03070 au

HOMO_eps= -0.23998 au

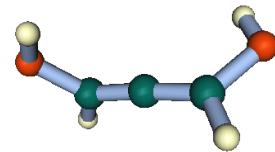
Dipole= 1.264 debye



8

C	0.656988	-0.482689	0.000000
C	0.000000	0.643879	0.000000
C	-0.646073	1.774994	0.000000
O	0.112787	-1.745853	0.000000
H	1.737890	-0.517886	0.000000
H	-0.928536	2.272014	0.922836
H	-0.928536	2.272014	-0.922836
H	-0.848607	-1.676418	0.000000

Molecule# 0657
propa-1,2-diene-1,3-diol
PointGroup: C2
E= -267.210984455 au
ZPE= 0.066552 au
LUMO_eps= -0.02775 au
HOMO_eps= -0.25113 au
Dipole= 0.558 debye



9
C 0.000000 0.000000 0.314636
C 0.000000 1.305048 0.357543
C 0.000000 -1.305048 0.357543
O 0.776928 2.146963 -0.393553
O -0.776928 -2.146963 -0.393553
H -0.646254 1.874974 1.014469
H 0.646254 -1.874974 1.014469
H 1.357245 1.618777 -0.955207
H -1.357245 -1.618777 -0.955207

Molecule# 0658

propanal

PointGroup: Cs

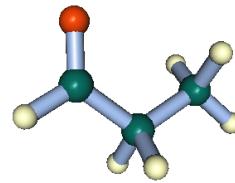
E= -193.225195869 au

ZPE= 0.083900 au

LUMO_eps= -0.03645 au

HOMO_eps= -0.26610 au

Dipole= 2.788 debye



10

C	0.996293	-0.222905	0.000000
C	-1.458518	0.470962	0.000000
C	0.000000	0.905538	0.000000
O	0.716194	-1.394736	0.000000
H	2.059410	0.097311	0.000000
H	-1.685732	-0.133233	0.877361
H	-1.685732	-0.133233	-0.877361
H	-2.117948	1.338361	0.000000
H	0.236898	1.533556	-0.867218
H	0.236898	1.533556	0.867218

Molecule# 0659

propanamide

PointGroup: C1

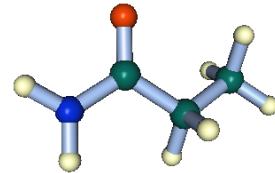
E= -248.635832668 au

ZPE= 0.101693 au

LUMO_eps= -0.02226 au

HOMO_eps= -0.26169 au

Dipole= 3.726 debye



12

H	-2.592675	-0.045641	-0.145798
H	-1.757839	-1.561246	-0.123394
N	-1.728931	-0.558727	-0.107702
O	-0.540022	1.352356	0.063774
C	-0.562261	0.136158	0.032402
H	0.704554	-1.095974	1.200102
H	0.596109	-1.605295	-0.469148
C	0.688051	-0.724248	0.170792
H	2.841756	-0.595111	0.039596
H	1.993138	0.372041	-1.170851
H	2.052216	0.921934	0.496008
C	1.971783	0.038345	-0.133659

Molecule# 0660

propane-1,2,3-triamine

PointGroup: C1

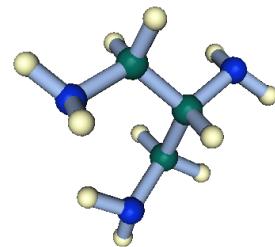
E= -285.303770602 au

ZPE= 0.156187 au

LUMO_eps= -0.01376 au

HOMO_eps= -0.23124 au

Dipole= 1.188 debye



17

C	-0.013757	-1.316234	0.197329
C	0.083647	1.251840	0.325748
C	0.646705	-0.029651	-0.312805
N	-1.467041	-1.338650	-0.018105
N	-1.231706	1.613642	-0.202973
N	2.093096	-0.186523	-0.116420
H	0.508805	-2.160172	-0.265080
H	0.158200	-1.387214	1.276005
H	0.104816	1.127108	1.421032
H	0.771050	2.067989	0.090551
H	0.474190	0.042447	-1.391124
H	-1.874954	-2.159342	0.411086
H	-1.678612	-1.389398	-1.008104
H	-1.536048	2.505919	0.164381
H	-1.910296	0.908416	0.058611
H	2.324036	-0.198746	0.871269
H	2.598800	0.587978	-0.527778

Molecule# 0661

propane-1,2,3-trithiol

PointGroup: C1

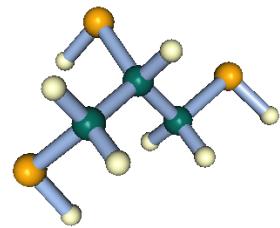
E= -1313.853105320 au

ZPE= 0.101986 au

LUMO_eps= -0.03044 au

HOMO_eps= -0.24365 au

Dipole= 2.871 debye



14

C	0.834198	-0.936571	-0.030495
C	-1.402371	-0.269951	0.991854
C	0.042139	0.149384	0.691781
S	2.619734	-0.495778	-0.173755
S	-2.501238	-0.563857	-0.452043
S	0.149502	1.790968	-0.137745
H	0.429951	-1.103433	-1.026573
H	0.765825	-1.867304	0.532760
H	-1.408866	-1.167657	1.610121
H	-1.897031	0.521267	1.550558
H	0.520127	0.338062	1.655473
H	3.083147	-1.750169	-0.026735
H	-2.037822	-1.781895	-0.783799
H	-0.587096	1.452627	-1.213971

Molecule# 0662

propane

PointGroup: C2v

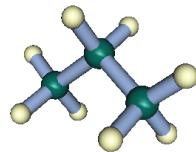
E= -119.192959509 au

ZPE= 0.102911 au

LUMO_eps= -0.00910 au

HOMO_eps= -0.33002 au

Dipole= 0.094 debye



11

C	0.000000	0.000000	0.584601
C	0.000000	1.273888	-0.259060
C	0.000000	-1.273888	-0.259060
H	0.880629	1.318580	-0.903482
H	-0.880629	1.318580	-0.903482
H	-0.880629	-1.318580	-0.903482
H	0.000000	2.168536	0.365318
H	0.880629	-1.318580	-0.903482
H	0.000000	-2.168536	0.365318
H	0.873365	0.000000	1.242204
H	-0.873365	0.000000	1.242204

Molecule# 0663

propanedial

PointGroup: C1

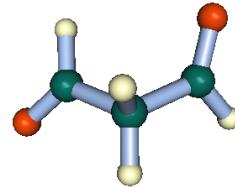
E= -267.250818545 au

ZPE= 0.065011 au

LUMO_eps= -0.07636 au

HOMO_eps= -0.27716 au

Dipole= 1.910 debye



9

C	1.070710	-0.368234	0.146305
C	-1.282848	0.323971	-0.320122
C	0.020532	0.716170	0.346563
O	2.179848	-0.153436	-0.260150
O	-1.960910	-0.597247	0.054811
H	0.734564	-1.388064	0.407927
H	-1.572330	0.919367	-1.206311
H	0.403972	1.666523	-0.018102
H	-0.168069	0.776197	1.422723

Molecule# 0664

propanenitrile

PointGroup: Cs

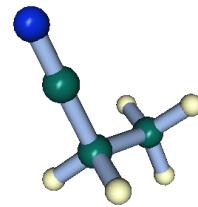
E= -172.136638432 au

ZPE= 0.074077 au

LUMO_eps= -0.02333 au

HOMO_eps= -0.33452 au

Dipole= 4.154 debye



9

C	0.771682	-0.432622	0.000000
C	-1.515437	0.563249	0.000000
C	0.000000	0.807103	0.000000
N	1.364991	-1.417770	0.000000
H	-1.819793	0.002200	0.881973
H	-2.041098	1.517131	0.000000
H	-1.819793	0.002200	-0.881973
H	0.294138	1.388238	0.876058
H	0.294138	1.388238	-0.876058

Molecule# 0665

propanoic acid

PointGroup: C1

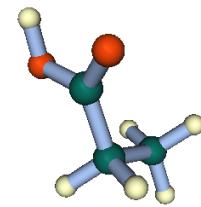
E= -268.512752614 au

ZPE= 0.090360 au

LUMO_eps= -0.01997 au

HOMO_eps= -0.28754 au

Dipole= 1.879 debye



11

H	-1.766142	-0.526208	-1.297472
C	-1.849296	0.110726	-0.416946
C	-0.795460	-0.266086	0.634887
C	0.604920	-0.137267	0.093049
O	1.306287	-1.044919	-0.274495
O	1.008287	1.158088	0.032116
H	-2.849620	-0.014338	-0.003869
H	-1.738498	1.147718	-0.730793
H	-0.895780	0.381920	1.506215
H	1.897322	1.160106	-0.352283
H	-0.924854	-1.298789	0.951287

Molecule# 0666

propargylamine

PointGroup: C1

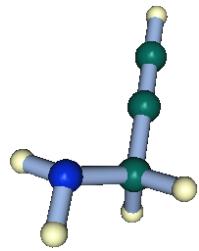
E= -172.069968092 au

ZPE= 0.073511 au

LUMO_eps= -0.01939 au

HOMO_eps= -0.25568 au

Dipole= 1.548 debye



9

N	-1.521190	-0.514806	-0.120022
C	-0.579874	0.602125	0.038950
C	0.805281	0.144140	-0.003594
C	1.943561	-0.232193	-0.014649
H	-1.375309	-1.207070	0.604410
H	-2.473718	-0.181419	-0.036708
H	-0.745639	1.300834	-0.784742
H	-0.721665	1.172303	0.967186
H	2.950856	-0.565445	-0.034238

Molecule# 0667

propenalol

PointGroup: Cs

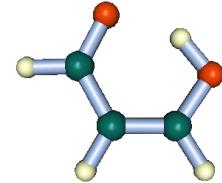
E= -267.264780753 au

ZPE= 0.067581 au

LUMO_eps= -0.07783 au

HOMO_eps= -0.26928 au

Dipole= 2.718 debye



9

C	0.000000	1.096648	0.000000
C	1.231022	0.361916	0.000000
C	-1.183818	0.424873	0.000000
O	1.286331	-0.874778	0.000000
O	-1.283038	-0.888616	0.000000
H	-0.346283	-1.239665	0.000000
H	0.009428	2.175177	0.000000
H	2.168876	0.938076	0.000000
H	-2.141591	0.932940	0.000000

Molecule# 0668

propene

PointGroup: Cs

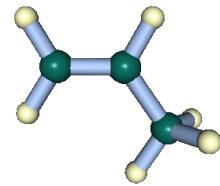
E= -117.958009477 au

ZPE= 0.079395 au

LUMO_eps= -0.00753 au

HOMO_eps= -0.26343 au

Dipole= 0.426 debye



9

C	1.288205	0.152169	0.000000
C	0.000000	0.471192	0.000000
C	-1.134493	-0.504884	0.000000
H	2.059749	0.910251	0.000000
H	1.617497	-0.880355	0.000000
H	-0.276862	1.521647	0.000000
H	-1.772629	-0.363826	0.876178
H	-0.777400	-1.534749	0.000000
H	-1.772629	-0.363826	-0.876178

Molecule# 0669

propiolic acid

PointGroup: C1

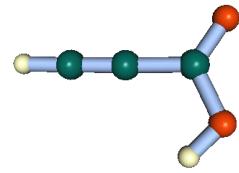
E= -266.007086192 au

ZPE= 0.042911 au

LUMO_eps= -0.07220 au

HOMO_eps= -0.30742 au

Dipole= 4.396 debye



7

O -1.140757 1.067901 -0.000039

O -1.122638 -1.159311 -0.000036

C -0.509953 -0.131001 -0.000019

C 0.939527 -0.050347 0.000023

C 2.137587 0.000371 0.000080

H -0.495557 1.786680 -0.000024

H 3.199749 0.030461 0.000128

Molecule# 0670
propiolonitrile
PointGroup: C(infinity)v
E= -169.639729406 au
ZPE= 0.027084 au
LUMO_eps= -0.06963 au
HOMO_eps= -0.32379 au
Dipole= 3.887 debye



5
N 0.000000 0.000000 1.892411
C 0.000000 0.000000 0.737350
C 0.000000 0.000000 -0.631058
C 0.000000 0.000000 -1.831727
H 0.000000 0.000000 -2.894266

Molecule# 0671

propyl butanoate

PointGroup: Cs

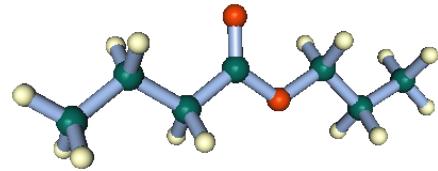
E= -425.817186146 au

ZPE= 0.202741 au

LUMO_eps= -0.01332 au

HOMO_eps= -0.27926 au

Dipole= 1.932 debye



23

C	0.000000	0.612118	0.000000
C	3.008130	3.090722	0.000000
C	-2.513916	-3.581102	0.000000
C	1.428318	1.107953	0.000000
C	1.552590	2.627842	0.000000
C	-1.172950	-2.848444	0.000000
C	-1.353001	-1.343669	0.000000
O	-0.985991	1.306773	0.000000
O	-0.041603	-0.736721	0.000000
H	3.073746	4.179115	0.000000
H	3.541696	2.727258	0.880860
H	3.541696	2.727258	-0.880860
H	-3.106341	-3.328029	-0.881190
H	-2.366530	-4.660890	0.000000
H	-3.106341	-3.328029	0.881190
H	1.929119	0.673098	0.869456
H	1.929119	0.673098	-0.869456
H	1.031923	3.030231	-0.870409
H	1.031923	3.030231	0.870409
H	-0.587970	-3.136322	-0.876168
H	-0.587970	-3.136322	0.876168
H	-1.899180	-1.001821	-0.880481
H	-1.899180	-1.001821	0.880481

Molecule# 0672

propyl nitrite

PointGroup: C1

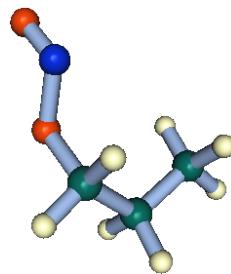
E= -323.770511834 au

ZPE= 0.104716 au

LUMO_eps= -0.08687 au

HOMO_eps= -0.28318 au

Dipole= 2.723 debye



13

H	0.523976	-2.089870	0.151478
N	-1.558037	0.145643	0.423258
O	-2.483813	0.541713	-0.169766
O	-0.642907	-0.522944	-0.431654
C	1.780908	-0.362548	-0.207690
H	1.873022	-0.557573	-1.278447
H	2.615550	-0.879811	0.273817
C	0.501420	-1.009602	0.298749
H	0.339389	-0.803022	1.358537
H	2.807723	1.545267	-0.303725
H	1.808716	1.348492	1.134869
H	1.057381	1.676612	-0.426643
C	1.866715	1.137191	0.065387

Molecule# 0673

propyl propanoate

PointGroup: Cs

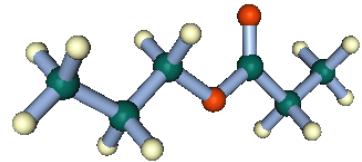
E= -386.489307610 au

ZPE= 0.174329 au

LUMO_eps= -0.01340 au

HOMO_eps= -0.27988 au

Dipole= 2.046 debye



20

C	-1.003940	-0.403757	0.000000
C	-3.525526	-0.680888	0.000000
C	3.764809	0.667909	0.000000
C	-2.349682	0.286562	0.000000
C	2.310162	1.136229	0.000000
C	1.344509	-0.032085	0.000000
O	-0.826705	-1.596688	0.000000
O	0.000000	0.497494	0.000000
H	-3.504242	-1.325262	0.877722
H	-4.466982	-0.131692	0.000000
H	-3.504242	-1.325262	-0.877722
H	3.988516	0.063792	-0.881154
H	4.446920	1.517824	0.000000
H	3.988516	0.063792	0.881154
H	-2.378363	0.948115	0.869070
H	-2.378363	0.948115	-0.869070
H	2.115703	1.758242	-0.876284
H	2.115703	1.758242	0.876284
H	1.474239	-0.663085	-0.880525
H	1.474239	-0.663085	0.880525

Molecule# 0674

propylbenzene

PointGroup: Cs

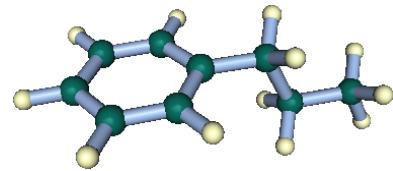
E= -350.322868362 au

ZPE= 0.184607 au

LUMO_eps= -0.01464 au

HOMO_eps= -0.24753 au

Dipole= 0.438 debye



21

C	0.386271	-2.839243	0.000000
C	0.387351	-2.138596	1.200339
C	0.387351	-2.138596	-1.200339
C	0.387351	-0.748944	1.197148
C	0.387351	-0.748944	-1.197148
C	0.385210	-0.031430	0.000000
C	-1.108485	3.575531	0.000000
C	0.345445	1.476802	0.000000
C	-1.082048	2.048572	0.000000
H	0.389739	-3.921015	0.000000
H	0.393022	-2.674365	2.140600
H	0.393022	-2.674365	-2.140600
H	0.394621	-0.211935	2.138121
H	0.394621	-0.211935	-2.138121
H	-0.604834	3.979341	0.880742
H	-0.604834	3.979341	-0.880742
H	-2.131197	3.954700	0.000000
H	0.878157	1.856658	0.875883
H	0.878157	1.856658	-0.875883
H	-1.617623	1.668007	-0.873416
H	-1.617623	1.668007	0.873416

Molecule# 0675

propylcyclopentane

PointGroup: C1

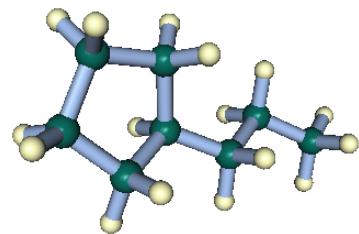
E= -314.615219891 au

ZPE= 0.224589 au

LUMO_eps= -0.01059 au

HOMO_eps= -0.30624 au

Dipole= 0.107 debye



24

C	-2.668057	-0.516202	-0.151817
C	-2.379219	0.990207	0.083732
C	-1.340914	-1.229360	0.139892
C	-0.838544	1.117468	0.194491
C	-0.268079	-0.224742	-0.304017
C	3.632805	-0.000756	0.134440
C	1.143001	-0.554336	0.179922
C	2.231894	0.390324	-0.333620
H	-3.488035	-0.885577	0.464020
H	-2.953947	-0.684716	-1.191912
H	-2.769755	1.593120	-0.736241
H	-2.864319	1.350360	0.991058
H	-1.236812	-1.414843	1.213997
H	-1.254830	-2.193162	-0.364168
H	-0.452275	1.972210	-0.360265
H	-0.546339	1.259696	1.238803
H	-0.259603	-0.208411	-1.401207
H	3.700615	0.007006	1.224348
H	3.895190	-1.005453	-0.203653
H	4.388824	0.686078	-0.248814
H	1.393620	-1.576741	-0.122604
H	1.150697	-0.552656	1.276131
H	2.014697	1.411417	-0.009971
H	2.204946	0.406052	-1.427659

Molecule# 0676

propylene glycol

PointGroup: C1

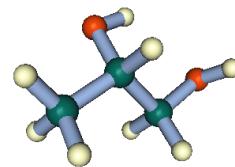
E= -269.690199032 au

ZPE= 0.112909 au

LUMO_eps= -0.02136 au

HOMO_eps= -0.27478 au

Dipole= 2.387 debye



13

O	-0.463972	1.384052	-0.155574
H	0.450340	1.692749	-0.148928
O	1.955994	-0.044939	0.007682
H	2.204193	-0.174878	0.928152
C	0.719569	-0.720388	-0.243068
H	0.626152	-0.767914	-1.328484
H	0.743413	-1.741843	0.148870
C	-0.461734	0.047680	0.337446
H	-0.352342	0.067485	1.432972
C	-1.793602	-0.587521	-0.016562
H	-1.917072	-0.637100	-1.099209
H	-1.865467	-1.596382	0.392217
H	-2.610789	0.006348	0.390648

Molecule# 0677

propylene oxide

PointGroup: C1

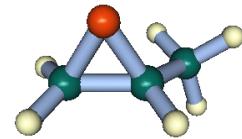
E= -193.188399647 au

ZPE= 0.085153 au

LUMO_eps= -0.00912 au

HOMO_eps= -0.27778 au

Dipole= 2.010 debye



10

O	0.828981	-0.789180	-0.238022
C	-1.508266	0.097281	-0.148770
H	-1.418953	0.320203	-1.211647
H	-2.074015	-0.829198	-0.038726
H	-2.076905	0.897311	0.329487
C	-0.152980	-0.033489	0.484726
H	-0.154020	-0.247472	1.550696
C	1.040125	0.616650	-0.061363
H	0.954099	1.210204	-0.965902
H	1.864673	0.879739	0.592713

Molecule# 0678

propyne

PointGroup: C3

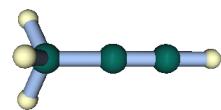
E= -116.704908501 au

ZPE= 0.055500 au

LUMO_eps= -0.01092 au

HOMO_eps= -0.27631 au

Dipole= 0.836 debye



7

C 0.000000 0.000000 1.417677

C 0.000000 0.000000 0.218758

C 0.000000 0.000000 -1.236142

H 0.000000 0.000000 2.478402

H 0.000000 1.018882 -1.626721

H 0.882377 -0.509441 -1.626721

H -0.882377 -0.509441 -1.626721

Molecule# 0679

propynyl propiolate

PointGroup: C1

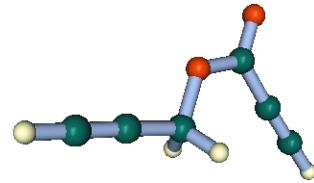
E= -381.482428675 au

ZPE= 0.079828 au

LUMO_eps= -0.07258 au

HOMO_eps= -0.29714 au

Dipole= 4.556 debye



12

O	0.219214	-0.692487	0.000002
O	-1.737049	-1.731787	0.000000
C	-1.131002	-0.695733	0.000000
C	-1.795334	0.594519	-0.000001
C	0.941706	0.562529	0.000002
C	2.364687	0.276671	0.000000
C	-2.399277	1.630600	-0.000004
C	3.545311	0.077874	0.000000
H	0.670540	1.140839	0.884807
H	0.670539	1.140839	-0.884803
H	-2.945518	2.542080	-0.000006
H	4.590571	-0.108328	-0.000001

Molecule# 0680

pyrazine-2-carboxylic acid

PointGroup: Cs

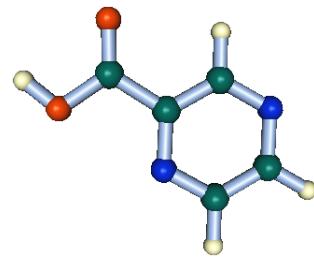
E= -453.060918936 au

ZPE= 0.091315 au

LUMO_eps= -0.09334 au

HOMO_eps= -0.27149 au

Dipole= 1.897 debye



13

C	0.136653	-2.474879	0.000000
C	-1.086113	-1.807655	0.000000
C	1.225830	-0.491905	0.000000
C	0.000000	0.176466	0.000000
C	-0.001608	1.673965	0.000000
N	1.295696	-1.820586	0.000000
N	-1.158456	-0.482162	0.000000
O	1.008915	2.334974	0.000000
O	-1.233924	2.207653	0.000000
H	0.179099	-3.557509	0.000000
H	-2.020706	-2.355520	0.000000
H	2.152353	0.065708	0.000000
H	-1.119931	3.169586	0.000000

Molecule# 0681

pyrazine

PointGroup: D2h

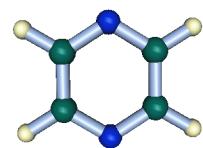
E= -264.413335734 au

ZPE= 0.076638 au

LUMO_eps= -0.06810 au

HOMO_eps= -0.26216 au

Dipole= 0.000 debye



10

C	0.000000	1.130554	0.695666
N	0.000000	0.000000	1.399240
C	0.000000	1.130554	-0.695666
C	0.000000	-1.130554	0.695666
N	0.000000	0.000000	-1.399240
C	0.000000	-1.130554	-0.695666
H	0.000000	-2.060631	-1.251616
H	0.000000	2.060631	-1.251616
H	0.000000	-2.060631	1.251616
H	0.000000	2.060631	1.251616

Molecule# 0682

pyrazino[2,3-b]pyrazine

PointGroup: D2h

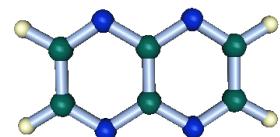
E= -450.188183096 au

ZPE= 0.099571 au

LUMO_eps= -0.11467 au

HOMO_eps= -0.25754 au

Dipole= 0.000 debye



14

C	0.000000	0.000000	0.712293
N	0.000000	1.158741	1.413954
N	0.000000	-1.158741	1.413954
C	0.000000	-2.261085	0.709672
C	0.000000	2.261085	0.709672
C	0.000000	-2.261085	-0.709672
N	0.000000	-1.158741	-1.413954
C	0.000000	0.000000	-0.712293
N	0.000000	1.158741	-1.413954
C	0.000000	2.261085	-0.709672
H	0.000000	3.201418	-1.250194
H	0.000000	-3.201418	1.250194
H	0.000000	3.201418	1.250194
H	0.000000	-3.201418	-1.250194

Molecule# 0683

pyridazine

PointGroup: C2v

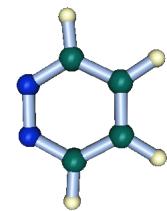
E= -264.384046854 au

ZPE= 0.076011 au

LUMO_eps= -0.06658 au

HOMO_eps= -0.24566 au

Dipole= 4.240 debye



10

C	0.000000	0.688857	1.174003
C	0.000000	-0.688857	1.174003
C	0.000000	-1.319429	-0.067431
C	0.000000	1.319429	-0.067431
H	0.000000	1.265199	2.088781
H	0.000000	-1.265199	2.088781
H	0.000000	-2.398824	-0.151216
H	0.000000	2.398824	-0.151216
N	0.000000	0.664263	-1.225286
N	0.000000	-0.664263	-1.225286

Molecule# 0684

pyridine-2,4-diol

PointGroup: Cs

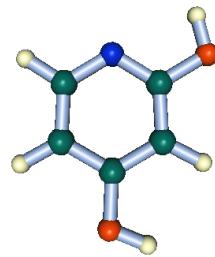
E= -398.903618153 au

ZPE= 0.097701 au

LUMO_eps= -0.03034 au

HOMO_eps= -0.25074 au

Dipole= 1.286 debye



13

C	-1.181319	-1.083539	0.000000
C	0.000000	1.010809	0.000000
C	0.048798	-1.709300	0.000000
C	-1.198215	0.314134	0.000000
C	1.176033	0.261682	0.000000
N	1.220451	-1.060717	0.000000
O	-2.406742	0.931648	0.000000
O	2.354509	0.926245	0.000000
H	-2.104345	-1.642803	0.000000
H	0.041008	2.091380	0.000000
H	0.107341	-2.790875	0.000000
H	-2.290414	1.887774	0.000000
H	3.049335	0.253679	0.000000

Molecule# 0685

pyridine-2,4-dithiol

PointGroup: Cs

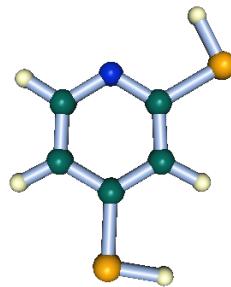
E= -1044.829386600 au

ZPE= 0.086425 au

LUMO_eps= -0.04790 au

HOMO_eps= -0.24209 au

Dipole= 1.321 debye



13

C	-1.178117	-1.374042	0.000000
C	0.000000	0.710936	0.000000
C	0.054673	-2.002123	0.000000
C	-1.206605	0.023456	0.000000
C	1.184142	-0.028878	0.000000
N	1.224295	-1.357495	0.000000
S	-2.784231	0.826539	0.000000
S	2.727524	0.857050	0.000000
H	-2.088791	-1.955558	0.000000
H	0.031617	1.791274	0.000000
H	0.111277	-3.084243	0.000000
H	-2.326622	2.090660	0.000000
H	3.485210	-0.253177	0.000000

Molecule# 0686

pyridine-3-carbaldehyde

PointGroup: Cs

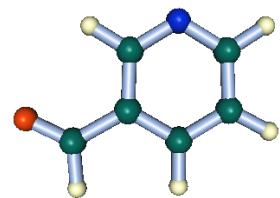
E= -361.741016493 au

ZPE= 0.097685 au

LUMO_eps= -0.09033 au

HOMO_eps= -0.26991 au

Dipole= 4.080 debye



13

C	1.610317	-1.209436	0.000000
C	1.329993	0.147978	0.000000
C	0.543915	-2.101297	0.000000
C	-0.997140	-0.422562	0.000000
C	0.000000	0.559527	0.000000
C	-0.339161	1.998058	0.000000
N	-0.739333	-1.725611	0.000000
O	-1.461675	2.444254	0.000000
H	2.627285	-1.575291	0.000000
H	2.126453	0.882601	0.000000
H	0.725761	-3.169850	0.000000
H	-2.037530	-0.121485	0.000000
H	0.539218	2.675668	0.000000

Molecule# 0687

pyridine-3-carbonitrile

PointGroup: Cs

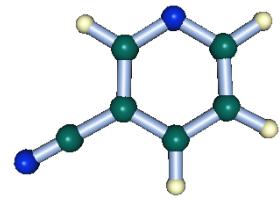
E= -340.648470985 au

ZPE= 0.087166 au

LUMO_eps= -0.08138 au

HOMO_eps= -0.29126 au

Dipole= 4.009 debye



12

C	-0.053693	2.019437	0.000000
C	1.204654	-1.469386	0.000000
C	1.220966	-0.085509	0.000000
C	-0.022972	-2.123259	0.000000
C	-1.181722	-0.159565	0.000000
C	0.000000	0.592498	0.000000
N	-0.100145	3.170672	0.000000
N	-1.195466	-1.486799	0.000000
H	2.124938	-2.035655	0.000000
H	2.150017	0.466484	0.000000
H	-0.067713	-3.205810	0.000000
H	-2.141358	0.342572	0.000000

Molecule# 0688

pyridine-4-carbaldehyde

PointGroup: Cs

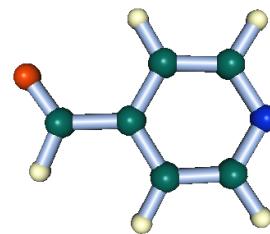
E= -361.740158310 au

ZPE= 0.097654 au

LUMO_eps= -0.09941 au

HOMO_eps= -0.27881 au

Dipole= 1.771 debye



13

C	1.317704	0.115038	0.000000
C	-1.022687	-0.385775	0.000000
C	1.558392	-1.254677	0.000000
C	-0.677231	-1.728443	0.000000
C	0.000000	0.561086	0.000000
C	-0.292864	2.016587	0.000000
N	0.586424	-2.165062	0.000000
O	-1.402646	2.490215	0.000000
H	2.141104	0.817975	0.000000
H	-2.055648	-0.068068	0.000000
H	2.573168	-1.634741	0.000000
H	-1.445137	-2.492744	0.000000
H	0.602825	2.668397	0.000000

Molecule# 0689

pyridine-4-carbonitrile

PointGroup: C2v

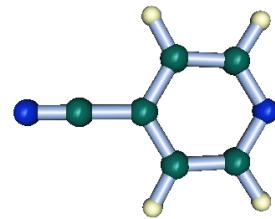
E= -340.647173582 au

ZPE= 0.087123 au

LUMO_eps= -0.08995 au

HOMO_eps= -0.29090 au

Dipole= 2.080 debye



12

C	0.000000	0.000000	2.029610
C	0.000000	1.200354	-0.112893
C	0.000000	-1.200354	-0.112893
C	0.000000	1.140883	-1.499716
C	0.000000	-1.140883	-1.499716
C	0.000000	0.000000	0.598544
N	0.000000	0.000000	3.181206
N	0.000000	0.000000	-2.189569
H	0.000000	2.149584	0.402220
H	0.000000	-2.149584	0.402220
H	0.000000	2.054587	-2.081755
H	0.000000	-2.054587	-2.081755

Molecule# 0690

pyridine

PointGroup: C2v

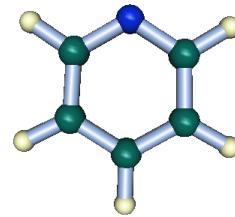
E= -248.376254473 au

ZPE= 0.088606 au

LUMO_eps= -0.04104 au

HOMO_eps= -0.26489 au

Dipole= 2.266 debye



11

C	0.000000	1.138944	0.719367
N	0.000000	0.000000	1.412722
C	0.000000	1.193219	-0.669712
C	0.000000	-1.138944	0.719367
C	0.000000	-1.193219	-0.669712
C	0.000000	0.000000	-1.378970
H	0.000000	-2.147907	-1.177548
H	0.000000	2.053255	1.302467
H	0.000000	2.147907	-1.177548
H	0.000000	-2.053255	1.302467
H	0.000000	0.000000	-2.460925

Molecule# 0691

pyrimidin-2-amine

PointGroup: Cs

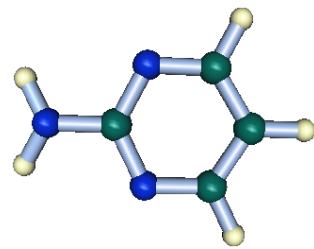
E= -319.820393438 au

ZPE= 0.093498 au

LUMO_eps= -0.04631 au

HOMO_eps= -0.23996 au

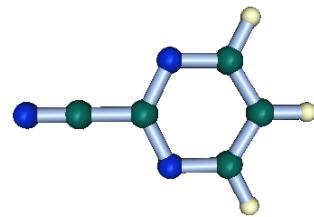
Dipole= 0.485 debye



12

C	-0.000845	-1.808309	0.000000
C	0.002500	-1.071896	1.177316
C	0.002500	-1.071896	-1.177316
C	-0.003688	0.863909	0.000000
N	0.002500	0.255572	1.197627
N	0.002500	0.255572	-1.197627
N	-0.041543	2.223054	0.000000
H	-0.000837	-2.887318	0.000000
H	0.007769	-1.564229	2.143784
H	0.007769	-1.564229	-2.143784
H	0.119153	2.702771	-0.866351
H	0.119153	2.702771	0.866351

Molecule# 0692
pyrimidine-2-carbonitrile
PointGroup: C2v
E= -356.685447605 au
ZPE= 0.075021 au
LUMO_eps= -0.09319 au
HOMO_eps= -0.29393 au
Dipole= 6.409 debye



11

C	0.000000	0.000000	1.983144
C	0.000000	0.000000	-2.114003
C	0.000000	1.182119	-1.386720
C	0.000000	-1.182119	-1.386720
C	0.000000	0.000000	0.536531
N	0.000000	0.000000	3.132944
N	0.000000	1.194621	-0.055327
N	0.000000	-1.194621	-0.055327
H	0.000000	0.000000	-3.193985
H	0.000000	2.147839	-1.877717
H	0.000000	-2.147839	-1.877717

Molecule# 0693

pyrrole

PointGroup: C2v

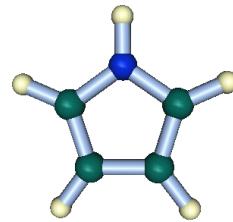
E= -210.252325997 au

ZPE= 0.082428 au

LUMO_eps= -0.01492 au

HOMO_eps= -0.21902 au

Dipole= 1.833 debye



10

C	0.000000	0.710696	-0.980035
C	0.000000	-0.710696	-0.980035
C	0.000000	1.121982	0.330484
C	0.000000	-1.121982	0.330484
N	0.000000	0.000000	1.118833
H	0.000000	1.356378	-1.841340
H	0.000000	-1.356378	-1.841340
H	0.000000	2.107246	0.761724
H	0.000000	-2.107246	0.761724
H	0.000000	0.000000	2.121999

Molecule# 0694

pyrrolidin-2-one

PointGroup: C1

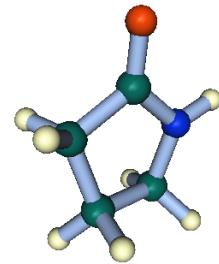
E= -286.745071828 au

ZPE= 0.110608 au

LUMO_eps= -0.01937 au

HOMO_eps= -0.25375 au

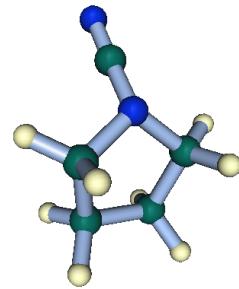
Dipole= 4.270 debye



13

C	-0.903175	0.001036	-0.006994
C	0.005478	1.220666	0.132987
C	1.412127	0.693606	-0.180358
C	1.324994	-0.815730	0.127683
N	-0.088155	-1.094127	-0.072504
O	-2.116544	-0.011504	-0.038990
H	-0.330880	2.020914	-0.521866
H	-0.083303	1.580279	1.160742
H	1.635799	0.834612	-1.237813
H	2.197405	1.180877	0.393609
H	1.945173	-1.412323	-0.541075
H	1.632814	-1.032529	1.156074
H	-0.484123	-2.018367	-0.030135

Molecule# 0695
pyrrolidine-1-carbonitrile
PointGroup: Cs
E= -304.932643435 au
ZPE= 0.127682 au
LUMO_eps= -0.02347 au
HOMO_eps= -0.25188 au
Dipole= 5.369 debye



15

H	0.006474	-0.227339	2.044374
H	-1.635546	-0.354899	1.408749
C	-0.624771	-0.007610	1.187918
H	0.006474	-0.227339	-2.044374
H	-1.635546	-0.354899	-1.408749
C	-0.624771	-0.007610	-1.187918
H	-1.486817	2.000076	-1.189456
H	0.267197	1.975221	-1.154715
C	-0.624771	1.478937	-0.776179
H	-1.486817	2.000076	1.189456
H	0.267197	1.975221	1.154715
C	-0.624771	1.478937	0.776179
N	-0.139113	-0.737456	0.000000
C	1.096623	-1.229239	0.000000
N	2.155136	-1.700631	0.000000

Molecule# 0696

pyrrolidine

PointGroup: Cs

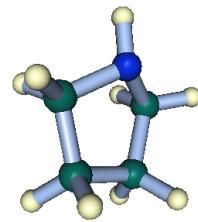
E= -212.666588032 au

ZPE= 0.129290 au

LUMO_eps= -0.01270 au

HOMO_eps= -0.22746 au

Dipole= 0.952 debye



14

C	0.098831	1.023382	0.776623
C	0.098831	1.023382	-0.776623
C	0.098831	-0.465440	1.163404
C	0.098831	-0.465440	-1.163404
N	-0.516767	-1.106166	0.000000
H	0.959997	1.544372	1.192744
H	-0.795896	1.513765	1.157193
H	-0.795896	1.513765	-1.157193
H	0.959997	1.544372	-1.192744
H	1.132013	-0.807155	1.332694
H	-0.473545	-0.671624	2.067900
H	-0.473545	-0.671624	-2.067900
H	1.132013	-0.807155	-1.332694
H	-0.399708	-2.110863	0.000000

Molecule# 0697

pyrrolo-1,2-oxadithiazole

PointGroup: C1

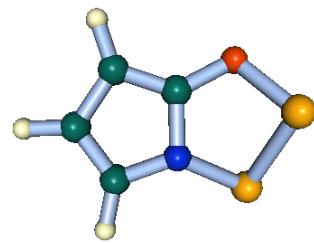
E= -1080.679021680 au

ZPE= 0.067295 au

LUMO_eps= -0.08404 au

HOMO_eps= -0.21953 au

Dipole= 1.076 debye



11

S	-1.051061	1.281881	-0.283900
S	-1.895278	-0.532601	0.338547
O	-0.614494	-1.427165	-0.363889
N	0.475661	0.575388	0.138694
C	0.558745	-0.776721	-0.091504
C	1.756359	1.099948	0.219774
C	1.870920	-1.154035	-0.105040
C	2.624545	0.047815	0.089137
H	1.921997	2.142592	0.418071
H	2.246994	-2.155899	-0.208071
H	3.695337	0.112379	0.181703

Molecule# 0698

quadricyclane

PointGroup: C2v

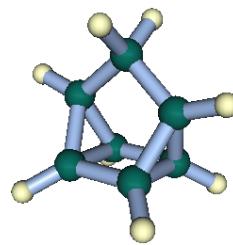
E= -271.539068746 au

ZPE= 0.127715 au

LUMO_eps= -0.00791 au

HOMO_eps= -0.22658 au

Dipole= 0.024 debye



15

C	-0.756547	0.773373	-0.707390
C	0.756547	0.773373	-0.707390
C	0.000000	1.149648	0.549230
C	-0.756547	-0.773373	-0.707390
C	0.756547	-0.773373	-0.707390
C	0.000000	-1.149648	0.549230
C	0.000000	0.000000	1.534441
H	-1.443256	1.422663	-1.227100
H	1.443256	1.422663	-1.227100
H	0.000000	2.180720	0.872633
H	-1.443256	-1.422663	-1.227100
H	1.443256	-1.422663	-1.227100
H	0.000000	-2.180720	0.872633
H	0.887300	0.000000	2.171546
H	-0.887300	0.000000	2.171546

Molecule# 0699

quinazoline

PointGroup: Cs

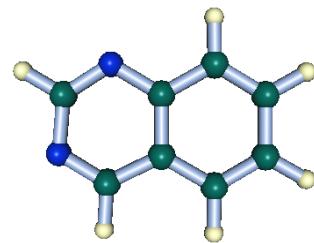
E= -418.116129504 au

ZPE= 0.123717 au

LUMO_eps= -0.08025 au

HOMO_eps= -0.25955 au

Dipole= 3.019 debye



16

C	0.039427	-0.709559	0.000000
N	1.218194	-1.390076	0.000000
C	-1.186285	-1.412578	0.000000
C	2.313681	-0.674653	0.000000
N	2.413160	0.680885	0.000000
C	1.283002	1.344715	0.000000
C	0.020191	0.710676	0.000000
C	-2.369673	-0.719355	0.000000
C	-2.387537	0.694079	0.000000
C	-1.212893	1.400081	0.000000
H	3.255001	-1.211833	0.000000
H	1.342186	2.429877	0.000000
H	-3.335479	1.214343	0.000000
H	-3.307696	-1.258260	0.000000
H	-1.215242	2.482785	0.000000
H	-1.157726	-2.493006	0.000000

Molecule# 0700

quinoline

PointGroup: Cs

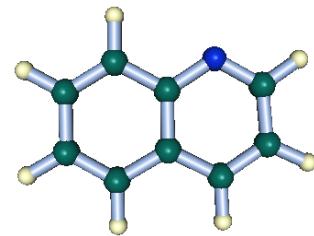
E= -402.071798819 au

ZPE= 0.135389 au

LUMO_eps= -0.06623 au

HOMO_eps= -0.24396 au

Dipole= 2.077 debye



17

C	0.000000	0.703651	0.000000
N	-1.128178	1.465945	0.000000
C	1.258493	1.350388	0.000000
C	-2.286918	0.851830	0.000000
C	-2.438097	-0.553100	0.000000
C	-1.316052	-1.335881	0.000000
C	-0.043208	-0.722482	0.000000
C	2.416244	0.616895	0.000000
C	2.373746	-0.794928	0.000000
C	1.170348	-1.450387	0.000000
H	-3.428480	-0.986603	0.000000
H	-3.168814	1.484250	0.000000
H	3.297826	-1.356965	0.000000
H	3.374149	1.119515	0.000000
H	-1.387749	-2.416474	0.000000
H	1.132723	-2.532563	0.000000
H	1.270259	2.431307	0.000000

Molecule# 0701

quinolizin-4-one

PointGroup: Cs

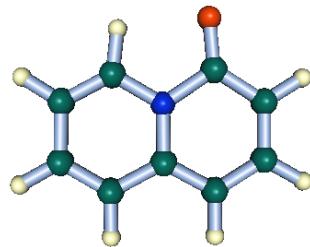
E= -477.321986878 au

ZPE= 0.139737 au

LUMO_eps= -0.06868 au

HOMO_eps= -0.20684 au

Dipole= 4.480 debye



18

C	2.686397	-0.273422	0.000000
C	-1.985691	-1.496841	0.000000
C	1.738404	-1.247442	0.000000
C	-2.345922	-0.171174	0.000000
C	2.286782	1.088692	0.000000
C	-0.649161	-1.894413	0.000000
C	0.967175	1.392721	0.000000
C	0.349704	-0.934931	0.000000
C	-1.385928	0.877093	0.000000
N	0.000000	0.414424	0.000000
O	-1.598324	2.082096	0.000000
H	3.736243	-0.531122	0.000000
H	-2.760364	-2.253013	0.000000
H	2.008743	-2.293604	0.000000
H	-3.380584	0.135967	0.000000
H	3.014749	1.885444	0.000000
H	-0.368672	-2.936075	0.000000
H	0.565928	2.392966	0.000000

Molecule# 0702

quinoxaline

PointGroup: C2v

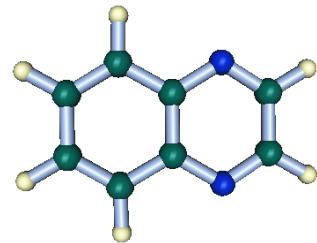
E= -418.111029499 au

ZPE= 0.123381 au

LUMO_eps= -0.08556 au

HOMO_eps= -0.25845 au

Dipole= 0.550 debye



16

C	0.000000	0.706926	2.368951
C	0.000000	-0.706926	2.368951
C	0.000000	1.406054	1.190448
C	0.000000	-1.406054	1.190448
C	0.000000	0.708403	-2.312800
C	0.000000	-0.708403	-2.312800
C	0.000000	0.712878	-0.041323
C	0.000000	-0.712878	-0.041323
N	0.000000	1.410993	-1.208183
N	0.000000	-1.410993	-1.208183
H	0.000000	1.237156	3.311638
H	0.000000	-1.237156	3.311638
H	0.000000	2.486877	1.166492
H	0.000000	-2.486877	1.166492
H	0.000000	1.250205	-3.252504
H	0.000000	-1.250205	-3.252504

Molecule# 0703

quinuclidine

PointGroup: C3v

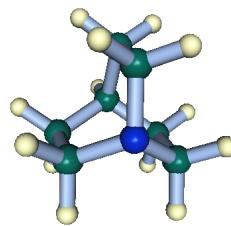
E= -329.427208484 au

ZPE= 0.194208 au

LUMO_eps= -0.01429 au

HOMO_eps= -0.21064 au

Dipole= 1.098 debye



21

N	0.000000	0.000000	1.286725
C	0.000000	1.384344	0.796964
C	-1.198877	-0.692172	0.796964
C	1.198877	-0.692172	0.796964
C	0.000000	1.443662	-0.760521
C	-1.250248	-0.721831	-0.760521
C	1.250248	-0.721831	-0.760521
C	0.000000	0.000000	-1.290089
H	0.877475	1.885976	1.207931
H	-0.877475	1.885976	1.207931
H	-2.072040	-0.183072	1.207931
H	-1.194565	-1.702903	1.207931
H	1.194565	-1.702903	1.207931
H	2.072040	-0.183072	1.207931
H	0.877284	1.977815	-1.131569
H	-0.877284	1.977815	-1.131569
H	-2.151480	-0.229157	-1.131569
H	-1.274196	-1.748657	-1.131569
H	1.274196	-1.748657	-1.131569
H	2.151480	-0.229157	-1.131569
H	0.000000	0.000000	-2.380678

Molecule# 0704

R,S-2,3-dichlorobutane

PointGroup: Ci

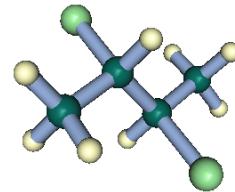
E= -1077.788713650 au

ZPE= 0.113655 au

LUMO_eps= -0.02206 au

HOMO_eps= -0.30076 au

Dipole= 0.000 debye



14

C1	-0.963836	1.196188	-1.568576
C1	0.963836	-1.196188	1.568576
C	-1.877280	-0.439478	0.405978
C	1.877280	0.439478	-0.405978
C	-0.655802	0.388883	0.056013
C	0.655802	-0.388883	-0.056013
H	-2.768750	0.184001	0.395510
H	2.768750	-0.184001	-0.395510
H	1.763930	0.869887	-1.399295
H	-1.763930	-0.869887	1.399295
H	-2.014805	-1.248691	-0.311234
H	2.014805	1.248691	0.311234
H	0.528989	-1.216949	-0.749644
H	-0.528989	1.216949	0.749644

Molecule# 0705

S-2-pyridinyl ethanethioate

PointGroup: C1

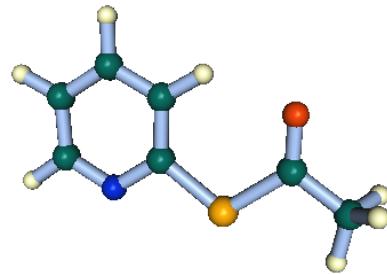
E= -799.308903871 au

ZPE= 0.126301 au

LUMO_eps= -0.05380 au

HOMO_eps= -0.25090 au

Dipole= 0.595 debye



17

C	2.274150	1.388749	-0.000069
C	3.234944	0.386128	0.000107
C	0.927785	1.052725	-0.000171
C	2.801859	-0.932997	0.000173
C	0.607018	-0.304386	-0.000074
C	-2.244819	0.347643	0.000025
C	-3.658489	-0.190391	0.000171
N	1.514712	-1.276021	0.000089
O	-1.993920	1.525908	0.000110
S	-1.049030	-0.997881	-0.000205
H	2.565776	2.430616	-0.000132
H	4.290895	0.616050	0.000187
H	0.153685	1.800661	-0.000305
H	3.511957	-1.751445	0.000302
H	-4.172879	0.194508	-0.880641
H	-4.172111	0.193012	0.882092
H	-3.699155	-1.277234	-0.000689

Molecule# 0706

S-ethyl ethanethioate

PointGroup: C1

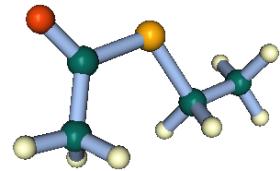
E= -630.791598177 au

ZPE= 0.113615 au

LUMO_eps= -0.02945 au

HOMO_eps= -0.25743 au

Dipole= 4.457 debye



14

O	-2.357106	-0.826508	0.000023
C	-1.415289	-0.075802	0.000085
S	0.232683	-0.804196	-0.000140
H	-1.076024	1.860038	0.880271
H	-2.611239	1.674996	0.000488
H	-1.076214	1.860311	-0.879564
C	-1.552652	1.427474	0.000338
H	1.252246	1.209742	-0.884316
H	1.252388	1.209438	0.884567
C	1.422814	0.598820	0.000007
H	3.026676	-0.571696	0.882060
H	3.561268	0.860316	-0.000120
H	3.026534	-0.571397	-0.882700
C	2.841508	0.040750	-0.000202

Molecule# 0707

S-hydroperoxy hexa-2,4-diynethioate

PointGroup: C1

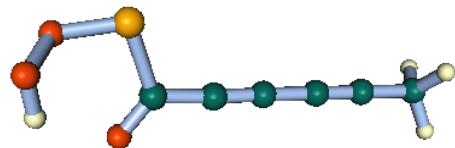
E= -854.890509906 au

ZPE= 0.084635 au

LUMO_eps= -0.10387 au

HOMO_eps= -0.27446 au

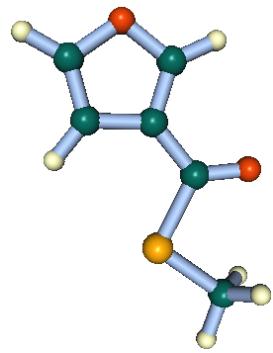
Dipole= 6.405 debye



14

S	1.777893	-1.017043	-0.098312
O	3.331071	-0.521658	-0.383927
O	1.564558	1.616301	-0.260640
O	3.903677	0.151691	0.784045
C	0.945852	0.577476	-0.185281
C	-0.473005	0.441711	-0.112433
C	-1.670367	0.263764	-0.051931
C	-3.011782	0.084916	0.015677
C	-4.208213	-0.073703	0.076329
C	-5.641659	-0.262465	0.148528
H	3.588858	1.056127	0.611506
H	-6.026208	-0.654858	-0.794688
H	-6.149180	0.680904	0.356636
H	-5.899149	-0.970358	0.938381

Molecule# 0708
 S-methyl-3-furancarbothioate
 PointGroup: Cs
 E= -781.049548521 au
 ZPE= 0.108393 au
 LUMO_eps= -0.06013 au
 HOMO_eps= -0.25580 au
 Dipole= 1.642 debye



15

C	-1.392165	1.170066	0.000000
C	-1.428012	2.519619	0.000000
C	0.691129	1.983502	0.000000
C	0.000000	0.807541	0.000000
C	0.635993	-0.516796	0.000000
C	0.661715	-3.268787	0.000000
O	1.835393	-0.684653	0.000000
O	-0.157808	3.030443	0.000000
S	-0.521930	-1.891204	0.000000
H	-2.241204	0.509673	0.000000
H	-2.223626	3.241441	0.000000
H	1.742596	2.204050	0.000000
H	1.285248	-3.226145	0.888112
H	1.285248	-3.226145	-0.888112
H	0.069983	-4.180792	0.000000

Molecule# 0709

S-methyl benzenecarbothioate

PointGroup: Cs

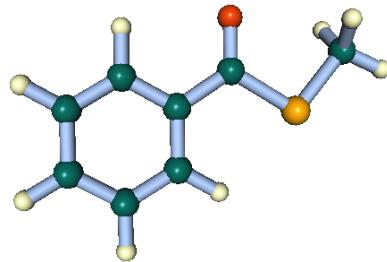
E= -783.271862163 au

ZPE= 0.138733 au

LUMO_eps= -0.07126 au

HOMO_eps= -0.25514 au

Dipole= 1.583 debye



18

C	1.333065	3.036686	0.000000
C	-0.058033	3.001626	0.000000
C	2.057969	1.849796	0.000000
C	-0.721944	1.784420	0.000000
C	1.395636	0.630072	0.000000
C	0.000000	0.587581	0.000000
C	-0.775412	-0.687600	0.000000
C	-1.161168	-3.408295	0.000000
O	-1.984399	-0.723520	0.000000
S	0.197665	-2.203581	0.000000
H	1.851085	3.986336	0.000000
H	-0.623442	3.923567	0.000000
H	3.139026	1.874086	0.000000
H	-1.801297	1.738555	0.000000
H	1.969563	-0.285827	0.000000
H	-1.773676	-3.283052	0.887927
H	-0.695712	-4.390868	0.000000
H	-1.773676	-3.283052	-0.887927

Molecule# 0710

S-methyl thioformate

PointGroup: Cs

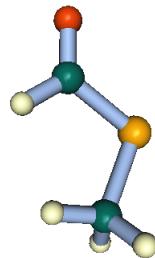
E= -552.126179653 au

ZPE= 0.056798 au

LUMO_eps= -0.04614 au

HOMO_eps= -0.27058 au

Dipole= 3.895 debye



8

C	-0.591523	-0.910088	0.000000
C	1.806424	0.511742	0.000000
O	-1.751511	-1.205927	0.000000
S	0.000000	0.769997	0.000000
H	0.228373	-1.652841	0.000000
H	2.021441	-0.556170	0.000000
H	2.236433	0.963278	0.889535
H	2.236433	0.963278	-0.889535

Molecule# 0711

S-methylsulfinylbenzene

PointGroup: C1

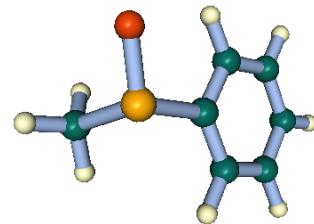
E= -745.104574156 au

ZPE= 0.132415 au

LUMO_eps= -0.04194 au

HOMO_eps= -0.23912 au

Dipole= 4.035 debye



17

C	-2.865077	0.100616	0.165518
C	-2.070507	1.223857	0.366327
C	-2.286294	-1.104138	-0.223924
C	-0.692839	1.148380	0.186907
C	-0.911773	-1.187321	-0.409725
C	-0.127095	-0.061385	-0.186065
C	2.115664	-0.968781	1.096612
O	2.191158	1.279499	-0.345256
S	1.671473	-0.126541	-0.469671
H	-3.936059	0.164368	0.301992
H	-2.522707	2.162209	0.657897
H	-2.905625	-1.974771	-0.391995
H	-0.051411	2.009136	0.320028
H	-0.461290	-2.117623	-0.732907
H	1.639276	-1.946560	1.131766
H	1.794165	-0.342110	1.925393
H	3.198354	-1.073357	1.090709

Molecule# 0712

S-nitrosocysteine

PointGroup: C1

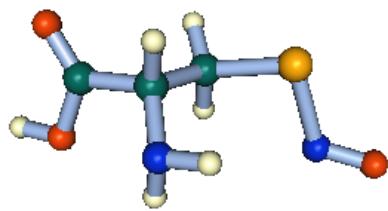
E= -851.448960976 au

ZPE= 0.105557 au

LUMO_eps= -0.11405 au

HOMO_eps= -0.26057 au

Dipole= 1.375 debye



15

S	-1.708055	-0.944543	0.238777
O	2.543314	1.082665	-0.736842
O	3.099840	-0.995616	-0.091408
O	-3.637533	0.704920	-0.308545
N	0.648212	1.175180	1.198357
N	-2.500457	0.538811	-0.543859
C	0.958154	-0.108039	0.596436
C	-0.057481	-0.638317	-0.450388
C	2.322002	-0.078776	-0.081186
H	1.047909	-0.847293	1.390980
H	0.293305	-1.573053	-0.885849
H	-0.196720	0.090629	-1.251576
H	-0.227541	1.132950	1.703394
H	0.584033	1.910377	0.505497
H	3.412596	1.016178	-1.159186

Molecule# 0713

sarcosine

PointGroup: C1

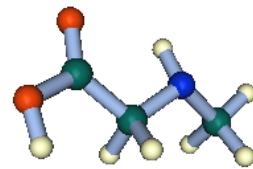
E= -323.864920209 au

ZPE= 0.107035 au

LUMO_eps= -0.02908 au

HOMO_eps= -0.24341 au

Dipole= 4.044 debye



13

H	-1.062995	1.233708	-0.007749
N	-1.287298	0.301061	-0.329906
H	-2.668450	-0.329662	1.188710
H	-2.886524	-1.049290	-0.414325
H	-3.337280	0.630006	-0.147704
C	-2.603422	-0.132820	0.107415
H	-0.323323	-1.023463	1.042073
H	-0.185290	-1.445839	-0.662916
C	-0.216255	-0.595054	0.027536
O	1.244161	1.313708	0.076402
C	1.122183	0.123838	0.016980
H	1.964442	-1.602938	-0.095392
O	2.217773	-0.675674	-0.014519

Molecule# 0714
sec-butylbenzene

PointGroup: C1

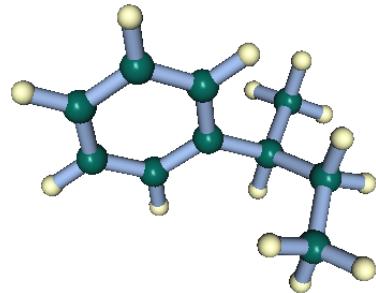
E= -389.649007507 au

ZPE= 0.212708 au

LUMO_eps= -0.01562 au

HOMO_eps= -0.24813 au

Dipole= 0.387 debye



24

C	2.857988	-0.186371	-0.233131
C	2.053766	0.384179	-1.214486
C	2.290498	-0.563987	0.976902
C	0.697008	0.573868	-0.984913
C	0.930680	-0.371454	1.200202
C	0.110355	0.199210	0.227134
C	-2.106231	-1.897819	-0.384502
C	-1.735472	1.906080	0.469313
C	-2.268736	-0.382193	-0.478594
C	-1.370680	0.413775	0.488686
H	3.914630	-0.333895	-0.411250
H	2.484835	0.682992	-2.161028
H	2.904128	-1.009341	1.748912
H	0.089544	1.020400	-1.761714
H	0.498685	-0.670061	2.147496
H	-2.781757	-2.406774	-1.073300
H	-1.088989	-2.207419	-0.625697
H	-2.330630	-2.254856	0.622994
H	-1.578291	2.339587	-0.519828
H	-2.785198	2.048697	0.731767
H	-1.128084	2.469271	1.178299
H	-2.072665	-0.053669	-1.503150
H	-3.308762	-0.116218	-0.270236
H	-1.572502	0.039560	1.497058

Molecule# 0715

serine

PointGroup: C1

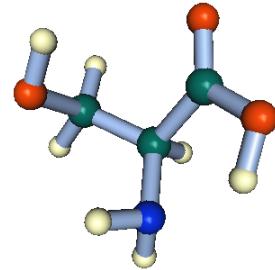
E= -399.133291251 au

ZPE= 0.113502 au

LUMO_eps= -0.03187 au

HOMO_eps= -0.27379 au

Dipole= 4.121 debye



14

N	-0.177991	1.757044	-0.045284
C	-0.174557	0.454696	0.630245
C	1.009523	-0.385808	0.110632
O	1.076352	-1.580041	0.246542
O	1.963473	0.331956	-0.488889
H	1.615569	1.250303	-0.522903
C	-1.479889	-0.332217	0.505893
O	-1.818406	-0.558856	-0.858546
H	0.029220	0.618593	1.692314
H	-2.295702	0.252625	0.931383
H	-1.398556	-1.270636	1.055345
H	-1.310349	-1.313636	-1.174889
H	-0.748545	1.709812	-0.883078
H	-0.547515	2.489126	0.545335

Molecule# 0716

spiro[4.4]nona-1,3,6,8-tetraene

PointGroup: D2d

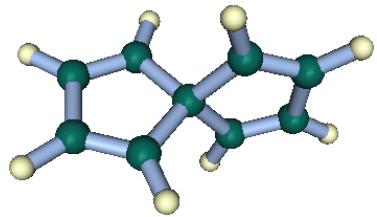
E= -347.811411331 au

ZPE= 0.137854 au

LUMO_eps= -0.03690 au

HOMO_eps= -0.21084 au

Dipole= 0.000 debye



17

C	0.000000	0.000000	0.000000
C	0.000000	1.177445	0.958848
C	0.000000	-1.177445	0.958848
C	1.177445	0.000000	-0.958848
C	-1.177445	0.000000	-0.958848
C	0.000000	0.734608	2.223211
C	0.000000	-0.734608	2.223211
C	0.734608	0.000000	-2.223211
C	-0.734608	0.000000	-2.223211
H	0.000000	2.201549	0.620322
H	0.000000	-2.201549	0.620322
H	2.201549	0.000000	-0.620322
H	-2.201549	0.000000	-0.620322
H	0.000000	1.348828	3.111832
H	0.000000	-1.348828	3.111832
H	1.348828	0.000000	-3.111832
H	-1.348828	0.000000	-3.111832

Molecule# 0717

spiropentane

PointGroup: D2d

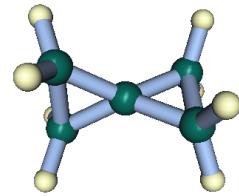
E= -195.345750460 au

ZPE= 0.114536 au

LUMO_eps= -0.00540 au

HOMO_eps= -0.27596 au

Dipole= 0.000 debye



13

C	0.000000	0.000000	0.000000
C	0.000000	0.763303	1.266524
C	0.000000	-0.763303	1.266524
C	-0.763303	0.000000	-1.266524
C	0.763303	0.000000	-1.266524
H	0.910461	1.264133	1.569347
H	-0.910461	1.264133	1.569347
H	-0.910461	-1.264133	1.569347
H	0.910461	-1.264133	1.569347
H	-1.264133	-0.910461	-1.569347
H	-1.264133	0.910461	-1.569347
H	1.264133	0.910461	-1.569347
H	1.264133	-0.910461	-1.569347

Molecule# 0718

styrene

PointGroup: Cs

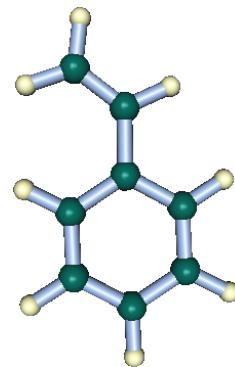
E= -309.763256985 au

ZPE= 0.133041 au

LUMO_eps= -0.04974 au

HOMO_eps= -0.23527 au

Dipole= 0.203 debye



16

C	0.646281	-2.178017	0.000000
C	1.654479	-1.222905	0.000000
C	-0.685207	-1.768319	0.000000
C	1.332018	0.128421	0.000000
C	-1.004470	-0.419868	0.000000
C	0.000000	0.557656	0.000000
C	-1.470206	2.598351	0.000000
C	-0.279787	1.999196	0.000000
H	0.891660	-3.231362	0.000000
H	2.692244	-1.528409	0.000000
H	-1.476757	-2.505897	0.000000
H	2.123019	0.867889	0.000000
H	-2.044665	-0.124640	0.000000
H	-1.545935	3.676443	0.000000
H	-2.403023	2.050610	0.000000
H	0.604810	2.628272	0.000000

Molecule# 0719

succinic acid

PointGroup: C1

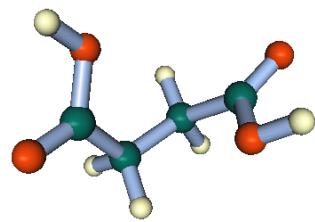
E= -457.158154780 au

ZPE= 0.105712 au

LUMO_eps= -0.02630 au

HOMO_eps= -0.29526 au

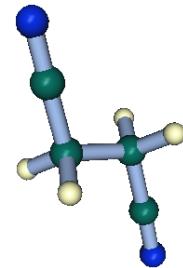
Dipole= 0.843 debye



14

O	-2.569105	-0.409889	-0.572480
C	-1.603311	-0.035392	0.038272
C	-0.692304	1.087981	-0.403001
C	0.695435	1.135208	0.232886
C	1.604629	-0.043381	-0.033539
O	2.579645	-0.312785	0.616746
O	1.230271	-0.763568	-1.119024
O	-1.243334	-0.568197	1.231448
H	-1.222247	2.014615	-0.166974
H	-0.636885	1.034304	-1.487924
H	0.640007	1.245840	1.313535
H	1.226901	2.014895	-0.139503
H	1.873901	-1.480386	-1.220794
H	-1.888183	-1.260241	1.440431

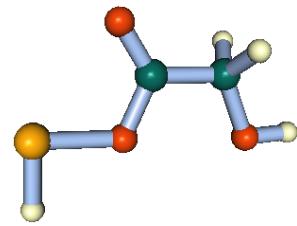
Molecule# 0720
succinonitrile
PointGroup: C2h
E= -264.402496197 au
ZPE= 0.073278 au
LUMO_eps= -0.03394 au
HOMO_eps= -0.35367 au
Dipole= 0.000 debye



10

C	0.422954	0.646920	0.000000
C	-0.422954	-0.646920	0.000000
C	-0.422954	1.834859	0.000000
C	0.422954	-1.834859	0.000000
N	1.107673	-2.757950	0.000000
N	-1.107673	2.757950	0.000000
H	1.069525	0.672423	0.877634
H	1.069525	0.672423	-0.877634
H	-1.069525	-0.672423	0.877634
H	-1.069525	-0.672423	-0.877634

Molecule# 0721
sulfanyl-2-hydroxyacetate
PointGroup: C1
E= -702.610471966 au
ZPE= 0.065008 au
LUMO_eps= -0.06300 au
HOMO_eps= -0.25927 au
Dipole= 2.485 debye



10

S	2.048400	-0.290055	-0.000004
O	0.344735	-0.570900	0.000028
O	0.114295	1.662368	-0.000031
O	-2.201166	-1.044702	-0.000050
C	-0.370001	0.558920	0.000004
C	-1.869456	0.327817	0.000042
H	2.266181	-1.618423	0.000025
H	-3.158635	-1.130729	0.000000
H	-2.254090	0.847812	-0.883395
H	-2.254023	0.847674	0.883591

Molecule# 0722

sulfanylacetyl chloride

PointGroup: C1

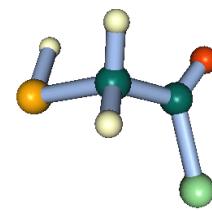
E= -1011.764772990 au

ZPE= 0.047238 au

LUMO_eps= -0.07150 au

HOMO_eps= -0.27342 au

Dipole= 2.260 debye



8

C1	1.676546	-0.809324	-0.064042
S	-1.948152	-0.418639	-0.243515
O	0.873755	1.670610	-0.356742
C	0.580777	0.624501	0.110504
C	-0.682958	0.310390	0.867857
H	-2.149817	0.689707	-0.979994
H	-1.058018	1.227789	1.313361
H	-0.499959	-0.434986	1.635345

Molecule# 0723

sulfanylacetylenol

PointGroup: C1

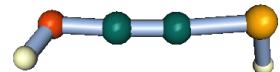
E= -550.834377099 au

ZPE= 0.032450 au

LUMO_eps= -0.03173 au

HOMO_eps= -0.23594 au

Dipole= 1.926 debye



6

S -1.717687 -0.094549 0.004331

O 2.473344 -0.005347 -0.104993

C -0.032037 0.049767 -0.007089

C 1.170348 0.011478 0.003985

H -2.024932 1.220216 0.023363

H 2.891302 -0.032124 0.765910

Molecule# 0724

sulfanyl methyl thiocyanate

PointGroup: C1

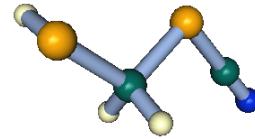
E= -929.240481375 au

ZPE= 0.046383 au

LUMO_eps= -0.05929 au

HOMO_eps= -0.27957 au

Dipole= 3.538 debye



8

S	-0.581423	0.778059	-0.046508
S	2.290563	-0.099694	-0.028882
N	-3.075461	-0.603242	0.072586
C	0.575090	-0.674352	-0.075835
C	-2.060382	-0.051436	0.023082
H	2.304288	0.255860	1.269161
H	0.444681	-1.205612	-1.013319
H	0.344772	-1.326672	0.758810

Molecule# 0725

syn-tricyclo[4.2.0.0_{2,5}]octane

PointGroup: C2v

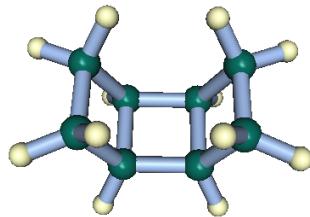
E= -312.083628716 au

ZPE= 0.179212 au

LUMO_eps= -0.01125 au

HOMO_eps= -0.25238 au

Dipole= 0.177 debye



20

C	-0.780890	0.782120	0.714182
C	0.780890	0.782120	0.714182
C	0.780890	-0.782120	0.714182
C	-0.780890	-0.782120	0.714182
C	-1.552994	0.779426	-0.630946
C	-1.552994	-0.779426	-0.630946
H	-1.230266	1.359101	1.520382
H	-1.230266	-1.359101	1.520382
H	-1.058422	1.259186	-1.474246
H	-2.550804	1.207825	-0.545553
H	-2.550804	-1.207825	-0.545553
H	-1.058422	-1.259186	-1.474246
C	1.552994	-0.779426	-0.630946
C	1.552994	0.779426	-0.630946
H	1.230266	1.359101	1.520382
H	1.230266	-1.359101	1.520382
H	2.550804	-1.207825	-0.545553
H	1.058422	-1.259186	-1.474246
H	2.550804	1.207825	-0.545553
H	1.058422	1.259186	-1.474246

Molecule# 0726

t-butylmethylsulfone

PointGroup: C1

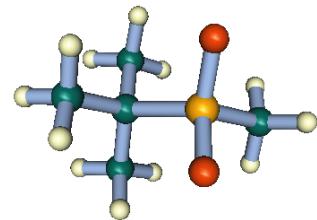
E= -746.545415514 au

ZPE= 0.168822 au

LUMO_eps= -0.02124 au

HOMO_eps= -0.28530 au

Dipole= 4.704 debye



20

C	-1.390811	0.856682	-1.268373
C	-1.015837	0.089879	-0.000005
C	-1.643181	-1.309663	-0.000111
C	-1.390836	0.856501	1.268466
S	0.822500	-0.225263	-0.000009
C	1.634089	1.387915	0.000134
O	1.168494	-0.878127	1.262513
O	1.168524	-0.877920	-1.262630
H	-1.046643	0.337279	-2.160653
H	-2.477629	0.942211	-1.319652
H	-0.985355	1.868581	-1.272654
H	-1.352891	-1.874065	0.884264
H	-2.728961	-1.202794	-0.000121
H	-1.352864	-1.873940	-0.884557
H	-0.985387	1.868403	1.272894
H	-2.477655	0.942016	1.319740
H	-1.046678	0.336974	2.160677
H	2.695942	1.152116	0.000133
H	1.370739	1.934035	-0.900315
H	1.370708	1.933886	0.900664

Molecule# 0727

terephthalonitrile

PointGroup: D2h

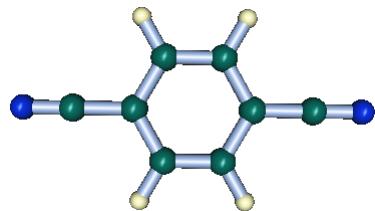
E= -416.880734531 au

ZPE= 0.097492 au

LUMO_eps= -0.10614 au

HOMO_eps= -0.29713 au

Dipole= 0.000 debye



14

C	0.000000	0.000000	2.819994
C	0.000000	0.000000	-2.819994
C	0.000000	1.212111	0.691573
C	0.000000	1.212111	-0.691573
C	0.000000	-1.212111	0.691573
C	0.000000	-1.212111	-0.691573
C	0.000000	0.000000	1.390135
C	0.000000	0.000000	-1.390135
N	0.000000	0.000000	3.971955
N	0.000000	0.000000	-3.971955
H	0.000000	2.144546	1.236677
H	0.000000	2.144546	-1.236677
H	0.000000	-2.144546	1.236677
H	0.000000	-2.144546	-1.236677

Molecule# 0728

tertbutylbenzene

PointGroup: Cs

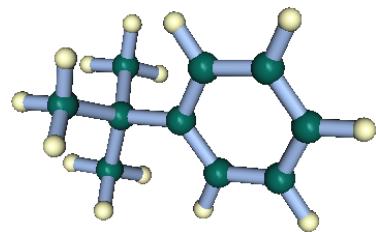
E= -389.645834486 au

ZPE= 0.212247 au

LUMO_eps= -0.01442 au

HOMO_eps= -0.24788 au

Dipole= 0.429 debye



24

C	1.016390	2.717163	0.000000
C	1.881445	1.628485	0.000000
C	-0.351319	2.489477	0.000000
C	1.378116	0.335664	0.000000
C	-0.850314	1.189521	0.000000
C	0.000795	0.083541	0.000000
C	0.000795	-2.093932	1.258284
C	0.000795	-2.093932	-1.258284
C	-2.048330	-1.439541	0.000000
C	-0.514092	-1.363859	0.000000
H	1.405258	3.726594	0.000000
H	2.952226	1.785794	0.000000
H	-1.040642	3.323885	0.000000
H	2.076582	-0.490211	0.000000
H	-1.921023	1.051194	0.000000
H	-0.357843	-3.125177	1.270861
H	1.089525	-2.120203	1.294620
H	-0.351283	-1.601521	2.165820
H	1.089525	-2.120203	-1.294620
H	-0.357843	-3.125177	-1.270861
H	-0.351283	-1.601521	-2.165820
H	-2.361319	-2.484481	0.000000
H	-2.478782	-0.967247	0.883628
H	-2.478782	-0.967247	-0.883628

Molecule# 0729

tertbutylcyclobutane

PointGroup: Cs

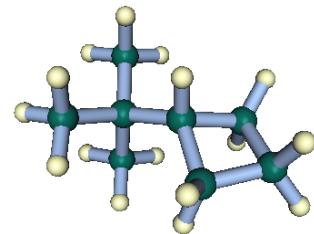
E= -314.585190738 au

ZPE= 0.222249 au

LUMO_eps= -0.01196 au

HOMO_eps= -0.28908 au

Dipole= 0.045 debye



24

C	-0.176910	-0.999418	0.000000
C	0.539789	0.364342	0.000000
C	0.254060	-1.777499	1.254087
C	-1.706916	-0.860851	0.000000
C	0.254060	1.442946	1.082409
C	0.254060	-1.777499	-1.254087
C	0.486107	2.526258	0.000000
H	-0.178689	3.388865	0.000000
H	0.895719	1.457716	1.962608
C	0.254060	1.442946	-1.082409
H	0.895719	1.457716	-1.962608
H	-2.173656	-1.847725	0.000000
H	-0.206452	-2.767279	-1.276969
H	-0.785006	1.429853	1.411389
H	-0.785006	1.429853	-1.411389
H	1.615876	0.164339	0.000000
H	-0.038955	-1.254061	-2.165956
H	-2.067434	-0.330830	0.882403
H	-2.067434	-0.330830	-0.882403
H	-0.206452	-2.767279	1.276969
H	1.337322	-1.913005	-1.279707
H	1.516228	2.882374	0.000000
H	1.337322	-1.913005	1.279707
H	-0.038955	-1.254061	2.165956

Molecule# 0730

tertbutylhydroperoxide

PointGroup: C1

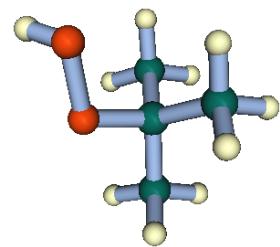
E= -308.934804974 au

ZPE= 0.138127 au

LUMO_eps= -0.01727 au

HOMO_eps= -0.26827 au

Dipole= 1.744 debye



16

C	-0.389046	-0.000005	0.034711
O	0.738307	-0.064366	-0.877245
O	1.978654	0.098687	-0.135089
C	-1.568549	-0.139826	-0.926939
C	-0.342451	-1.161836	1.025628
C	-0.410298	1.351768	0.745235
H	2.385379	-0.765132	-0.282112
H	-1.561837	0.664179	-1.661962
H	-2.504086	-0.091572	-0.369874
H	-1.529057	-1.092846	-1.453933
H	-0.427183	2.162831	0.017417
H	0.469173	1.471463	1.374999
H	-1.297114	1.433058	1.375024
H	-0.300458	-2.114938	0.496791
H	-1.234525	-1.159418	1.652852
H	0.526087	-1.082798	1.677660

Molecule# 0731

tetrabromomethane

PointGroup: Td

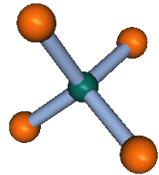
E= -10335.001911900 au

ZPE= 0.006686 au

LUMO_eps= -0.11251 au

HOMO_eps= -0.29566 au

Dipole= 0.000 debye



5

C 0.000000 0.000000 0.000000

Br 1.129855 1.129855 1.129855

Br -1.129855 -1.129855 1.129855

Br 1.129855 -1.129855 -1.129855

Br -1.129855 1.129855 -1.129855

Molecule# 0732

tetrachloroethylene

PointGroup: D2h

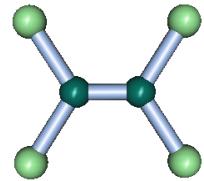
E= -1917.133885510 au

ZPE= 0.015170 au

LUMO_eps= -0.04923 au

HOMO_eps= -0.26580 au

Dipole= 0.000 debye



6

C 0.000000 0.000000 0.669101

C 0.000000 0.000000 -0.669101

Cl 0.000000 1.454916 1.595675

Cl 0.000000 -1.454916 1.595675

Cl 0.000000 -1.454916 -1.595675

Cl 0.000000 1.454916 -1.595675

Molecule# 0733

tetrachloromethane

PointGroup: Td

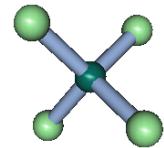
E= -1879.027329030 au

ZPE= 0.009109 au

LUMO_eps= -0.07821 au

HOMO_eps= -0.32634 au

Dipole= 0.000 debye



5

C 0.000000 0.000000 0.000000

Cl 1.030607 1.030607 1.030607

Cl -1.030607 -1.030607 1.030607

Cl 1.030607 -1.030607 -1.030607

Cl -1.030607 1.030607 -1.030607

Molecule# 0734

tetracyanoethylene

PointGroup: D2h

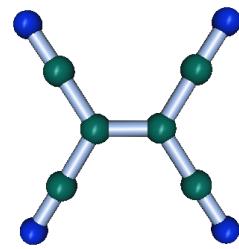
E= -447.679089629 au

ZPE= 0.046452 au

LUMO_eps= -0.19240 au

HOMO_eps= -0.34790 au

Dipole= 0.000 debye



10

C	0.000000	0.000000	0.681974
C	0.000000	0.000000	-0.681974
C	0.000000	1.213865	1.428575
C	0.000000	-1.213865	1.428575
C	0.000000	1.213865	-1.428575
C	0.000000	-1.213865	-1.428575
N	0.000000	2.183501	2.049472
N	0.000000	-2.183501	2.049472
N	0.000000	2.183501	-2.049472
N	0.000000	-2.183501	-2.049472

Molecule# 0735

tetracyanomethane

PointGroup: Td

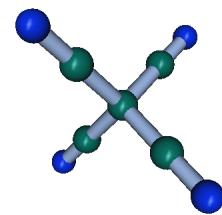
E= -409.539759111 au

ZPE= 0.040539 au

LUMO_eps= -0.08377 au

HOMO_eps= -0.40925 au

Dipole= 0.000 debye



9

C	0.000000	0.000000	0.000000
C	0.856146	0.856146	0.856146
C	-0.856146	-0.856146	0.856146
C	-0.856146	0.856146	-0.856146
C	0.856146	-0.856146	-0.856146
N	1.518318	1.518318	1.518318
N	-1.518318	-1.518318	1.518318
N	-1.518318	1.518318	-1.518318
N	1.518318	-1.518318	-1.518318

Molecule# 0736

tetracyclo-undecane

PointGroup: C1

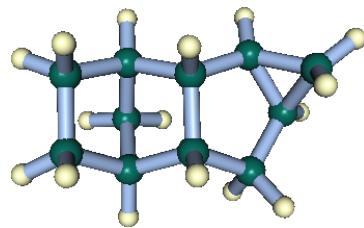
E= -428.919749929 au

ZPE= 0.245956 au

LUMO_eps= -0.01091 au

HOMO_eps= -0.26677 au

Dipole= 0.197 debye



27

C	-2.401528	0.502518	-0.667526
C	-2.260633	-1.021826	-0.364232
C	-1.222072	1.126694	0.106636
C	-0.997200	-1.082851	0.518924
C	-1.144453	0.209527	1.343374
C	0.221275	-0.773296	-0.380965
C	0.094854	0.782700	-0.624847
C	1.349485	1.451766	0.000179
C	1.581769	-0.992045	0.255521
C	2.270694	0.335229	0.459780
C	2.775082	-0.620972	-0.585328
H	-3.352715	0.889677	-0.300403
H	-2.352143	0.725742	-1.733924
H	-2.158654	-1.624292	-1.267296
H	-3.129856	-1.394619	0.178895
H	-1.339901	2.191878	0.303109
H	-0.899022	-2.008675	1.084603
H	-0.291880	0.414655	1.989396
H	-2.051980	0.229391	1.948912
H	0.145237	-1.338197	-1.312928
H	0.018474	1.024497	-1.684640
H	1.840307	2.119123	-0.711691
H	1.063396	2.066804	0.856481
H	1.694152	-1.794885	0.972678
H	2.893858	0.506385	1.327317
H	2.609293	-0.379963	-1.628590
H	3.707801	-1.132180	-0.391015

Molecule# 0737

tetrafluorocyclobutadiene

PointGroup: C2h

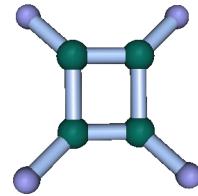
E= -551.819386621 au

ZPE= 0.031266 au

LUMO_eps= -0.10512 au

HOMO_eps= -0.23506 au

Dipole= 0.000 debye



8

C 0.135333 0.760964 0.664678

C -0.135333 -0.760964 0.664678

C -0.135333 -0.760964 -0.664678

C 0.135333 0.760964 -0.664678

F -0.135333 1.670444 1.579297

F 0.135333 -1.670444 1.579297

F 0.135333 -1.670444 -1.579297

F -0.135333 1.670444 -1.579297

Molecule# 0738

tetrafluoroethylene

PointGroup: D2h

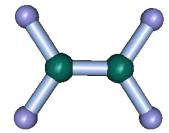
E= -475.711462027 au

ZPE= 0.021428 au

LUMO_eps= -0.00966 au

HOMO_eps= -0.27680 au

Dipole= 0.000 debye



6

C 0.000000 0.000000 0.660447

C 0.000000 0.000000 -0.660447

F 0.000000 1.100779 1.387647

F 0.000000 -1.100779 1.387647

F 0.000000 -1.100779 -1.387647

F 0.000000 1.100779 -1.387647

Molecule# 0739

tetrafluoromethane

PointGroup: Td

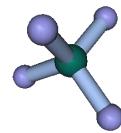
E= -437.669270177 au

ZPE= 0.016710 au

LUMO_eps= 0.00324 au

HOMO_eps= -0.45463 au

Dipole= 0.000 debye



5

C 0.000000 0.000000 0.000000

F 0.765982 0.765982 0.765982

F -0.765982 -0.765982 0.765982

F 0.765982 -0.765982 -0.765982

F -0.765982 0.765982 -0.765982

Molecule# 0740

tetrahydro-2-methylthiophene

PointGroup: C1

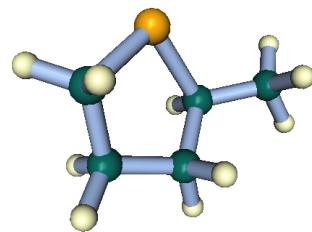
E= -594.861075775 au

ZPE= 0.141260 au

LUMO_eps= -0.01307 au

HOMO_eps= -0.21827 au

Dipole= 2.083 debye



16

C	-2.277189	0.125824	0.212360
H	-2.220830	0.016412	1.295791
H	-2.855694	1.024383	-0.016248
H	-2.824192	-0.729215	-0.185129
S	0.123265	-1.298216	-0.068974
C	1.676730	-0.364875	0.283148
H	2.502112	-0.834989	-0.246639
H	1.880084	-0.410297	1.352120
C	-0.886248	0.229699	-0.395836
H	-0.974067	0.321657	-1.479581
C	1.420648	1.071535	-0.176011
H	1.587312	1.148737	-1.252546
H	2.105520	1.766873	0.312872
C	-0.039816	1.384131	0.141919
H	-0.360577	2.332565	-0.294901
H	-0.176661	1.457447	1.224367

Molecule# 0741

tetrahydro-2H-pyran

PointGroup: Cs

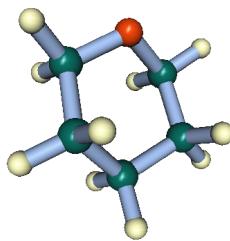
E= -271.875496636 au

ZPE= 0.145700 au

LUMO_eps= -0.01084 au

HOMO_eps= -0.25539 au

Dipole= 1.516 debye



16

C	-0.621065	1.325981	0.000000
C	0.020904	0.729584	1.256731
C	0.020904	0.729584	-1.256731
C	0.020904	-0.794091	1.182195
C	0.020904	-0.794091	-1.182195
O	0.655923	-1.267487	0.000000
H	-1.692321	1.099091	0.000000
H	-0.531769	2.413763	0.000000
H	1.053246	1.077801	1.346976
H	-0.509437	1.050894	2.156429
H	-0.509437	1.050894	-2.156429
H	1.053246	1.077801	-1.346976
H	0.568763	-1.234712	2.014395
H	-1.011867	-1.171361	1.218225
H	-1.011867	-1.171361	-1.218225
H	0.568763	-1.234712	-2.014395

Molecule# 0742

tetrahydro-2H-thiopyran-2-one

PointGroup: C1

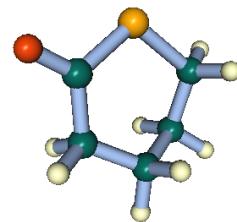
E= -668.910142124 au

ZPE= 0.123383 au

LUMO_eps= -0.03526 au

HOMO_eps= -0.25616 au

Dipole= 4.649 debye



15

C	1.198990	0.282455	-0.007474
C	0.320745	1.512346	-0.137212
C	-1.130694	1.395994	0.326233
C	-1.862920	0.229297	-0.332913
C	-1.354109	-1.115286	0.160621
O	2.401259	0.353705	0.028692
S	0.466431	-1.359194	-0.017043
H	0.844846	2.313553	0.384969
H	0.347720	1.769982	-1.201227
H	-1.165948	1.279754	1.413293
H	-1.641074	2.333623	0.100488
H	-2.931348	0.287651	-0.110885
H	-1.760809	0.292350	-1.419347
H	-1.596178	-1.250293	1.214503
H	-1.802248	-1.937986	-0.394177

Molecule# 0743

tetrahydro-2H-thiopyran

PointGroup: Cs

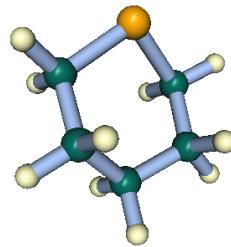
E= -594.861314192 au

ZPE= 0.142170 au

LUMO_eps= -0.01289 au

HOMO_eps= -0.22076 au

Dipole= 1.897 debye

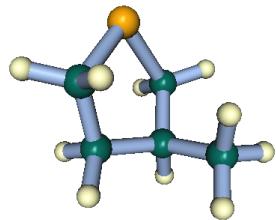


16

S	-0.747974	-1.318207	0.000000
C	0.805831	1.524574	0.000000
C	0.139507	1.011430	1.280779
C	0.139507	1.011430	-1.280779
C	0.139507	-0.511309	1.383433
C	0.139507	-0.511309	-1.383433
H	0.797332	2.616416	0.000000
H	1.859810	1.225806	0.000000
H	1.161031	-0.896509	1.416773
H	1.161031	-0.896509	-1.416773
H	0.661931	1.421155	2.150299
H	0.661931	1.421155	-2.150299
H	-0.890910	1.371982	1.328857
H	-0.890910	1.371982	-1.328857
H	-0.368406	-0.846533	-2.286830
H	-0.368406	-0.846533	2.286830

Molecule# 0744
tetrahydro-3-methylthiophene
PointGroup: C1

E= -594.858774156 au
ZPE= 0.141309 au
LUMO_eps= -0.01582 au
HOMO_eps= -0.21823 au
Dipole= 2.156 debye



16

S	-1.476701	-0.452025	-0.259302
C	1.913232	-0.302099	-0.804682
H	1.265426	-0.226374	-1.678866
H	2.683844	0.466120	-0.886402
H	2.406718	-1.274145	-0.844759
C	-0.015272	-1.169321	0.615996
H	0.232350	-2.124200	0.156285
H	-0.282085	-1.344028	1.657022
C	1.122948	-0.146438	0.496930
H	1.809247	-0.288791	1.336203
C	-0.761847	1.249024	-0.311830
H	-1.519110	1.960559	0.008816
H	-0.481066	1.483947	-1.337013
C	0.449983	1.229470	0.621149
H	0.115459	1.375949	1.649963
H	1.142169	2.039539	0.382198

Molecule# 0745

tetrahydrofuran

PointGroup: C2

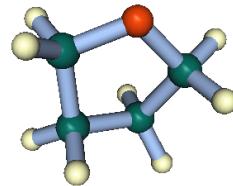
E= -232.541590312 au

ZPE= 0.116240 au

LUMO_eps= -0.01242 au

HOMO_eps= -0.25132 au

Dipole= 1.843 debye



13

C	0.000000	0.766501	-0.994198
C	0.000000	-0.766501	-0.994198
C	0.461326	1.081053	0.428368
C	-0.461326	-1.081053	0.428368
O	0.000000	0.000000	1.249603
H	0.652460	1.198961	-1.751443
H	-1.009869	1.145990	-1.159921
H	-0.652460	-1.198961	-1.751443
H	1.009869	-1.145990	-1.159921
H	1.553740	1.135699	0.488606
H	0.050023	2.012637	0.819323
H	-1.553740	-1.135699	0.488606
H	-0.050023	-2.012637	0.819323

Molecule# 0746

tetrahydropyran-2-one

PointGroup: C1

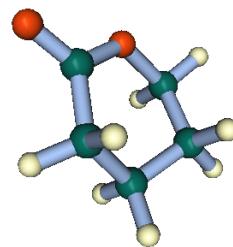
E= -345.939224776 au

ZPE= 0.127008 au

LUMO_eps= -0.02355 au

HOMO_eps= -0.27326 au

Dipole= 4.968 debye



15

C	-1.136499	-0.015675	-0.013358
C	-0.351177	1.282015	-0.109345
C	1.121374	1.196395	0.288033
C	1.730375	-0.061094	-0.320692
C	0.967631	-1.274376	0.171548
O	-2.337675	-0.038845	0.011767
O	-0.460963	-1.190435	-0.035842
H	-0.435798	1.586810	-1.156969
H	-0.898296	2.025035	0.467869
H	1.649445	2.092882	-0.038416
H	1.214168	1.154900	1.376777
H	1.688686	-0.010986	-1.412045
H	2.779640	-0.174267	-0.041841
H	1.269887	-2.184408	-0.342725
H	1.131141	-1.419315	1.242831

Molecule# 0747

tetrahydrothiophene

PointGroup: C2

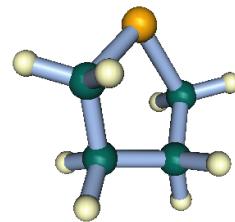
E= -555.531151315 au

ZPE= 0.113466 au

LUMO_eps= -0.01441 au

HOMO_eps= -0.21865 au

Dipole= 2.145 debye



13

H	0.727709	2.103092	0.342737
H	-0.986957	1.809222	0.025908
C	0.000000	1.349368	0.050917
H	1.422074	0.557865	-1.364380
H	0.016317	1.302538	-2.122147
C	0.340403	0.685094	-1.282406
H	-0.016317	-1.302538	-2.122147
H	-1.422074	-0.557865	-1.364380
C	-0.340403	-0.685094	-1.282406
H	0.986957	-1.809222	0.025908
H	-0.727709	-2.103092	0.342737
C	0.000000	-1.349368	0.050917
S	0.000000	0.000000	1.313352

Molecule# 0748
tetramethylbutane

PointGroup: C1

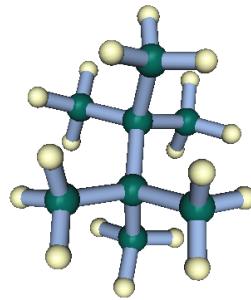
E= -315.820802155 au

ZPE= 0.243412 au

LUMO_eps= -0.01303 au

HOMO_eps= -0.30129 au

Dipole= 0.001 debye



26

C	-0.793806	0.000318	0.000712
C	0.794117	-0.000302	-0.000582
C	-1.356708	-0.190381	-1.421764
C	-1.354984	-1.136464	0.877663
C	-1.354681	1.328013	0.546448
C	1.357091	-0.075244	1.432659
C	1.353535	-1.204868	-0.782754
C	1.355771	1.278820	-0.652338
H	-2.441884	-0.073265	-1.406406
H	-1.144492	-1.183517	-1.816507
H	-0.962417	0.543192	-2.125265
H	-2.440034	-1.182634	0.768829
H	-1.142299	-0.980842	1.934840
H	-0.959235	-2.112026	0.594245
H	-2.439863	1.257189	0.639872
H	-1.140724	2.165686	-0.116604
H	-0.960397	1.570217	1.533667
H	2.442714	0.035395	1.406956
H	1.140854	-1.031082	1.908797
H	0.966525	0.716279	2.072656
H	2.439259	-1.240178	-0.675973
H	1.134677	-1.138294	-1.847977
H	0.961030	-2.153714	-0.416363
H	2.441259	1.201912	-0.736986
H	1.139195	2.167901	-0.060992
H	0.963822	1.438426	-1.657047

Molecule# 0749

tetrinitromethane

PointGroup: S4

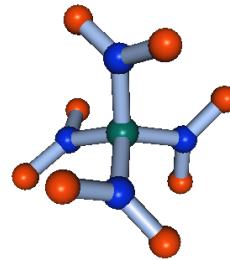
E= -858.762224373 au

ZPE= 0.054731 au

LUMO_eps= -0.16332 au

HOMO_eps= -0.37353 au

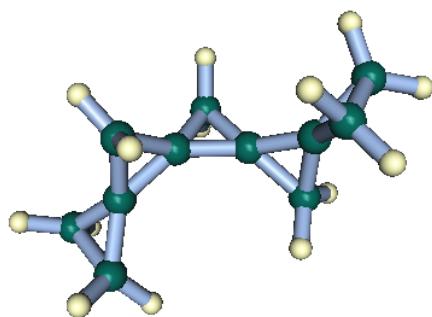
Dipole= 0.000 debye



13

C	0.000000	0.000000	0.000000
N	0.447266	-1.152752	0.927023
O	1.211160	-0.804270	1.793232
N	-0.447266	1.152752	0.927023
O	0.000000	2.247297	0.698711
O	-1.211160	0.804270	1.793232
N	-1.152752	-0.447266	-0.927023
O	-2.247297	0.000000	-0.698711
O	-0.804270	-1.211160	-1.793232
N	1.152752	0.447266	-0.927023
O	0.804270	1.211160	-1.793232
O	2.247297	0.000000	-0.698711
O	0.000000	-2.247297	0.698711

Molecule# 0750
 tetraspiro[2.0.0.0.2.1.1.1]undecane
 PointGroup: C2
 E= -427.552941284 au
 ZPE= 0.214587 au
 LUMO_eps= -0.00825 au
 HOMO_eps= -0.25813 au
 Dipole= 0.033 debye



25

C	0.413406	2.700298	-1.134720
C	0.000000	3.315092	0.199170
C	-0.395103	1.934856	-0.158726
C	-1.657201	1.128232	-0.172530
C	-0.395289	0.613063	0.456739
C	0.000000	0.000000	1.767022
C	0.395289	-0.613063	0.456739
C	1.657201	-1.128232	-0.172530
C	0.395103	-1.934856	-0.158726
C	0.000000	-3.315092	0.199170
C	-0.413406	-2.700298	-1.134720
H	-0.070461	3.069979	-2.029417
H	1.454651	2.435395	-1.262890
H	0.769193	3.453264	0.948163
H	-0.755429	4.089910	0.182539
H	-2.465963	1.433064	0.481413
H	-1.971867	0.689861	-1.112222
H	0.765446	0.497373	2.351754
H	-0.765446	-0.497373	2.351754
H	1.971867	-0.689861	-1.112222
H	2.465963	-1.433064	0.481413
H	-0.769193	-3.453264	0.948163
H	0.755429	-4.089910	0.182539
H	-1.454651	-2.435395	-1.262890
H	0.070461	-3.069979	-2.029417

Molecule# 0751

theophylline

PointGroup: C1

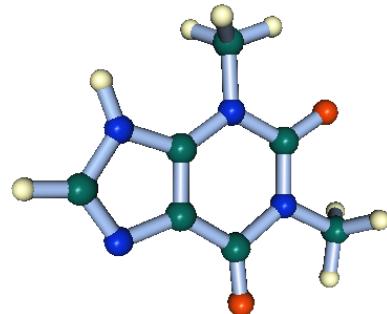
E= -641.289474681 au

ZPE= 0.159762 au

LUMO_eps= -0.03788 au

HOMO_eps= -0.23585 au

Dipole= 7.065 debye



21

O	-0.702493	-2.681831	-0.000062
C	-0.427456	-1.502083	-0.000033
C	0.890406	-0.915681	-0.000045
C	1.039767	0.449836	-0.000006
C	0.269702	2.790611	0.000072
N	0.022247	1.356401	0.000047
C	-1.294568	0.876674	0.000053
N	-1.455705	-0.502781	0.000017
C	-2.848272	-0.963109	0.000032
O	-2.241746	1.641359	0.000089
N	2.127187	-1.527354	-0.000091
C	2.991264	-0.559718	-0.000081
N	2.381227	0.689357	-0.000031
H	4.063530	-0.659977	-0.000108
H	2.840421	1.583267	-0.000003
H	0.825941	3.084691	0.892129
H	-0.692999	3.289743	0.000154
H	0.825822	3.084747	-0.892040
H	-3.364115	-0.590499	0.882301
H	-2.830297	-2.046278	0.000011
H	-3.364145	-0.590467	-0.882207

Molecule# 0752

thiadiazolidine-4-thione

PointGroup: C1

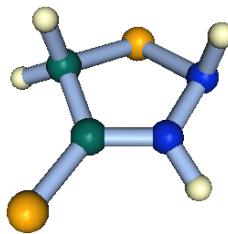
E= -984.591491620 au

ZPE= 0.068912 au

LUMO_eps= -0.06936 au

HOMO_eps= -0.22906 au

Dipole= 2.821 debye



10

S	-1.849048	-0.498034	-0.251110
S	2.347895	-0.118777	-0.102268
N	0.029899	1.184602	0.018376
N	-1.384596	1.156257	0.116381
C	0.716388	0.030291	0.085786
C	-0.237505	-1.118129	0.367886
H	0.445368	2.022351	-0.358482
H	-1.620549	1.333484	1.090140
H	0.061019	-2.005332	-0.179311
H	-0.257812	-1.340511	1.436386

Molecule# 0753

thiazole

PointGroup: Cs

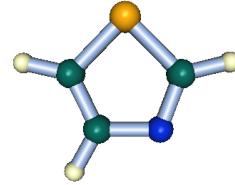
E= -569.148985987 au

ZPE= 0.055023 au

LUMO_eps= -0.04177 au

HOMO_eps= -0.26359 au

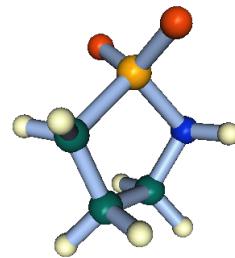
Dipole= 1.589 debye



8

C	0.639432	-1.264100	0.000000
C	1.220264	-0.033712	0.000000
C	-1.203295	-0.069611	0.000000
N	-0.732370	-1.277174	0.000000
S	0.000000	1.184691	0.000000
H	1.176233	-2.200416	0.000000
H	2.266607	0.216808	0.000000
H	-2.254655	0.173318	0.000000

Molecule# 0754
 thiazolidine-1,1-dioxide
 PointGroup: C1
 E= -722.042954418 au
 ZPE= 0.111308 au
 LUMO_eps= -0.02711 au
 HOMO_eps= -0.29094 au
 Dipole= 5.832 debye



14

C	1.834252	0.658103	-0.170078
C	1.649901	-0.833890	0.185441
C	0.498294	1.346797	0.118872
N	0.326076	-1.259222	-0.291458
O	-1.335449	-0.168992	1.339154
O	-1.629458	0.146059	-1.144584
S	-0.765053	0.008844	0.017322
H	2.646117	1.108508	0.400152
H	2.080033	0.749839	-1.228760
H	2.410975	-1.464557	-0.268110
H	1.690040	-0.982698	1.264866
H	0.427121	1.743751	1.127834
H	0.219725	2.107908	-0.603766
H	0.308880	-1.432296	-1.291141

Molecule# 0755

thietane

PointGroup: Cs

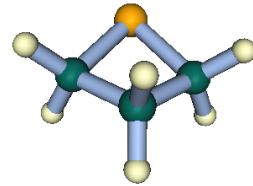
E= -516.176519983 au

ZPE= 0.083984 au

LUMO_eps= -0.01957 au

HOMO_eps= -0.22461 au

Dipole= 1.990 debye



10

S	0.340727	1.046092	0.000000
C	-0.205833	-0.304647	1.150622
C	-0.205833	-0.304647	-1.150622
C	-0.205833	-1.328854	0.000000
H	-1.195905	-0.094659	1.550789
H	0.484953	-0.493732	1.967693
H	-1.195905	-0.094659	-1.550789
H	0.484953	-0.493732	-1.967693
H	-1.043401	-2.027484	0.000000
H	0.718680	-1.904316	0.000000

Molecule# 0756

thirane

PointGroup: C2v

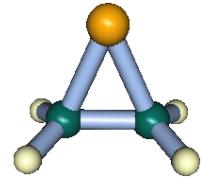
E= -476.851352951 au

ZPE= 0.054843 au

LUMO_eps= -0.01357 au

HOMO_eps= -0.23377 au

Dipole= 1.963 debye



7

S 0.000000 0.000000 0.871858

C 0.000000 0.738462 -0.803990

C 0.000000 -0.738462 -0.803990

H -0.912020 1.251798 -1.075460

H 0.912020 1.251798 -1.075460

H 0.912020 -1.251798 -1.075460

H -0.912020 -1.251798 -1.075460

Molecule# 0757

thioacetaldehyde

PointGroup: Cs

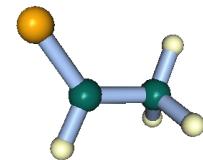
E= -476.855056965 au

ZPE= 0.053360 au

LUMO_eps= -0.08827 au

HOMO_eps= -0.23150 au

Dipole= 2.545 debye



7

C 0.000000 0.619383 0.000000

C -1.485214 0.718099 0.000000

S 0.874031 -0.744703 0.000000

H 0.520354 1.577729 0.000000

H -1.957612 -0.260850 0.000000

H -1.817979 1.286739 0.874315

H -1.817979 1.286739 -0.874315

Molecule# 0758

thioacetone

PointGroup: C2v

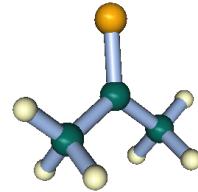
E= -516.191431489 au

ZPE= 0.081365 au

LUMO_eps= -0.07925 au

HOMO_eps= -0.22386 au

Dipole= 2.946 debye



10

C	0.000000	0.000000	-0.255900
S	0.000000	0.000000	1.375571
C	0.000000	1.266131	-1.062046
C	0.000000	-1.266131	-1.062046
H	0.000000	2.147096	-0.427764
H	0.000000	-2.147096	-0.427764
H	0.875313	1.291889	-1.718417
H	-0.875313	1.291889	-1.718417
H	-0.875313	-1.291889	-1.718417
H	0.875313	-1.291889	-1.718417

Molecule# 0759

thiobenzamide

PointGroup: C1

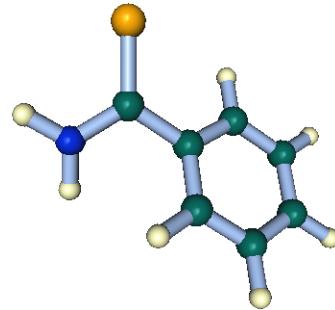
E= -724.065163010 au

ZPE= 0.125168 au

LUMO_eps= -0.07257 au

HOMO_eps= -0.21706 au

Dipole= 4.306 debye



16

N	-1.772399	1.554665	0.469600
C	-1.366140	0.325170	0.092859
S	-2.456819	-0.860510	-0.315837
C	0.106704	0.129865	0.044612
C	0.966492	1.187191	-0.276202
C	2.340741	0.991999	-0.324842
C	2.877285	-0.257721	-0.040450
C	2.030458	-1.315064	0.278402
C	0.657396	-1.126729	0.311776
H	-2.760372	1.733207	0.530743
H	-1.135771	2.217677	0.877192
H	0.563130	2.157313	-0.533805
H	2.990082	1.814218	-0.593305
H	3.947644	-0.409333	-0.073904
H	2.441819	-2.290833	0.498199
H	-0.008244	-1.945015	0.544143

Molecule# 0760

thiocyanatoacetic acid

PointGroup: C1

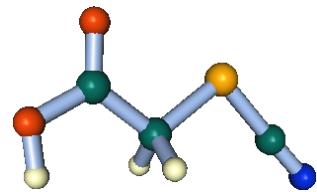
E= -719.655383461 au

ZPE= 0.061571 au

LUMO_eps= -0.06138 au

HOMO_eps= -0.28614 au

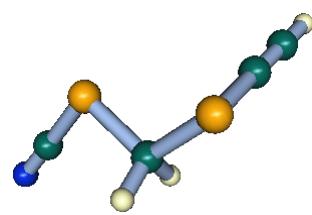
Dipole= 3.633 debye



10

S	-0.904941	-0.785080	-0.000054
O	2.696807	0.929615	0.000054
O	1.923496	-1.150439	-0.000102
N	-3.304099	0.760189	0.000086
C	0.294332	0.611111	0.000040
C	1.693547	0.022896	-0.000011
C	-2.320544	0.152967	0.000030
H	0.138262	1.224382	0.886861
H	0.138251	1.224511	-0.886690
H	2.364788	1.835806	0.000127

Molecule# 0761
thiocyanatomethylsulfanylacetylene
PointGroup: C1
E= -1005.401789510 au
ZPE= 0.057214 au
LUMO_eps= -0.06473 au
HOMO_eps= -0.26397 au
Dipole= 3.373 debye



10

S	-1.101935	0.129883	0.766287
S	1.586860	-1.013699	0.024402
N	-3.556241	0.444182	-0.651748
C	-0.110750	-0.717112	-0.552454
C	-2.556688	0.312656	-0.085241
C	2.264315	0.527879	-0.112470
C	2.817305	1.593553	-0.189220
H	-0.109558	-0.111181	-1.451631
H	-0.538550	-1.696769	-0.745449
H	3.297908	2.537882	-0.255392

Molecule# 0762

thioformaldehyde

PointGroup: C2v

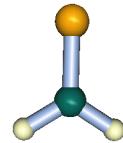
E= -437.514969744 au

ZPE= 0.024645 au

LUMO_eps= -0.10456 au

HOMO_eps= -0.24019 au

Dipole= 1.763 debye



4

S 0.000000 0.000000 0.585088

C 0.000000 0.000000 -1.025466

H 0.000000 0.920769 -1.604308

H 0.000000 -0.920769 -1.604308

Molecule# 0763

thiolane-1-oxide

PointGroup: C1

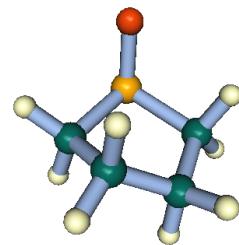
E= -630.751324563 au

ZPE= 0.116600 au

LUMO_eps= -0.01974 au

HOMO_eps= -0.23304 au

Dipole= 4.409 debye



14

C	1.387883	-0.811682	0.479852
C	1.678206	0.633319	0.061765
C	0.258572	-1.279223	-0.428050
C	0.330814	1.347067	-0.089120
O	-1.798582	-0.049523	0.835116
S	-1.000813	0.079000	-0.439396
H	2.269472	-1.447422	0.387147
H	1.059693	-0.849628	1.519688
H	2.312291	1.147645	0.784708
H	2.210285	0.636734	-0.891921
H	0.589747	-1.411400	-1.460234
H	-0.266524	-2.172907	-0.098828
H	-0.021163	1.794675	0.838932
H	0.315012	2.097602	-0.876757

Molecule# 0764

thiolane-1,1-dioxide

PointGroup: C2

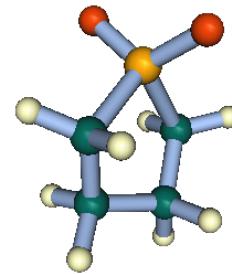
E= -706.002040110 au

ZPE= 0.122223 au

LUMO_eps= -0.02340 au

HOMO_eps= -0.28884 au

Dipole= 5.418 debye



15

C	0.000000	0.770224	-1.780388
C	0.000000	-0.770224	-1.780388
C	-0.597986	1.220604	-0.448931
C	0.597986	-1.220604	-0.448931
O	-1.137264	-0.551302	1.517439
O	1.137264	0.551302	1.517439
S	0.000000	0.000000	0.784354
H	1.022518	1.140282	-1.873334
H	-0.569407	1.169658	-2.618789
H	-1.022518	-1.140282	-1.873334
H	0.569407	-1.169658	-2.618789
H	-0.277102	2.202041	-0.111847
H	-1.683808	1.153218	-0.434458
H	0.277102	-2.202041	-0.111847
H	1.683808	-1.153218	-0.434458

Molecule# 0765

thiophene-1-oxide

PointGroup: C1

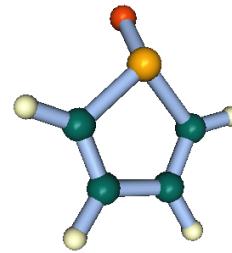
E= -628.281565200 au

ZPE= 0.069440 au

LUMO_eps= -0.08750 au

HOMO_eps= -0.24561 au

Dipole= 4.362 debye



10

C	1.612095	-0.729797	0.125254
C	1.612095	0.729797	0.125254
C	0.390198	-1.266356	0.004379
C	0.390198	1.266356	0.004379
O	-2.034840	0.000000	0.503621
S	-0.812350	0.000000	-0.367403
H	2.522887	-1.308036	0.196077
H	2.522887	1.308036	0.196077
H	0.101515	-2.302731	-0.049137
H	0.101515	2.302731	-0.049137

Molecule# 0766

thiophene

PointGroup: C2v

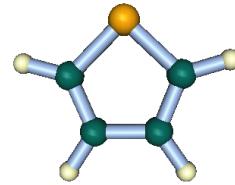
E= -553.100390309 au

ZPE= 0.066535 au

LUMO_eps= -0.02549 au

HOMO_eps= -0.24611 au

Dipole= 0.527 debye



9

C	0.000000	0.711523	-1.267123
C	0.000000	-0.711523	-1.267123
C	0.000000	1.238059	-0.009487
C	0.000000	-1.238059	-0.009487
S	0.000000	0.000000	1.192594
H	0.000000	1.314467	-2.162845
H	0.000000	-1.314467	-2.162845
H	0.000000	2.274447	0.281757
H	0.000000	-2.274447	0.281757

Molecule# 0767

thiophosgene

PointGroup: C2v

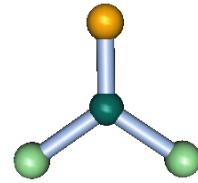
E= -1356.786159680 au

ZPE= 0.007876 au

LUMO_eps= -0.11743 au

HOMO_eps= -0.26961 au

Dipole= 0.499 debye



4

C1 0.000000 1.435076 -0.846417

C 0.000000 0.000000 0.142885

C1 0.000000 -1.435076 -0.846417

S 0.000000 0.000000 1.745054

Molecule# 0768

thiosemicarbazide

PointGroup: C1

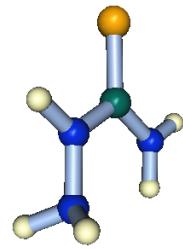
E= -603.668416894 au

ZPE= 0.077997 au

LUMO_eps= -0.03375 au

HOMO_eps= -0.21038 au

Dipole= 5.727 debye



10

S	-1.756434	-0.365803	-0.000188
N	0.863151	-0.693485	0.000281
N	0.167197	1.487661	-0.000079
N	2.197899	-0.268846	0.000181
C	-0.173325	0.187895	0.000004
H	0.618610	-1.671311	0.000117
H	1.137120	1.757055	0.000069
H	-0.566962	2.169753	-0.000192
H	2.678241	-0.603657	0.827164
H	2.678150	-0.603667	-0.826856

Molecule# 0769

thiourea

PointGroup: C2

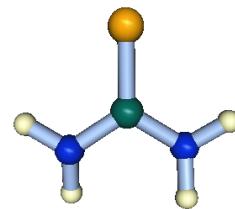
E= -548.325021712 au

ZPE= 0.060868 au

LUMO_eps= -0.03224 au

HOMO_eps= -0.21577 au

Dipole= 5.046 debye



8

C	0.000000	0.000000	-0.316883
S	0.000000	0.000000	1.353097
N	0.000000	1.146987	-1.046835
N	0.000000	-1.146987	-1.046835
H	0.128543	2.000926	-0.533905
H	0.285536	1.143343	-2.012373
H	-0.128543	-2.000926	-0.533905
H	-0.285536	-1.143343	-2.012373

Molecule# 0770

threonine

PointGroup: C1

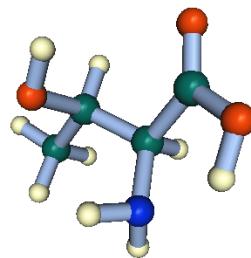
E= -438.465665691 au

ZPE= 0.141163 au

LUMO_eps= -0.03132 au

HOMO_eps= -0.27153 au

Dipole= 4.248 debye



17

N	-0.051147	1.703848	0.244380
C	-0.043314	0.431492	-0.483504
C	-1.376086	-0.303235	-0.228367
O	-1.530938	-1.479219	-0.435919
O	-2.351637	0.487074	0.227525
H	-1.928124	1.363089	0.369080
C	1.141533	-0.499575	-0.166921
O	1.167043	-0.778126	1.238261
C	2.485110	0.099679	-0.539476
H	-0.035888	0.649255	-1.555103
H	0.984216	-1.425674	-0.722324
H	0.509733	-1.457032	1.425652
H	3.279834	-0.613026	-0.325853
H	2.518013	0.345316	-1.601845
H	2.686599	1.005623	0.033605
H	0.347974	1.576034	1.168534
H	0.476463	2.421484	-0.231731

Molecule# 0771

thymine

PointGroup: C1

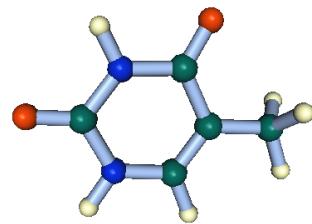
E= -454.318274789 au

ZPE= 0.114529 au

LUMO_eps= -0.05675 au

HOMO_eps= -0.25588 au

Dipole= 4.426 debye



15

N	-0.726579	1.028726	-0.000001
C	0.669751	0.895487	0.000064
O	1.378069	1.884236	0.000131
C	1.153712	-0.486497	0.000042
C	2.632341	-0.716781	0.000106
C	0.240400	-1.474972	-0.000038
N	-1.115294	-1.239106	-0.000094
C	-1.675291	0.026086	-0.000082
O	-2.872270	0.222918	-0.000137
H	-1.085233	1.972913	0.000012
H	3.096734	-0.258658	0.874392
H	2.863608	-1.781203	0.000091
H	3.096819	-0.258616	-0.874114
H	0.522304	-2.518618	-0.000059
H	-1.773003	-2.000335	-0.000157

Molecule# 0772

toluene

PointGroup: C1

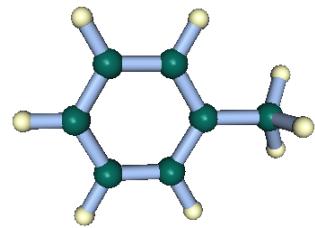
E= -271.666929235 au

ZPE= 0.127517 au

LUMO_eps= -0.01604 au

HOMO_eps= -0.24809 au

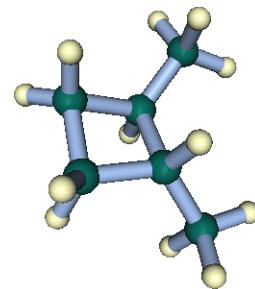
Dipole= 0.406 debye



15

C	-1.897971	-0.000097	0.008691
C	-1.196697	1.200136	0.001975
C	-1.196435	-1.200271	0.001973
C	0.193419	1.197285	-0.008982
C	0.193595	-1.197195	-0.008976
C	0.910843	0.000147	-0.011486
C	2.417290	0.000075	0.009328
H	-2.979553	-0.000212	0.014466
H	-1.731919	2.140543	0.001706
H	-1.731521	-2.140756	0.001687
H	0.729597	2.138337	-0.018405
H	0.729920	-2.138174	-0.018405
H	2.822376	-0.877771	-0.494005
H	2.822189	0.887290	-0.477332
H	2.794646	-0.009730	1.035147

Molecule# 0773
 trans-1,2-dimethylcyclobutane
 PointGroup: C2
 E= -235.934903010 au
 ZPE= 0.165935 au
 LUMO_eps= -0.00810 au
 HOMO_eps= -0.29087 au
 Dipole= 0.089 debye



18

C	-0.126624	0.767713	-0.173969
C	0.126624	-0.767713	-0.173969
C	0.126624	0.763654	1.356240
C	-0.126624	-0.763654	1.356240
C	0.714435	1.661716	-1.066390
C	-0.714435	-1.661716	-1.066390
H	-1.188759	0.949185	-0.364152
H	1.188759	-0.949185	-0.364152
H	1.167412	0.999661	1.584849
H	-0.514312	1.387012	1.978811
H	-1.167412	-0.999661	1.584849
H	0.514312	-1.387012	1.978811
H	1.780030	1.498868	-0.888391
H	0.519941	1.467661	-2.123812
H	0.505264	2.718063	-0.882589
H	-1.780030	-1.498868	-0.888391
H	-0.519941	-1.467661	-2.123812
H	-0.505264	-2.718063	-0.882589

Molecule# 0774

trans-1,3-dimethylcyclobutane

PointGroup: Cs

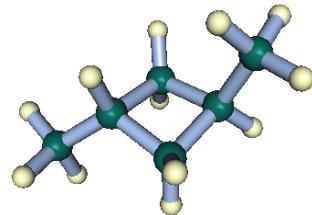
E= -235.933129346 au

ZPE= 0.166016 au

LUMO_eps= -0.00947 au

HOMO_eps= -0.28867 au

Dipole= 0.021 debye



18

C	0.244705	0.078242	1.082742
C	0.244705	0.078242	-1.082742
C	0.834997	-0.869296	0.000000
C	-0.656207	0.731128	0.000000
C	0.244705	-2.272702	0.000000
C	-0.820584	2.239722	0.000000
H	-0.252168	-0.391852	1.932537
H	0.988396	0.780747	1.462896
H	-0.252168	-0.391852	-1.932537
H	0.988396	0.780747	-1.462896
H	1.923688	-0.935418	0.000000
H	-1.640735	0.259122	0.000000
H	-0.847355	-2.246577	0.000000
H	0.151583	2.738338	0.000000
H	0.561618	-2.832501	-0.882519
H	0.561618	-2.832501	0.882519
H	-1.368402	2.579864	-0.881781
H	-1.368402	2.579864	0.881781

Molecule# 0775

trans-2-butenal

PointGroup: Cs

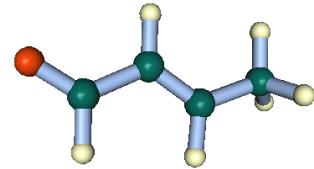
E= -231.328847532 au

ZPE= 0.089225 au

LUMO_eps= -0.06889 au

HOMO_eps= -0.26304 au

Dipole= 4.256 debye



11

C	0.000000	0.336443	0.000000
C	-0.894961	-0.655241	0.000000
C	1.437530	0.059783	0.000000
C	-2.376114	-0.496353	0.000000
O	2.302239	0.907893	0.000000
H	-0.296890	1.379137	0.000000
H	-0.520454	-1.676347	0.000000
H	1.704005	-1.017594	0.000000
H	-2.814656	-0.983507	0.874815
H	-2.814656	-0.983507	-0.874815
H	-2.673991	0.550880	0.000000

Molecule# 0776
trans-2,3-dimethylnorborane

PointGroup: C1

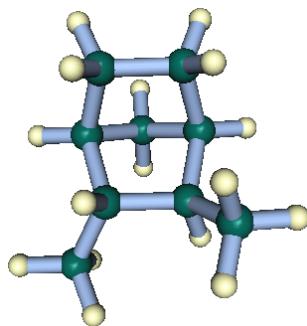
E= -352.721058931 au

ZPE= 0.231887 au

LUMO_eps= -0.01139 au

HOMO_eps= -0.28748 au

Dipole= 0.067 debye



25

C	0.707742	-0.940168	1.191925
C	0.805573	0.571081	0.911672
C	0.286298	-1.294617	-0.248550
C	1.813009	0.594515	-0.256246
C	-0.630377	0.862567	0.409362
C	-0.961973	-0.400731	-0.457716
C	1.455724	-0.696655	-1.057146
H	-0.041153	-1.191218	1.943754
H	1.658013	-1.391146	1.482484
H	1.098896	1.197400	1.754117
H	0.105962	-2.349691	-0.452928
H	2.832978	0.547501	0.127018
C	-2.278499	-1.071176	-0.071401
H	2.300532	-1.386094	-1.086752
H	-1.280255	0.846643	1.290316
H	1.172461	-0.486382	-2.089154
C	-0.854203	2.196159	-0.296344
H	1.744295	1.498504	-0.859168
H	-1.027284	-0.113838	-1.511063
H	-3.112889	-0.370708	-0.150666
H	-2.254833	-1.436327	0.957417
H	-2.497120	-1.920640	-0.721600
H	-0.581866	3.037107	0.345146
H	-1.905142	2.317448	-0.566598
H	-0.272369	2.275590	-1.215659

Molecule# 0777

trans-2,3,4-hexatriene

PointGroup: C2h

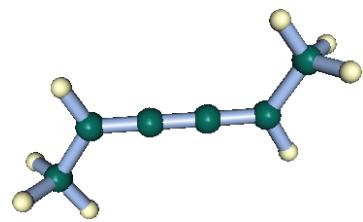
E= -233.460910680 au

ZPE= 0.116673 au

LUMO_eps= -0.04742 au

HOMO_eps= -0.22697 au

Dipole= 0.000 debye



14

C	1.233554	-2.804366	0.000000
H	1.251117	-3.456614	0.877469
H	1.251117	-3.456614	-0.877469
H	2.138991	-2.200941	0.000000
C	-1.233554	2.804366	0.000000
H	-1.251117	3.456614	-0.877469
H	-1.251117	3.456614	0.877469
H	-2.138991	2.200941	0.000000
C	0.001866	-1.946573	0.000000
H	-0.953142	-2.465454	0.000000
C	-0.001866	1.946573	0.000000
H	0.953142	2.465454	0.000000
C	0.001866	0.631609	0.000000
C	-0.001866	-0.631609	0.000000

Molecule# 0778

trans-decalin

PointGroup: C2h

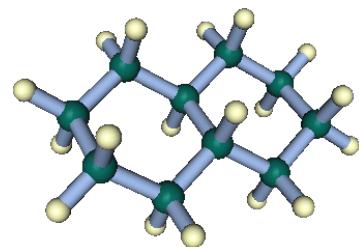
E= -392.071969436 au

ZPE= 0.262768 au

LUMO_eps= -0.00935 au

HOMO_eps= -0.28060 au

Dipole= 0.000 debye



28

C	-0.225728	0.731655	2.543314
C	0.225728	-0.731655	2.543314
C	0.225728	1.456661	1.272775
C	-0.225728	-1.456661	1.272775
C	-0.231499	0.735086	0.000000
C	0.231499	-0.735086	0.000000
C	0.225728	1.456661	-1.272775
C	-0.225728	0.731655	-2.543314
C	0.225728	-0.731655	-2.543314
C	-0.225728	-1.456661	-1.272775
H	0.156998	1.245982	-3.427820
H	-0.156998	-1.245982	3.427820
H	0.150668	-2.483241	-1.270085
H	-0.156998	-1.245982	-3.427820
H	1.318123	-0.770907	-2.610688
H	-0.150668	2.483241	1.270085
H	0.156998	1.245982	3.427820
H	-0.150668	2.483241	-1.270085
H	0.150668	-2.483241	1.270085
H	-1.318123	0.770907	2.610688
H	1.319276	1.529769	-1.266570
H	1.319276	1.529769	1.266570
H	1.318123	-0.770907	2.610688
H	-1.318123	0.770907	-2.610688
H	-1.319276	-1.529769	1.266570
H	-1.319276	-1.529769	-1.266570
H	-1.330699	0.726592	0.000000
H	1.330699	-0.726592	0.000000

Molecule# 0779

trans-dithiocyanatoethene

PointGroup: C1

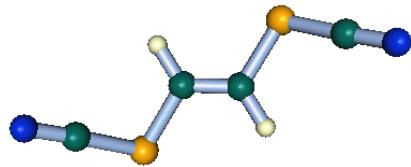
E= -1059.594960020 au

ZPE= 0.051484 au

LUMO_eps= -0.07709 au

HOMO_eps= -0.27592 au

Dipole= 3.222 debye



10

S	2.050341	0.742508	-0.499891
S	-2.050342	-0.742503	-0.499907
N	3.923970	-0.715598	1.081612
N	-3.923966	0.715581	1.081626
C	0.603325	-0.276815	-0.332055
C	-0.603328	0.276827	-0.332072
C	3.140682	-0.141456	0.456341
C	-3.140681	0.141447	0.456343
H	0.769347	-1.345261	-0.318590
H	-0.769353	1.345273	-0.318638

Molecule# 0780

tribromochloromethane

PointGroup: C3v

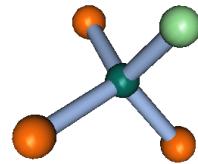
E= -8221.008318790 au

ZPE= 0.007318 au

LUMO_eps= -0.10707 au

HOMO_eps= -0.29589 au

Dipole= 0.074 debye



5

C 0.000000 0.000000 0.303323

Cl 0.000000 0.000000 2.077798

Br 0.000000 1.848334 -0.353738

Br 1.600704 -0.924167 -0.353738

Br -1.600704 -0.924167 -0.353738

Molecule# 0781

tribromofluoromethane

PointGroup: C3v

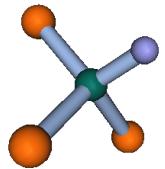
E= -7860.663967180 au

ZPE= 0.009033 au

LUMO_eps= -0.10151 au

HOMO_eps= -0.29813 au

Dipole= 0.453 debye



5

C 0.000000 0.000000 0.433853

F 0.000000 0.000000 1.771869

Br 0.000000 1.859061 -0.176666

Br 1.609994 -0.929531 -0.176666

Br -1.609994 -0.929531 -0.176666

Molecule# 0782

tribromomethane

PointGroup: C3v

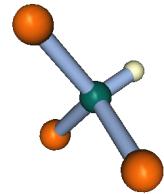
E= -7761.395813970 au

ZPE= 0.017841 au

LUMO_eps= -0.08706 au

HOMO_eps= -0.29120 au

Dipole= 0.865 debye



5

C 0.000000 0.000000 0.519257

Br 0.000000 1.862001 -0.044887

Br -1.612540 -0.931001 -0.044887

Br 1.612540 -0.931001 -0.044887

H 0.000000 0.000000 1.597626

Molecule# 0783

trichloroacetaldehyde

PointGroup: Cs

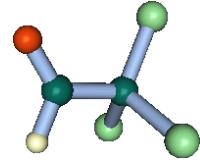
E= -1532.764979660 au

ZPE= 0.027738 au

LUMO_eps= -0.08760 au

HOMO_eps= -0.30813 au

Dipole= 1.573 debye



7

C 0.038452 0.035580 0.000000

C 0.922994 -1.233024 0.000000

O 0.496614 -2.344783 0.000000

Cl -1.683707 -0.338809 0.000000

Cl 0.496614 0.961332 1.470611

Cl 0.496614 0.961332 -1.470611

H 1.996540 -0.982605 0.000000

Molecule# 0784

trichloroethylene

PointGroup: Cs

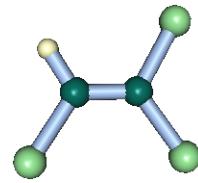
E= -1457.512555340 au

ZPE= 0.024617 au

LUMO_eps= -0.04272 au

HOMO_eps= -0.26685 au

Dipole= 0.855 debye



6

C -1.034580 -0.395303 0.000000

C 0.000000 0.438157 0.000000

H -2.045695 -0.022811 0.000000

Cl -0.896263 -2.113950 0.000000

Cl -0.268366 2.154033 0.000000

Cl 1.650109 -0.053866 0.000000

Molecule# 0785

trichlorofluoromethane

PointGroup: C3v

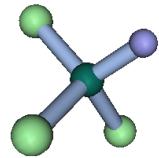
E= -1518.684794240 au

ZPE= 0.010898 au

LUMO_eps= -0.06811 au

HOMO_eps= -0.32863 au

Dipole= 0.372 debye



5

C 0.000000 0.000000 0.251893

F 0.000000 0.000000 1.591574

Cl 0.000000 1.691025 -0.310500

Cl 1.464470 -0.845512 -0.310500

Cl -1.464470 -0.845512 -0.310500

Molecule# 0786

trichloromethane

PointGroup: C3v

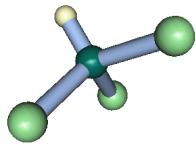
E= -1419.413620110 au

ZPE= 0.019660 au

LUMO_eps= -0.05479 au

HOMO_eps= -0.31916 au

Dipole= 1.085 debye



5

C 0.000000 0.000000 0.456698

Cl 0.000000 1.697300 -0.083852

Cl -1.469905 -0.848650 -0.083852

Cl 1.469905 -0.848650 -0.083852

H 0.000000 0.000000 1.536281

Molecule# 0787

tricyclo[3.2.1.0(1,5)]octane

PointGroup: Cs

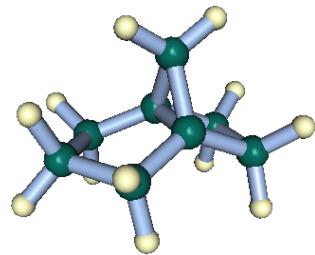
E= -312.114584377 au

ZPE= 0.179816 au

LUMO_eps= -0.01017 au

HOMO_eps= -0.22899 au

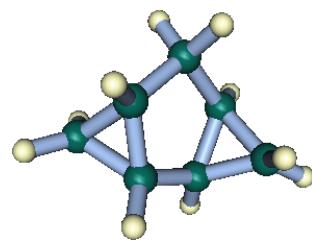
Dipole= 0.458 debye



20

C	-0.091009	0.344069	0.762763
C	-0.091009	0.344069	-0.762763
C	-1.274798	0.863593	0.000000
C	1.043254	1.383282	0.782434
C	-0.091009	-1.088216	1.246819
C	1.043254	1.383282	-0.782434
C	-0.091009	-1.088216	-1.246819
C	-0.542343	-1.905205	0.000000
H	-2.164538	0.249662	0.000000
H	-1.477867	1.927933	0.000000
H	1.969402	0.987255	1.196949
H	0.820737	2.329837	1.278331
H	-0.731511	-1.283950	2.109647
H	0.926511	-1.368063	1.532126
H	0.820737	2.329837	-1.278331
H	1.969402	0.987255	-1.196949
H	0.926511	-1.368063	-1.532126
H	-0.731511	-1.283950	-2.109647
H	-1.627719	-2.012526	0.000000
H	-0.132150	-2.915184	0.000000

Molecule# 0788
 tricyclo[4.1.0.0]heptane
 PointGroup: C2
 E= -272.800444953 au
 ZPE= 0.151335 au
 LUMO_eps= -0.00716 au
 HOMO_eps= -0.26221 au
 Dipole= 0.038 debye



17

C	0.000000	1.212629	0.508884
C	1.216393	1.420165	-0.356202
C	0.000000	0.000000	1.437632
C	-0.001233	0.749275	-0.932390
C	0.001233	-0.749275	-0.932390
C	-1.216393	-1.420165	-0.356202
H	-0.565029	2.087185	0.799175
H	2.090716	0.811351	-0.162580
H	1.434669	2.428532	-0.679316
H	-0.877843	0.008372	2.088558
H	0.877843	-0.008372	2.088558
H	-0.578811	1.277641	-1.680483
H	0.578811	-1.277641	-1.680483
H	-1.434669	-2.428532	-0.679316
H	-2.090716	-0.811351	-0.162580
C	0.000000	-1.212629	0.508884
H	0.565029	-2.087185	0.799175

Molecule# 0789

triethylamine

PointGroup: C3

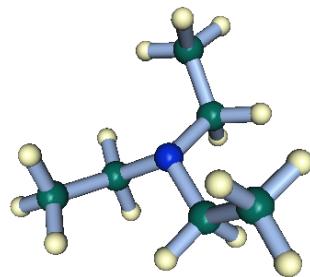
E= -292.529312917 au

ZPE= 0.204501 au

LUMO_eps= -0.00838 au

HOMO_eps= -0.21608 au

Dipole= 0.521 debye



22

C	0.303046	2.442712	-0.429029
C	-2.266973	-0.958910	-0.429029
C	1.963927	-1.483802	-0.429029
C	-0.336477	1.361557	0.436145
C	-1.010905	-0.972176	0.436145
C	1.347381	-0.389381	0.436145
N	0.000000	0.000000	0.013396
H	1.392234	2.405845	-0.399061
H	-0.007763	2.331357	-1.467880
H	0.000000	3.431615	-0.080419
H	-2.779640	0.002788	-0.399061
H	-2.015133	-1.172401	-1.467880
H	-2.971866	-1.715807	-0.080419
H	1.387406	-2.408633	-0.399061
H	2.022896	-1.158955	-1.467880
H	2.971866	-1.715807	-0.080419
H	-1.418618	1.473387	0.378135
H	-0.069001	1.520307	1.495273
H	-0.566682	-1.965253	0.378135
H	-1.282124	-0.819910	1.495273
H	1.985300	0.491866	0.378135
H	1.351125	-0.700397	1.495273

Molecule# 0790

trifluoroacetaldehyde

PointGroup: Cs

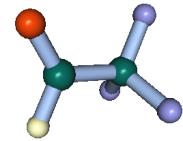
E= -451.730237471 au

ZPE= 0.032876 au

LUMO_eps= -0.09438 au

HOMO_eps= -0.31680 au

Dipole= 1.726 debye



7

C 0.015025 0.360286 0.000000

C 0.501815 -1.106329 0.000000

O -0.245494 -2.035813 0.000000

F -1.307957 0.464386 0.000000

F 0.501815 0.987853 1.088479

F 0.501815 0.987853 -1.088479

H 1.601854 -1.198064 0.000000

Molecule# 0791

trifluoroacetic acid

PointGroup: Cs

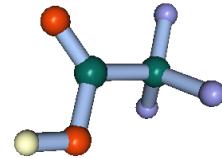
E= -527.014756135 au

ZPE= 0.038633 au

LUMO_eps= -0.05872 au

HOMO_eps= -0.33356 au

Dipole= 2.229 debye



8

C	0.085896	0.594059	0.000000
C	-0.294386	-0.910548	0.000000
O	0.812941	-1.659252	0.000000
O	-1.420191	-1.307503	0.000000
F	-1.007987	1.348927	0.000000
F	0.812941	0.893583	1.087792
F	0.812941	0.893583	-1.087792
H	0.547878	-2.591865	0.000000

Molecule# 0792

trifluoroacetonitrile

PointGroup: C3v

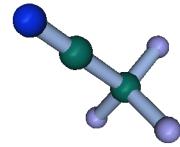
E= -430.628345072 au

ZPE= 0.022424 au

LUMO_eps= -0.04623 au

HOMO_eps= -0.40168 au

Dipole= 1.311 debye



6

C 0.000000 0.000000 -0.320697

C 0.000000 0.000000 1.160968

N 0.000000 0.000000 2.307595

F 0.000000 1.253146 -0.784992

F 1.085256 -0.626573 -0.784992

F -1.085256 -0.626573 -0.784992

Molecule# 0793

trifluoroacetylchloride

PointGroup: Cs

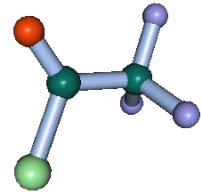
E= -911.373927511 au

ZPE= 0.024220 au

LUMO_eps= -0.09826 au

HOMO_eps= -0.34451 au

Dipole= 0.810 debye



7

C 0.542207 -0.688625 0.000000

C 0.081178 0.798349 0.000000

O 0.821365 1.714338 0.000000

F 1.870099 -0.749751 0.000000

F 0.081178 -1.316809 1.087399

F 0.081178 -1.316809 -1.087399

Cl -1.682548 0.945722 0.000000

Molecule# 0794

trifluoromethane

PointGroup: C3v

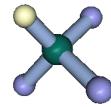
E= -338.381378940 au

ZPE= 0.024983 au

LUMO_eps= -0.00946 au

HOMO_eps= -0.41325 au

Dipole= 1.639 debye



5

C 0.000000 0.000000 0.340441

F 0.000000 1.256469 -0.128588

F -1.088134 -0.628234 -0.128588

F 1.088134 -0.628234 -0.128588

H 0.000000 0.000000 1.429227

Molecule# 0795

trifluoromethanol

PointGroup: Cs

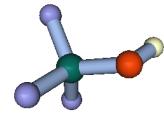
E= -413.647048120 au

ZPE= 0.028459 au

LUMO_eps= -0.02634 au

HOMO_eps= -0.38163 au

Dipole= 1.974 debye



6

C	0.001401	0.023882	0.000000
O	-1.039480	0.879467	0.000000
F	1.127698	0.728595	0.000000
F	0.001401	-0.784388	1.081319
F	0.001401	-0.784388	-1.081319
H	-1.867070	0.382602	0.000000

Molecule# 0796

trifluoromethylbenzene

PointGroup: C1

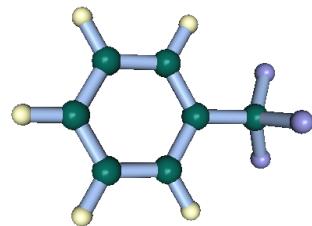
E= -569.515919953 au

ZPE= 0.104913 au

LUMO_eps= -0.04663 au

HOMO_eps= -0.28109 au

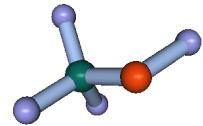
Dipole= 2.947 debye



15

C	-2.830605	-0.004894	0.011148
C	-2.141181	1.201669	0.001644
C	-2.130097	-1.206446	0.001574
C	-0.751864	1.211198	-0.016805
C	-0.742127	-1.203364	-0.017162
C	-0.054399	0.007588	-0.027137
C	1.449778	0.003678	-0.003578
F	1.974663	1.157149	-0.464769
F	1.932309	-0.167372	1.251571
F	1.967606	-0.995256	-0.750684
H	-3.912035	-0.009776	0.023540
H	-2.683315	2.137140	0.005948
H	-2.664442	-2.146382	0.005924
H	-0.213065	2.147199	-0.028956
H	-0.195372	-2.135445	-0.029626

Molecule# 0797
trifluoromethylhypofluorite
PointGroup: Cs
E= -512.786577968 au
ZPE= 0.019717 au
LUMO_eps= -0.11039 au
HOMO_eps= -0.37675 au
Dipole= 0.381 debye



6
C 0.328492 0.194175 0.000000
O -1.058695 0.337244 0.000000
F 0.765646 1.447109 0.000000
F 0.765646 -0.443615 1.077970
F 0.765646 -0.443615 -1.077970
F -1.574869 -0.989103 0.000000

Molecule# 0798

trimethoxymethylbenzene

PointGroup: C1

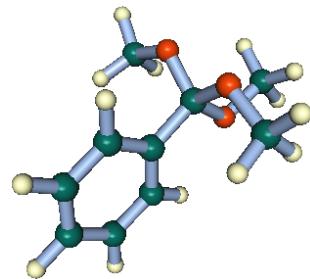
E= -615.369148963 au

ZPE= 0.225465 au

LUMO_eps= -0.02503 au

HOMO_eps= -0.25800 au

Dipole= 1.212 debye



27

C	-3.388472	-0.000044	0.286846
C	-2.807439	0.000148	-0.978192
C	-2.578343	-0.000206	1.414731
C	-1.425809	0.000177	-1.109541
C	-1.192222	-0.000179	1.283865
C	-0.608039	0.000014	0.021203
C	1.023124	2.379898	-0.470319
C	1.023043	-2.379763	-0.470812
C	2.948244	-0.000221	1.058956
C	0.905320	0.000039	-0.194792
O	1.326351	1.086368	-0.980293
O	1.326380	-1.086139	-0.980478
O	1.520552	-0.000056	1.068131
H	-4.465338	-0.000067	0.390194
H	-3.431913	0.000275	-1.861615
H	-3.022627	-0.000356	2.401202
H	-0.970398	0.000327	-2.090355
H	-0.562616	-0.000306	2.160548
H	1.487995	3.084722	-1.155242
H	1.431223	2.525679	0.531882
H	-0.053609	2.559742	-0.444154
H	1.430937	-2.525742	0.531445
H	1.488048	-3.084462	-1.155774
H	-0.053696	-2.559606	-0.444897
H	3.344275	0.885053	0.560867
H	3.344088	-0.886340	0.562212
H	3.250946	0.000524	2.103146

Molecule# 0799

trimethylamine

PointGroup: Cs

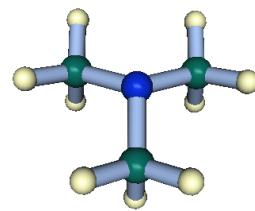
E= -174.544562920 au

ZPE= 0.119571 au

LUMO_eps= -0.01204 au

HOMO_eps= -0.21872 au

Dipole= 0.506 debye



13

C	0.000000	1.388631	-0.059542
C	1.202590	-0.694316	-0.059542
C	-1.202590	-0.694316	-0.059542
N	0.000000	0.000000	0.366212
H	-0.882915	1.895599	0.330609
H	0.000000	1.499929	-1.158458
H	0.882915	1.895599	0.330609
H	2.083094	-0.183172	0.330609
H	1.298977	-0.749964	-1.158458
H	1.200179	-1.712426	0.330609
H	-1.200179	-1.712426	0.330609
H	-1.298977	-0.749964	-1.158458
H	-2.083094	-0.183172	0.330609

Molecule# 0800

trimethylenecyclopropane

PointGroup: C3v

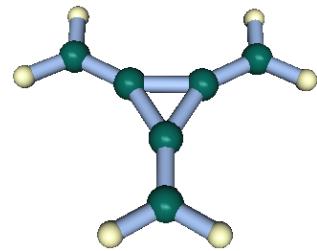
E= -232.202050112 au

ZPE= 0.094045 au

LUMO_eps= -0.08963 au

HOMO_eps= -0.25467 au

Dipole= 0.000 debye



12

C	0.000000	0.830500	0.000000
C	0.719234	-0.415250	0.000000
C	-0.719234	-0.415250	0.000000
C	0.000000	2.159401	0.000000
C	1.870096	-1.079700	0.000000
C	-1.870096	-1.079700	0.000000
H	-0.925056	2.719957	0.000000
H	0.925056	2.719957	0.000000
H	2.818080	-0.558856	0.000000
H	1.893024	-2.161100	0.000000
H	-1.893024	-2.161100	0.000000
H	-2.818080	-0.558856	0.000000

Molecule# 0801

trimethylorthoformate

PointGroup: C1

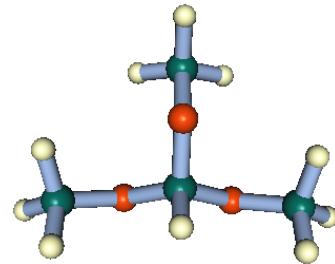
E= -384.241060537 au

ZPE= 0.145084 au

LUMO_eps= -0.01043 au

HOMO_eps= -0.27971 au

Dipole= 1.080 debye



17

C	0.000002	-0.367307	0.256085
O	-0.000002	0.965131	0.702169
C	-0.000007	1.956470	-0.327711
O	-1.098087	-0.677695	-0.536994
C	-2.334659	-0.671033	0.163443
O	1.098092	-0.677688	-0.536995
C	2.334663	-0.671026	0.163443
H	0.000003	-0.955286	1.185152
H	-0.000019	2.916553	0.181998
H	0.887101	1.876333	-0.957416
H	-0.887109	1.876316	-0.957423
H	-2.319311	-1.383477	0.994703
H	-2.574558	0.320771	0.552376
H	-3.094725	-0.974563	-0.551733
H	2.574558	0.320777	0.552383
H	2.319318	-1.383476	0.994698
H	3.094731	-0.974549	-0.551734

Molecule# 0802

trioxidanyl methane

PointGroup: C1

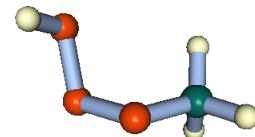
E= -266.113450943 au

ZPE= 0.058109 au

LUMO_eps= -0.02147 au

HOMO_eps= -0.30271 au

Dipole= 1.229 debye



8

O	0.614839	-0.531311	0.412981
O	-0.558693	-0.562512	-0.398497
O	1.453969	0.529309	-0.061717
C	-1.474009	0.413749	0.097467
H	1.911049	0.100315	-0.801444
H	-1.737810	0.202807	1.133973
H	-2.351255	0.313601	-0.540435
H	-1.058850	1.416901	0.000969

Molecule# 0803
tris-(methylsulfanyl)methane

PointGroup: C3

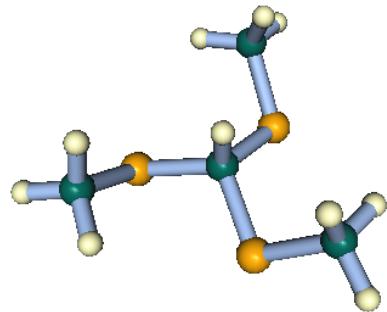
E= -1353.179496530 au

ZPE= 0.132901 au

LUMO_eps= -0.01566 au

HOMO_eps= -0.23017 au

Dipole= 3.171 debye



17

C	-0.299347	2.755142	0.647638
C	2.535697	-1.118329	0.647638
C	-2.236350	-1.636813	0.647638
C	0.000000	0.000000	0.150368
S	0.610957	1.615429	-0.447444
S	1.093524	-1.336819	-0.447444
S	-1.704481	-0.278610	-0.447444
H	0.000000	3.759716	0.355248
H	-0.029337	2.594355	1.690157
H	-1.372452	2.645233	0.513627
H	2.261446	-1.271771	1.690157
H	2.977065	-0.134038	0.513627
H	3.256010	-1.879858	0.355248
H	-3.256010	-1.879858	0.355248
H	-2.232109	-1.322585	1.690157
H	-1.604613	-2.511195	0.513627
H	0.000000	0.000000	1.240520

Molecule# 0804

trispiro[2.0.0.2.1.1]nonane

PointGroup: C2

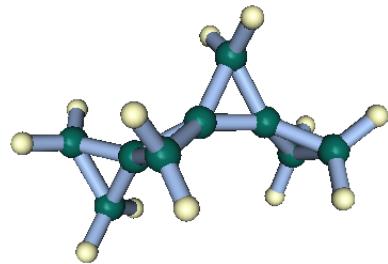
E= -350.150545873 au

ZPE= 0.181197 au

LUMO_eps= -0.00779 au

HOMO_eps= -0.26146 au

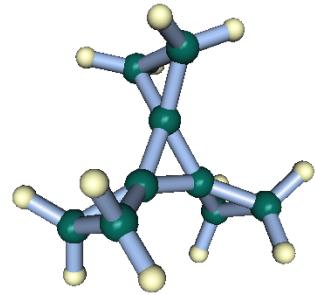
Dipole= 0.012 debye



21

C	0.000000	2.646312	-0.153625
C	-0.783823	1.911812	-1.237462
C	-0.502659	1.272733	0.068369
C	0.000000	0.000000	0.571930
C	-1.280621	0.550204	1.125888
C	0.502659	-1.272733	0.068369
C	1.280621	-0.550204	1.125888
C	0.783823	-1.911812	-1.237462
C	0.000000	-2.646312	-0.153625
H	1.061695	2.787753	-0.310710
H	-0.492162	3.465471	0.354450
H	-1.792102	2.247544	-1.442544
H	-0.237243	1.571736	-2.107218
H	-1.270911	0.951885	2.132470
H	-2.207587	0.066955	0.838743
H	1.270911	-0.951885	2.132470
H	2.207587	-0.066955	0.838743
H	0.237243	-1.571736	-2.107218
H	1.792102	-2.247544	-1.442544
H	0.492162	-3.465471	0.354450
H	-1.061695	-2.787753	-0.310710

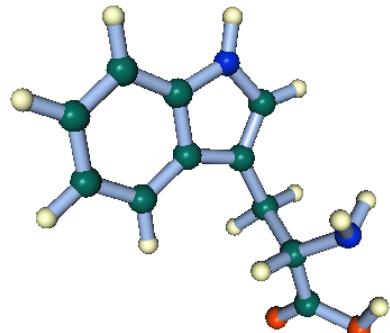
Molecule# 0805
 trispiro[2.0.2.0.2.0]nonane
 PointGroup: D3h
 E= -350.150726509 au
 ZPE= 0.181129 au
 LUMO_eps= -0.01010 au
 HOMO_eps= -0.26603 au
 Dipole= 0.000 debye



21

C	0.000000	0.851770	0.000000
C	0.737655	-0.425885	0.000000
C	-0.737655	-0.425885	0.000000
C	1.836386	-1.060238	0.763078
C	1.836386	-1.060238	-0.763078
C	0.000000	2.120476	-0.763078
C	0.000000	2.120476	0.763078
C	-1.836386	-1.060238	-0.763078
C	-1.836386	-1.060238	0.763078
H	2.551440	-0.422252	1.266347
H	1.641401	-1.998486	1.266347
H	1.641401	-1.998486	-1.266347
H	2.551440	-0.422252	-1.266347
H	-0.910039	2.420738	-1.266347
H	0.910039	2.420738	-1.266347
H	0.910039	2.420738	1.266347
H	-0.910039	2.420738	1.266347
H	-2.551440	-0.422252	-1.266347
H	-1.641401	-1.998486	-1.266347
H	-1.641401	-1.998486	1.266347
H	-2.551440	-0.422252	1.266347

Molecule# 0806
tryptophan
PointGroup: C1
E= -686.631771465 au
ZPE= 0.218667 au
LUMO_eps= -0.03542 au
HOMO_eps= -0.22133 au
Dipole= 6.986 debye



27

N	2.144383	0.943689	1.387392
C	1.971739	-0.048913	0.317057
C	3.347538	-0.585408	-0.126533
O	3.499669	-1.288634	-1.089817
O	4.357944	-0.224123	0.675223
H	3.948061	0.342244	1.365987
C	1.161509	0.438981	-0.901876
C	-0.257433	0.783250	-0.580119
C	-0.805706	2.035533	-0.532908
N	-2.138822	1.958860	-0.185729
C	-2.481917	0.638427	-0.006198
C	-1.318044	-0.133672	-0.246754
C	-1.401983	-1.529651	-0.146912
C	-2.612554	-2.107991	0.190616
C	-3.751206	-1.320897	0.431315
C	-3.702578	0.059180	0.334532
H	1.461495	-0.911416	0.750748
H	1.667652	1.311632	-1.324861
H	1.212237	-0.340971	-1.662152
H	-0.349483	2.989906	-0.737807
H	-2.764965	2.739256	-0.115895
H	-0.538307	-2.151734	-0.341881
H	-2.688793	-3.183992	0.266850
H	-4.683614	-1.802505	0.692328
H	-4.582950	0.662376	0.513597
H	2.105789	1.887369	1.020285
H	1.416855	0.869019	2.084595

Molecule# 0807

tyrosine

PointGroup: C1

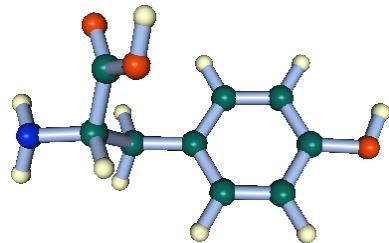
E= -630.265671436 au

ZPE= 0.193080 au

LUMO_eps= -0.02596 au

HOMO_eps= -0.23005 au

Dipole= 1.393 debye



24

C	0.892185	0.423300	-1.115386
C	1.127635	-1.387733	0.424444
C	2.194801	0.827052	-0.845555
C	2.427792	-0.998183	0.705423
C	0.332695	-0.688148	-0.487319
C	2.965844	0.116591	0.068362
C	-2.186401	0.883216	0.310248
C	-1.089329	-1.109749	-0.762062
C	-2.127374	-0.636628	0.291467
N	-3.490056	-1.105655	0.051276
O	-2.617114	1.551395	-0.596087
O	4.254274	0.460267	0.375386
O	-1.697499	1.415760	1.446528
H	0.304511	0.985498	-1.829904
H	0.725773	-2.261652	0.922750
H	2.610134	1.691457	-1.350405
H	3.037227	-1.547870	1.408931
H	-1.411636	-0.739805	-1.736775
H	-1.153616	-2.200087	-0.793954
H	-1.814661	-0.977674	1.277619
H	-3.514304	-2.114400	-0.027753
H	-3.850384	-0.712728	-0.810813
H	4.512609	1.239394	-0.126667
H	-1.759650	2.379779	1.363694

Molecule# 0808

undecan-2-one

PointGroup: C1

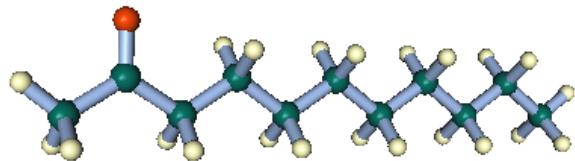
E= -507.860713822 au

ZPE= 0.310261 au

LUMO_eps= -0.02473 au

HOMO_eps= -0.25462 au

Dipole= 2.776 debye



34

C	-4.806157	0.164946	-0.005623
C	-6.062810	-0.680870	0.015204
C	6.725592	-0.280291	-0.006395
C	-3.487345	-0.589442	-0.010665
C	5.426775	0.524067	0.007880
C	-2.245230	0.293358	0.007034
C	4.172804	-0.350971	-0.004536
C	-0.944153	-0.509724	-0.005659
C	2.867501	0.444990	0.008804
C	0.309146	0.366142	0.008951
C	1.614054	-0.430731	-0.003842
O	-4.857865	1.374419	-0.015761
H	-6.066233	-1.383636	-0.820306
H	-6.941478	-0.043492	-0.036220
H	-6.097895	-1.276478	0.930151
H	6.792162	-0.936999	0.863557
H	6.790716	-0.908018	-0.897593
H	7.599872	0.372101	0.003614
H	-3.487195	-1.243242	-0.890607
H	-3.492921	-1.273880	0.845326
H	5.404779	1.195795	-0.855539
H	5.406736	1.168164	0.892173
H	-2.273858	0.968070	-0.851145
H	-2.275701	0.936898	0.889030
H	4.193680	-0.996496	-0.889181
H	4.195186	-1.023399	0.859786
H	-0.922432	-1.183317	0.857933
H	-0.922105	-1.154301	-0.891131
H	2.847599	1.090299	0.893334
H	2.846263	1.117212	-0.855399
H	0.287614	1.010598	0.893780
H	0.287855	1.038888	-0.854540
H	1.635068	-1.102846	0.860594
H	1.634146	-1.076122	-0.888446

Molecule# 0809

uracil

PointGroup: Cs

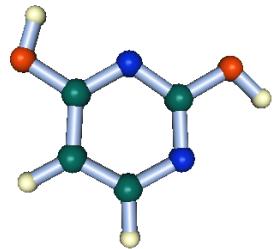
E= -414.964575752 au

ZPE= 0.086643 au

LUMO_eps= -0.04696 au

HOMO_eps= -0.26555 au

Dipole= 1.199 debye



12

C	-1.137324	0.318072	0.000000
O	-2.279401	1.022074	0.000000
C	-1.190713	-1.078014	0.000000
C	0.031924	-1.715471	0.000000
N	1.199468	-1.061094	0.000000
C	1.110451	0.264069	0.000000
O	2.256714	0.960746	0.000000
N	0.000000	0.995036	0.000000
H	-2.038605	1.959714	0.000000
H	-2.128722	-1.608922	0.000000
H	0.091249	-2.797105	0.000000
H	2.975267	0.314212	0.000000

Molecule# 0810

urea

PointGroup: C2

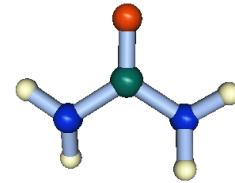
E= -225.370399655 au

ZPE= 0.063395 au

LUMO_eps= -0.02700 au

HOMO_eps= -0.27001 au

Dipole= 3.860 debye



8

C 0.000000 0.000000 0.141895

O 0.000000 0.000000 1.357923

N 0.000000 1.161700 -0.607409

N 0.000000 -1.161700 -0.607409

H 0.198783 1.990644 -0.072919

H 0.395193 1.143037 -1.532593

H -0.198783 -1.990644 -0.072919

H -0.395193 -1.143037 -1.532593

Molecule# 0811

urethane

PointGroup: C1

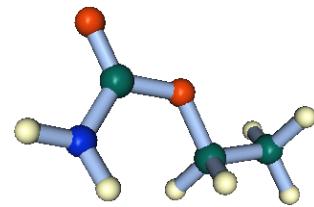
E= -323.886052282 au

ZPE= 0.107026 au

LUMO_eps= -0.02642 au

HOMO_eps= -0.28063 au

Dipole= 5.182 debye



13

C	2.562959	-0.246263	0.024431
H	2.684739	-0.856591	-0.869433
H	3.378057	0.477039	0.064926
H	2.630633	-0.894805	0.896772
C	1.233789	0.476855	0.001020
H	1.104781	1.083961	0.900241
H	1.171235	1.127632	-0.877417
O	0.198136	-0.516463	-0.060443
N	-1.408351	1.154815	0.055718
H	-0.750537	1.856650	-0.229457
H	-2.382975	1.377652	-0.044925
C	-1.116122	-0.185256	-0.006501
O	-1.955791	-1.049445	0.017389

Molecule# 0812

valine

PointGroup: C1

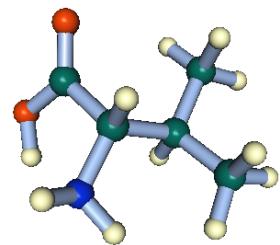
E= -402.537705593 au

ZPE= 0.164287 au

LUMO_eps= -0.02663 au

HOMO_eps= -0.26951 au

Dipole= 5.126 debye



19

N	-0.204180	1.865921	-0.165122
C	-0.044385	0.433011	-0.462275
C	-1.370928	-0.271392	-0.129443
O	-1.723843	-1.301180	-0.637826
O	-2.103030	0.357938	0.804964
H	-1.646282	1.209604	0.969437
C	1.128185	-0.162775	0.360267
C	2.465222	0.464609	-0.056758
C	1.217327	-1.687377	0.244479
H	0.147500	0.235377	-1.520887
H	0.941461	0.092091	1.408810
H	3.277525	0.032580	0.528053
H	2.673618	0.266976	-1.110595
H	2.508562	1.543790	0.096919
H	0.318428	-2.184121	0.600700
H	1.371984	-1.994000	-0.791577
H	2.062337	-2.049689	0.830873
H	0.683380	2.321499	-0.008696
H	-0.666802	2.353922	-0.921910

Molecule# 0813

vinyl acetate

PointGroup: C1

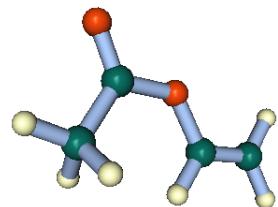
E= -306.586478278 au

ZPE= 0.093758 au

LUMO_eps= -0.03131 au

HOMO_eps= -0.26664 au

Dipole= 3.950 debye



12

C	-1.357401	1.261636	-0.000015
C	-1.021256	-0.208745	0.000007
O	0.300018	-0.575884	-0.000304
C	1.343345	0.319637	0.000014
C	2.594789	-0.109974	0.000104
O	-1.841186	-1.081285	0.000173
H	-0.954127	1.760057	0.881924
H	-0.953586	1.760128	-0.881661
H	-2.438358	1.353144	-0.000324
H	1.083879	1.367562	0.000051
H	2.832057	-1.163725	0.000004
H	3.402610	0.604869	0.000394

Molecule# 0814

vinyl ether

PointGroup: C2v

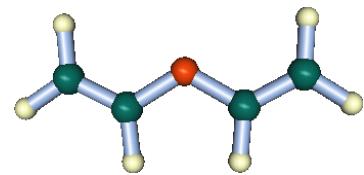
E= -231.294881479 au

ZPE= 0.088854 au

LUMO_eps= -0.00819 au

HOMO_eps= -0.23167 au

Dipole= 1.187 debye



11

O	0.000000	0.000000	0.327847
C	0.000000	1.173022	-0.371331
C	0.000000	-1.173022	-0.371331
C	0.000000	2.350479	0.235228
C	0.000000	-2.350479	0.235228
H	0.000000	1.065115	-1.450457
H	0.000000	-1.065115	-1.450457
H	0.000000	3.252035	-0.356369
H	0.000000	2.435055	1.312056
H	0.000000	-3.252035	-0.356369
H	0.000000	-2.435055	1.312056

Molecule# 0815

vinylsulfonylbenzene

PointGroup: C1

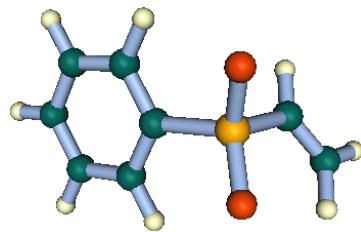
E= -858.443857779 au

ZPE= 0.143174 au

LUMO_eps= -0.06859 au

HOMO_eps= -0.28339 au

Dipole= 5.051 debye



19

C	-2.760426	-1.207325	1.207306
C	-1.942526	-0.170313	1.165936
S	-1.209568	0.357864	-0.377660
O	-1.661482	-0.546197	-1.429486
O	-1.432644	1.796435	-0.478409
C	0.549958	0.093229	-0.128571
C	1.327317	1.134136	0.365938
C	2.688495	0.926492	0.555460
C	3.254893	-0.306208	0.249360
C	2.466154	-1.336958	-0.253252
C	1.104750	-1.142081	-0.445145
H	-2.971203	-1.781796	0.315349
H	-3.245923	-1.496562	2.129835
H	-1.694653	0.461090	2.008205
H	0.872163	2.091493	0.574475
H	3.306169	1.729235	0.933931
H	4.315074	-0.462596	0.395508
H	2.912325	-2.289975	-0.502003
H	0.480456	-1.924459	-0.851784

Molecule# 0816

Z-1-chloro-1-propene

PointGroup: Cs

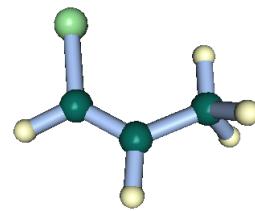
E= -577.592120528 au

ZPE= 0.070773 au

LUMO_eps= -0.01264 au

HOMO_eps= -0.25834 au

Dipole= 1.746 debye



9

C	0.000000	0.915171	0.000000
C	-1.234906	0.436582	0.000000
C	-1.665685	-0.992435	0.000000
Cl	1.445564	-0.071997	0.000000
H	0.228804	1.968959	0.000000
H	-2.020171	1.186064	0.000000
H	-0.816904	-1.671987	0.000000
H	-2.281387	-1.207498	0.876786
H	-2.281387	-1.207498	-0.876786

Molecule# 0817

Z-1-methylprop-1-enyl acetate

PointGroup: C1

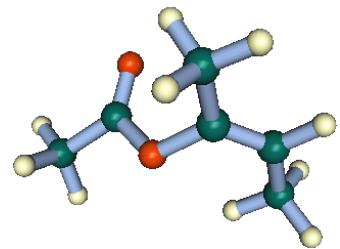
E= -385.260103997 au

ZPE= 0.149497 au

LUMO_eps= -0.01395 au

HOMO_eps= -0.24931 au

Dipole= 1.848 debye



18

C	-1.951735	-0.180434	0.100405
C	-0.883932	0.542857	-0.210248
C	1.381983	-0.094680	0.182826
C	-2.041959	-1.672002	0.148175
C	-0.803865	2.031933	-0.270242
C	2.547078	-0.777270	-0.480474
O	1.391725	0.406289	1.275264
O	0.290604	-0.118487	-0.630137
H	-2.849211	0.374513	0.346595
H	-2.835495	-2.034166	-0.509960
H	-1.110051	-2.145591	-0.151752
H	-2.289315	-2.012966	1.156589
H	-1.765809	2.473463	-0.017477
H	-0.524541	2.360081	-1.274356
H	-0.054472	2.408994	0.426265
H	2.828171	-0.232808	-1.382252
H	2.270172	-1.786382	-0.783928
H	3.386497	-0.809977	0.206602

Molecule# 0818

Z-1,2-dichloroethene

PointGroup: C2v

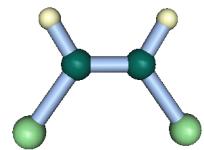
E= -997.888029109 au

ZPE= 0.034006 au

LUMO_eps= -0.03035 au

HOMO_eps= -0.26752 au

Dipole= 1.879 debye



6

C 0.000000 0.661946 0.959662

C 0.000000 -0.661946 0.959662

Cl 0.000000 1.660082 -0.449807

Cl 0.000000 -1.660082 -0.449807

H 0.000000 1.210752 1.888744

H 0.000000 -1.210752 1.888744

Molecule# 0819

Z-1,2-difluoroethene

PointGroup: C2v

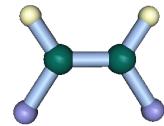
E= -277.169145066 au

ZPE= 0.036930 au

LUMO_eps= -0.01480 au

HOMO_eps= -0.27625 au

Dipole= 2.327 debye



6

C 0.000000 0.660572 0.578468

C 0.000000 -0.660572 0.578468

F 0.000000 1.383039 -0.550638

F 0.000000 -1.383039 -0.550638

H 0.000000 1.245818 1.484934

H 0.000000 -1.245818 1.484934

Molecule# 0820

Z-1,2,3-trifluoropropene

PointGroup: Cs

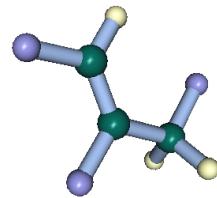
E= -415.772916139 au

ZPE= 0.057725 au

LUMO_eps= -0.01316 au

HOMO_eps= -0.27320 au

Dipole= 1.557 debye



9

C	-0.894816	-0.631696	0.000000
H	-0.633553	-1.676755	0.000000
F	-2.212388	-0.376299	0.000000
C	0.000000	0.341550	0.000000
F	-0.371902	1.637064	0.000000
C	1.486201	0.188572	0.000000
F	1.834576	-1.152835	0.000000
H	1.916333	0.657416	0.888334
H	1.916333	0.657416	-0.888334

Molecule# 0821

Z-1,3-hexadiene

PointGroup: Cs

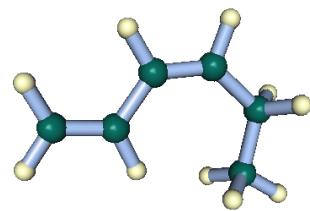
E= -234.711175116 au

ZPE= 0.142123 au

LUMO_eps= -0.03249 au

HOMO_eps= -0.22950 au

Dipole= 0.813 debye



16

H	-2.046077	1.260629	0.000000
C	-1.219389	0.555593	0.000000
H	0.021554	2.201006	0.000000
C	0.000000	1.114678	0.000000
H	1.392911	-0.573551	0.000000
C	1.319865	0.504047	0.000000
H	3.420124	0.739387	0.000000
H	2.436778	2.299849	0.000000
C	2.450226	1.216544	0.000000
H	-2.367696	-0.977943	0.864681
H	-2.367696	-0.977943	-0.864681
C	-1.702301	-0.867901	0.000000
H	-1.238007	-2.971360	0.000000
H	-0.064100	-2.005323	-0.883366
H	-0.064100	-2.005323	0.883366
C	-0.702350	-2.021198	0.000000

Molecule# 0822

Z-1,3,3-trifluoropropene

PointGroup: Cs

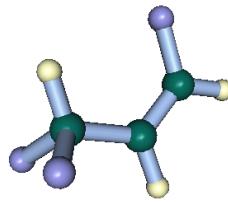
E= -415.790755354 au

ZPE= 0.057915 au

LUMO_eps= -0.03579 au

HOMO_eps= -0.30279 au

Dipole= 2.309 debye



9

C	-0.795540	-1.498083	0.000000
F	0.356729	-2.191946	0.000000
H	-1.660114	-2.146002	0.000000
C	-0.829762	-0.177917	0.000000
H	-1.791395	0.315467	0.000000
C	0.375366	0.693448	0.000000
H	1.319452	0.152643	0.000000
F	0.356729	1.516706	1.098964
F	0.356729	1.516706	-1.098964

Molecule# 0823

Z-1,3,5-hexatriene

PointGroup: C2v

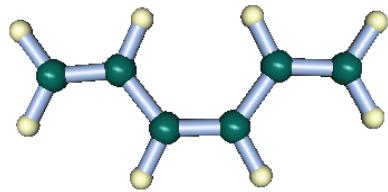
E= -233.489556684 au

ZPE= 0.118579 au

LUMO_eps= -0.05965 au

HOMO_eps= -0.22451 au

Dipole= 0.031 debye



14

C	0.000000	0.674455	0.756935
C	0.000000	-0.674455	0.756935
C	0.000000	1.546499	-0.398566
C	0.000000	-1.546499	-0.398566
C	0.000000	2.881171	-0.319932
C	0.000000	-2.881171	-0.319932
H	0.000000	1.175747	1.719147
H	0.000000	-1.175747	1.719147
H	0.000000	1.087294	-1.380064
H	0.000000	-1.087294	-1.380064
H	0.000000	3.391009	0.635734
H	0.000000	-3.391009	0.635734
H	0.000000	3.500756	-1.205438
H	0.000000	-3.500756	-1.205438

Molecule# 0824

Z-1,4-hexadiene

PointGroup: C1

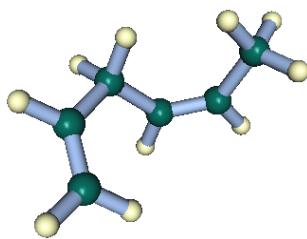
E= -234.708271484 au

ZPE= 0.141345 au

LUMO_eps= -0.01098 au

HOMO_eps= -0.25109 au

Dipole= 0.581 debye



16

C	-2.336058	0.040054	-0.754448
H	-3.277485	0.507889	-0.453946
H	-1.772566	0.765717	-1.337617
H	-2.599402	-0.788479	-1.416868
C	-1.586968	-0.461683	0.442081
H	-2.107557	-1.217663	1.022372
C	-0.380120	-0.094692	0.868817
H	0.005574	-0.582736	1.758463
C	0.533363	0.933703	0.270646
H	0.042346	1.473818	-0.542976
H	0.746217	1.697623	1.028760
C	1.855390	0.410014	-0.232532
H	2.574553	1.177611	-0.503227
C	2.197298	-0.864315	-0.374253
H	3.172382	-1.142407	-0.750747
H	1.518518	-1.669861	-0.126075

Molecule# 0825

Z-2-butene

PointGroup: C2v

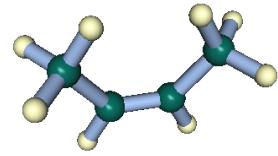
E= -157.288811534 au

ZPE= 0.107559 au

LUMO_eps= -0.01044 au

HOMO_eps= -0.24668 au

Dipole= 0.262 debye



12

C	0.000000	0.665985	0.661718
C	0.000000	-0.665985	0.661718
C	0.000000	1.586665	-0.520621
C	0.000000	-1.586665	-0.520621
H	0.000000	1.161212	1.627911
H	0.000000	-1.161212	1.627911
H	0.000000	1.057812	-1.471692
H	0.000000	-1.057812	-1.471692
H	-0.875737	2.240903	-0.501401
H	0.875737	2.240903	-0.501401
H	0.875737	-2.240903	-0.501401
H	-0.875737	-2.240903	-0.501401

Molecule# 0826

Z-2-butenenitrile

PointGroup: Cs

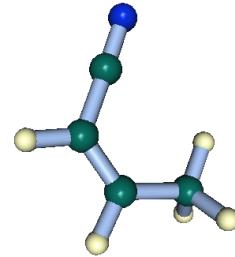
E= -210.235905806 au

ZPE= 0.078880 au

LUMO_eps= -0.05931 au

HOMO_eps= -0.28567 au

Dipole= 4.339 debye



10

C	-1.222725	0.248264	0.000000
N	-2.224302	-0.323411	0.000000
C	0.000000	0.979779	0.000000
H	-0.097533	2.057310	0.000000
C	1.206868	0.404586	0.000000
H	2.065769	1.066361	0.000000
C	1.490613	-1.057531	0.000000
H	0.580711	-1.654271	0.000000
H	2.086316	-1.328056	0.875372
H	2.086316	-1.328056	-0.875372

Molecule# 0827

Z-2-chloro-2-butene

PointGroup: Cs

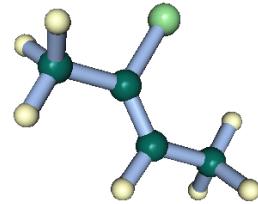
E= -616.926557136 au

ZPE= 0.098604 au

LUMO_eps= -0.01393 au

HOMO_eps= -0.24949 au

Dipole= 1.761 debye



12

H	0.296999	2.638501	0.000000
Cl	-1.282302	-0.692895	0.000000
C	1.865985	-1.198419	0.000000
C	-0.527300	1.925834	0.000000
H	-1.148337	2.109135	0.878732
H	-1.148337	2.109135	-0.878732
C	0.000000	0.528312	0.000000
C	1.279580	0.174679	0.000000
H	1.985598	0.999563	0.000000
H	1.099594	-1.969354	0.000000
H	2.502012	-1.345103	-0.876739
H	2.502012	-1.345103	0.876739

Molecule# 0828

Z-2-chloro-2-butenedinitrile

PointGroup: C1

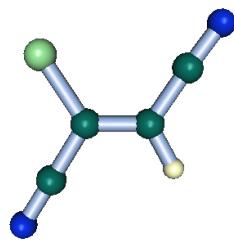
E= -722.791908608 au

ZPE= 0.040377 au

LUMO_eps= -0.13073 au

HOMO_eps= -0.31449 au

Dipole= 0.533 debye



8

C1	-0.219933	1.550529	-0.000002
N	-2.880130	-0.962984	0.000001
N	3.077266	-0.391223	0.000000
C	-0.432054	-0.165225	0.000000
C	0.591544	-1.033696	0.000001
C	-1.783875	-0.609615	0.000001
C	1.955445	-0.655823	0.000001
H	0.372561	-2.093385	0.000003

Molecule# 0829

Z-2-pentene

PointGroup: C1

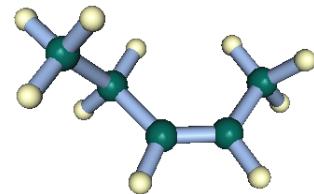
E= -196.616398788 au

ZPE= 0.136268 au

LUMO_eps= -0.01093 au

HOMO_eps= -0.24688 au

Dipole= 0.301 debye



15

C	1.302290	0.615163	-0.139445
C	0.013355	0.809181	0.136131
C	2.074570	-0.668347	-0.088094
C	-2.202655	-0.271676	-0.404781
C	-1.010350	-0.203515	0.558717
H	1.881490	1.484329	-0.436504
H	-0.366648	1.822918	0.039577
H	2.535067	-0.880541	-1.056528
H	1.460917	-1.524351	0.185335
H	2.891800	-0.598640	0.634949
H	-2.954741	-0.977144	-0.048720
H	-1.884282	-0.587950	-1.398923
H	-2.681767	0.703860	-0.505963
H	-1.381230	0.065717	1.553563
H	-0.563862	-1.193034	0.658048

Molecule# 0830

Z-2-pentenenitrile

PointGroup: C1

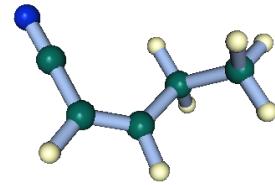
E= -249.563614688 au

ZPE= 0.107552 au

LUMO_eps= -0.05948 au

HOMO_eps= -0.28439 au

Dipole= 4.350 debye



13

C	-1.766341	-0.115464	-0.079800
N	-2.492129	-1.010435	-0.031960
C	-0.894931	1.009998	-0.149808
H	-1.357106	1.941241	-0.450071
C	0.411013	0.955887	0.131841
H	0.972979	1.879716	0.039002
C	1.185347	-0.249154	0.551313
H	0.526822	-1.114981	0.622590
H	1.581474	-0.068108	1.556020
C	2.357367	-0.548639	-0.394504
H	2.000836	-0.775983	-1.399184
H	3.038423	0.301062	-0.463225
H	2.926753	-1.405678	-0.035660

Molecule# 0831

Z-3-amino-2,4-difluorobut-2-enenitrile

PointGroup: C1

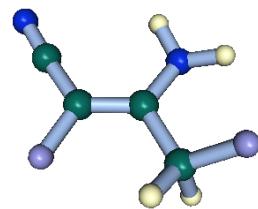
E= -464.158579956 au

ZPE= 0.081128 au

LUMO_eps= -0.05854 au

HOMO_eps= -0.24799 au

Dipole= 3.627 debye



12

F	2.712836	-0.183297	-0.382192
F	-0.780636	1.809141	-0.002362
N	0.499090	-1.575311	0.231574
N	-3.035226	-0.748871	-0.138204
C	0.398551	-0.217436	0.121358
C	1.691625	0.542189	0.236949
C	-0.771372	0.445989	0.008802
C	-2.034053	-0.175673	-0.069809
H	1.624059	1.515903	-0.239488
H	1.970850	0.661136	1.285812
H	1.376086	-1.979329	-0.052815
H	-0.316350	-2.131455	0.030091

Molecule# 0832

Z-3-methyl-2-pentene

PointGroup: C1

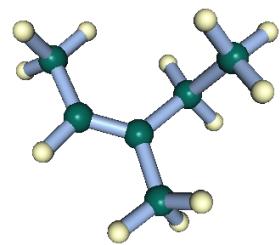
E= -235.947142038 au

ZPE= 0.164035 au

LUMO_eps= -0.01163 au

HOMO_eps= -0.23582 au

Dipole= 0.220 debye



18

C	1.701604	-1.275001	-0.436236
H	2.374174	-0.561889	-0.914203
H	2.313484	-2.070904	-0.008931
H	1.074007	-1.711323	-1.214157
C	0.842683	-0.605101	0.647356
H	1.502107	-0.227760	1.434975
H	0.212380	-1.360114	1.116333
C	0.743877	1.839260	-0.066279
H	0.096872	2.613381	-0.477032
H	1.149562	2.202250	0.882755
H	1.594614	1.719062	-0.742276
C	-2.193807	-0.745612	-0.035612
H	-3.043183	-0.530327	0.618671
H	-2.614514	-1.013203	-1.008980
H	-1.686431	-1.625328	0.355250
C	0.004778	0.540753	0.128637
C	-1.296904	0.449290	-0.156534
H	-1.786454	1.344617	-0.530396

Molecule# 0833

Z-3-penten-1-yne

PointGroup: Cs

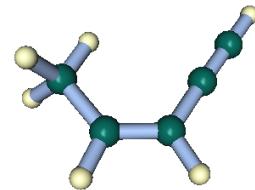
E= -194.134273520 au

ZPE= 0.089149 au

LUMO_eps= -0.03542 au

HOMO_eps= -0.24484 au

Dipole= 0.897 debye



11

H	3.165275	-0.906366	0.000000
C	2.248373	-0.372188	0.000000
C	1.205752	0.228394	0.000000
H	0.114647	2.056770	0.000000
C	0.000000	0.978779	0.000000
H	-2.064969	1.154769	0.000000
C	-1.233830	0.458318	0.000000
H	-0.691320	-1.620929	0.000000
H	-2.183701	-1.244462	0.875775
H	-2.183701	-1.244462	-0.875775
C	-1.579666	-0.992523	0.000000

Molecule# 0834

Z-azodioxymethane

PointGroup: C2

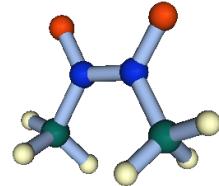
E= -339.752264717 au

ZPE= 0.093617 au

LUMO_eps= -0.05728 au

HOMO_eps= -0.21723 au

Dipole= 6.838 debye

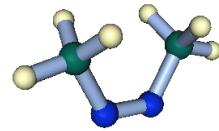


12

N	-0.000879	0.657327	-0.156908
N	0.000879	-0.657327	-0.156908
O	0.011007	1.297461	-1.232955
O	-0.011007	-1.297461	-1.232955
C	0.000879	1.397974	1.121153
C	-0.000879	-1.397974	1.121153
H	-0.261515	2.413654	0.851840
H	-0.729762	0.994639	1.816917
H	0.995166	1.380452	1.566321
H	0.261515	-2.413654	0.851840
H	0.729762	-0.994639	1.816917
H	-0.995166	-1.380452	1.566321

Molecule# 0835
Z-dimethyldiazine
PointGroup: C2v

E= -189.335524287 au
ZPE= 0.083460 au
LUMO_eps= -0.04966 au
HOMO_eps= -0.22680 au
Dipole= 3.200 debye



10

C	0.000000	1.361719	0.498953
N	0.000000	0.616634	-0.777570
N	0.000000	-0.616634	-0.777570
C	0.000000	-1.361719	0.498953
H	0.885227	1.126165	1.094742
H	-0.885227	1.126165	1.094742
H	0.000000	2.420611	0.259791
H	0.885227	-1.126165	1.094742
H	-0.885227	-1.126165	1.094742
H	0.000000	-2.420611	0.259791

Molecule# 0836

Z-hex-2-ene

PointGroup: C1

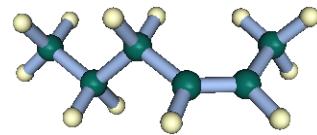
E= -235.944634719 au

ZPE= 0.164654 au

LUMO_eps= -0.01083 au

HOMO_eps= -0.24615 au

Dipole= 0.256 debye



18

C	2.504241	0.931319	-0.085192
C	1.998142	-0.478800	-0.128417
C	0.769296	-0.918216	0.140008
C	-0.434805	-0.119302	0.542445
C	-1.601727	-0.257472	-0.447654
C	-2.851525	0.501404	-0.006889
H	1.734783	1.651980	0.184380
H	3.319775	1.027195	0.636764
H	2.913879	1.224357	-1.055460
H	2.738677	-1.220567	-0.412233
H	0.595713	-1.987355	0.051531
H	-0.185051	0.936381	0.659414
H	-0.776153	-0.463279	1.525879
H	-1.278423	0.098753	-1.429077
H	-1.840844	-1.317309	-0.573189
H	-3.661297	0.386912	-0.728721
H	-3.213611	0.139892	0.957916
H	-2.649176	1.569437	0.096993

Molecule# 0837

Z-hexa-1,5-diyne-3-ene

PointGroup: C2v

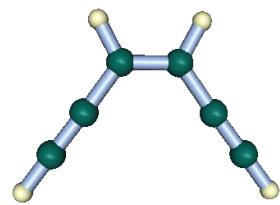
E= -230.975132333 au

ZPE= 0.070699 au

LUMO_eps= -0.07135 au

HOMO_eps= -0.24595 au

Dipole= 0.156 debye



10

C	0.000000	0.673836	1.076580
C	0.000000	-0.673836	1.076580
C	0.000000	1.493940	-0.073575
C	0.000000	-1.493940	-0.073575
H	0.000000	1.184203	2.032282
H	0.000000	-1.184203	2.032282
C	0.000000	2.225403	-1.028515
C	0.000000	-2.225403	-1.028515
H	0.000000	2.859977	-1.879220
H	0.000000	-2.859977	-1.879220

Molecule# 0838

1'H-1,2'-bipyrrole

PointGroup: C1

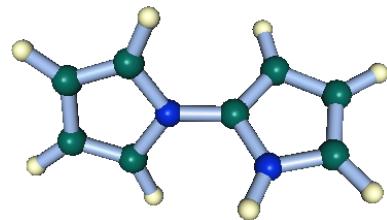
E= -419.294691925 au

ZPE= 0.145049 au

LUMO_eps= -0.01608 au

HOMO_eps= -0.21447 au

Dipole= 1.712 debye



18

C	2.841297	0.623378	-0.306532
C	2.814080	-0.667434	0.287849
C	-2.861574	0.594094	0.254885
C	-1.540425	1.066662	0.485810
C	-2.766925	-0.654559	-0.305131
C	1.541870	1.032508	-0.460978
C	1.498859	-1.002720	0.481775
C	-0.682616	0.087435	0.048268
N	-1.432507	-0.956411	-0.430976
N	0.716428	0.038300	0.020394
H	3.714040	1.183550	-0.595045
H	3.662216	-1.274837	0.553684
H	-3.776525	1.109760	0.489826
H	-1.248499	1.997823	0.938908
H	-3.525636	-1.349731	-0.616531
H	1.122489	1.926638	-0.885807
H	1.048662	-1.865483	0.939940
H	-1.051588	-1.777123	-0.866575

Molecule# 0839

1-(ethylsulfanyl)-2-(methylsulfanyl)ethane

PointGroup: C1

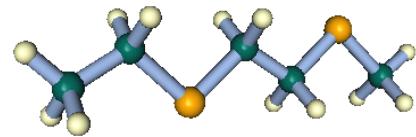
E= -994.289299207 au

ZPE= 0.161560 au

LUMO_eps= -0.01257 au

HOMO_eps= -0.22181 au

Dipole= 0.219 debye



19

C	4.257269	-0.037794	0.000030
C	-3.949908	-0.598011	0.000036
C	2.887553	0.627975	0.000013
C	-1.167307	-0.413074	-0.000018
C	0.091194	0.440608	-0.000020
S	-2.645575	0.670998	-0.000005
S	1.568672	-0.643862	-0.000022
H	4.392436	-0.663324	0.882566
H	4.392468	-0.663306	-0.882513
H	5.042030	0.719953	0.000052
H	-3.889650	-1.219817	-0.891752
H	-4.901476	-0.070840	0.000059
H	-3.889600	-1.219808	0.891826
H	2.763247	1.254670	-0.883576
H	2.763215	1.254650	0.883612
H	-1.197075	-1.048863	0.885008
H	-1.197083	-1.048856	-0.885049
H	0.119565	1.076575	-0.884964
H	0.119567	1.076572	0.884926

Molecule# 0840

1-2-3-5-tetrazole

PointGroup: Cs

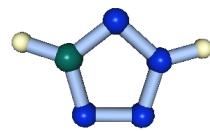
E= -258.354118229 au

ZPE= 0.047407 au

LUMO_eps= -0.04854 au

HOMO_eps= -0.31230 au

Dipole= 2.236 debye



7

N 1.116569 0.323298 0.000000

N 0.000000 1.033096 0.000000

N -1.109966 0.315745 0.000000

N -0.722852 -0.930666 0.000000

C 0.629718 -0.907123 0.000000

H -0.009536 2.040913 0.000000

H 1.244977 -1.788487 0.000000

Molecule# 0841

1-3-difluoropyrrole

PointGroup: C1

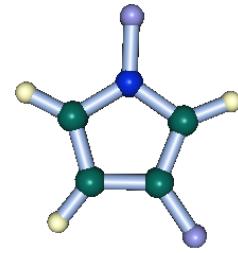
E= -408.711433125 au

ZPE= 0.064668 au

LUMO_eps= -0.01394 au

HOMO_eps= -0.24334 au

Dipole= 1.383 debye



10

F	2.330214	-0.536042	0.000001
F	-2.393334	-0.522974	-0.000003
N	1.036400	-0.102187	0.000000
C	-1.116301	-0.113298	0.000000
C	-0.028009	-0.957326	-0.000003
C	0.691209	1.205519	0.000003
C	-0.693561	1.228172	0.000003
H	0.078795	-2.024555	-0.000006
H	1.428370	1.986186	0.000006
H	-1.313902	2.106420	0.000004

Molecule# 0842

1-amino-1,2-dicyanoethene

PointGroup: C1

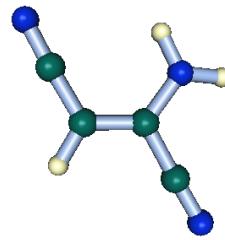
E= -318.559283258 au

ZPE= 0.066478 au

LUMO_eps= -0.09506 au

HOMO_eps= -0.26854 au

Dipole= 2.246 debye



10

N	-0.215113	1.497969	-0.037148
N	-2.925719	-0.543036	0.011247
N	2.995579	-0.108089	0.011842
C	-0.435847	0.155615	-0.006082
C	0.526381	-0.803968	-0.007016
C	-1.814276	-0.244776	-0.000475
C	1.891978	-0.450754	0.001475
H	0.725085	1.844501	0.057268
H	-0.969933	2.136882	0.130733
H	0.252209	-1.846001	-0.016996

Molecule# 0843

1-azido-2-chloroethane

PointGroup: C1

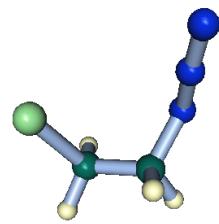
E= -703.135992822 au

ZPE= 0.070391 au

LUMO_eps= -0.04497 au

HOMO_eps= -0.27148 au

Dipole= 3.204 debye



10

C1	1.571721	-0.909942	0.008496
N	-1.173896	0.820814	-0.448314
N	-1.762173	-0.193172	-0.081847
N	-2.396372	-1.096686	0.152096
C	-0.060470	1.285982	0.393333
C	1.295650	0.872078	-0.145488
H	-0.103030	2.376437	0.375286
H	-0.177806	0.958752	1.427891
H	2.090432	1.359964	0.413029
H	1.387147	1.108808	-1.201250

Molecule# 0844

1-azido-3-chloro-2-propanol

PointGroup: C1

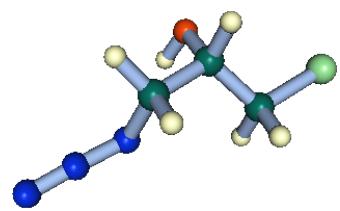
E= -817.712614224 au

ZPE= 0.103123 au

LUMO_eps= -0.05539 au

HOMO_eps= -0.28403 au

Dipole= 2.295 debye



14

C1	2.984399	-0.417879	-0.152987
O	0.545008	1.604346	-0.451726
N	-1.674474	-0.203357	-0.321610
N	-2.891489	-0.320120	-0.222649
N	-4.011018	-0.462784	-0.239944
C	0.486114	0.564884	0.505089
C	-0.961721	0.258054	0.891001
C	1.212507	-0.698086	0.052682
H	0.985966	0.954778	1.392928
H	-1.421537	1.170797	1.275391
H	-0.999608	-0.510498	1.668236
H	1.110587	-1.489064	0.791667
H	0.836499	-1.050422	-0.903648
H	0.010714	1.348290	-1.213192

Molecule# 0845

1-bromo-1-fluoroethene

PointGroup: Cs

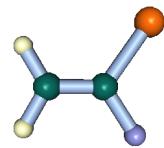
E= -2751.525605330 au

ZPE= 0.034331 au

LUMO_eps= -0.02739 au

HOMO_eps= -0.27326 au

Dipole= 1.350 debye



6

Br	0.000000	0.944463	0.000000
F	-1.164488	-1.479903	0.000000
C	0.059373	-0.946597	0.000000
C	1.154128	-1.680158	0.000000
H	1.072609	-2.757376	0.000000
H	2.126778	-1.219186	0.000000

Molecule# 0846

1-bromo-1,2-dicyanoethane

PointGroup: C1

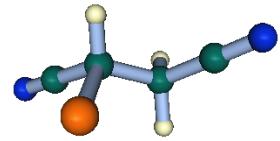
E= -2838.017065870 au

ZPE= 0.063280 au

LUMO_eps= -0.08511 au

HOMO_eps= -0.32321 au

Dipole= 0.764 debye



10

Br	0.484161	-1.250284	0.042825
N	2.403295	1.993003	0.037945
N	-3.263844	0.248113	-0.220851
C	0.212892	0.659505	-0.397179
C	-0.947883	1.262384	0.413056
C	1.447752	1.383866	-0.156347
C	-2.239957	0.683654	0.064803
H	-0.012194	0.667867	-1.460128
H	-0.982969	2.336793	0.216444
H	-0.763464	1.131030	1.479162

Molecule# 0847

1-bromo-2-chloroethane

PointGroup: Cs

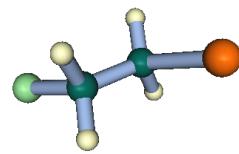
E= -3113.123692270 au

ZPE= 0.057291 au

LUMO_eps= -0.03971 au

HOMO_eps= -0.29544 au

Dipole= 0.080 debye



8

C	1.240203	-0.212740	0.000000
C	0.000000	0.644652	0.000000
Cl	2.702933	0.863781	0.000000
Br	-1.595912	-0.518012	0.000000
H	1.306850	-0.832496	0.887890
H	1.306850	-0.832496	-0.887890
H	-0.073922	1.259830	-0.889431
H	-0.073922	1.259830	0.889431

Molecule# 0848

1-bromo-2-methylpropane

PointGroup: C1

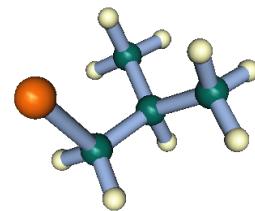
E= -2732.148973990 au

ZPE= 0.122086 au

LUMO_eps= -0.01958 au

HOMO_eps= -0.27646 au

Dipole= 2.290 debye



14

C	-1.834533	1.268289	-0.400426
C	-1.834533	-1.268288	-0.400426
C	-0.216545	0.000000	1.098319
C	-1.577154	0.000000	0.414555
Br	1.331761	0.000000	-0.150889
H	-1.161986	1.326133	-1.256561
H	-2.858396	1.279544	-0.775600
H	-1.687919	2.166121	0.202464
H	-1.161987	-1.326133	-1.256561
H	-2.858396	-1.279543	-0.775600
H	-1.687920	-2.166121	0.202463
H	-0.068439	-0.887671	1.705388
H	-0.068439	0.887670	1.705389
H	-2.281566	0.000000	1.257593

Molecule# 0849

1-bromobutane

PointGroup: Cs

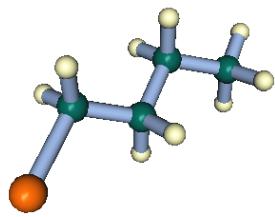
E= -2732.149345560 au

ZPE= 0.122552 au

LUMO_eps= -0.02199 au

HOMO_eps= -0.27791 au

Dipole= 2.455 debye



14

C	-3.641893	-0.591266	0.000000
C	-2.496939	0.420603	0.000000
C	-1.117874	-0.250006	0.000000
C	0.000000	0.772896	0.000000
Br	1.788178	-0.077333	0.000000
H	-3.599505	-1.234516	0.880844
H	-4.610970	-0.091293	0.000000
H	-3.599505	-1.234516	-0.880844
H	-2.584638	1.071178	0.874826
H	-2.584638	1.071178	-0.874826
H	-1.021525	-0.894784	0.876074
H	-1.021525	-0.894784	-0.876074
H	-0.011837	1.400411	0.886249
H	-0.011837	1.400411	-0.886249

Molecule# 0850

1-bromoheptane

PointGroup: Cs

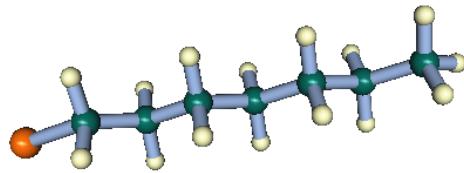
E= -2850.133647960 au

ZPE= 0.207677 au

LUMO_eps= -0.02149 au

HOMO_eps= -0.27712 au

Dipole= 2.539 debye



23

C	1.764781	-5.617581	0.000000
C	2.028889	-4.112926	0.000000
C	0.750440	-3.274006	0.000000
C	1.007520	-1.766974	0.000000
C	-0.272667	-0.929505	0.000000
C	0.000000	0.579454	0.000000
C	-1.288109	1.377306	0.000000
Br	-0.956194	3.330314	0.000000
H	2.696175	-6.185285	0.000000
H	1.193700	-5.918250	0.880782
H	1.193700	-5.918250	-0.880782
H	2.631895	-3.849152	-0.874055
H	2.631895	-3.849152	0.874055
H	0.146800	-3.538224	0.874765
H	0.146800	-3.538224	-0.874765
H	1.610373	-1.502874	-0.874726
H	1.610373	-1.502874	0.874726
H	-0.875444	-1.190887	0.875500
H	-0.875444	-1.190887	-0.875500
H	0.593789	0.847801	0.876114
H	0.593789	0.847801	-0.876114
H	-1.888361	1.196425	-0.886534
H	-1.888361	1.196425	0.886534

Molecule# 0851

1-bromohexane

PointGroup: Cs

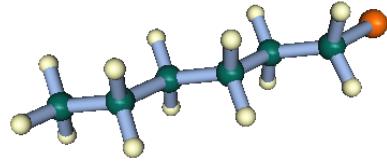
E= -2810.805459110 au

ZPE= 0.178937 au

LUMO_eps= -0.02144 au

HOMO_eps= -0.27731 au

Dipole= 2.547 debye



20

C	-4.936568	1.465145	0.000000
C	-3.922526	0.322511	0.000000
C	-2.471384	0.804576	0.000000
C	-1.450102	-0.334338	0.000000
C	0.000000	0.164093	0.000000
C	0.985477	-0.987102	0.000000
Br	2.863952	-0.359390	0.000000
H	-4.816817	2.099428	0.880736
H	-5.960401	1.088998	0.000000
H	-4.816817	2.099428	-0.880736
H	-4.090369	-0.313716	0.874123
H	-4.090369	-0.313716	-0.874123
H	-2.302394	1.440928	0.874604
H	-2.302394	1.440928	-0.874604
H	-1.617587	-0.969807	-0.875461
H	-1.617587	-0.969807	0.875461
H	0.175058	0.791780	0.876000
H	0.175058	0.791780	-0.876000
H	0.898455	-1.608448	0.886264
H	0.898455	-1.608448	-0.886264

Molecule# 0852

1-bromoisothiocyanatoethane

PointGroup: C1

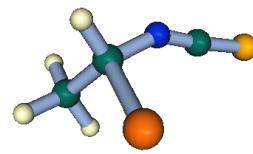
E= -3143.993391160 au

ZPE= 0.066893 au

LUMO_eps= -0.07306 au

HOMO_eps= -0.26781 au

Dipole= 2.678 debye



10

Br	-1.611959	-0.676707	-0.060437
S	3.188561	-0.473831	-0.212178
N	0.804766	0.605290	0.683249
C	-0.543122	0.946003	0.504531
C	-0.745641	2.059764	-0.506152
C	1.810058	0.133187	0.252507
H	-0.983142	1.183265	1.466702
H	-1.802666	2.302122	-0.586938
H	-0.372012	1.764535	-1.484569
H	-0.201719	2.945380	-0.173108

Molecule# 0853

1-bromoocane

PointGroup: C1

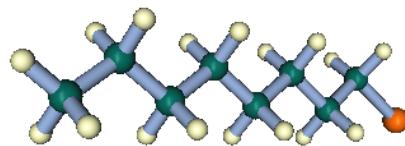
E= -2889.461663440 au

ZPE= 0.235973 au

LUMO_eps= -0.02132 au

HOMO_eps= -0.27700 au

Dipole= 2.590 debye



26

C	-6.534030	-0.514996	0.000019
C	-5.302372	0.389014	-0.000013
C	-3.983974	-0.386062	0.000155
C	-2.745486	0.510646	-0.000145
C	-1.428074	-0.265911	-0.000090
C	-0.191349	0.634712	-0.000033
C	1.123907	-0.153976	0.000007
C	2.324734	0.770374	0.000180
Br	4.036420	-0.226015	-0.000020
H	-6.549451	-1.160327	0.880807
H	-7.456740	0.066937	-0.000174
H	-6.549247	-1.160608	-0.880564
H	-5.332736	1.046867	0.873861
H	-5.332634	1.046608	-0.874087
H	-3.953841	-1.044491	0.874820
H	-3.953918	-1.044948	-0.874172
H	-2.776580	1.168716	-0.874892
H	-2.776413	1.169083	0.874338
H	-1.395055	-0.923423	-0.874681
H	-1.395117	-0.923380	0.874535
H	-0.222551	1.291283	-0.875362
H	-0.222632	1.291268	0.875305
H	1.165253	-0.804347	-0.876140
H	1.165131	-0.804516	0.876036
H	2.365848	1.396665	-0.885997
H	2.365863	1.396332	0.886591

Molecule# 0854

1-bromopentane

PointGroup: Cs

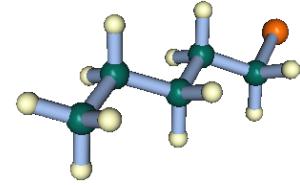
E= -2771.477422420 au

ZPE= 0.150732 au

LUMO_eps= -0.02180 au

HOMO_eps= -0.27754 au

Dipole= 2.485 debye



17

C	-1.988098	4.012180	0.000000
C	-0.792968	3.060598	0.000000
C	-1.200752	1.586022	0.000000
C	0.000000	0.632126	0.000000
C	-0.443162	-0.816706	0.000000
Br	1.091819	-2.068589	0.000000
H	-1.665993	5.054165	0.000000
H	-2.614435	3.858712	0.880998
H	-2.614435	3.858712	-0.880998
H	-0.166691	3.259922	-0.874218
H	-0.166691	3.259922	0.874218
H	-1.826464	1.385353	0.875522
H	-1.826464	1.385353	-0.875522
H	0.622908	0.822511	-0.876270
H	0.622908	0.822511	0.876270
H	-1.014215	-1.075935	-0.886408
H	-1.014215	-1.075935	0.886408

Molecule# 0855

1-bromopropane

PointGroup: Cs

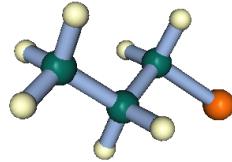
E= -2692.821280280 au

ZPE= 0.094128 au

LUMO_eps= -0.02512 au

HOMO_eps= -0.27855 au

Dipole= 2.350 debye



11

C	-2.200637	2.059738	0.000000
C	-1.508543	0.693752	0.000000
C	0.000000	0.843650	0.000000
Br	0.922931	-0.907372	0.000000
H	-3.284264	1.940493	0.000000
H	-1.931173	2.643611	0.881907
H	-1.931173	2.643611	-0.881907
H	-1.815296	0.119503	-0.875518
H	-1.815296	0.119503	0.875518
H	0.364857	1.354220	0.886426
H	0.364857	1.354220	-0.886426

Molecule# 0856

1-butanamine

PointGroup: C1

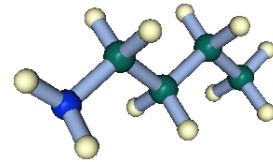
E= -213.890458266 au

ZPE= 0.149103 au

LUMO_eps= -0.01252 au

HOMO_eps= -0.24289 au

Dipole= 1.232 debye



16

C	2.533757	-0.306220	-0.014186
C	1.251222	0.522342	0.039823
C	-0.016716	-0.327791	-0.039403
C	-1.300133	0.493422	0.015850
N	-2.480785	-0.370083	-0.090337
H	3.420315	0.326593	0.045198
H	2.578190	-1.017755	0.812928
H	2.594900	-0.877280	-0.942685
H	1.237543	1.111057	0.961985
H	1.251521	1.245452	-0.781337
H	-0.017096	-0.915524	-0.961024
H	-0.018900	-1.049862	0.785140
H	-1.293033	1.109193	0.926922
H	-1.321845	1.185998	-0.829220
H	-3.332664	0.176428	-0.103509
H	-2.542214	-0.994236	0.705456

Molecule# 0857

1-butanol

PointGroup: C1

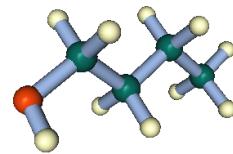
E= -233.765868525 au

ZPE= 0.136455 au

LUMO_eps= -0.01402 au

HOMO_eps= -0.27839 au

Dipole= 1.773 debye



15

C	2.514552	-0.302534	-0.010159
C	1.228558	0.521535	0.028293
C	-0.036512	-0.336644	-0.027812
C	-1.316665	0.487981	0.016814
O	-2.500646	-0.301127	-0.092060
H	2.565348	-0.993371	0.833797
H	2.575280	-0.895054	-0.925011
H	3.397647	0.336304	0.030805
H	1.214362	1.130960	0.936793
H	1.223025	1.225237	-0.809202
H	-0.039872	-0.939383	-0.939874
H	-0.034575	-1.041035	0.812011
H	-1.343796	1.095071	0.929885
H	-1.352146	1.175054	-0.829661
H	-2.539703	-0.906796	0.654122

Molecule# 0858

1-buten-3-yne

PointGroup: Cs

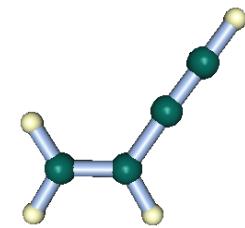
E= -154.799560423 au

ZPE= 0.060984 au

LUMO_eps= -0.04710 au

HOMO_eps= -0.25742 au

Dipole= 0.413 debye



8

C	0.575831	-0.555754	0.000000
C	0.000000	0.742606	0.000000
C	-0.120645	-1.693322	0.000000
C	-0.451906	1.856856	0.000000
H	1.660286	-0.592176	0.000000
H	0.382293	-2.649906	0.000000
H	-1.201790	-1.696289	0.000000
H	-0.860469	2.836051	0.000000

Molecule# 0859

1-butene

PointGroup: C1

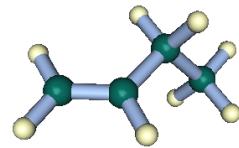
E= -157.285738172 au

ZPE= 0.108010 au

LUMO_eps= -0.01013 au

HOMO_eps= -0.26337 au

Dipole= 0.429 debye



12

C	-1.857174	0.019065	-0.276434
C	-0.721381	-0.297100	0.333323
C	1.726840	-0.243467	-0.291830
C	0.536972	0.517277	0.306749
H	-2.729067	-0.618792	-0.220189
H	-1.956005	0.931088	-0.853592
H	-0.671041	-1.224905	0.898141
H	2.633033	0.362779	-0.261767
H	1.534052	-0.514731	-1.330436
H	1.923869	-1.164107	0.260591
H	0.363340	1.438791	-0.253243
H	0.790277	0.815231	1.329652

Molecule# 0860

1-butoxybutane

PointGroup: C2v

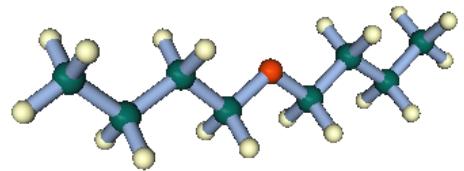
E= -391.071047175 au

ZPE= 0.249369 au

LUMO_eps= -0.01062 au

HOMO_eps= -0.25959 au

Dipole= 1.058 debye



27

C	0.000000	4.931161	0.525769
C	0.000000	-4.931161	0.525769
C	0.000000	3.717960	-0.402856
C	0.000000	-3.717960	-0.402856
C	0.000000	2.388987	0.353309
C	0.000000	-2.388987	0.353309
C	0.000000	1.184688	-0.571073
C	0.000000	-1.184688	-0.571073
O	0.000000	0.000000	0.205597
H	-0.880623	4.932775	1.171072
H	0.880623	4.932775	1.171072
H	0.000000	5.864641	-0.038469
H	0.880623	-4.932775	1.171072
H	-0.880623	-4.932775	1.171072
H	0.000000	-5.864641	-0.038469
H	-0.874418	3.763393	-1.058921
H	0.874418	3.763393	-1.058921
H	0.874418	-3.763393	-1.058921
H	-0.874418	-3.763393	-1.058921
H	0.876326	2.331130	1.004232
H	-0.876326	2.331130	1.004232
H	-0.876326	-2.331130	1.004232
H	0.876326	-2.331130	1.004232
H	-0.884669	1.203511	-1.223789
H	0.884669	1.203511	-1.223789
H	0.884669	-1.203511	-1.223789
H	-0.884669	-1.203511	-1.223789

Molecule# 0861

1-butylsulfonylbutane

PointGroup: C1

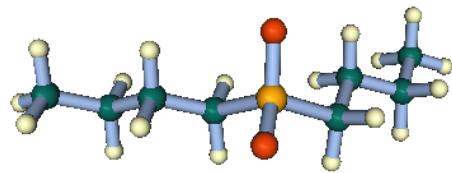
E= -864.529930040 au

ZPE= 0.255261 au

LUMO_eps= -0.02087 au

HOMO_eps= -0.28505 au

Dipole= 4.817 debye



29

C	-4.547650	-1.705638	0.272597
C	-3.795689	-0.553081	-0.390005
C	-2.349515	-0.430093	0.100464
C	-1.615268	0.722413	-0.573309
S	0.037748	1.077404	0.089018
O	0.541910	2.249760	-0.624888
C	1.055947	-0.348493	-0.390800
C	2.496572	-0.170036	0.080449
C	3.378082	-1.358055	-0.315035
C	4.824517	-1.194420	0.147764
O	-0.048573	1.105880	1.548995
H	-4.067320	-2.663473	0.063479
H	-4.581440	-1.582093	1.356437
H	-5.575090	-1.764796	-0.087565
H	-4.320256	0.386228	-0.194738
H	-3.803321	-0.687023	-1.475548
H	-1.826735	-1.371038	-0.089908
H	-2.336575	-0.275264	1.180431
H	-2.130655	1.672755	-0.422484
H	-1.487390	0.579358	-1.646641
H	0.990394	-0.416247	-1.477160
H	0.591980	-1.227121	0.056620
H	2.505188	-0.047615	1.164989
H	2.901550	0.749170	-0.346134
H	3.354143	-1.481736	-1.401693
H	2.960814	-2.276931	0.107216
H	5.277008	-0.300011	-0.284003
H	4.882665	-1.102883	1.233779
H	5.432396	-2.050455	-0.146968

Molecule# 0862

1-butyne

PointGroup: Cs

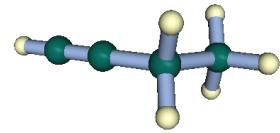
E= -156.032679751 au

ZPE= 0.084382 au

LUMO_eps= -0.01232 au

HOMO_eps= -0.27420 au

Dipole= 0.850 debye



10

C	1.328756	-1.459271	0.000000
C	0.738939	-0.414592	0.000000
C	-1.523500	0.649784	0.000000
C	0.000000	0.843190	0.000000
H	1.855678	-2.379936	0.000000
H	-1.844031	0.095387	0.881353
H	-1.844031	0.095387	-0.881353
H	-2.027340	1.616676	0.000000
H	0.297280	1.428911	0.873961
H	0.297280	1.428911	-0.873961

Molecule# 0863

1-carboxymethylamino-2-diazenioethenolate

PointGroup: C1

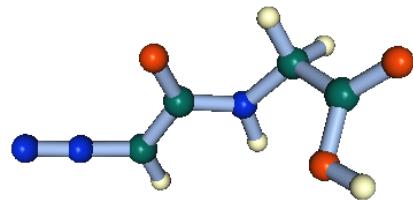
E= -545.550364031 au

ZPE= 0.103472 au

LUMO_eps= -0.07778 au

HOMO_eps= -0.25393 au

Dipole= 4.836 debye



15

O	2.042882	1.386061	-0.306059
O	-0.918032	-1.066477	-0.827288
O	3.605054	-0.221660	-0.468251
N	0.250255	-0.222810	0.941283
N	-3.135574	0.325904	-0.031872
N	-4.076826	0.233940	-0.637842
C	1.503935	-0.802214	0.535266
C	-0.876835	-0.354541	0.164605
C	2.504443	0.128212	-0.134773
C	-2.026017	0.411410	0.648141
H	2.017669	-1.255971	1.383817
H	1.288572	-1.598028	-0.176598
H	0.261728	0.487240	1.652644
H	-2.050184	1.041177	1.521965
H	2.744845	1.885755	-0.749461

Molecule# 0864

1-chloro-1-cyano-2-isocyanatoethane

PointGroup: C1

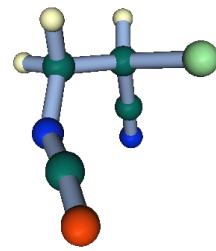
E= -799.293909459 au

ZPE= 0.069192 au

LUMO_eps= -0.05895 au

HOMO_eps= -0.31360 au

Dipole= 4.613 debye



11

C1	-0.676413	1.647673	-0.198839
O	2.973312	-0.003864	-0.788694
N	1.171490	-0.909893	0.447772
N	-2.183834	-1.569197	-1.071477
C	0.125081	-0.508516	1.336558
C	-1.098061	0.085661	0.622655
C	-1.695846	-0.827966	-0.341528
C	2.065665	-0.383032	-0.161385
H	0.479121	0.224746	2.062267
H	-0.217303	-1.388512	1.882361
H	-1.843922	0.340978	1.373321

Molecule# 0865

1-chloro-1-ethyl-3-nitrosourea

PointGroup: C1

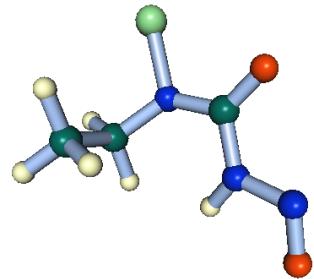
E= -892.925821159 au

ZPE= 0.105691 au

LUMO_eps= -0.09319 au

HOMO_eps= -0.27053 au

Dipole= 5.628 debye



15

C1	2.286656	-0.909638	-0.094329
O	-0.348592	-1.741340	0.570157
O	-3.591259	0.368778	-0.156789
N	0.834131	-0.041900	-0.440896
N	-1.480456	0.074394	-0.263918
N	-2.680962	-0.317585	0.233515
C	1.034960	1.411899	-0.556362
C	1.208429	2.133260	0.774373
C	-0.314225	-0.670944	0.029846
H	0.193913	1.822214	-1.115508
H	1.908061	1.546450	-1.191269
H	1.383554	3.194973	0.597832
H	0.320409	2.034185	1.398486
H	2.061221	1.735025	1.322072
H	-1.505481	0.861831	-0.903010

Molecule# 0866

1-chloro-1-fluoroethane

PointGroup: C1

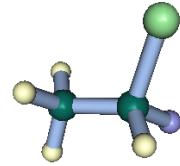
E= -638.775504118 au

ZPE= 0.058573 au

LUMO_eps= -0.01452 au

HOMO_eps= -0.31383 au

Dipole= 2.316 debye



8

C	0.416411	0.100268	0.386308
C	1.263415	-1.037984	-0.112361
H	0.427859	0.216469	1.466770
F	0.842920	1.284656	-0.164507
Cl	-1.324878	-0.129863	-0.054942
H	1.189287	-1.116293	-1.195399
H	2.302538	-0.853754	0.163176
H	0.938014	-1.974348	0.336348

Molecule# 0867

1-chloro-1-fluoroethene

PointGroup: C1

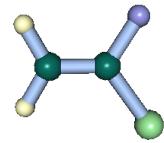
E= -637.532795980 au

ZPE= 0.034910 au

LUMO_eps= -0.02174 au

HOMO_eps= -0.27718 au

Dipole= 1.375 debye



6

C1	1.271311	-0.098836	0.000000
F	-0.891537	1.237652	0.000000
C	-0.455870	-0.024081	0.000000
C	-1.271818	-1.059179	0.000002
H	-0.883625	-2.063137	0.000003
H	-2.338704	-0.895953	0.000003

Molecule# 0868

1-chloro-1,1-difluoroethane

PointGroup: Cs

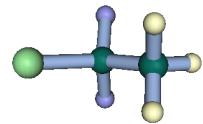
E= -738.060793072 au

ZPE= 0.050217 au

LUMO_eps= -0.01520 au

HOMO_eps= -0.33406 au

Dipole= 2.270 debye



8

C	-0.355891	0.007246	0.000000
C	-0.817838	1.438371	0.000000
Cl	1.445175	-0.130990	0.000000
F	-0.817838	-0.654552	1.085396
F	-0.817838	-0.654552	-1.085396
H	-1.907414	1.446254	0.000000
H	-0.448549	1.944401	0.887913
H	-0.448549	1.944401	-0.887913

Molecule# 0869

1-chloro-1,3-butadiene

PointGroup: Cs

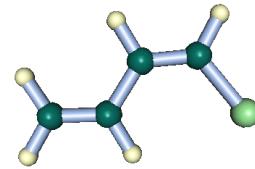
E= -615.690964728 au

ZPE= 0.076376 au

LUMO_eps= -0.05404 au

HOMO_eps= -0.24434 au

Dipole= 1.471 debye



10

C	0.000000	1.019263	0.000000
C	1.348969	0.492686	0.000000
C	-1.138067	0.325279	0.000000
C	2.440288	1.261794	0.000000
H	-0.108466	2.099001	0.000000
H	1.454409	-0.585078	0.000000
H	-2.111345	0.788809	0.000000
Cl	-1.232208	-1.416011	0.000000
H	3.432030	0.832553	0.000000
H	2.373763	2.342770	0.000000

Molecule# 0870

1-chloro-2-butene

PointGroup: C1

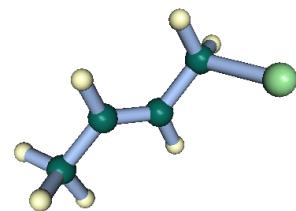
E= -616.923013618 au

ZPE= 0.099268 au

LUMO_eps= -0.02627 au

HOMO_eps= -0.26846 au

Dipole= 2.601 debye



12

C	2.920911	-0.389382	0.000288
H	2.911727	-0.857297	0.984172
H	3.712820	0.363693	-0.014052
H	3.197836	-1.147075	-0.737175
C	0.524673	0.206787	0.450874
H	1.523663	0.702405	-1.305710
C	1.597085	0.217659	-0.335522
H	-1.130829	1.516651	0.856898
H	-0.715930	1.362140	-0.864008
C	-0.765272	0.842040	0.087533
Cl	-2.101674	-0.407151	-0.091662
H	0.564791	-0.281572	1.419098

Molecule# 0871

1-chloro-2-ethoxyethane

PointGroup: Cs

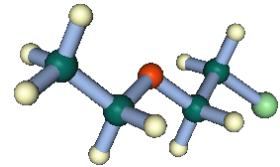
E= -693.390351263 au

ZPE= 0.127431 au

LUMO_eps= -0.01379 au

HOMO_eps= -0.27606 au

Dipole= 2.133 debye



15

C	-1.364294	-0.257422	0.000000
Cl	-2.663967	1.000357	0.000000
C	0.000000	0.402791	0.000000
C	3.235965	-1.355048	0.000000
C	2.301786	-0.163749	0.000000
O	0.959835	-0.634578	0.000000
H	4.273451	-1.018738	0.000000
H	-1.508982	-0.865324	0.887556
H	-1.508982	-0.865324	-0.887556
H	0.111166	1.038659	-0.886420
H	0.111166	1.038659	0.886420
H	3.073565	-1.971524	-0.883887
H	3.073565	-1.971524	0.883887
H	2.471534	0.463118	0.884863
H	2.471534	0.463118	-0.884863

Molecule# 0872

1-chloro-2-methylbenzene

PointGroup: Cs

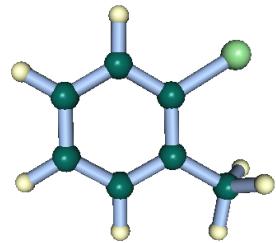
E= -731.299600914 au

ZPE= 0.118410 au

LUMO_eps= -0.02738 au

HOMO_eps= -0.25137 au

Dipole= 1.550 debye



15

C	1.683448	-1.663575	0.000000
C	2.220125	-0.382943	0.000000
C	0.305726	-1.835687	0.000000
C	1.373807	0.717619	0.000000
C	-0.573870	-0.751190	0.000000
C	0.000000	0.522425	0.000000
C	-2.061411	-0.960930	0.000000
Cl	-1.036566	1.943162	0.000000
H	2.334268	-2.527315	0.000000
H	3.291363	-0.235053	0.000000
H	-0.108141	-2.835976	0.000000
H	1.769429	1.722783	0.000000
H	-2.526446	-0.504646	0.875379
H	-2.526446	-0.504646	-0.875379
H	-2.299351	-2.023197	0.000000

Molecule# 0873

1-chloro-3-diazo-2-propanone

PointGroup: C1

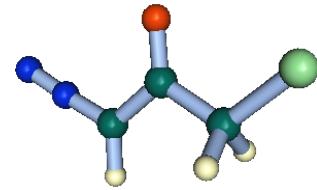
E= -761.140433492 au

ZPE= 0.061854 au

LUMO_eps= -0.08847 au

HOMO_eps= -0.26874 au

Dipole= 4.617 debye



10

C1	2.615902	-0.172641	-0.000080
O	-0.165508	-1.237912	0.000142
N	-2.509366	0.187022	-0.000312
N	-3.469270	-0.391475	-0.000476
C	-0.149899	-0.026948	0.000164
C	-1.350968	0.797979	-0.000120
C	1.130742	0.811941	0.000604
H	-1.378265	1.874748	-0.000193
H	1.151566	1.448971	-0.881951
H	1.151625	1.447808	0.884002

Molecule# 0874

1-chloro-4-isothiocyanato-2-butyne

PointGroup: C1

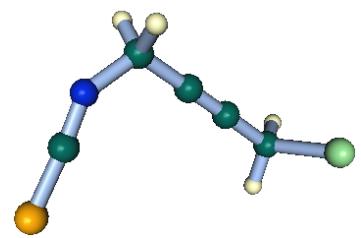
E= -1106.162985170 au

ZPE= 0.077662 au

LUMO_eps= -0.04890 au

HOMO_eps= -0.25942 au

Dipole= 2.613 debye



12

C1	-3.572987	-0.567278	-0.510317
S	3.299035	-1.317260	-0.006901
N	2.079494	1.156701	-0.250864
C	0.857173	1.910593	-0.125215
C	-2.394964	-0.380030	0.871471
C	-0.304421	1.103913	0.230165
C	-1.256817	0.432000	0.515067
C	2.559311	0.073133	-0.131631
H	0.675175	2.422451	-1.072973
H	1.016661	2.691477	0.622020
H	-2.961711	0.058649	1.688357
H	-2.092050	-1.387238	1.145296

Molecule# 0875

1-chloro-4,5-dihydro-1H-1,2,3-triazole

PointGroup: C1

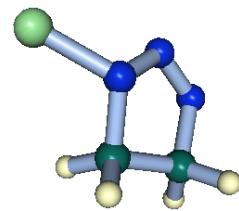
E= -703.095257992 au

ZPE= 0.070897 au

LUMO_eps= -0.06723 au

HOMO_eps= -0.26570 au

Dipole= 3.604 debye



10

C1	-1.920947	0.002248	0.086589
N	-0.262504	0.015809	-0.439109
N	0.411868	-1.174015	-0.049153
N	1.602483	-0.955892	0.169301
C	0.539461	1.153832	0.050933
C	1.913135	0.495408	0.023525
H	0.436411	1.995512	-0.626647
H	0.234666	1.446107	1.058692
H	2.588289	0.800194	0.817850
H	2.418220	0.623228	-0.935934

Molecule# 0876

1-chloroallyl isothiocyanate

PointGroup: C1

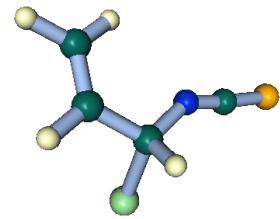
E= -1068.087482570 au

ZPE= 0.072300 au

LUMO_eps= -0.06926 au

HOMO_eps= -0.27137 au

Dipole= 2.481 debye



11

C1	1.206649	1.711643	-0.227494
S	-3.019563	-0.139639	-0.082460
N	-0.291654	-0.495146	0.196818
C	0.951475	0.047369	0.568780
C	2.117266	-0.819228	0.224719
C	2.032356	-1.986494	-0.395802
C	-1.463636	-0.293893	0.095615
H	0.943371	0.294738	1.629473
H	3.072452	-0.416382	0.534896
H	2.918954	-2.568416	-0.603567
H	1.082018	-2.394155	-0.711641

Molecule# 0877

1-chlorobutane

PointGroup: Cs

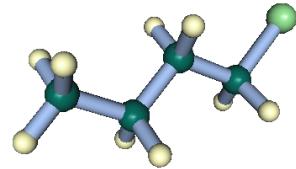
E= -618.153937589 au

ZPE= 0.123219 au

LUMO_eps= -0.01499 au

HOMO_eps= -0.29616 au

Dipole= 2.413 debye



14

C	1.161089	2.783469	0.000000
C	1.336413	1.265667	0.000000
C	0.000000	0.516511	0.000000
C	0.195757	-0.987200	0.000000
Cl	-1.389892	-1.875231	0.000000
H	0.609343	3.116554	0.880936
H	2.125518	3.292440	0.000000
H	0.609343	3.116554	-0.880936
H	1.921195	0.966651	0.874698
H	1.921195	0.966651	-0.874698
H	-0.585899	0.802883	0.876235
H	-0.585899	0.802883	-0.876235
H	0.726910	-1.328188	0.885109
H	0.726910	-1.328188	-0.885109

Molecule# 0878

1-chlorohexane

PointGroup: C1

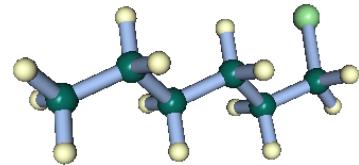
E= -696.809800572 au

ZPE= 0.179779 au

LUMO_eps= -0.01353 au

HOMO_eps= -0.29477 au

Dipole= 2.168 debye



20

C	4.107657	-0.250205	-0.215211
C	2.717325	-0.521399	0.356513
C	1.636426	0.390420	-0.225173
C	0.242168	0.120079	0.340479
C	-0.829692	1.038232	-0.244879
C	-2.225201	0.823188	0.309411
Cl	-2.919780	-0.797045	-0.154599
H	4.124179	-0.394646	-1.297420
H	4.854124	-0.916596	0.218969
H	4.423588	0.775876	-0.015423
H	2.443823	-1.564425	0.172169
H	2.740755	-0.402685	1.443977
H	1.613418	0.271434	-1.313552
H	1.909906	1.435111	-0.040928
H	0.262024	0.239696	1.428936
H	-0.032215	-0.919987	0.150936
H	-0.857119	0.939470	-1.332660
H	-0.568928	2.082139	-0.035424
H	-2.240983	0.846311	1.396326
H	-2.928401	1.556175	-0.074565

Molecule# 0879

1-chloronaphthalene

PointGroup: Cs

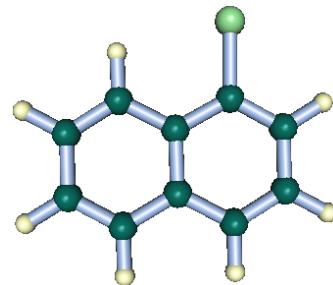
E= -845.659967429 au

ZPE= 0.137709 au

LUMO_eps= -0.06145 au

HOMO_eps= -0.23046 au

Dipole= 1.734 debye



18

C	1.134283	-0.569029	0.000000
C	1.016492	-1.932922	0.000000
C	-0.261594	-2.526193	0.000000
C	-1.387179	-1.747660	0.000000
C	-2.441560	0.487066	0.000000
C	-2.335638	1.852213	0.000000
C	-1.064302	2.461445	0.000000
C	0.074645	1.699051	0.000000
C	0.000000	0.285851	0.000000
C	-1.289332	-0.336021	0.000000
Cl	2.747884	0.124724	0.000000
H	1.904173	-2.548108	0.000000
H	-0.340512	-3.604770	0.000000
H	-2.369483	-2.201792	0.000000
H	-3.414600	0.012616	0.000000
H	-3.225734	2.466898	0.000000
H	-0.988024	3.540457	0.000000
H	1.045261	2.171590	0.000000

Molecule# 0880

1-chloropentane

PointGroup: C1

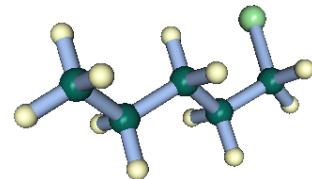
E= -657.481752806 au

ZPE= 0.151526 au

LUMO_eps= -0.01347 au

HOMO_eps= -0.29508 au

Dipole= 2.214 debye



17

C	3.289623	-0.683161	0.151762
C	2.227943	0.295481	-0.346814
C	0.848628	0.047344	0.264611
C	-0.212368	1.027510	-0.233040
C	-1.589905	0.838545	0.373045
Cl	-2.363950	-0.734686	-0.125608
H	3.018596	-1.713424	-0.086887
H	3.409472	-0.616939	1.235067
H	4.260930	-0.481964	-0.301814
H	2.544221	1.319704	-0.126280
H	2.154297	0.228978	-1.436338
H	0.918418	0.115557	1.355563
H	0.530695	-0.973458	0.040898
H	-0.289842	0.977813	-1.321766
H	0.095882	2.051249	0.008963
H	-1.558172	0.815998	1.459589
H	-2.280876	1.611830	0.050962

Molecule# 0881

1-chloropropane

PointGroup: C1

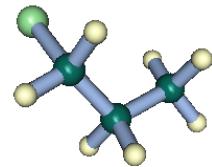
E= -578.825678418 au

ZPE= 0.094784 au

LUMO_eps= -0.01420 au

HOMO_eps= -0.29666 au

Dipole= 2.217 debye



11

C	-1.818641	-0.717279	0.144096
C	-1.150092	0.559242	-0.358350
C	0.172758	0.883165	0.310034
Cl	1.464599	-0.345613	-0.067396
H	-2.003786	-0.667711	1.219027
H	-2.776988	-0.872261	-0.351812
H	-1.195361	-1.589705	-0.048379
H	-1.001591	0.509688	-1.438752
H	-1.806916	1.416179	-0.174399
H	0.089223	0.894421	1.394122
H	0.573090	1.834040	-0.028754

Molecule# 0882

1-chloropyrazole

PointGroup: C1

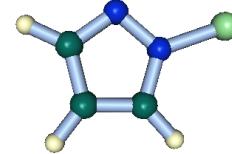
E= -685.870986804 au

ZPE= 0.060559 au

LUMO_eps= -0.05849 au

HOMO_eps= -0.26663 au

Dipole= 2.163 debye



9

C1	-1.906509	-0.012464	-0.000003
N	-0.208360	0.009411	0.000000
N	0.477354	-1.136970	0.000000
C	0.568717	1.122667	0.000002
C	1.748562	-0.743730	0.000002
C	1.865057	0.659271	0.000004
H	0.143298	2.109292	0.000002
H	2.528586	-1.486330	0.000002
H	2.761801	1.252584	0.000006

Molecule# 0883

1-cyano-1-bromoethene

PointGroup: Cs

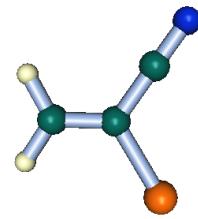
E= -2744.519275110 au

ZPE= 0.040960 au

LUMO_eps= -0.08518 au

HOMO_eps= -0.29270 au

Dipole= 3.607 debye



7

Br	-0.528269	-1.001303	0.000000
N	2.548987	1.195833	0.000000
C	0.000000	0.834859	0.000000
C	1.407533	1.038004	0.000000
C	-0.884708	1.825293	0.000000
H	-0.543534	2.851220	0.000000
H	-1.946908	1.634614	0.000000

Molecule# 0884

1-cyano-1,1-difluoroethane

PointGroup: C1

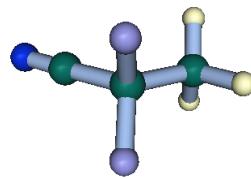
E= -370.684345292 au

ZPE= 0.057856 au

LUMO_eps= -0.02904 au

HOMO_eps= -0.37660 au

Dipole= 3.297 debye



9

F	-0.675349	-0.769946	1.097109
F	-0.675515	-0.770081	-1.096910
N	2.321971	0.174000	-0.000189
C	-0.299060	-0.045692	0.000026
C	-0.986636	1.297029	-0.000005
C	1.181140	0.048530	-0.000093
H	-2.061714	1.126864	0.000085
H	-0.703552	1.858035	-0.887970
H	-0.703421	1.858143	0.887851

Molecule# 0885

1-cyano-1,2-difluoroethane

PointGroup: C1

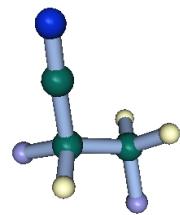
E= -370.670675795 au

ZPE= 0.059131 au

LUMO_eps= -0.03892 au

HOMO_eps= -0.36148 au

Dipole= 1.907 debye



9

F	-0.068610	1.517102	-0.198375
F	-2.172960	-0.385347	0.136936
N	2.539942	-0.590490	-0.068123
C	0.095496	0.250121	0.339624
C	-0.898581	-0.714336	-0.288536
C	1.473579	-0.202694	0.110068
H	-0.088862	0.322052	1.413853
H	-0.677638	-1.735688	0.024438
H	-0.861929	-0.637279	-1.375414

Molecule# 0886

1-cyano-2-fluoroethene

PointGroup: C1

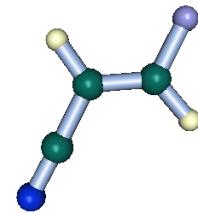
E= -270.174484285 au

ZPE= 0.043249 au

LUMO_eps= -0.07139 au

HOMO_eps= -0.30038 au

Dipole= 2.840 debye



7

F 2.208132 0.011420 0.000000

N -2.522866 -0.216097 0.000001

C -0.054551 0.505268 0.000000

C 0.934896 -0.381578 0.000000

C -1.412545 0.093056 0.000000

H 0.158393 1.565950 0.000001

H 0.821683 -1.456525 0.000000

Molecule# 0887

1-cyclohexylethanone

PointGroup: C1

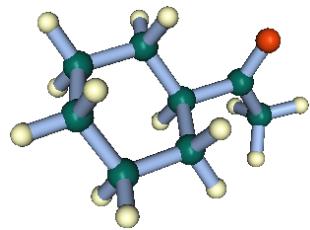
E= -388.665845212 au

ZPE= 0.206479 au

LUMO_eps= -0.02349 au

HOMO_eps= -0.24966 au

Dipole= 2.917 debye



23

C	1.811591	-0.159551	-0.096424
C	-2.556321	0.066825	-0.240521
C	-1.751190	1.356259	-0.059733
C	-1.921204	-1.099327	0.521490
C	-0.281229	1.164125	-0.442828
C	-0.451165	-1.293520	0.140424
C	0.359157	-0.006631	0.338914
C	2.843613	0.624195	0.685597
O	2.127563	-0.861400	-1.032000
H	-3.586727	0.217570	0.088357
H	-2.602212	-0.181621	-1.305799
H	-2.183986	2.161109	-0.657926
H	-1.812407	1.678111	0.985184
H	-1.997578	-0.910144	1.597770
H	-2.475926	-2.020574	0.331373
H	-0.204618	0.946364	-1.511824
H	0.274902	2.088076	-0.268004
H	-0.011128	-2.101922	0.728414
H	-0.371415	-1.596118	-0.905549
H	0.351723	0.262560	1.401185
H	2.520697	1.654562	0.843527
H	2.957113	0.173697	1.675299
H	3.801543	0.605286	0.172476

Molecule# 0888

1-decanol

PointGroup: Cs

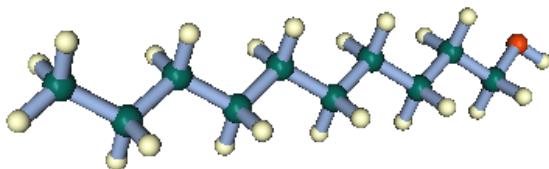
E= -469.734292450 au

ZPE= 0.306555 au

LUMO_eps= -0.01331 au

HOMO_eps= -0.27943 au

Dipole= 1.546 debye



33

C	-6.348463	-0.676838	0.000000
C	-5.115500	0.225307	0.000000
C	-3.797980	-0.550892	0.000000
C	-2.557416	0.342637	0.000000
C	-1.240689	-0.434878	0.000000
C	0.000000	0.458845	0.000000
C	1.316086	-0.319402	0.000000
C	2.556349	0.575341	0.000000
C	3.868290	-0.209696	0.000000
C	5.092393	0.687237	0.000000
O	6.258306	-0.139839	0.000000
H	-6.364365	-1.322364	0.880634
H	-6.364365	-1.322364	-0.880634
H	-7.270587	-0.093915	0.000000
H	-5.145071	0.883042	-0.873992
H	-5.145071	0.883042	0.873992
H	-3.769111	-1.209699	0.874515
H	-3.769111	-1.209699	-0.874515
H	-2.587308	1.001155	0.874567
H	-2.587308	1.001155	-0.874567
H	-1.210788	-1.093366	0.874472
H	-1.210788	-1.093366	-0.874472
H	-0.029832	1.117282	0.874617
H	-0.029832	1.117282	-0.874617
H	1.346921	-0.977463	-0.874449
H	1.346921	-0.977463	0.874449
H	2.524211	1.232959	0.875019
H	2.524211	1.232959	-0.875019
H	3.914692	-0.861511	0.876340
H	3.914692	-0.861511	-0.876340
H	5.083448	1.333838	0.885549
H	5.083448	1.333838	-0.885549
H	7.040122	0.418909	0.000000

Molecule# 0889

1-dichloroamino-oxy-1-methoxyethene

PointGroup: C1

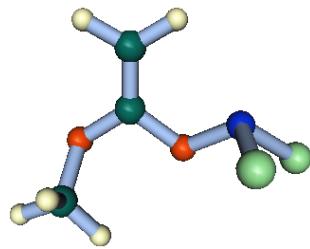
E= -1242.952704250 au

ZPE= 0.084233 au

LUMO_eps= -0.10988 au

HOMO_eps= -0.25814 au

Dipole= 1.493 debye



13

C1	-2.228128	-1.021501	-0.416681
C1	-1.176042	1.636902	0.087881
O	0.217710	-0.557728	-0.248136
O	2.451588	-0.549725	-0.247351
N	-0.936161	-0.161967	0.426500
C	1.373759	-0.430493	0.538916
C	1.403284	-0.296492	1.855640
C	2.597789	0.411824	-1.311164
H	0.502906	-0.317994	2.444647
H	2.358608	-0.182888	2.340675
H	3.551083	0.185303	-1.778270
H	1.794461	0.315767	-2.038707
H	2.613575	1.422361	-0.900703

Molecule# 0890

1-difluoroaminoethanol

PointGroup: C1

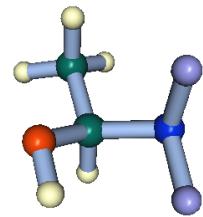
E= -408.920544831 au

ZPE= 0.079452 au

LUMO_eps= -0.02076 au

HOMO_eps= -0.30301 au

Dipole= 2.199 debye



11

F	-1.669344	0.483858	-0.453523
F	-0.788373	-1.103319	0.767200
O	0.629635	1.223624	0.727671
N	-0.619879	-0.472984	-0.472184
C	0.621002	0.357868	-0.363789
C	1.814672	-0.567909	-0.285540
H	-0.126057	1.819060	0.668820
H	0.599329	0.897393	-1.316545
H	2.723091	0.026037	-0.362124
H	1.817974	-1.095028	0.666070
H	1.793148	-1.290166	-1.099425

Molecule# 0891

1-ethoxy-2-methoxyethane

PointGroup: C1

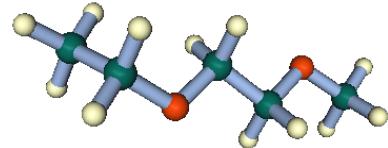
E= -348.316279038 au

ZPE= 0.168982 au

LUMO_eps= -0.00892 au

HOMO_eps= -0.26201 au

Dipole= 0.197 debye



19

C	3.132473	0.770972	0.253731
C	-3.489777	0.102524	0.120232
C	2.463060	-0.488339	-0.280821
C	-1.182999	-0.374018	0.214782
C	0.153763	0.132123	-0.293733
O	-2.191518	0.483645	-0.283274
O	1.158560	-0.710687	0.238596
H	4.155816	0.833282	-0.120982
H	2.611059	1.675762	-0.058785
H	3.167460	0.751844	1.343340
H	-4.186566	0.819251	-0.309463
H	-3.589678	0.116485	1.212175
H	-3.741954	-0.902048	-0.239929
H	3.038609	-1.367952	0.008601
H	2.422491	-0.463753	-1.377404
H	-1.184178	-0.379223	1.312052
H	-1.345961	-1.404224	-0.125418
H	0.289010	1.172957	0.018531
H	0.168426	0.104380	-1.390449

Molecule# 0892

1-ethoxyethoxyethane

PointGroup: C1

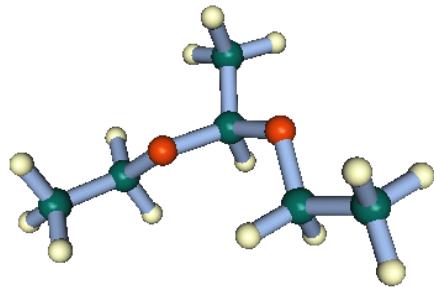
E= -387.663916866 au

ZPE= 0.196549 au

LUMO_eps= -0.01143 au

HOMO_eps= -0.26488 au

Dipole= 1.812 debye



22

C	2.945747	-1.326432	-0.272137
C	-3.205462	-0.965279	-0.174465
C	0.235796	2.251178	-0.163046
C	2.118990	-0.257690	0.413385
C	-1.783395	-0.782436	0.311995
C	-0.023554	0.819576	0.264379
O	0.911871	-0.083840	-0.314715
O	-1.302450	0.472628	-0.168283
H	3.881046	-1.483282	0.266831
H	2.403192	-2.271186	-0.304900
H	3.182130	-1.032240	-1.294481
H	-3.603189	-1.917908	0.177985
H	-3.848536	-0.165468	0.192996
H	-3.241225	-0.960448	-1.263778
H	0.138687	2.326594	-1.245260
H	1.239390	2.563008	0.124892
H	-0.483643	2.921348	0.306118
H	2.680904	0.683225	0.457447
H	1.890021	-0.550298	1.446690
H	-1.139904	-1.586590	-0.051523
H	-1.743586	-0.787738	1.409110
H	0.040618	0.717179	1.361201

Molecule# 0893

1-ethoxypropane

PointGroup: Cs

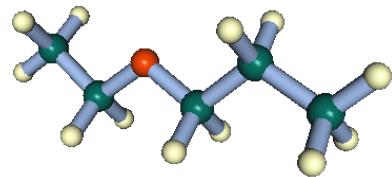
E= -273.087478167 au

ZPE= 0.164192 au

LUMO_eps= -0.01013 au

HOMO_eps= -0.26072 au

Dipole= 1.008 debye



18

C	0.989190	2.876892	0.000000
H	1.934526	3.421126	0.000000
H	0.422313	3.170372	0.883513
H	0.422313	3.170372	-0.883513
C	1.244016	1.383759	0.000000
H	1.827047	1.091952	-0.884410
H	1.827047	1.091952	0.884410
O	0.000000	0.704770	0.000000
C	0.125303	-0.705775	0.000000
H	0.691231	-1.031792	-0.884779
H	0.691231	-1.031792	0.884779
C	-1.257913	-1.331654	0.000000
H	-1.802831	-0.972980	0.875837
H	-1.802831	-0.972980	-0.875837
C	-1.205589	-2.858427	0.000000
H	-0.685547	-3.239386	-0.881267
H	-0.685547	-3.239386	0.881267
H	-2.208990	-3.284394	0.000000

Molecule# 0894

1-ethyl-1H-imidazole

PointGroup: C1

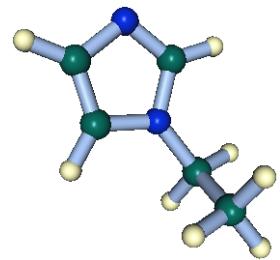
E= -304.958860727 au

ZPE= 0.127196 au

LUMO_eps= -0.01890 au

HOMO_eps= -0.23390 au

Dipole= 4.295 debye



15

N	1.951229	-0.653592	0.274179
C	-1.544566	-0.217982	-0.577174
C	0.599777	1.081360	-0.202261
H	0.156334	2.041637	-0.396652
C	1.871547	0.709910	0.140798
H	2.728958	1.343392	0.292022
H	0.434363	-2.128670	0.020356
C	0.743448	-1.095776	0.014974
N	-0.123330	-0.087560	-0.284887
H	-1.720891	-1.257639	-0.851818
H	-1.770847	0.387341	-1.456142
C	-2.439557	0.181938	0.592297
H	-2.233726	-0.434183	1.467321
H	-3.488111	0.054549	0.320622
H	-2.285276	1.224935	0.867450

Molecule# 0895

1-ethyl-2-methylbenzene

PointGroup: C1

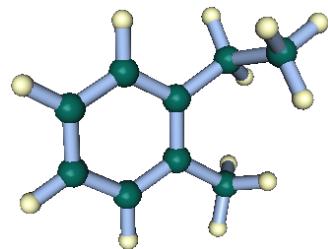
E= -350.323630876 au

ZPE= 0.183939 au

LUMO_eps= -0.01582 au

HOMO_eps= -0.24139 au

Dipole= 0.660 debye



21

C	2.405659	-0.121060	0.246773
C	1.838083	-1.367505	0.021924
C	1.605620	1.013405	0.195074
C	0.478870	-1.458493	-0.249138
C	0.238294	0.935373	-0.073405
C	-0.337705	-0.327932	-0.297810
C	-0.578927	2.201942	-0.131830
C	-2.647406	-0.664207	0.717826
C	-1.815959	-0.498821	-0.563287
H	3.462852	-0.029350	0.457059
H	2.446720	-2.261366	0.052064
H	2.051065	1.985879	0.364968
H	0.037240	-2.430840	-0.432374
H	-1.016171	2.353512	-1.121381
H	-1.404257	2.191747	0.581999
H	0.039631	3.069984	0.091030
H	-2.324469	-1.542269	1.278281
H	-3.705954	-0.783854	0.481579
H	-2.545656	0.200048	1.374935
H	-2.198729	0.349580	-1.132566
H	-1.961452	-1.379284	-1.192367

Molecule# 0896

1-ethyl-4-methylbenzene

PointGroup: C1

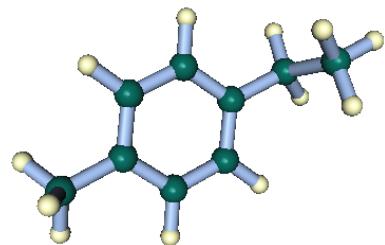
E= -350.325638356 au

ZPE= 0.183446 au

LUMO_eps= -0.01456 au

HOMO_eps= -0.23745 au

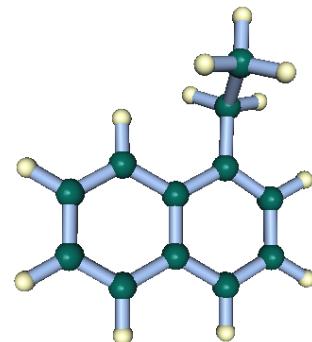
Dipole= 0.064 debye



21

C	1.146241	1.193842	-0.045431
C	1.145772	-1.192583	-0.047381
C	-0.230006	1.193850	-0.240696
C	-0.229569	-1.192065	-0.242263
C	1.860578	0.000971	0.058338
C	-0.945645	0.001362	-0.341139
C	3.348664	-0.001567	0.293250
C	-3.212526	-0.002676	0.806592
C	-2.443952	0.001078	-0.522341
H	1.673704	2.137762	0.019717
H	1.673111	-2.136822	0.016045
H	-0.753713	2.138576	-0.325696
H	-0.753659	-2.136478	-0.328520
H	3.832697	-0.827825	-0.228257
H	3.806428	0.927029	-0.047139
H	3.579777	-0.109506	1.356230
H	-2.964444	-0.884319	1.399104
H	-4.290020	-0.003069	0.634112
H	-2.965687	0.876560	1.403176
H	-2.738175	0.877564	-1.103946
H	-2.737362	-0.872740	-1.108399

Molecule# 0897
 1-ethylnaphthalene
 PointGroup: C1
 E= -464.685475931 au
 ZPE= 0.203499 au
 LUMO_eps= -0.04933 au
 HOMO_eps= -0.22036 au
 Dipole= 0.401 debye



24

C	2.843382	-0.911793	0.095853
C	1.865295	-1.900259	-0.134234
C	-0.579750	2.511077	0.033711
C	2.473262	0.403278	0.193327
C	0.543571	-1.555480	-0.257841
C	0.733917	2.152826	0.165181
C	-1.562211	1.527220	-0.196166
C	1.117464	0.793908	0.069366
C	0.119466	-0.205263	-0.160726
C	-1.248770	0.190590	-0.290811
C	-2.802522	-1.523090	0.785080
C	-2.351636	-0.819638	-0.504417
H	3.882886	-1.194986	0.192496
H	2.160956	-2.937871	-0.214193
H	-0.872273	3.550458	0.101606
H	3.218207	1.169736	0.366401
H	-0.186369	-2.331752	-0.434482
H	1.496318	2.901125	0.340027
H	-2.595290	1.834475	-0.303229
H	-1.982937	-2.067541	1.253974
H	-3.604229	-2.233272	0.576827
H	-3.173490	-0.797867	1.510083
H	-3.209005	-0.305295	-0.941733
H	-2.043584	-1.567462	-1.237707

Molecule# 0898

1-ethylsulfinylpropane

PointGroup: C1

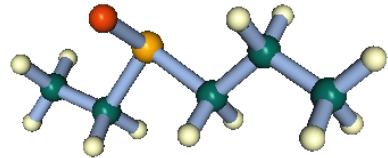
E= -671.292611905 au

ZPE= 0.164314 au

LUMO_eps= -0.01616 au

HOMO_eps= -0.23199 au

Dipole= 3.877 debye



19

C	3.493846	-0.421699	0.204243
C	-3.184549	-0.384832	0.026086
C	2.208239	0.268987	-0.251395
C	-1.762741	-0.898519	0.195965
C	0.966634	-0.554479	0.069940
O	-0.668107	1.544752	0.490797
S	-0.558033	0.349232	-0.423484
H	4.366226	0.187832	-0.033018
H	3.490187	-0.590172	1.282549
H	3.622266	-1.390088	-0.283365
H	-3.313566	0.561793	0.548967
H	-3.430342	-0.232732	-1.025459
H	-3.894890	-1.102230	0.438056
H	2.251096	0.456272	-1.327242
H	2.117148	1.242262	0.233126
H	-1.584775	-1.813954	-0.371007
H	-1.518743	-1.069941	1.245101
H	0.880940	-0.746643	1.141226
H	0.959278	-1.504876	-0.468592

Molecule# 0899

1-ethylsulfonylpropane

PointGroup: Cs

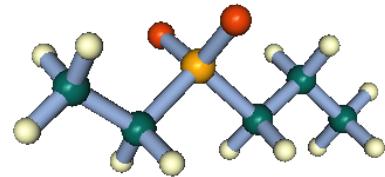
E= -746.546038616 au

ZPE= 0.170212 au

LUMO_eps= -0.02178 au

HOMO_eps= -0.28899 au

Dipole= 4.411 debye



20

C	-2.143446	-2.929295	0.000000
C	1.157418	2.955149	0.000000
C	-0.838198	-2.133417	0.000000
C	-0.055932	2.033897	0.000000
C	-1.094835	-0.628266	0.000000
O	1.157418	0.026179	1.262499
O	1.157418	0.026179	-1.262499
S	0.468746	0.293929	0.000000
H	-1.938473	-3.999896	0.000000
H	-2.746355	-2.706824	0.882228
H	-2.746355	-2.706824	-0.882228
H	0.824711	3.992976	0.000000
H	1.770380	2.790531	0.884210
H	1.770380	2.790531	-0.884210
H	-0.242657	-2.391528	-0.876212
H	-0.242657	-2.391528	0.876212
H	-0.670671	2.165871	-0.889878
H	-0.670671	2.165871	0.889878
H	-1.638152	-0.309656	-0.890168
H	-1.638152	-0.309656	0.890168

Molecule# 0900

1-heptanamine

PointGroup: Cs

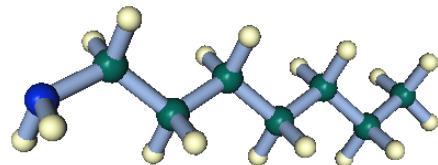
E= -331.874793928 au

ZPE= 0.234162 au

LUMO_eps= -0.01305 au

HOMO_eps= -0.24050 au

Dipole= 1.399 debye



25

C	2.858294	3.448276	0.000000
C	1.443396	2.872081	0.000000
C	1.412286	1.343354	0.000000
C	0.000000	0.757661	0.000000
C	-0.030717	-0.771281	0.000000
C	-1.443246	-1.357334	0.000000
C	-1.465482	-2.889128	0.000000
N	-2.786976	-3.518510	0.000000
H	3.416468	3.123539	0.880618
H	3.416468	3.123539	-0.880618
H	2.845446	4.539098	0.000000
H	0.899109	3.242456	0.874013
H	0.899109	3.242456	-0.874013
H	1.957625	0.972748	0.874556
H	1.957625	0.972748	-0.874556
H	-0.544592	1.128853	0.874555
H	-0.544592	1.128853	-0.874555
H	0.514279	-1.142144	-0.874488
H	0.514279	-1.142144	0.874488
H	-1.990914	-0.993618	0.876239
H	-1.990914	-0.993618	-0.876239
H	-0.922544	-3.259922	-0.873380
H	-0.922544	-3.259922	0.873380
H	-3.321330	-3.237562	-0.813570
H	-3.321330	-3.237562	0.813570

Molecule# 0901

1-heptanol

PointGroup: C1

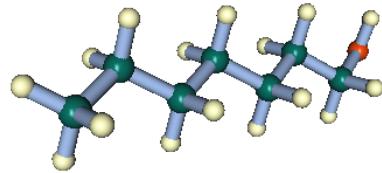
E= -351.750084522 au

ZPE= 0.221573 au

LUMO_eps= -0.01414 au

HOMO_eps= -0.27696 au

Dipole= 1.817 debye



24

C	4.455953	0.270233	0.013128
C	3.156486	-0.532657	-0.014810
C	1.903604	0.343655	0.011250
C	0.597863	-0.451106	-0.015679
C	-0.653922	0.427229	0.009040
C	-1.958782	-0.370300	-0.022500
C	-3.196862	0.516964	0.008447
O	-4.418615	-0.215524	-0.077873
H	4.523173	0.941403	-0.845601
H	5.329459	-0.382837	-0.007953
H	4.521716	0.882668	0.914818
H	3.133472	-1.218292	0.837586
H	3.136119	-1.162088	-0.909563
H	1.926908	1.029567	-0.842248
H	1.924665	0.974859	0.906112
H	0.577344	-1.082187	-0.910093
H	0.574572	-1.136132	0.838283
H	-0.629327	1.112199	-0.844708
H	-0.633266	1.057787	0.903988
H	-1.987895	-1.054978	0.832841
H	-1.997124	-0.992014	-0.920763
H	-3.202967	1.185677	-0.853276
H	-3.189897	1.145038	0.907556
H	-4.484069	-0.800583	0.682753

Molecule# 0902

1-heptene

PointGroup: C1

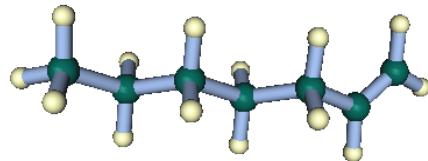
E= -275.270040070 au

ZPE= 0.193026 au

LUMO_eps= -0.00967 au

HOMO_eps= -0.26152 au

Dipole= 0.483 debye



21

C	-3.718906	0.008129	-0.494379
C	-2.699428	0.209382	0.331599
C	3.687893	-0.207825	-0.120495
C	-1.396675	-0.530695	0.303389
C	2.358809	0.545407	-0.139559
C	-0.186173	0.386338	0.074430
C	1.148183	-0.358947	0.093708
H	-4.631597	0.584270	-0.421349
H	-3.677416	-0.743766	-1.273896
H	-2.790163	0.977233	1.096030
H	3.716728	-0.976298	-0.895791
H	3.846764	-0.703368	0.839542
H	4.530129	0.464536	-0.289388
H	-1.260508	-1.052629	1.257535
H	-1.428811	-1.300599	-0.471834
H	2.244636	1.058481	-1.099103
H	2.373926	1.330018	0.622906
H	-0.176694	1.167721	0.841095
H	-0.305655	0.900978	-0.883282
H	1.134469	-1.144791	-0.669046
H	1.261978	-0.872523	1.054419

Molecule# 0903

1-heptyne

PointGroup: Cs

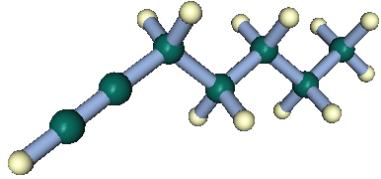
E= -274.017198198 au

ZPE= 0.169394 au

LUMO_eps= -0.01193 au

HOMO_eps= -0.27248 au

Dipole= 0.987 debye



19

C	2.257879	3.177876	0.000000
C	1.939719	2.020940	0.000000
C	-2.330524	-2.718125	0.000000
C	1.527217	0.622766	0.000000
C	-1.925506	-1.245234	0.000000
C	0.000000	0.434858	0.000000
C	-0.410473	-1.036234	0.000000
H	2.546918	4.198732	0.000000
H	-3.415229	-2.832921	0.000000
H	-1.942770	-3.234004	0.880832
H	-1.942770	-3.234004	-0.880832
H	1.956087	0.124043	-0.874253
H	1.956087	0.124043	0.874253
H	-2.356942	-0.748038	-0.873782
H	-2.356942	-0.748038	0.873782
H	-0.418718	0.938863	0.874266
H	-0.418718	0.938863	-0.874266
H	0.021563	-1.534311	-0.874638
H	0.021563	-1.534311	0.874638

Molecule# 0904

1-hexanamine

PointGroup: Cs

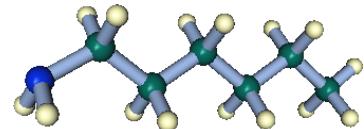
E= -292.546743082 au

ZPE= 0.205923 au

LUMO_eps= -0.01307 au

HOMO_eps= -0.24064 au

Dipole= 1.339 debye



22

C	3.802935	-0.490610	0.000000
C	2.559112	0.396474	0.000000
C	1.251338	-0.396094	0.000000
C	0.000000	0.482704	0.000000
C	-1.308018	-0.309699	0.000000
C	-2.556134	0.578683	0.000000
N	-3.845546	-0.114188	0.000000
H	4.717679	0.103723	0.000000
H	3.826861	-1.135787	0.880692
H	3.826861	-1.135787	-0.880692
H	2.580491	1.054451	0.873988
H	2.580491	1.054451	-0.873988
H	1.230295	-1.055016	0.874553
H	1.230295	-1.055016	-0.874553
H	0.022835	1.141535	-0.874500
H	0.022835	1.141535	0.874500
H	-1.338505	-0.966435	0.876192
H	-1.338505	-0.966435	-0.876192
H	-2.533944	1.235791	0.873348
H	-2.533944	1.235791	-0.873348
H	-3.935161	-0.711119	0.813635
H	-3.935161	-0.711119	-0.813635

Molecule# 0905

1-hexanol

PointGroup: C1

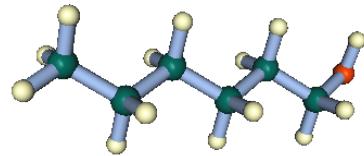
E= -312.422028067 au

ZPE= 0.193201 au

LUMO_eps= -0.01417 au

HOMO_eps= -0.27725 au

Dipole= 1.804 debye



21

C	3.803979	-0.333546	-0.007335
C	2.523952	0.499934	0.021358
C	1.251148	-0.346744	-0.014028
C	-0.035517	0.479205	0.013309
C	-1.306448	-0.371112	-0.025050
C	-2.580107	0.464187	0.009234
O	-3.770500	-0.317449	-0.083397
H	4.692588	0.298478	0.020787
H	3.852231	-1.011503	0.847324
H	3.858181	-0.941543	-0.912719
H	2.519811	1.190707	-0.827105
H	2.515487	1.124471	0.919783
H	1.255049	-1.037842	0.835498
H	1.259420	-0.972533	-0.912499
H	-0.037623	1.169441	-0.836563
H	-0.042076	1.104927	0.911889
H	-1.308490	-1.061289	0.826320
H	-1.317911	-0.988628	-0.926931
H	-2.600079	1.086487	0.912165
H	-2.612653	1.137348	-0.848433
H	-3.811971	-0.910475	0.672738

Molecule# 0906

1-hexene

PointGroup: C1

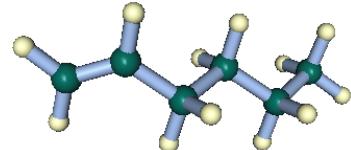
E= -235.942000663 au

ZPE= 0.164706 au

LUMO_eps= -0.00938 au

HOMO_eps= -0.26175 au

Dipole= 0.488 debye



18

C	3.083882	-0.164653	-0.435306
C	2.038689	-0.211887	0.381630
C	-3.012649	-0.378385	-0.169663
C	0.775189	0.578680	0.225667
C	-1.771338	0.499840	-0.023071
C	-0.474243	-0.302353	0.082056
H	3.964976	-0.769042	-0.266002
H	3.096130	0.483870	-1.303601
H	2.074756	-0.880467	1.238236
H	-2.952804	-0.999751	-1.065528
H	-3.919711	0.223030	-0.243990
H	-3.127075	-1.046179	0.686669
H	0.861213	1.241498	-0.639318
H	0.645805	1.223387	1.102645
H	-1.704688	1.181440	-0.876345
H	-1.875165	1.133412	0.863013
H	-0.537082	-0.981633	0.938389
H	-0.363539	-0.937015	-0.802044

Molecule# 0907

1-hexyne

PointGroup: Cs

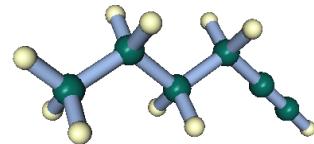
E= -234.689153439 au

ZPE= 0.141132 au

LUMO_eps= -0.01181 au

HOMO_eps= -0.27282 au

Dipole= 0.989 debye



16

C	-2.312498	-2.277578	0.000000
C	-1.228339	-1.763422	0.000000
C	1.311092	2.604422	0.000000
C	0.077794	-1.116147	0.000000
C	1.378741	1.078321	0.000000
C	0.000000	0.420250	0.000000
H	-3.268709	-2.737512	0.000000
H	2.308010	3.046780	0.000000
H	0.783276	2.975425	0.880761
H	0.783276	2.975425	-0.880761
H	0.642365	-1.452734	0.874593
H	0.642365	-1.452734	-0.874593
H	1.941609	0.738131	-0.874478
H	1.941609	0.738131	0.874478
H	-0.567271	0.747005	0.874792
H	-0.567271	0.747005	-0.874792

Molecule# 0908

1-hydroperoxy-N-nitrosodimethylamine

PointGroup: C1

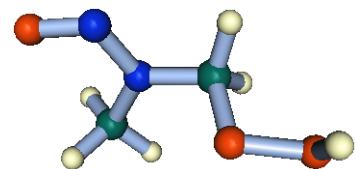
E= -414.988053368 au

ZPE= 0.097225 au

LUMO_eps= -0.05990 au

HOMO_eps= -0.25028 au

Dipole= 2.829 debye



13

O	1.527751	-0.041787	-0.537922
O	2.903656	-0.081519	-0.081598
O	-2.550243	-0.648905	-0.302870
N	-0.622833	0.129378	0.252599
N	-1.430434	-0.925890	0.075880
C	0.715920	-0.171147	0.638713
C	-1.072890	1.482292	-0.050054
H	1.075986	0.533849	1.388665
H	0.743524	-1.191858	1.019263
H	-0.254370	2.165555	0.153369
H	-1.938584	1.731739	0.562219
H	-1.363685	1.558623	-1.097009
H	3.202517	-0.911507	-0.478692

Molecule# 0909

1-hydroxy-1,3-dibutyne

PointGroup: C1

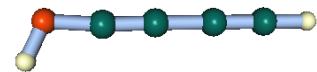
E= -228.790422130 au

ZPE= 0.041882 au

LUMO_eps= -0.03624 au

HOMO_eps= -0.24603 au

Dipole= 2.061 debye



7

O -2.416628 -0.098841 -0.000028

C 0.087033 -0.011100 0.000005

C -1.117057 -0.002424 -0.000010

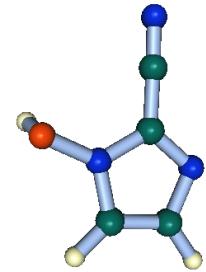
C 1.449836 0.001422 0.000013

C 2.655112 0.011669 0.000023

H -2.832487 0.773856 0.000005

H 3.715965 0.019465 0.000027

Molecule# 0910
1-hydroxy-1H-imidazole-2-carbonitrile
PointGroup: C1
E= -393.762559270 au
ZPE= 0.072834 au
LUMO_eps= -0.06296 au
HOMO_eps= -0.27049 au
Dipole= 5.328 debye



11

O	-0.027776	1.986911	-0.109462
N	0.447489	0.699855	0.009592
N	0.482610	-1.505368	0.002437
N	-2.871050	-0.377420	0.004695
C	-0.304395	-0.445800	-0.010178
C	1.764045	0.350395	0.006510
C	1.757719	-1.024291	0.007880
C	-1.719987	-0.424794	-0.008428
H	-0.325015	2.249084	0.774101
H	2.543576	1.089605	-0.002664
H	2.606018	-1.686508	0.012487

Molecule# 0911

1-hydroxy-3,4-dihydroquinolin-2-one

PointGroup: C1

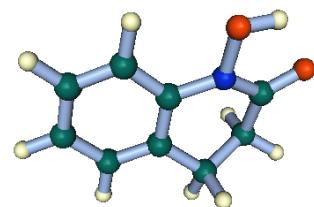
E= -553.755145311 au

ZPE= 0.166973 au

LUMO_eps= -0.03656 au

HOMO_eps= -0.22580 au

Dipole= 3.071 debye



21

C	3.077395	0.196598	-0.111658
C	2.666570	-1.128501	-0.161156
C	2.129143	1.205688	0.034852
C	1.317412	-1.453527	-0.078360
C	0.776833	0.911753	0.133669
C	0.382349	-0.432412	0.060180
C	-2.008325	0.164976	-0.109593
C	-0.286188	1.954073	0.363802
C	-1.588515	1.593777	-0.354663
N	-0.990799	-0.704017	0.145273
O	-3.161157	-0.254175	-0.157240
O	-1.361171	-2.042198	0.243835
H	4.126728	0.446250	-0.182912
H	3.395360	-1.919947	-0.269911
H	2.445503	2.240189	0.082160
H	0.987299	-2.479262	-0.120828
H	-0.484242	2.028309	1.438806
H	0.064034	2.934551	0.042685
H	-1.473721	1.707651	-1.437370
H	-2.413797	2.234873	-0.051575
H	-2.332996	-1.968059	0.126836

Molecule# 0912

1-hydroxyguanidine

PointGroup: C1

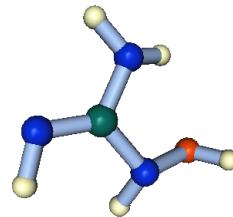
E= -280.658477309 au

ZPE= 0.079775 au

LUMO_eps= -0.02550 au

HOMO_eps= -0.24241 au

Dipole= 2.770 debye



10

O	1.787242	0.003282	-0.184204
N	0.624265	-0.739187	0.193069
N	-1.728663	-0.614242	-0.065776
N	-0.477517	1.325874	0.083465
C	-0.595184	-0.035554	0.023160
H	2.301487	0.044235	0.629806
H	0.630705	-1.583507	-0.364470
H	-1.653756	-1.625649	-0.018118
H	-1.320486	1.821828	-0.150356
H	0.388624	1.723041	-0.237498

Molecule# 0913

1-isocyanato-1,1,2-ethanetriol

PointGroup: C1

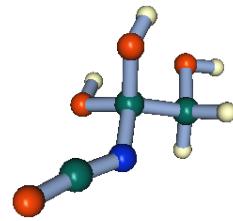
E= -473.163969733 au

ZPE= 0.092347 au

LUMO_eps= -0.03535 au

HOMO_eps= -0.30062 au

Dipole= 5.142 debye



13

O	-0.307443	-0.870123	-1.164144
O	-0.307406	-0.869880	1.164290
O	-2.627780	0.100056	0.000029
O	3.229423	0.053522	0.000030
N	0.941114	0.662461	-0.000117
C	-0.281383	-0.078177	-0.000011
C	-1.450502	0.910137	-0.000090
C	2.088626	0.280911	-0.000031
H	-1.215065	-1.172916	-1.295790
H	-1.215054	-1.172515	1.296121
H	-3.410450	0.656719	-0.000033
H	-1.390992	1.532924	0.893801
H	-1.391037	1.532728	-0.894121

Molecule# 0914

1-isocyanato-1,2,2-ethanetriol

PointGroup: C1

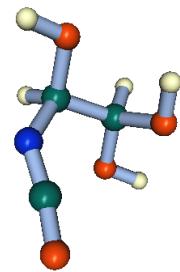
E= -473.162623581 au

ZPE= 0.092808 au

LUMO_eps= -0.02600 au

HOMO_eps= -0.29325 au

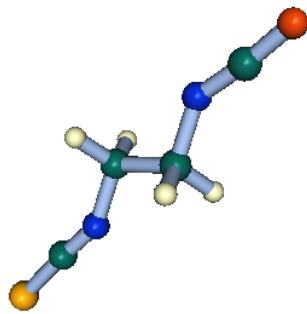
Dipole= 3.064 debye



13

O	-1.482146	-1.542331	0.230188
O	-0.780161	0.943861	1.241654
O	-0.288525	1.618368	-0.871586
O	2.697279	0.071265	0.337982
N	0.716696	-0.999336	-0.393493
C	-0.677117	-0.691619	-0.564145
C	-1.055012	0.730034	-0.123074
C	1.681516	-0.387203	-0.003450
H	-1.203672	-2.453161	0.090455
H	-1.228041	0.256337	1.750743
H	-0.405482	2.503660	-0.509998
H	-0.919496	-0.810808	-1.623032
H	-2.128076	0.862744	-0.315611

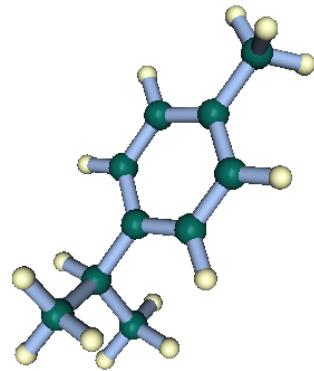
Molecule# 0915
1-isocyanato-2-isothiocyanatoethane
PointGroup: C1
E= -737.905674371 au
ZPE= 0.080720 au
LUMO_eps= -0.04792 au
HOMO_eps= -0.26205 au
Dipole= 0.349 debye



12

S	-3.986894	-0.049708	-0.000087
O	4.775654	-0.113191	-0.000147
N	-1.218888	-0.119564	0.000118
N	2.439468	0.263192	0.000069
C	0.039669	0.560667	0.000057
C	1.185169	-0.449890	0.000115
C	-2.404278	-0.042911	0.000025
C	3.612272	0.010529	-0.000044
H	0.112187	1.198876	-0.883098
H	0.112207	1.198992	0.883127
H	1.109813	-1.086449	-0.883060
H	1.109821	-1.086333	0.883374

Molecule# 0916
 1-isopropyl-4-methylbenzene
 PointGroup: C1
 E= -389.652750457 au
 ZPE= 0.211318 au
 LUMO_eps= -0.01373 au
 HOMO_eps= -0.23752 au
 Dipole= 0.021 debye



24

C	1.600593	1.193755	0.000030
C	1.362015	-1.179084	-0.000623
C	0.214960	1.329237	0.000273
C	-0.018274	-1.043342	-0.000385
C	2.201025	-0.061784	-0.000327
C	-0.622831	0.217224	0.000106
C	3.699139	-0.219727	0.000340
C	-2.774529	-0.208537	1.265773
C	-2.774681	-0.207345	-1.265700
C	-2.132337	0.379225	0.000275
H	2.220883	2.081689	0.000055
H	1.797012	-2.171508	-0.001121
H	-0.219605	2.321673	0.000499
H	-0.631041	-1.935901	-0.000690
H	4.039551	-0.780061	-0.872912
H	4.199664	0.747760	-0.008810
H	4.040365	-0.763522	0.883764
H	-2.623372	-1.288055	1.321226
H	-3.850322	-0.023817	1.272330
H	-2.347796	0.233736	2.166427
H	-2.348059	0.235781	-2.165987
H	-3.850477	-0.022626	-1.271955
H	-2.623518	-1.286809	-1.322188
H	-2.333765	1.453939	0.000792

Molecule# 0917

1-methoxybut-2-yne

PointGroup: C1

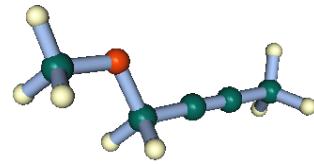
E= -270.598079772 au

ZPE= 0.116951 au

LUMO_eps= -0.01217 au

HOMO_eps= -0.25570 au

Dipole= 0.998 debye



14

C	-1.854995	0.059212	0.000286
C	-0.682965	0.318398	0.000121
C	-3.272404	-0.269344	-0.000016
C	2.908916	-0.231355	-0.000182
C	0.731823	0.658966	0.000000
O	1.525377	-0.520062	0.000268
H	-3.785213	0.196056	-0.843401
H	-3.757047	0.068458	0.917494
H	-3.416982	-1.348358	-0.076266
H	3.201339	0.338694	0.890135
H	3.200880	0.338009	-0.891089
H	3.434078	-1.183772	0.000063
H	0.968850	1.268307	0.883485
H	0.968823	1.267833	-0.883814

Molecule# 0918

1-methoxybutane

PointGroup: Cs

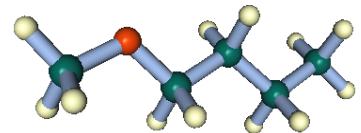
E= -273.082140860 au

ZPE= 0.164293 au

LUMO_eps= -0.01035 au

HOMO_eps= -0.26246 au

Dipole= 1.166 debye



18

C	1.485110	2.778995	0.000000
C	1.429424	1.252245	0.000000
C	-1.555601	-2.629031	0.000000
O	-1.408397	-1.225844	0.000000
C	-0.054114	-0.808031	0.000000
C	0.000000	0.708683	0.000000
H	-2.622301	-2.844448	0.000000
H	2.514453	3.139718	0.000000
H	0.988352	3.190751	0.880627
H	0.988352	3.190751	-0.880627
H	1.964404	0.869962	0.874461
H	1.964404	0.869962	-0.874461
H	-1.100454	-3.081175	0.889958
H	-1.100454	-3.081175	-0.889958
H	-0.538951	1.078011	-0.876368
H	-0.538951	1.078011	0.876368
H	0.459702	-1.210388	-0.884985
H	0.459702	-1.210388	0.884985

Molecule# 0919

1-methoxyethanimine

PointGroup: Cs

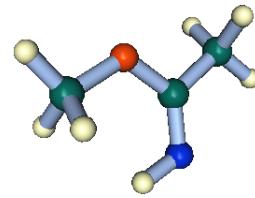
E= -248.598421746 au

ZPE= 0.101667 au

LUMO_eps= -0.01490 au

HOMO_eps= -0.27919 au

Dipole= 2.191 debye



12

C	0.000000	0.513378	0.000000
C	1.126362	1.500699	0.000000
C	-0.434875	-1.838472	0.000000
N	-1.214300	0.871560	0.000000
O	0.493529	-0.759900	0.000000
H	1.755164	1.352520	0.878602
H	1.755164	1.352520	-0.878602
H	0.727889	2.509956	0.000000
H	0.161301	-2.746313	0.000000
H	-1.064794	-1.818499	-0.892116
H	-1.064794	-1.818499	0.892116
H	-1.866987	0.092961	0.000000

Molecule# 0920

1-methoxypropane

PointGroup: Cs

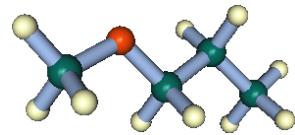
E= -233.754234588 au

ZPE= 0.136001 au

LUMO_eps= -0.01043 au

HOMO_eps= -0.26283 au

Dipole= 1.093 debye



15

C	2.489725	-0.124251	0.000000
C	-2.342568	0.613953	0.000000
C	1.086798	-0.728805	0.000000
C	0.000000	0.330652	0.000000
O	-1.268327	-0.300846	0.000000
H	2.655854	0.498469	0.881326
H	3.251026	-0.904383	0.000000
H	2.655854	0.498469	-0.881326
H	-2.324263	1.255246	0.889932
H	-3.263750	0.034649	0.000000
H	-2.324263	1.255246	-0.889932
H	0.951134	-1.366811	0.875899
H	0.951134	-1.366811	-0.875899
H	0.095077	0.976700	0.885030
H	0.095077	0.976700	-0.885030

Molecule# 0921

1-methyl-1H-imidazole

PointGroup: Cs

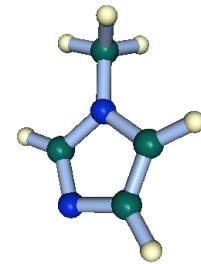
E= -265.628290864 au

ZPE= 0.098739 au

LUMO_eps= -0.01800 au

HOMO_eps= -0.23574 au

Dipole= 4.137 debye



12

C	0.645337	-1.483107	0.000000
C	1.115639	-0.197648	0.000000
C	-1.077575	-0.225768	0.000000
C	-0.022919	2.058005	0.000000
N	-0.726800	-1.489807	0.000000
N	0.000000	0.608310	0.000000
H	1.214722	-2.396921	0.000000
H	2.111503	0.208433	0.000000
H	-2.087758	0.150798	0.000000
H	0.471699	2.452768	0.887470
H	0.471699	2.452768	-0.887470
H	-1.057157	2.393731	0.000000

Molecule# 0922

1-methyl-1H-pyrrole

PointGroup: Cs

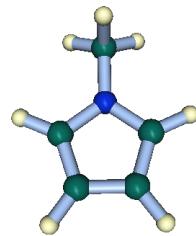
E= -249.574412357 au

ZPE= 0.109957 au

LUMO_eps= -0.01270 au

HOMO_eps= -0.21538 au

Dipole= 2.147 debye



13

C	-0.016408	-1.487716	0.709392
C	-0.016408	-1.487716	-0.709392
C	-0.016408	-0.174043	1.115752
C	-0.016408	-0.174043	-1.115752
C	0.066679	2.069240	0.000000
N	-0.023110	0.623459	0.000000
H	-0.026850	-2.347321	1.357432
H	-0.026850	-2.347321	-1.357432
H	-0.017376	0.257756	2.101616
H	-0.017376	0.257756	-2.101616
H	-0.430683	2.466938	0.882657
H	1.105307	2.406717	0.000000
H	-0.430683	2.466938	-0.882657

Molecule# 0923

1-methyl-1H-tetrazole

PointGroup: Cs

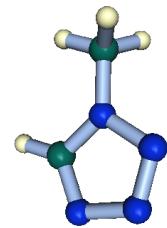
E= -297.677737340 au

ZPE= 0.074442 au

LUMO_eps= -0.03365 au

HOMO_eps= -0.29593 au

Dipole= 5.993 debye



10

C	-0.115632	2.015647	0.000000
H	-0.652547	2.342305	0.887714
H	-0.652547	2.342305	-0.887714
H	0.882425	2.445220	0.000000
N	0.000000	0.569086	0.000000
N	-1.090343	-0.221557	0.000000
N	-0.666004	-1.437578	0.000000
H	2.096573	0.126082	0.000000
C	1.080585	-0.227007	0.000000
N	0.690116	-1.479630	0.000000

Molecule# 0924

1-methyl-2-nitro-benzene

PointGroup: C1

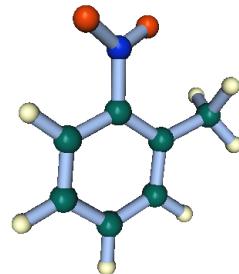
E= -476.245484208 au

ZPE= 0.130636 au

LUMO_eps= -0.09769 au

HOMO_eps= -0.27839 au

Dipole= 4.399 debye



17

C	2.555199	-0.206184	-0.030002
C	1.904094	-1.432601	-0.092797
C	1.822358	0.969098	0.049255
C	0.521008	-1.464364	-0.071553
C	0.424347	0.981756	0.050347
C	-0.196494	-0.273992	-0.013060
C	-0.290301	2.302138	0.145550
N	-1.666810	-0.404509	-0.018623
O	-2.143297	-1.460414	0.374057
O	-2.328126	0.540642	-0.426159
H	3.635895	-0.163364	-0.037093
H	2.465502	-2.353997	-0.153385
H	2.342694	1.915301	0.114787
H	-0.021103	-2.396371	-0.103663
H	-0.772031	2.558749	-0.796957
H	-1.076089	2.289354	0.898913
H	0.422924	3.084965	0.398137

Molecule# 0925

1-methyl-3-nitro-benzene

PointGroup: Cs

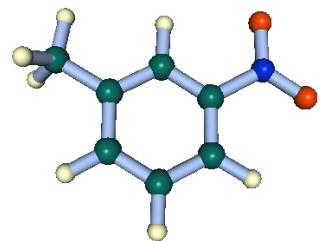
E= -476.249963160 au

ZPE= 0.130135 au

LUMO_eps= -0.10155 au

HOMO_eps= -0.27822 au

Dipole= 5.079 debye



17

C	-2.057620	-0.570893	0.000000
C	-1.349473	-1.765667	0.000000
C	-1.385262	0.643953	0.000000
C	0.722393	-0.566463	0.000000
C	0.048829	-1.783697	0.000000
C	0.000000	0.619586	0.000000
C	0.801538	-3.087682	0.000000
N	0.736402	1.899710	0.000000
O	0.081540	2.932000	0.000000
O	1.958229	1.853894	0.000000
H	-3.138638	-0.583862	0.000000
H	-1.890749	-2.703493	0.000000
H	-1.907623	1.587184	0.000000
H	1.800839	-0.524533	0.000000
H	1.877726	-2.925062	0.000000
H	0.551524	-3.685088	0.878569
H	0.551524	-3.685088	-0.878569

Molecule# 0926

1-methyl-4-methylsulfonylbenzene

PointGroup: Cs

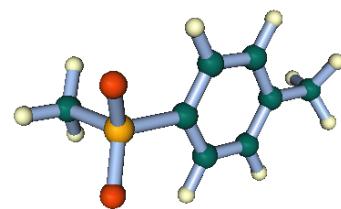
E= -859.689054504 au

ZPE= 0.165137 au

LUMO_eps= -0.05251 au

HOMO_eps= -0.27566 au

Dipole= 5.644 debye



21

C	-1.656245	-2.355698	0.000000
S	0.088738	-1.905377	0.000000
O	0.654560	-2.357841	1.267005
O	0.654560	-2.357841	-1.267005
C	0.080334	-0.110707	0.000000
C	0.087584	0.574569	-1.208898
C	0.087584	1.962499	-1.199749
C	0.081470	2.677518	0.000000
C	0.055105	4.182111	0.000000
C	0.087584	1.962499	1.199749
C	0.087584	0.574569	1.208898
H	-2.123209	-1.961947	-0.898464
H	-1.678863	-3.443534	0.000000
H	-2.123209	-1.961947	0.898464
H	0.119138	0.024829	-2.138786
H	0.104503	2.498591	-2.139961
H	0.546532	4.588743	0.883175
H	-0.973845	4.550449	0.000000
H	0.546532	4.588743	-0.883175
H	0.104503	2.498591	2.139961
H	0.119138	0.024829	2.138786

Molecule# 0927

1-methyl-4-vinylsulfonylbenzene

PointGroup: C1

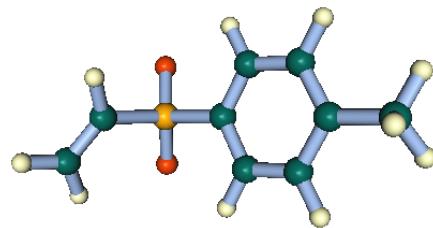
E= -897.776226377 au

ZPE= 0.170333 au

LUMO_eps= -0.06441 au

HOMO_eps= -0.27223 au

Dipole= 5.539 debye



22

C	-3.078529	-1.367977	1.210348
C	-2.305286	-0.296520	1.197245
S	-1.653876	0.347458	-0.339227
O	-2.103694	-0.521011	-1.422004
O	-1.949843	1.776690	-0.353711
C	0.119813	0.156743	-0.166060
C	0.875233	1.211605	0.329411
C	2.250170	1.058628	0.455227
C	2.880484	-0.132464	0.093069
C	4.367008	-0.302232	0.252868
C	2.095867	-1.173407	-0.412746
C	0.722573	-1.038461	-0.544117
H	-3.301679	-1.900515	0.295654
H	-3.514621	-1.728332	2.132549
H	-2.049479	0.296576	2.064631
H	0.392477	2.143116	0.587644
H	2.842356	1.882699	0.831571
H	4.794103	-0.860951	-0.579957
H	4.597393	-0.855973	1.166365
H	4.873811	0.659644	0.314839
H	2.568975	-2.098441	-0.716657
H	0.122971	-1.838083	-0.954756

Molecule# 0928

1-methylcyclohexene

PointGroup: C1

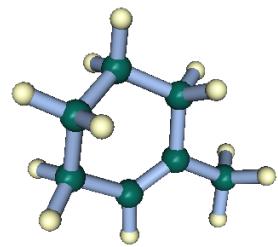
E= -274.068992350 au

ZPE= 0.173315 au

LUMO_eps= -0.01183 au

HOMO_eps= -0.23458 au

Dipole= 0.285 debye



19

C	-0.310382	1.216690	-0.089709
C	-1.007899	0.083990	0.004985
C	1.192425	1.294994	-0.102231
C	-0.326807	-1.262539	0.080273
C	1.847130	-0.015210	0.343539
C	1.153813	-1.212625	-0.305738
C	-2.509324	0.066544	0.050173
H	-0.847383	2.157642	-0.160153
H	1.536186	1.559736	-1.109789
H	1.519991	2.116878	0.540709
H	-0.437051	-1.659080	1.097370
H	-0.858397	-1.969943	-0.563834
H	2.911702	-0.007513	0.101968
H	1.771087	-0.104427	1.431482
H	1.646877	-2.144880	-0.023372
H	1.239620	-1.129025	-1.393390
H	-2.926173	1.072864	0.023793
H	-2.868014	-0.426133	0.959054
H	-2.922178	-0.497189	-0.791594

Molecule# 0929

1-methylcyclohexylhydroperoxide

PointGroup: C1

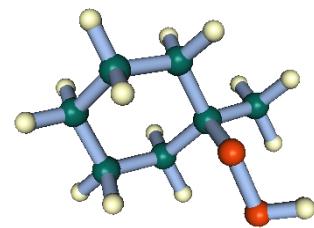
E= -425.708112227 au

ZPE= 0.204491 au

LUMO_eps= -0.01667 au

HOMO_eps= -0.26537 au

Dipole= 1.487 debye



23

O	-2.016926	-1.216020	-0.772187
O	-1.054020	-0.153372	-1.018473
C	-0.594460	0.399667	0.242789
C	-1.748089	1.091571	0.961695
C	0.047512	-0.692223	1.111646
C	1.271993	-1.337332	0.459293
C	2.312818	-0.289435	0.056807
C	1.699456	0.775969	-0.855005
C	0.461929	1.417906	-0.220985
H	-2.812365	-0.822759	-1.154034
H	-2.514347	0.371918	1.247143
H	-2.198490	1.849073	0.318379
H	-1.393009	1.581890	1.868465
H	0.337697	-0.229451	2.059796
H	-0.704912	-1.445089	1.346701
H	0.955390	-1.894817	-0.424991
H	1.710071	-2.062943	1.147967
H	3.159370	-0.767676	-0.440398
H	2.711283	0.189455	0.958403
H	1.423587	0.321303	-1.808390
H	2.433947	1.553119	-1.077801
H	-0.005539	2.120714	-0.913867
H	0.757931	1.993648	0.660473

Molecule# 0930

1-methylcyclopentene

PointGroup: C1

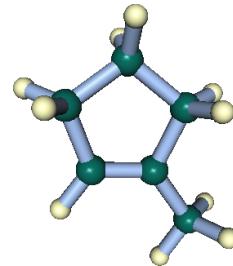
E= -234.735550831 au

ZPE= 0.143979 au

LUMO_eps= -0.01077 au

HOMO_eps= -0.23356 au

Dipole= 0.255 debye



16

C	-0.756198	0.073934	-0.002520
H	-0.343604	2.171486	-0.066463
C	0.023743	1.153783	-0.022376
H	-2.647844	-0.452806	0.859762
H	-2.606606	-0.553100	-0.889410
H	-2.679983	1.029419	-0.103430
C	-2.248786	0.030965	-0.036722
H	-0.043702	-1.617124	1.120770
H	-0.250301	-1.964412	-0.582053
C	0.069948	-1.188503	0.117983
H	1.780513	-0.916913	-1.185058
H	2.249118	-1.218041	0.478619
C	1.515599	-0.711239	-0.147209
H	1.879408	1.089875	1.069321
H	2.101884	1.357766	-0.645531
C	1.489213	0.820035	0.081422

Molecule# 0931

1-methylcyclopropene

PointGroup: Cs

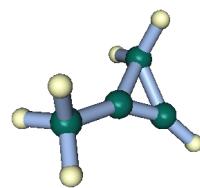
E= -156.005583942 au

ZPE= 0.084055 au

LUMO_eps= -0.00905 au

HOMO_eps= -0.24479 au

Dipole= 0.919 debye



10

H	-2.225998	-0.334426	0.000000
C	-1.153291	-0.397233	0.000000
C	0.000000	0.177369	0.000000
H	0.299785	-1.863186	0.910841
H	0.299785	-1.863186	-0.910841
C	0.031359	-1.328906	0.000000
H	1.501616	1.388241	0.877063
H	0.254349	2.293402	0.000000
H	1.501616	1.388241	-0.877063
C	0.850074	1.380589	0.000000

Molecule# 0932

1-methylethyl hydroperoxide

PointGroup: C1

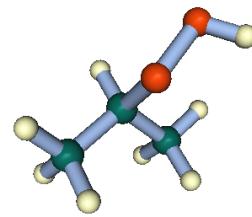
E= -269.604542396 au

ZPE= 0.110636 au

LUMO_eps= -0.01551 au

HOMO_eps= -0.26871 au

Dipole= 1.721 debye



13

O	-1.918563	-0.173683	-0.195389
H	-2.312775	0.187830	0.609427
O	-0.661485	-0.686944	0.324121
C	1.651684	-0.787137	0.026852
H	1.820412	-0.777766	1.104424
H	1.554045	-1.821145	-0.300398
H	2.523590	-0.349504	-0.459304
C	0.487776	1.469705	0.103519
H	0.672394	1.540668	1.177022
H	1.301951	1.974955	-0.418152
H	-0.436230	1.995634	-0.131444
C	0.408750	0.013954	-0.330908
H	0.227738	-0.044785	-1.408201

Molecule# 0933

1-methylnaphthalene

PointGroup: Cs

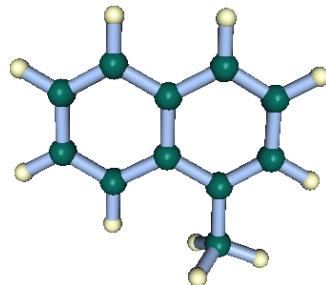
E= -425.359397038 au

ZPE= 0.174951 au

LUMO_eps= -0.04963 au

HOMO_eps= -0.22112 au

Dipole= 0.371 debye



21

C	-2.758791	-0.172612	0.000000
C	-2.313124	1.163832	0.000000
C	1.829384	-1.714992	0.000000
C	-1.848501	-1.196478	0.000000
C	-0.971197	1.448460	0.000000
C	0.490238	-1.990790	0.000000
C	2.279504	-0.378590	0.000000
C	-0.456728	-0.938145	0.000000
C	0.000000	0.416294	0.000000
C	1.404403	0.681449	0.000000
C	1.923415	2.094613	0.000000
H	-3.819371	-0.385993	0.000000
H	-3.035349	1.969463	0.000000
H	2.552742	-2.519609	0.000000
H	-2.183645	-2.226203	0.000000
H	-0.648971	2.479854	0.000000
H	0.135898	-3.013788	0.000000
H	3.344718	-0.184205	0.000000
H	1.585124	2.649218	0.878154
H	3.012098	2.103795	0.000000
H	1.585124	2.649218	-0.878154

Molecule# 0934

1-methylpiperazine

PointGroup: Cs

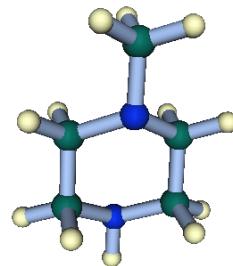
E= -307.359140991 au

ZPE= 0.174588 au

LUMO_eps= -0.01095 au

HOMO_eps= -0.21908 au

Dipole= 0.468 debye



19

C	-0.104320	-1.183383	1.206556
C	-0.104320	-1.183383	-1.206556
C	-0.104320	0.339172	1.204675
C	-0.104320	0.339172	-1.204675
C	0.628275	2.299249	0.000000
N	-0.769930	-1.666118	0.000000
N	0.541509	0.851074	0.000000
H	0.937429	-1.532481	1.281318
H	-0.646488	-1.547447	2.080373
H	-0.646488	-1.547447	-2.080373
H	0.937429	-1.532481	-1.281318
H	-1.145389	0.697953	1.285374
H	0.442711	0.708091	2.074318
H	0.442711	0.708091	-2.074318
H	-1.145389	0.697953	-1.285374
H	1.171992	2.637024	0.883042
H	-0.360624	2.789441	0.000000
H	1.171992	2.637024	-0.883042
H	-0.826919	-2.675387	0.000000

Molecule# 0935

1-methylpiperidine

PointGroup: Cs

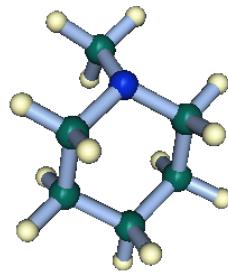
E= -291.318110570 au

ZPE= 0.185735 au

LUMO_eps= -0.01231 au

HOMO_eps= -0.20468 au

Dipole= 0.824 debye



20

C	0.965240	1.519566	0.000000
C	0.317239	0.938668	1.261849
C	0.317239	0.938668	-1.261849
C	0.317239	-0.596952	1.207472
C	0.317239	-0.596952	-1.207472
C	-1.745453	-1.132476	0.000000
N	-0.291486	-1.154914	0.000000
H	0.900662	2.609587	0.000000
H	2.032300	1.270920	0.000000
H	0.848574	1.272756	2.156437
H	-0.708429	1.307685	1.352481
H	-0.708429	1.307685	-1.352481
H	0.848574	1.272756	-2.156437
H	1.353737	-0.949519	1.247433
H	-0.193487	-1.015270	2.076593
H	-0.193487	-1.015270	-2.076593
H	1.353737	-0.949519	-1.247433
H	-2.112988	-1.660457	-0.881168
H	-2.199834	-0.129627	0.000000
H	-2.112988	-1.660457	0.881168

Molecule# 0936

1-methylsulfanylethanamine

PointGroup: Cs

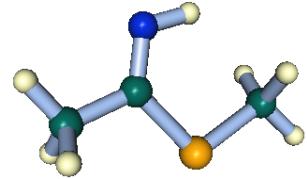
E= -571.574492498 au

ZPE= 0.097494 au

LUMO_eps= -0.01931 au

HOMO_eps= -0.24870 au

Dipole= 1.712 debye



12

C	0.000000	0.825176	0.000000
C	1.158271	1.785300	0.000000
C	-1.007571	-1.801949	0.000000
N	-1.193183	1.247338	0.000000
S	0.556958	-0.883144	0.000000
H	1.784741	1.632779	0.879911
H	1.784741	1.632779	-0.879911
H	0.775934	2.802688	0.000000
H	-0.737538	-2.855412	0.000000
H	-1.589589	-1.586821	-0.894274
H	-1.589589	-1.586821	0.894274
H	-1.891951	0.508598	0.000000

Molecule# 0937

1-methylsulfanylethanone

PointGroup: C1

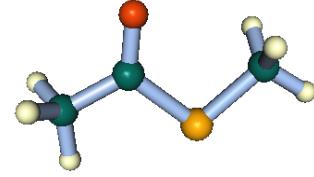
E= -591.470123647 au

ZPE= 0.084870 au

LUMO_eps= -0.03194 au

HOMO_eps= -0.26254 au

Dipole= 1.361 debye



11

C	0.754145	0.274218	-0.000001
C	2.080251	-0.448669	0.000000
C	-2.006474	0.397153	0.000001
O	0.648332	1.474901	0.000000
S	-0.661464	-0.824798	0.000000
H	1.966836	-1.530536	-0.000035
H	2.644386	-0.141223	0.880822
H	2.644418	-0.141166	-0.880780
H	-1.944496	1.019312	0.888116
H	-2.937384	-0.164322	0.000020
H	-1.944520	1.019289	-0.888133

Molecule# 0938

1-methylsulfonylbutane

PointGroup: C1

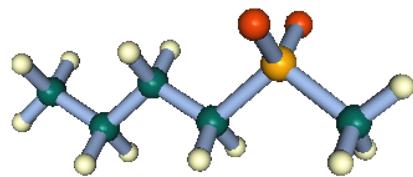
E= -746.545054072 au

ZPE= 0.170033 au

LUMO_eps= -0.02172 au

HOMO_eps= -0.29343 au

Dipole= 4.621 debye



20

C	3.923243	-0.294842	0.000054
C	2.698256	0.617692	-0.000087
C	1.382566	-0.165828	0.000024
C	0.168891	0.759188	-0.000133
S	-1.375513	-0.194329	0.000033
C	-2.659703	1.068823	-0.000208
O	-1.466231	-0.923301	-1.262796
O	-1.466246	-0.922837	1.263128
H	3.934055	-0.938927	0.881033
H	3.934060	-0.939189	-0.880734
H	4.846873	0.284744	-0.000030
H	2.730480	1.272993	-0.875356
H	2.730472	1.273253	0.874988
H	1.338291	-0.814008	0.877013
H	1.338307	-0.814284	-0.876761
H	0.138588	1.388271	-0.890317
H	0.138590	1.388574	0.889838
H	-3.601690	0.525093	-0.000121
H	-2.569767	1.670989	0.899941
H	-2.569747	1.670664	-0.900573

Molecule# 0939

1-methylsulfonylpropane

PointGroup: C1

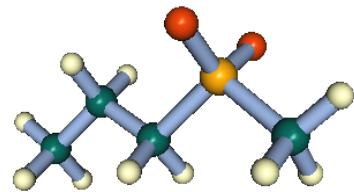
E= -707.216830721 au

ZPE= 0.141683 au

LUMO_eps= -0.02233 au

HOMO_eps= -0.29441 au

Dipole= 4.572 debye



17

O	1.052746	-0.884054	1.262930
S	0.899001	-0.165953	0.000000
O	1.052746	-0.884054	-1.262930
C	2.067344	1.204889	0.000000
C	-0.723417	0.647846	0.000000
C	-1.851316	-0.380647	0.000000
C	-3.225240	0.289975	0.000000
H	3.053274	0.745574	0.000000
H	1.925580	1.797049	-0.900169
H	1.925580	1.797049	0.900169
H	-0.749135	1.277504	0.890070
H	-0.749135	1.277504	-0.890070
H	-1.747958	-1.021292	-0.876349
H	-1.747958	-1.021292	0.876349
H	-3.362963	0.917670	0.882223
H	-3.362963	0.917671	-0.882223
H	-4.016488	-0.459710	0.000000

Molecule# 0940

1-methylthiobutane

PointGroup: Cs

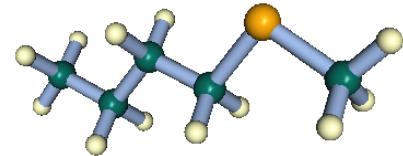
E= -596.069409246 au

ZPE= 0.160639 au

LUMO_eps= -0.01213 au

HOMO_eps= -0.22115 au

Dipole= 1.645 debye



18

C	-2.900530	-2.061190	0.000000
C	-2.210491	-0.698205	0.000000
C	2.318193	2.117672	0.000000
S	1.820699	0.367544	0.000000
C	0.000000	0.560581	0.000000
C	-0.683216	-0.803015	0.000000
H	3.406072	2.138869	0.000000
H	-3.986273	-1.956738	0.000000
H	-2.623158	-2.643745	0.880787
H	-2.623158	-2.643745	-0.880787
H	-2.533340	-0.125846	0.874655
H	-2.533340	-0.125846	-0.874655
H	1.955763	2.628694	0.891218
H	1.955763	2.628694	-0.891218
H	-0.357222	-1.371028	-0.875684
H	-0.357222	-1.371028	0.875684
H	-0.289402	1.132982	-0.883547
H	-0.289402	1.132982	0.883547

Molecule# 0941

1-nitrobutane

PointGroup: Cs

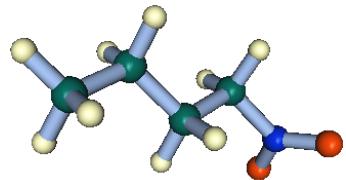
E= -363.103391020 au

ZPE= 0.135256 au

LUMO_eps= -0.08003 au

HOMO_eps= -0.30587 au

Dipole= 4.164 debye



16

C	0.536731	3.223064	0.000000
C	-0.454928	2.061221	0.000000
C	0.239825	0.697977	0.000000
C	-0.768764	-0.447146	0.000000
N	-0.044489	-1.768093	0.000000
O	0.239825	-2.250342	1.084249
O	0.239825	-2.250342	-1.084249
H	0.018030	4.181913	0.000000
H	1.179997	3.192827	0.881142
H	1.179997	3.192827	-0.881142
H	-1.106167	2.136482	0.875255
H	-1.106167	2.136482	-0.875255
H	0.880107	0.607526	-0.879899
H	0.880107	0.607526	0.879899
H	-1.384437	-0.442080	0.895216
H	-1.384437	-0.442080	-0.895216

Molecule# 0942

1-nitropentane

PointGroup: C1

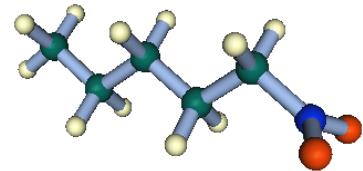
E= -402.431510898 au

ZPE= 0.163555 au

LUMO_eps= -0.07970 au

HOMO_eps= -0.30548 au

Dipole= 4.205 debye



19

C	-3.998201	-0.032014	0.092137
C	-2.629647	0.130528	-0.566038
C	-1.467215	-0.100900	0.400376
C	-0.099316	0.063086	-0.264256
C	1.038289	-0.173687	0.725014
N	2.364390	-0.001301	0.031077
O	2.905108	-1.004150	-0.406070
O	2.792402	1.136336	-0.078101
H	-4.802943	0.140790	-0.623098
H	-4.125783	-1.037723	0.497305
H	-4.128535	0.674598	0.914043
H	-2.547318	1.133724	-0.993858
H	-2.543271	-0.565696	-1.405148
H	-1.548032	-1.105658	0.827165
H	-1.550790	0.596612	1.239848
H	-0.003675	1.068374	-0.678690
H	-0.002303	-0.642032	-1.092626
H	1.032650	-1.187298	1.115133
H	1.025724	0.553854	1.532353

Molecule# 0943

1-nitropropan-2-ynitrile

PointGroup: C1

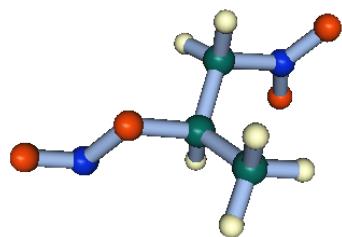
E= -528.350978880 au

ZPE= 0.107231 au

LUMO_eps= -0.10976 au

HOMO_eps= -0.30461 au

Dipole= 1.641 debye



15

O	-1.586677	0.242823	-0.452011
O	2.127839	-0.895530	1.082740
O	2.980961	0.036614	-0.679653
O	-3.549446	-0.597000	-0.150032
N	2.051118	-0.418864	-0.038076
N	-2.519406	-0.492165	0.375228
C	-0.310700	0.372479	0.201478
C	0.684193	-0.397131	-0.672929
C	0.022761	1.846227	0.352622
H	-0.376425	-0.112909	1.175395
H	0.382088	-1.438003	-0.762724
H	0.800672	0.053603	-1.652876
H	0.997303	1.974383	0.824190
H	-0.723135	2.333423	0.978516
H	0.038585	2.342002	-0.617938

Molecule# 0944

1-nitropropane

PointGroup: C1

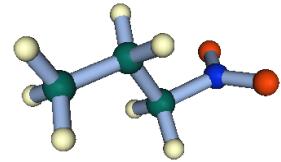
E= -323.775210667 au

ZPE= 0.106891 au

LUMO_eps= -0.08085 au

HOMO_eps= -0.30671 au

Dipole= 4.030 debye



13

C	-2.640949	-0.019049	0.026517
C	-1.209042	0.058303	-0.500284
C	-0.194938	-0.085420	0.631445
N	1.205024	-0.003386	0.081039
O	1.765014	-1.053167	-0.189400
O	1.672267	1.111046	-0.088501
H	-2.833745	-0.973366	0.519100
H	-2.844646	0.776897	0.744558
H	-3.353672	0.081711	-0.791461
H	-1.043315	1.011913	-1.003038
H	-1.035929	-0.731717	-1.232936
H	-0.270535	-1.051673	1.121825
H	-0.282005	0.723902	1.351821

Molecule# 0945

1-nitropyrrole-3-carbonitrile

PointGroup: C1

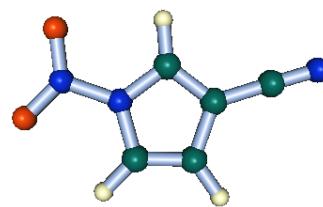
E= -507.075312503 au

ZPE= 0.083072 au

LUMO_eps= -0.12498 au

HOMO_eps= -0.28267 au

Dipole= 2.835 debye



13

O	-2.903943	0.542304	0.000007
O	-2.224534	-1.527721	-0.000004
N	-0.718011	0.114913	0.000001
N	-2.064664	-0.328750	0.000001
N	3.923133	-0.694141	-0.000009
C	1.475503	0.087120	0.000000
C	0.370315	-0.724286	-0.000004
C	-0.330392	1.446894	0.000007
C	1.027257	1.456025	0.000005
C	2.822191	-0.353769	-0.000005
H	0.260075	-1.791459	-0.000009
H	-1.062361	2.231220	0.000012
H	1.657653	2.327515	0.000009

Molecule# 0946

1-nitroso-2-imidazolidinethione

PointGroup: C1

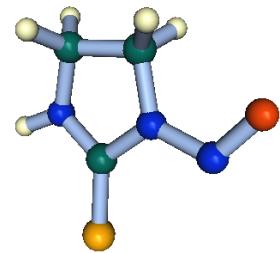
E= -755.089376910 au

ZPE= 0.093498 au

LUMO_eps= -0.08853 au

HOMO_eps= -0.22969 au

Dipole= 6.641 debye



13

S	-2.085780	-0.900716	0.006105
O	2.215947	-1.569659	0.000507
N	0.569237	-0.210430	0.014654
N	-0.824348	1.471103	-0.076104
N	1.006426	-1.480170	0.031513
C	-0.797846	0.120492	-0.016313
C	1.454352	0.955921	-0.068349
C	0.468196	2.125120	0.088754
H	-1.707844	1.945974	-0.009085
H	1.968507	0.956565	-1.029568
H	2.206495	0.910570	0.715423
H	0.550123	2.589299	1.074075
H	0.620197	2.893610	-0.667587

Molecule# 0947

1-nitrosopyrazolidin-3-one

PointGroup: C1

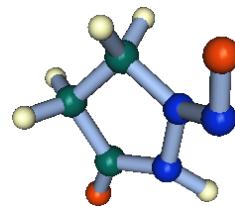
E= -432.093918615 au

ZPE= 0.094633 au

LUMO_eps= -0.07059 au

HOMO_eps= -0.25611 au

Dipole= 2.363 debye



13

O	2.708104	-0.570601	-0.088239
O	-2.779924	0.006037	-0.197353
N	-0.704809	-0.238358	0.294109
N	0.460380	-0.985720	0.109260
N	-1.836329	-0.763921	-0.182698
C	-0.379980	1.203560	0.320132
C	1.049525	1.244702	-0.232188
C	1.565924	-0.183314	-0.071158
H	-0.441868	1.572185	1.343414
H	-1.126052	1.719833	-0.277729
H	1.701720	1.927919	0.304039
H	1.078298	1.509182	-1.289948
H	0.514950	-1.886298	0.559549

Molecule# 0948

1-octanol

PointGroup: C1

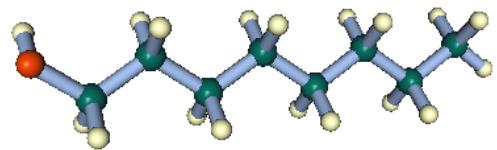
E= -391.078128614 au

ZPE= 0.249921 au

LUMO_eps= -0.01417 au

HOMO_eps= -0.27675 au

Dipole= 1.820 debye



27

C	5.089909	-0.352288	-0.006234
C	3.812557	0.485486	0.017342
C	2.536468	-0.356683	-0.009704
C	1.252161	0.472558	0.012261
C	-0.022805	-0.371121	-0.013333
C	-1.306858	0.459456	0.007688
C	-2.580564	-0.387028	-0.021920
C	-3.851423	0.452738	0.005891
O	-5.044544	-0.325727	-0.078454
H	5.140854	-0.967918	-0.906694
H	5.136911	-1.023546	0.853797
H	5.980865	0.276784	0.015618
H	3.809761	1.169734	-0.836459
H	3.807307	1.117177	0.910784
H	2.542544	-0.990137	-0.903143
H	2.539557	-1.041269	0.845242
H	1.249543	1.155909	-0.843424
H	1.247470	1.106707	0.905111
H	-0.018787	-1.005273	-0.905757
H	-0.021131	-1.053901	0.842702
H	-1.307512	1.142029	-0.848333
H	-1.310614	1.093278	0.900561
H	-2.584132	-1.069525	0.835632
H	-2.594832	-1.012605	-0.918195
H	-3.868468	1.083342	0.903101
H	-3.882554	1.118124	-0.857873
H	-5.087108	-0.911803	0.683019

Molecule# 0949

1-p-tolylethanone

PointGroup: C1

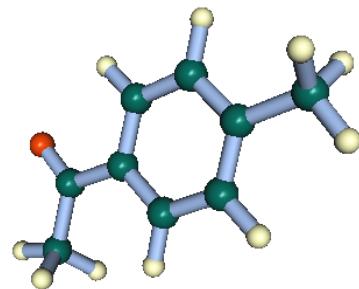
E= -424.371617131 au

ZPE= 0.164671 au

LUMO_eps= -0.06535 au

HOMO_eps= -0.25694 au

Dipole= 3.592 debye



20

C	0.024001	1.160298	-0.000002
C	-0.073857	-1.238567	0.000000
C	-1.364579	1.212066	-0.000005
C	-1.455060	-1.181361	-0.000003
C	0.690181	-0.065845	0.000000
C	-2.127814	0.046194	-0.000004
C	2.180603	-0.178189	0.000001
C	-3.631473	0.095804	0.000006
C	3.009944	1.089796	0.000003
O	2.722996	-1.266717	0.000000
H	0.581498	2.086205	-0.000003
H	0.442720	-2.187841	0.000000
H	-1.861326	2.173886	-0.000007
H	-2.027249	-2.100948	-0.000006
H	-4.040560	-0.408087	0.877954
H	-3.997196	1.121343	-0.000134
H	-4.040584	-0.408339	-0.877785
H	2.792622	1.698643	0.879269
H	2.792624	1.698642	-0.879264
H	4.061815	0.819045	0.000004

Molecule# 0950

1-pantanethiol

PointGroup: Cs

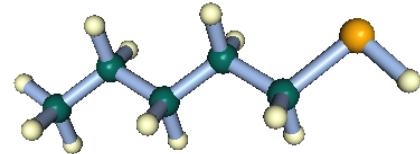
E= -596.070236239 au

ZPE= 0.159747 au

LUMO_eps= -0.01556 au

HOMO_eps= -0.23966 au

Dipole= 1.726 debye



18

S	-2.422026	1.676358	0.000000
H	-3.662177	1.155548	0.000000
C	-1.499663	0.079993	0.000000
H	-1.784672	-0.487365	0.884633
H	-1.784672	-0.487365	-0.884633
C	0.000000	0.354619	0.000000
H	0.257208	0.956252	-0.876062
H	0.257208	0.956252	0.876062
C	0.830343	-0.930799	0.000000
H	0.566953	-1.533496	0.875311
H	0.566953	-1.533496	-0.875311
C	2.338563	-0.676984	0.000000
H	2.601518	-0.074233	0.874144
H	2.601518	-0.074233	-0.874144
C	3.164445	-1.962117	0.000000
H	2.948285	-2.570045	0.880892
H	2.948285	-2.570045	-0.880892
H	4.233868	-1.747784	0.000000

Molecule# 0951

1-pentanol

PointGroup: C1

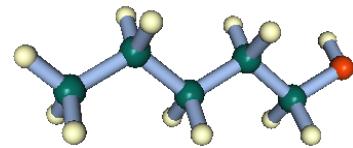
E= -273.093988342 au

ZPE= 0.164863 au

LUMO_eps= -0.01401 au

HOMO_eps= -0.27775 au

Dipole= 1.795 debye



18

C	-3.174894	0.221356	0.015832
C	-1.854161	-0.545307	-0.021865
C	-0.626182	0.365737	0.013037
C	0.699506	-0.395753	-0.027955
C	1.913737	0.523470	0.013334
O	3.154194	-0.175719	-0.081422
H	-3.256954	0.821962	0.924087
H	-3.261939	0.899200	-0.835780
H	-4.029566	-0.455825	-0.011540
H	-1.816621	-1.163702	-0.923412
H	-1.810925	-1.238981	0.823068
H	-0.670781	1.059963	-0.832589
H	-0.664660	0.985038	0.915426
H	0.754149	-1.005560	-0.933536
H	0.747184	-1.089540	0.819209
H	1.890619	1.140743	0.919619
H	1.902039	1.201994	-0.840618
H	3.235868	-0.766559	0.673146

Molecule# 0952

1-pentene

PointGroup: C1

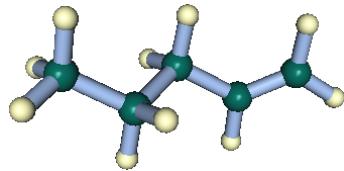
E= -196.613962957 au

ZPE= 0.136417 au

LUMO_eps= -0.00879 au

HOMO_eps= -0.26229 au

Dipole= 0.449 debye



15

C	2.480915	-0.213181	-0.298890
C	1.414749	0.338000	0.268186
C	-2.425591	-0.196397	-0.076523
C	0.075276	-0.316078	0.421811
C	-1.056864	0.450771	-0.277621
H	3.419178	0.318761	-0.382304
H	2.453489	-1.220352	-0.698261
H	1.492545	1.352012	0.652650
H	-2.441485	-1.215257	-0.468708
H	-3.209396	0.366453	-0.584990
H	-2.686714	-0.246940	0.982557
H	0.119287	-1.338660	0.037811
H	-0.166785	-0.392388	1.488258
H	-0.832514	0.519273	-1.344984
H	-1.078509	1.478406	0.096191

Molecule# 0953

1-phenylethanimine

PointGroup: Cs

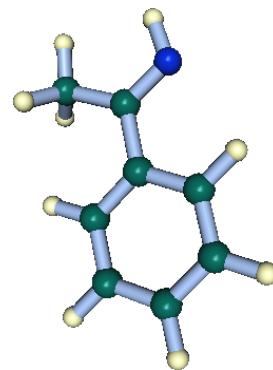
E= -365.150184140 au

ZPE= 0.150364 au

LUMO_eps= -0.05506 au

HOMO_eps= -0.25325 au

Dipole= 2.097 debye



18

C	-0.695065	-2.506553	0.000000
C	0.640810	-2.129667	0.000000
C	-1.686417	-1.527721	0.000000
C	0.985096	-0.782121	0.000000
C	-1.343694	-0.185795	0.000000
C	0.000000	0.209408	0.000000
C	0.343826	1.660851	0.000000
C	1.805185	2.046442	0.000000
N	-0.606615	2.511330	0.000000
H	-0.964675	-3.554227	0.000000
H	1.418044	-2.881961	0.000000
H	-2.729354	-1.815347	0.000000
H	2.031257	-0.512617	0.000000
H	-2.104187	0.580888	0.000000
H	2.317686	1.650451	0.878477
H	1.909909	3.129766	0.000000
H	2.317686	1.650451	-0.878477
H	-0.248508	3.464218	0.000000

Molecule# 0954

1-propanamine

PointGroup: Cs

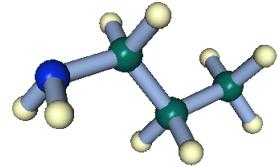
E= -174.562699408 au

ZPE= 0.120668 au

LUMO_eps= -0.01252 au

HOMO_eps= -0.24194 au

Dipole= 1.359 debye



13

C	1.426873	1.298590	0.000000
C	0.000000	0.751500	0.000000
C	-0.052657	-0.779459	0.000000
N	-1.385423	-1.383272	0.000000
H	1.978422	0.962964	0.880677
H	1.978422	0.962964	-0.880677
H	1.436602	2.389035	0.000000
H	-0.539820	1.125120	-0.875744
H	-0.539820	1.125120	0.875744
H	0.483988	-1.159679	0.873422
H	0.483988	-1.159679	-0.873422
H	-1.914561	-1.093363	-0.813803
H	-1.914561	-1.093363	0.813803

Molecule# 0955

1-propanethiol

PointGroup: C1

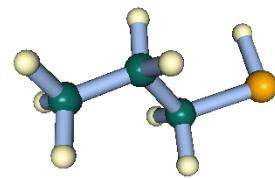
E= -517.414960571 au

ZPE= 0.102858 au

LUMO_eps= -0.01789 au

HOMO_eps= -0.24140 au

Dipole= 1.767 debye



12

C	-2.422945	0.072738	0.011279
C	-1.009653	-0.506476	-0.070522
C	0.062858	0.567077	0.075523
S	1.788351	-0.046408	-0.074553
H	-2.599612	0.799976	-0.783540
H	-3.173192	-0.712674	-0.085709
H	-2.591811	0.576633	0.964916
H	-0.869677	-1.024388	-1.021039
H	-0.874102	-1.257605	0.711730
H	-0.023659	1.307679	-0.720627
H	-0.038300	1.098518	1.021239
H	1.775172	-0.845654	1.008202

Molecule# 0956

1-propanol

PointGroup: C1

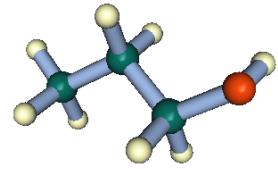
E= -194.437987807 au

ZPE= 0.108094 au

LUMO_eps= -0.01369 au

HOMO_eps= -0.27956 au

Dipole= 1.751 debye



12

C	1.897976	-0.126622	0.018618
C	0.516931	0.524551	-0.044771
C	-0.613059	-0.494853	0.024012
O	-1.909274	0.090322	-0.086974
H	2.048829	-0.814819	-0.815272
H	2.688867	0.622294	-0.024744
H	2.029572	-0.693014	0.942713
H	0.411143	1.099907	-0.967085
H	0.407044	1.234976	0.781380
H	-0.541025	-1.193082	-0.811207
H	-0.535151	-1.082893	0.946811
H	-2.046169	0.685602	0.656039

Molecule# 0957

1-propoxypyropane

PointGroup: C2v

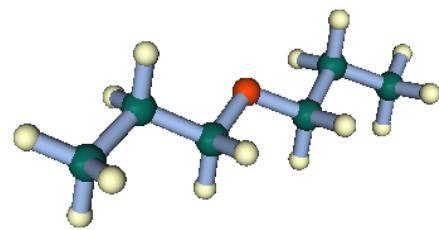
E= -312.415226151 au

ZPE= 0.192603 au

LUMO_eps= -0.01067 au

HOMO_eps= -0.26029 au

Dipole= 0.913 debye



21

C	0.000000	3.710922	-0.232233
C	0.000000	-3.710922	-0.232233
C	0.000000	2.389208	0.533807
C	0.000000	-2.389208	0.533807
C	0.000000	1.184713	-0.390496
C	0.000000	-1.184713	-0.390496
O	0.000000	0.000000	0.385340
H	-0.881297	3.802170	-0.870295
H	0.000000	4.559288	0.452278
H	0.881297	3.802170	-0.870295
H	0.881297	-3.802170	-0.870295
H	0.000000	-4.559288	0.452278
H	-0.881297	-3.802170	-0.870295
H	-0.875832	2.330147	1.183540
H	0.875832	2.330147	1.183540
H	0.875832	-2.330147	1.183540
H	-0.875832	-2.330147	1.183540
H	-0.884755	1.205018	-1.043297
H	0.884755	1.205018	-1.043297
H	0.884755	-1.205018	-1.043297
H	-0.884755	-1.205018	-1.043297

Molecule# 0958

1-propylsulfanylpropane

PointGroup: C2v

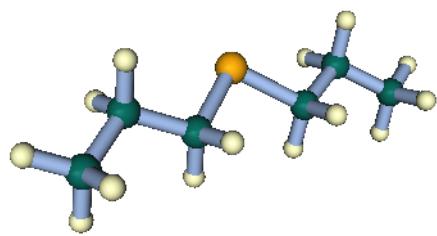
E= -635.397934436 au

ZPE= 0.189166 au

LUMO_eps= -0.01260 au

HOMO_eps= -0.21917 au

Dipole= 1.495 debye



21

C	0.000000	3.930707	-0.592405
C	0.000000	-3.930707	-0.592405
C	0.000000	2.732696	0.357453
C	0.000000	-2.732696	0.357453
C	0.000000	1.402662	-0.390073
C	0.000000	-1.402662	-0.390073
S	0.000000	0.000000	0.786742
H	-0.881478	3.925924	-1.236374
H	0.000000	4.869546	-0.037529
H	0.881478	3.925924	-1.236374
H	0.881478	-3.925924	-1.236374
H	0.000000	-4.869546	-0.037529
H	-0.881478	-3.925924	-1.236374
H	-0.875086	2.778860	1.009600
H	0.875086	2.778860	1.009600
H	0.875086	-2.778860	1.009600
H	-0.875086	-2.778860	1.009600
H	-0.883620	1.324451	-1.026352
H	0.883620	1.324451	-1.026352
H	0.883620	-1.324451	-1.026352
H	-0.883620	-1.324451	-1.026352

Molecule# 0959

1-propylsulfonylpropane

PointGroup: C1

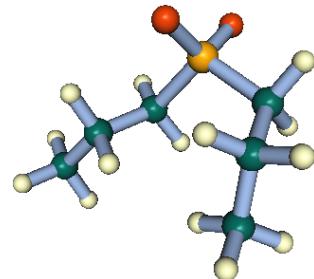
E= -785.867835060 au

ZPE= 0.198552 au

LUMO_eps= -0.02237 au

HOMO_eps= -0.28631 au

Dipole= 5.005 debye



23

C	-0.801844	2.711310	-0.338818
C	-1.556490	1.634435	0.440931
C	-1.752233	0.321404	-0.321811
S	-0.564304	-1.020795	0.008601
O	-0.486101	-1.205289	1.457548
C	1.079145	-0.500005	-0.592572
C	1.950093	0.217261	0.432281
C	3.350553	0.492327	-0.118099
O	-0.983323	-2.133534	-0.842642
H	0.202285	2.392866	-0.619062
H	-0.702543	3.619858	0.255426
H	-1.332410	2.972547	-1.256124
H	-2.546727	2.017284	0.694565
H	-1.068499	1.426270	1.394331
H	-1.766872	0.450649	-1.403970
H	-2.678996	-0.177479	-0.036482
H	0.908147	0.085211	-1.496916
H	1.520929	-1.450450	-0.895032
H	2.010961	-0.398610	1.328781
H	1.485259	1.155553	0.736171
H	3.854470	-0.434566	-0.397124
H	3.316961	1.131141	-1.002632
H	3.965955	0.992641	0.629730

Molecule# 0960

1-propyn-1-yl thiocyanate

PointGroup: C1

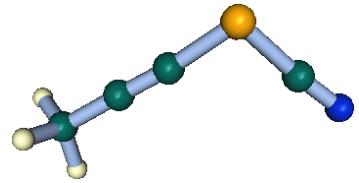
E= -607.188427290 au

ZPE= 0.056322 au

LUMO_eps= -0.04033 au

HOMO_eps= -0.26145 au

Dipole= 4.463 debye



9

S	-0.919300	-0.968615	0.000000
N	-2.596878	1.348222	0.000000
C	3.166496	0.507266	0.000001
C	1.788843	0.050261	0.000001
C	0.640017	-0.308782	0.000000
C	-1.880155	0.442903	0.000000
H	3.698733	0.156257	0.885244
H	3.198185	1.598130	-0.000150
H	3.698808	0.156014	-0.885101

Molecule# 0961

1-pyrazin-2-yethanone

PointGroup: Cs

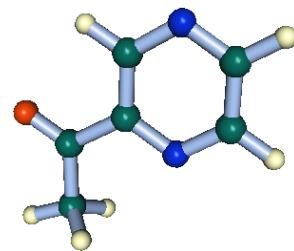
E= -417.117704847 au

ZPE= 0.113391 au

LUMO_eps= -0.09439 au

HOMO_eps= -0.25972 au

Dipole= 3.091 debye



15

C	0.787546	-2.366357	0.000000
C	-0.561033	-2.023230	0.000000
C	1.353155	-0.175015	0.000000
C	0.000000	0.175622	0.000000
C	-0.407656	1.626191	0.000000
C	-1.879880	1.940275	0.000000
N	1.749484	-1.444574	0.000000
N	-0.957273	-0.754759	0.000000
O	0.445137	2.489136	0.000000
H	1.096738	-3.404743	0.000000
H	-1.330829	-2.785557	0.000000
H	2.112882	0.594562	0.000000
H	-2.362568	1.497437	0.871986
H	-2.362568	1.497437	-0.871986
H	-2.013020	3.018193	0.000000

Molecule# 0962

1-pyrrolidin-1-ylethanone

PointGroup: C1

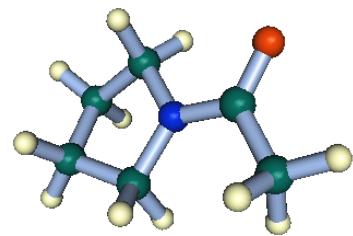
E= -365.393794193 au

ZPE= 0.166642 au

LUMO_eps= -0.02041 au

HOMO_eps= -0.24269 au

Dipole= 4.377 debye



19

C	1.450960	-0.211024	-0.011521
C	-2.167694	-0.617691	0.265295
C	-2.071854	0.820259	-0.260051
C	-0.795643	-1.209168	-0.064247
C	-0.629862	1.220730	0.068588
C	2.289731	1.049920	0.075090
N	0.101430	-0.048120	-0.007516
O	1.961184	-1.322156	-0.085316
H	-2.323362	-0.611690	1.345899
H	-2.982362	-1.182603	-0.184363
H	-2.222111	0.835109	-1.341119
H	-2.800072	1.494779	0.187414
H	-0.466604	-1.973381	0.637241
H	-0.772611	-1.654471	-1.062577
H	-0.232266	1.952833	-0.633874
H	-0.563031	1.651531	1.073408
H	2.013722	1.662081	0.934901
H	2.163330	1.663339	-0.818914
H	3.332065	0.758403	0.158197

Molecule# 0963

1-sulfanyl-5,6-dihydro-1,3,5-triazine-2(1H)-thione

PointGroup: C1

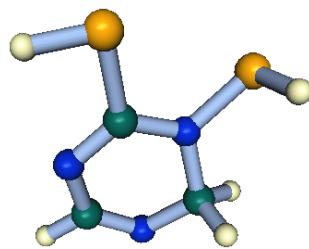
E= -1078.092587560 au

ZPE= 0.086017 au

LUMO_eps= -0.05740 au

HOMO_eps= -0.24436 au

Dipole= 2.380 debye



13

S	-1.343024	1.653778	-0.188507
S	-1.672982	-1.441915	0.055760
N	0.022233	0.641827	-0.044011
N	0.993395	-1.482659	0.024447
N	2.446897	0.418854	-0.082676
C	-0.052767	-0.722709	0.020912
C	1.336826	1.254097	0.292287
C	2.209200	-0.831052	-0.160281
H	-1.575475	1.878237	1.129449
H	-1.161932	-2.687349	0.059929
H	1.376602	1.458299	1.372225
H	1.387735	2.206582	-0.231409
H	3.031951	-1.493748	-0.408073

Molecule# 0964

1-thiazolidine-1-oxide

PointGroup: C1

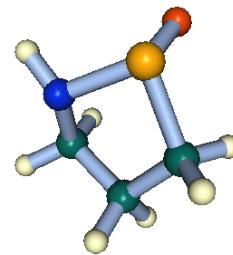
E= -646.795812885 au

ZPE= 0.105735 au

LUMO_eps= -0.01829 au

HOMO_eps= -0.24471 au

Dipole= 3.549 debye



13

C	-1.663197	0.594398	0.145760
C	-1.313787	-0.870942	0.411302
C	-0.347274	1.331041	-0.152189
N	-0.238792	-1.138186	-0.555395
O	1.706481	-0.033622	0.889358
S	0.987654	0.059920	-0.421492
H	-2.320976	0.654479	-0.720214
H	-2.180873	1.039574	0.994418
H	-0.990263	-1.021403	1.445604
H	-2.153940	-1.534637	0.209646
H	-0.400187	1.966309	-1.033577
H	0.034328	1.907959	0.686849
H	0.174693	-2.061706	-0.495193

Molecule# 0965

1-vinylsulfonylethylene

PointGroup: C1

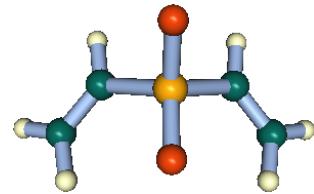
E= -704.733527926 au

ZPE= 0.094926 au

LUMO_eps= -0.07380 au

HOMO_eps= -0.29892 au

Dipole= 4.658 debye



13

C	2.237512	-1.080208	-0.077675
C	1.403583	-0.280902	-0.719892
S	0.000000	0.441332	0.117731
O	0.000000	-0.012068	1.503955
C	-1.403588	-0.280896	-0.719890
C	-2.237510	-1.080210	-0.077674
O	0.000003	1.864598	-0.204444
H	2.063322	-1.347346	0.955947
H	3.118409	-1.474130	-0.566836
H	1.522477	0.047345	-1.743611
H	-1.522490	0.047360	-1.743604
H	-2.063312	-1.347358	0.955944
H	-3.118410	-1.474129	-0.566832

Molecule# 0966

1,1-diacetoxyethane

PointGroup: C1

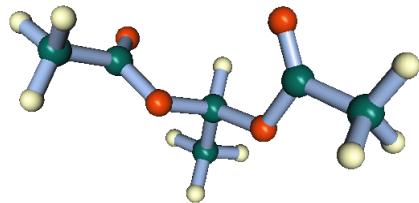
E= -535.806094262 au

ZPE= 0.159300 au

LUMO_eps= -0.01574 au

HOMO_eps= -0.28711 au

Dipole= 3.177 debye



20

C	1.958541	-0.478093	0.193954
C	-1.985911	-0.370129	0.044281
C	3.315328	-0.651679	-0.427177
C	-2.706370	-1.406200	-0.772082
C	-0.282027	2.350782	-0.151313
C	0.025654	0.906381	0.152375
O	1.466249	-1.192700	1.024364
O	-2.348571	0.063105	1.107404
O	1.336474	0.624435	-0.316945
O	-0.847020	0.027067	-0.577278
H	3.206350	-0.834642	-1.496483
H	3.901786	0.259171	-0.311364
H	3.823877	-1.488732	0.040209
H	-2.793777	-1.084287	-1.808678
H	-2.130275	-2.332268	-0.762710
H	-3.688403	-1.585106	-0.345883
H	0.418059	2.997677	0.375816
H	-1.291702	2.583448	0.181303
H	-0.200399	2.536528	-1.221464
H	-0.053858	0.666591	1.208658

Molecule# 0967

1,1-dichloro-1-fluoroethane

PointGroup: Cs

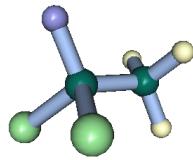
E= -1098.402136600 au

ZPE= 0.048549 au

LUMO_eps= -0.03421 au

HOMO_eps= -0.31879 au

Dipole= 2.086 debye



8

C	0.016027	0.345002	0.000000
C	-1.158543	1.289602	0.000000
F	1.179679	1.042816	0.000000
Cl	0.016027	-0.698667	1.468731
Cl	0.016027	-0.698667	-1.468731
H	-2.090468	0.731884	0.000000
H	-1.108226	1.914914	0.889721
H	-1.108226	1.914914	-0.889721

Molecule# 0968

1,1-dichloro-1-nitropropane

PointGroup: C1

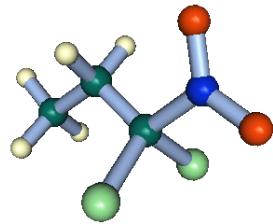
E= -1243.015691930 au

ZPE= 0.086895 au

LUMO_eps= -0.10455 au

HOMO_eps= -0.32237 au

Dipole= 3.314 debye



13

C1	0.249784	-0.974350	1.469255
C1	0.249795	-0.974958	-1.468853
O	-2.276486	-0.317705	0.000014
O	-1.578642	1.732450	-0.000305
N	-1.417338	0.529360	-0.000112
C	1.046188	1.203382	-0.000248
C	0.088165	0.027254	-0.000009
C	2.523780	0.818478	-0.000164
H	0.809962	1.806954	0.875296
H	0.809968	1.806595	-0.876042
H	3.125160	1.726672	-0.000357
H	2.787839	0.239740	-0.883469
H	2.787837	0.240117	0.883389

Molecule# 0969

1,1-dichloro-2,2,2-trifluoroethane

PointGroup: Cs

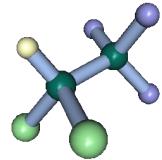
E= -1296.961764190 au

ZPE= 0.033827 au

LUMO_eps= -0.04275 au

HOMO_eps= -0.33406 au

Dipole= 1.328 debye



8

C	0.566910	-0.338873	0.000000
C	-0.170872	1.010509	0.000000
H	1.633086	-0.144099	0.000000
Cl	0.182082	-1.256529	1.476575
Cl	0.182082	-1.256529	-1.476575
F	-1.497512	0.873510	0.000000
F	0.182082	1.720816	1.083344
F	0.182082	1.720816	-1.083344

Molecule# 0970

1,1-dichloro-3,3-dimethylurea

PointGroup: C1

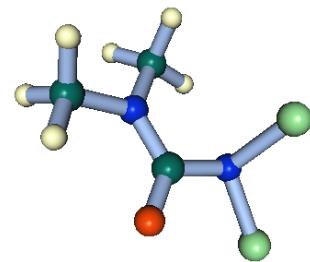
E= -1223.168811250 au

ZPE= 0.098709 au

LUMO_eps= -0.09278 au

HOMO_eps= -0.26744 au

Dipole= 3.960 debye



14

C1	-2.158879	-0.834991	0.460362
C1	-0.993288	1.532997	-0.682534
O	0.277220	-1.678178	-0.719199
N	-0.722342	0.149580	0.402406
N	1.607764	-0.059256	0.184479
C	0.425703	-0.637266	-0.128512
C	2.825179	-0.632336	-0.375066
C	1.787743	1.109351	1.035518
H	3.457133	-1.029550	0.422266
H	2.565217	-1.434482	-1.056315
H	3.383450	0.138196	-0.910345
H	2.037010	1.992083	0.442264
H	2.608475	0.914416	1.727449
H	0.888095	1.307890	1.605352

Molecule# 0971

1,1-dichloro-tetrafluoroethane

PointGroup: Cs

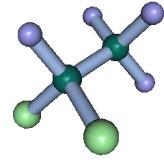
E= -1396.230801390 au

ZPE= 0.025107 au

LUMO_eps= -0.05136 au

HOMO_eps= -0.34246 au

Dipole= 0.636 debye



8

C 0.396947 -0.334365 0.000000

C -0.354044 1.033767 0.000000

F 1.717331 -0.069343 0.000000

Cl -0.012320 -1.251697 1.466556

Cl -0.012320 -1.251697 -1.466556

F -1.674751 0.856796 0.000000

F -0.012320 1.737455 1.082744

F -0.012320 1.737455 -1.082744

Molecule# 0972

1,1-dichloroethane

PointGroup: Cs

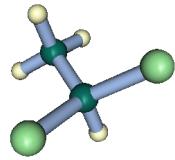
E= -999.126028280 au

ZPE= 0.057123 au

LUMO_eps= -0.02480 au

HOMO_eps= -0.30942 au

Dipole= 2.162 debye



8

C	0.965471	1.453203	0.000000
C	-0.209585	0.507329	0.000000
Cl	-0.209585	-0.525034	1.479700
Cl	-0.209585	-0.525034	-1.479700
H	1.903270	0.901560	0.000000
H	0.925876	2.084439	-0.887319
H	0.925876	2.084439	0.887319
H	-1.164450	1.017543	0.000000

Molecule# 0973

1,1-dichloroethene

PointGroup: C2v

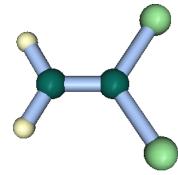
E= -997.885471617 au

ZPE= 0.033465 au

LUMO_eps= -0.03676 au

HOMO_eps= -0.27423 au

Dipole= 1.373 debye



6

C 0.000000 0.000000 1.747016

C 0.000000 0.000000 0.425505

H 0.000000 0.930182 2.293878

H 0.000000 -0.930182 2.293878

Cl 0.000000 1.459069 -0.518320

Cl 0.000000 -1.459069 -0.518320

Molecule# 0974

1,1-difluoro-1-hydroperoxyethane

PointGroup: C1

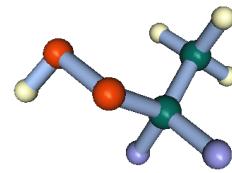
E= -428.848238819 au

ZPE= 0.067371 au

LUMO_eps= -0.03149 au

HOMO_eps= -0.33068 au

Dipole= 1.694 debye



10

F	-0.357644	-0.471312	1.292576
F	-1.367380	-0.721561	-0.632011
O	0.767788	-0.495627	-0.659306
O	1.909998	0.165753	-0.077280
C	-0.382758	-0.035679	-0.006307
C	-0.624405	1.447497	-0.059329
H	2.203516	-0.500296	0.562031
H	-0.689198	1.760727	-1.098748
H	-1.559522	1.670655	0.449572
H	0.191108	1.972855	0.428559

Molecule# 0975

1,1-difluoro-2-isocyanatoethane

PointGroup: C1

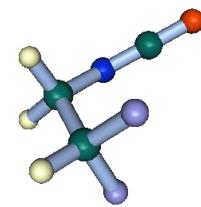
E= -445.962119243 au

ZPE= 0.064627 au

LUMO_eps= -0.02451 au

HOMO_eps= -0.30237 au

Dipole= 3.995 debye



10

F	0.892126	-1.165198	-0.729105
F	1.581051	-0.215516	1.129974
O	-2.608785	-0.637675	0.169502
N	-0.853328	0.946099	0.096004
C	1.403870	-0.009908	-0.206195
C	0.452351	1.146753	-0.457655
C	-1.702891	0.095842	0.092826
H	2.382805	0.162893	-0.658127
H	0.888228	2.041357	-0.014086
H	0.393969	1.304768	-1.537510

Molecule# 0976

1,1-difluoro-2-isothiocyanatoethane

PointGroup: C1

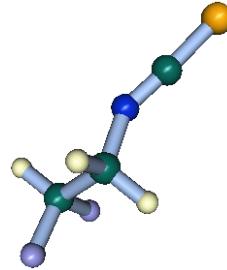
E= -768.923202170 au

ZPE= 0.061841 au

LUMO_eps= -0.05038 au

HOMO_eps= -0.26674 au

Dipole= 1.894 debye



10

S	3.207011	0.103485	-0.057042
F	-1.915460	1.328253	-0.160483
F	-3.079188	-0.540242	-0.097326
N	0.482209	-0.239691	0.285694
C	-1.923576	0.054593	0.324835
C	-0.750694	-0.732182	-0.236127
C	1.650101	-0.112516	0.094338
H	-1.934452	0.106448	1.414038
H	-0.774486	-0.657000	-1.325535
H	-0.881854	-1.778836	0.046326

Molecule# 0977

1,1-difluoro-2,2-ethanediol

PointGroup: C1

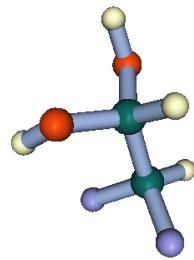
E= -428.928275976 au

ZPE= 0.070020 au

LUMO_eps= -0.02040 au

HOMO_eps= -0.31659 au

Dipole= 1.868 debye



10

F	0.936726	-0.752395	1.002357
F	1.646645	0.548458	-0.624816
O	-1.587352	-0.834466	-0.382371
O	-0.934596	1.174393	0.623606
C	-0.691510	0.252835	-0.394390
C	0.702183	-0.374100	-0.292984
H	-0.754108	0.816515	-1.328274
H	0.817745	-1.249022	-0.931294
H	-2.484848	-0.486276	-0.414125
H	-0.717580	0.762386	1.470180

Molecule# 0978

1,1-difluoroethane

PointGroup: Cs

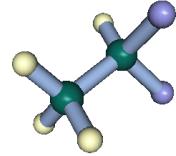
E= -278.428539330 au

ZPE= 0.060112 au

LUMO_eps= -0.01212 au

HOMO_eps= -0.35104 au

Dipole= 2.336 debye



8

C	0.898943	1.042679	0.000000
C	-0.321603	0.166943	0.000000
F	-0.321603	-0.652153	1.102135
F	-0.321603	-0.652153	-1.102135
H	1.793325	0.421274	0.000000
H	0.899762	1.674835	-0.886681
H	0.899762	1.674835	0.886681
H	-1.268028	0.710080	0.000000

Molecule# 0979

1,1-difluoroethene

PointGroup: C2v

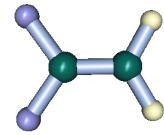
E= -277.183069831 au

ZPE= 0.036530 au

LUMO_eps= -0.01089 au

HOMO_eps= -0.28125 au

Dipole= 1.335 debye



6

F 0.000000 1.080780 -0.696531

F 0.000000 -1.080780 -0.696531

C 0.000000 0.000000 0.067620

C 0.000000 0.000000 1.382761

H 0.000000 0.934350 1.917633

H 0.000000 -0.934350 1.917633

Molecule# 0980

1,1-diisocyanato-2-sulfanylethane

PointGroup: C1

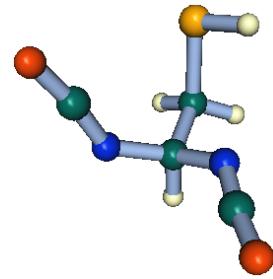
E= -813.167264431 au

ZPE= 0.082737 au

LUMO_eps= -0.04228 au

HOMO_eps= -0.26703 au

Dipole= 3.274 debye



13

S	-1.960908	-0.984786	-0.704762
O	-0.911149	2.680262	-0.504844
O	3.424680	-0.179183	-0.597952
N	-0.053917	1.049338	0.982459
N	1.194387	-0.739778	-0.030324
C	0.229652	-0.361475	0.989131
C	-1.027868	-1.225362	0.844298
C	-0.515341	1.815052	0.167561
C	2.331372	-0.414621	-0.267512
H	-1.018139	-1.475813	-1.529627
H	0.662672	-0.584117	1.965684
H	-1.719705	-0.969386	1.644141
H	-0.748716	-2.271237	0.952542

Molecule# 0981

1,1-dimethoxyethane

PointGroup: Cs

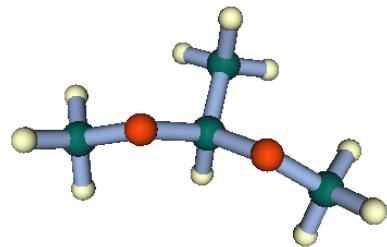
E= -308.990987297 au

ZPE= 0.139715 au

LUMO_eps= -0.01319 au

HOMO_eps= -0.26291 au

Dipole= 2.440 debye



16

O	-0.475052	-0.494394	1.113221
O	-0.475052	-0.494394	-1.113221
C	-0.475052	0.274157	2.299349
C	-0.475052	0.274157	-2.299349
C	0.108864	0.139234	0.000000
C	1.624653	-0.011059	0.000000
H	0.536031	0.457395	2.678474
H	0.536031	0.457395	-2.678474
H	-1.025623	-0.297309	3.043115
H	-1.025623	-0.297309	-3.043115
H	-0.974551	1.238607	2.149797
H	-0.974551	1.238607	-2.149797
H	-0.175109	1.205677	0.000000
H	1.876897	-1.070780	0.000000
H	2.063428	0.459549	-0.880282
H	2.063428	0.459549	0.880282

Molecule# 0982

1,1-dimethoxyethene

PointGroup: C2v

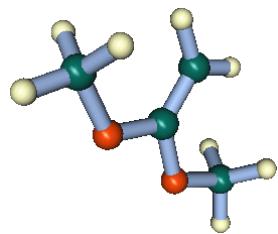
E= -307.770960682 au

ZPE= 0.117862 au

LUMO_eps= -0.01119 au

HOMO_eps= -0.22522 au

Dipole= 1.087 debye



14

C	0.000000	0.000000	1.419313
C	0.000000	0.000000	0.079174
H	0.000000	0.919976	1.976204
H	0.000000	-0.919976	1.976204
O	0.000000	1.079169	-0.727837
O	0.000000	-1.079169	-0.727837
C	0.000000	2.361498	-0.117979
C	0.000000	-2.361498	-0.117979
H	0.000000	3.078298	-0.933962
H	0.000000	-3.078298	-0.933962
H	-0.891567	2.503674	0.496436
H	0.891567	2.503674	0.496436
H	0.891567	-2.503674	0.496436
H	-0.891567	-2.503674	0.496436

Molecule# 0983

1,1-dimethylcyclopropane

PointGroup: C2v

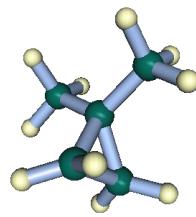
E= -196.604810324 au

ZPE= 0.136692 au

LUMO_eps= -0.00982 au

HOMO_eps= -0.27242 au

Dipole= 0.122 debye



15

C	0.000000	0.000000	0.149260
C	0.755342	0.000000	-1.153405
C	-0.755342	0.000000	-1.153405
C	0.000000	1.272527	0.969653
C	0.000000	-1.272527	0.969653
H	1.261720	0.908062	-1.451789
H	1.261720	-0.908062	-1.451789
H	-1.261720	-0.908062	-1.451789
H	-1.261720	0.908062	-1.451789
H	-0.882277	1.324395	1.612690
H	-0.882277	-1.324395	1.612690
H	0.882277	-1.324395	1.612690
H	0.882277	1.324395	1.612690
H	0.000000	2.158152	0.332929
H	0.000000	-2.158152	0.332929

Molecule# 0984

1,1-dimethylhydrazine

PointGroup: Cs

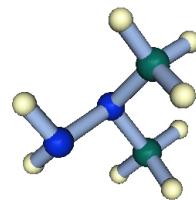
E= -190.562318078 au

ZPE= 0.108606 au

LUMO_eps= -0.01474 au

HOMO_eps= -0.20282 au

Dipole= 0.584 debye



12

C	0.327267	-0.588904	1.198224
N	0.327267	0.236816	0.000000
N	-0.931112	0.994972	0.000000
H	-0.869402	1.616300	0.803103
H	-0.869402	1.616300	-0.803103
H	0.334815	0.048085	2.083911
H	-0.549984	-1.250736	1.251362
H	1.234428	-1.191485	1.209716
C	0.327267	-0.588904	-1.198224
H	0.334815	0.048085	-2.083911
H	-0.549984	-1.250736	-1.251362
H	1.234428	-1.191485	-1.209716

Molecule# 0985

1,1-dithiocyanatoethane

PointGroup: C1

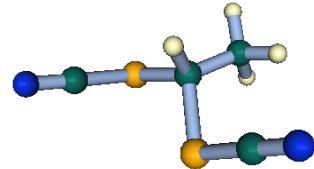
E= -1060.829698630 au

ZPE= 0.074718 au

LUMO_eps= -0.07964 au

HOMO_eps= -0.29212 au

Dipole= 4.428 debye



12

S	-0.941719	-0.587939	0.768936
S	1.669768	0.756964	0.287950
N	-3.415090	-0.760915	-0.639976
N	2.817085	-1.701635	-0.585142
C	-0.056728	0.618916	-0.342704
C	-2.408367	-0.687899	-0.075952
C	2.320508	-0.717745	-0.238832
C	-0.677159	2.004219	-0.337138
H	-0.021035	0.185721	-1.337080
H	-1.717428	1.940023	-0.652532
H	-0.647908	2.449729	0.656902
H	-0.145903	2.653030	-1.033882

Molecule# 0986

1,1-dithiocyanatoethene

PointGroup: C1

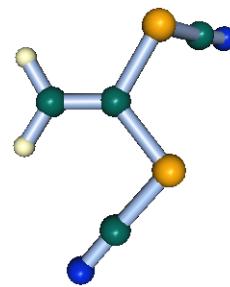
E= -1059.591055030 au

ZPE= 0.051379 au

LUMO_eps= -0.07986 au

HOMO_eps= -0.28793 au

Dipole= 3.690 debye



10

S	0.913405	-0.731150	-0.602876
S	-1.659560	0.749648	-0.498267
N	3.513666	-0.356225	0.501355
N	-2.753361	-1.506382	0.868888
C	0.061580	0.725895	0.003060
C	2.453147	-0.497661	0.065289
C	-2.270244	-0.603474	0.334802
C	0.589938	1.764744	0.634480
H	1.649607	1.825737	0.840445
H	-0.039790	2.579515	0.960377

Molecule# 0987

1,1-ethenediyl dicyanate

PointGroup: C1

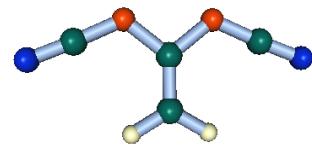
E= -413.609174762 au

ZPE= 0.057856 au

LUMO_eps= -0.05177 au

HOMO_eps= -0.30962 au

Dipole= 0.178 debye



10

O	1.086627	-0.768894	-0.000019
O	-1.086627	-0.768894	-0.000018
N	3.344570	0.172429	0.000005
N	-3.344570	0.172429	0.000011
C	0.000000	0.087074	-0.000001
C	2.270510	-0.244533	-0.000005
C	-2.270510	-0.244533	-0.000002
C	0.000000	1.401601	0.000027
H	-0.931172	1.945319	0.000038
H	0.931172	1.945319	0.000038

Molecule# 0988

1,1,1-propellane

PointGroup: C3v

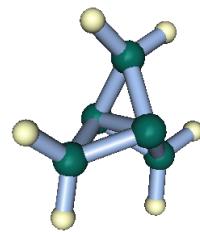
E= -194.078413103 au

ZPE= 0.093007 au

LUMO_eps= -0.00752 au

HOMO_eps= -0.26896 au

Dipole= 0.000 debye



11

C	0.000000	1.297147	0.000000
C	0.000000	0.000000	0.783698
C	0.000000	0.000000	-0.783698
C	-1.123362	-0.648574	0.000000
C	1.123362	-0.648574	0.000000
H	0.913369	1.877008	0.000000
H	-0.913369	1.877008	0.000000
H	-2.082221	-0.147503	0.000000
H	-1.168852	-1.729505	0.000000
H	2.082221	-0.147503	0.000000
H	1.168852	-1.729505	0.000000

Molecule# 0989

1,1,1-tribromoethane

PointGroup: C3

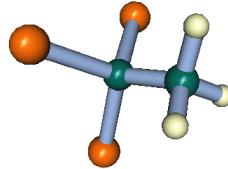
E= -7800.726683130 au

ZPE= 0.045218 au

LUMO_eps= -0.08372 au

HOMO_eps= -0.28490 au

Dipole= 1.672 debye



8

C	0.000000	0.000000	0.464722
C	0.000000	0.000000	1.977905
Br	0.000000	1.851460	-0.206566
Br	1.603411	-0.925730	-0.206566
Br	-1.603411	-0.925730	-0.206566
H	0.000000	-1.024993	2.344564
H	0.887670	0.512496	2.344564
H	-0.887670	0.512496	2.344564

Molecule# 0990

1,1,1-tribromopropane

PointGroup: Cs

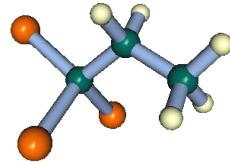
E= -7840.053948640 au

ZPE= 0.073446 au

LUMO_eps= -0.08116 au

HOMO_eps= -0.28272 au

Dipole= 1.937 debye



11

C	2.132498	1.845617	0.000000
C	0.610943	1.726691	0.000000
C	0.044563	0.310664	0.000000
Br	-1.926607	0.414369	0.000000
Br	0.610943	-0.684612	1.604449
Br	0.610943	-0.684612	-1.604449
H	2.571229	1.384883	-0.883343
H	2.403459	2.901508	0.000000
H	2.571229	1.384883	0.883343
H	0.195648	2.225398	-0.877219
H	0.195648	2.225398	0.877219

Molecule# 0991

1,1,1-trichloroethane

PointGroup: C3

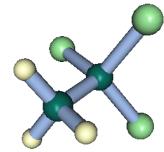
E= -1458.746443430 au

ZPE= 0.047016 au

LUMO_eps= -0.05032 au

HOMO_eps= -0.31188 au

Dipole= 1.875 debye



8

C 0.000000 0.000000 1.770041

C 0.000000 0.000000 0.257391

Cl 0.000000 1.689350 -0.363984

Cl 1.463020 -0.844675 -0.363984

Cl -1.463020 -0.844675 -0.363984

H 0.000000 -1.025689 2.132856

H 0.888273 0.512844 2.132856

H -0.888273 0.512844 2.132856

Molecule# 0992

1,1,1-trichloropropane

PointGroup: Cs

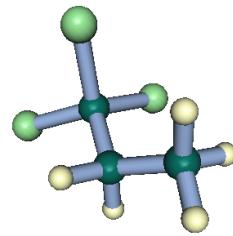
E= -1498.073980500 au

ZPE= 0.075338 au

LUMO_eps= -0.04783 au

HOMO_eps= -0.30967 au

Dipole= 2.096 debye



11

C	2.201897	-1.170837	0.000000
C	1.510358	0.188385	0.000000
C	-0.014350	0.152620	0.000000
Cl	-0.646271	1.840726	0.000000
Cl	-0.646271	-0.685884	1.463336
Cl	-0.646271	-0.685884	-1.463336
H	1.942156	-1.751560	-0.883333
H	3.281345	-1.020850	0.000000
H	1.942156	-1.751560	0.883333
H	1.803357	0.765336	-0.877934
H	1.803357	0.765336	0.877934

Molecule# 0993

1,1,1-trifluoro-2,2,2-trimethoxyethane

PointGroup: C1

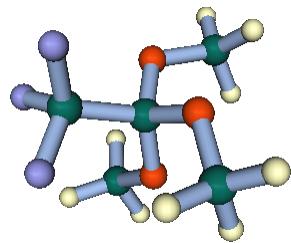
E= -721.411963064 au

ZPE= 0.149073 au

LUMO_eps= -0.01225 au

HOMO_eps= -0.29745 au

Dipole= 2.792 debye



20

C	0.258550	2.382485	0.824917
C	2.419735	-0.329563	-1.144869
C	0.651202	-1.608396	1.651249
C	0.344674	0.105814	-0.045876
C	-1.170238	-0.211734	-0.324776
O	0.585595	1.459026	-0.221890
O	1.018793	-0.603637	-1.020083
O	0.713817	-0.233280	1.257402
F	-1.581732	0.353567	-1.464232
F	-1.943092	0.265655	0.672940
F	-1.406607	-1.532928	-0.413131
H	-0.817668	2.438539	0.985805
H	0.620817	3.344736	0.473213
H	0.757167	2.116247	1.753875
H	2.924788	-0.411858	-0.181994
H	2.583857	0.662861	-1.559989
H	2.802661	-1.084794	-1.825432
H	1.042909	-2.260936	0.872164
H	-0.370179	-1.902674	1.893061
H	1.269351	-1.687276	2.541803

Molecule# 0994

1,1,1-trifluoroethane

PointGroup: C3v

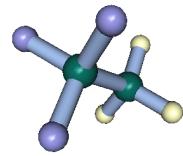
E= -377.722034954 au

ZPE= 0.051997 au

LUMO_eps= -0.01373 au

HOMO_eps= -0.39620 au

Dipole= 2.395 debye



8

C	0.000000	0.000000	1.478573
C	0.000000	0.000000	-0.023472
H	0.000000	-1.026225	1.838151
H	0.888737	0.513112	1.838151
H	-0.888737	0.513112	1.838151
F	0.000000	1.253973	-0.527595
F	-1.085973	-0.626987	-0.527595
F	1.085973	-0.626987	-0.527595

Molecule# 0995

1,1,1-trifluoropropane

PointGroup: Cs

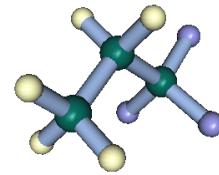
E= -417.050024973 au

ZPE= 0.080517 au

LUMO_eps= -0.01471 au

HOMO_eps= -0.37281 au

Dipole= 2.516 debye



11

C	-1.755788	-1.135628	0.000000
C	-1.135780	0.259439	0.000000
C	0.373557	0.244819	0.000000
F	0.879802	-0.382880	1.085643
F	0.879802	1.498257	0.000000
F	0.879802	-0.382880	-1.085643
H	-1.459013	-1.700292	0.882744
H	-2.842020	-1.057015	0.000000
H	-1.459013	-1.700292	-0.882744
H	-1.443277	0.826675	0.878962
H	-1.443277	0.826675	-0.878962

Molecule# 0996

1,1,1-trimethoxyethane

PointGroup: C1

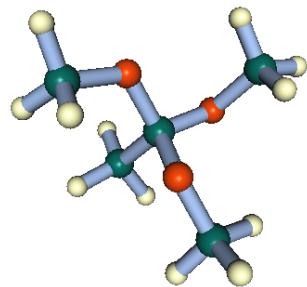
E= -423.571741218 au

ZPE= 0.172246 au

LUMO_eps= -0.01025 au

HOMO_eps= -0.27552 au

Dipole= 1.267 debye



20

C	0.396763	-0.849410	1.557707
C	-1.307595	1.844297	-0.284042
C	-1.397054	-1.675296	-0.631754
C	2.299456	0.075180	-0.646213
C	0.083784	-0.016254	0.319117
O	-0.932476	0.864857	0.686795
O	-0.287293	-0.804780	-0.801289
O	1.175176	0.756275	-0.102867
H	1.120921	-1.627964	1.326124
H	0.801114	-0.194836	2.326325
H	-0.507613	-1.314379	1.943099
H	-0.521991	2.587274	-0.415187
H	-2.202110	2.321102	0.109521
H	-1.531943	1.383740	-1.247020
H	-1.666306	-2.024172	-1.626421
H	-2.250042	-1.156136	-0.190361
H	-1.144456	-2.540690	-0.013310
H	2.776750	-0.573021	0.093646
H	3.004868	0.850810	-0.935557
H	2.025435	-0.513636	-1.520874

Molecule# 0997

1,1,1,2-tetrafluorochloroethane

PointGroup: C1

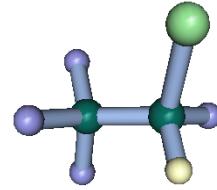
E= -936.610132351 au

ZPE= 0.035457 au

LUMO_eps= -0.02579 au

HOMO_eps= -0.34301 au

Dipole= 1.434 debye



8

C	0.451706	0.483657	-0.467135
C	-0.861674	-0.168523	-0.001224
H	0.454491	0.558887	-1.551837
F	0.530176	1.727520	0.073771
Cl	1.858333	-0.488147	0.023923
F	-0.920875	-0.298900	1.324534
F	-1.892087	0.597920	-0.396345
F	-1.004585	-1.376672	-0.562482

Molecule# 0998

1,1,1,2-tetrafluoroethane

PointGroup: Cs

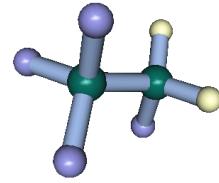
E= -476.984136640 au

ZPE= 0.044992 au

LUMO_eps= -0.01427 au

HOMO_eps= -0.38234 au

Dipole= 2.064 debye



8

C	0.361772	0.190165	0.000000
C	-1.157274	0.243325	0.000000
F	0.843210	1.450981	0.000000
F	0.843210	-0.436999	1.084078
F	0.843210	-0.436999	-1.084078
F	-1.667677	-1.036067	0.000000
H	-1.492284	0.765414	0.895748
H	-1.492284	0.765414	-0.895748

Molecule# 0999

1,1,1,2-tetramethoxyethane

PointGroup: C1

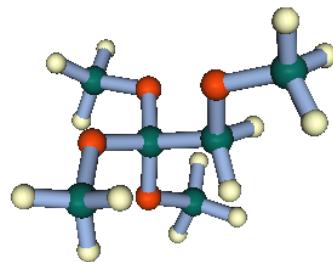
E= -538.125535785 au

ZPE= 0.205167 au

LUMO_eps= -0.01285 au

HOMO_eps= -0.26705 au

Dipole= 1.989 debye



24

C	-3.230761	-0.667661	0.267528
C	1.613648	-1.548109	-1.362053
C	1.930118	0.028520	1.827269
C	-0.095597	2.218883	-0.923603
C	-0.975112	-0.563177	-0.371630
C	0.386263	0.049656	-0.003455
O	-1.977896	-0.047508	0.468903
O	1.332271	-0.191322	-1.040678
O	0.777361	-0.532375	1.194775
O	0.352154	1.427453	0.171175
H	-3.588767	-0.528974	-0.760344
H	-3.934183	-0.201346	0.953910
H	-3.183230	-1.742606	0.478392
H	1.786633	-2.144110	-0.464434
H	2.519368	-1.537660	-1.964779
H	0.811054	-2.004198	-1.948597
H	2.760884	0.121924	1.126655
H	2.196807	-0.665495	2.620743
H	1.704697	1.005239	2.252683
H	-1.160540	2.065114	-1.111288
H	0.478256	2.010258	-1.826711
H	0.061973	3.253034	-0.626958
H	-0.901685	-1.650429	-0.263497
H	-1.193741	-0.339419	-1.423512

Molecule# 1000

1,1,2-trichloro-1,2,2-trifluoroethane

PointGroup: C1

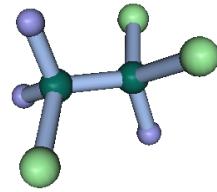
E= -1756.569748600 au

ZPE= 0.023144 au

LUMO_eps= -0.05438 au

HOMO_eps= -0.33566 au

Dipole= 0.465 debye



8

C	0.578488	0.148776	0.311897
C	-0.726971	-0.530081	-0.225129
F	0.477526	0.252431	1.648651
Cl	1.977285	-0.887503	-0.077159
Cl	0.788750	1.767240	-0.389497
Cl	-2.180351	0.394434	0.227356
F	-0.665283	-0.645666	-1.555470
F	-0.819545	-1.759329	0.300984

Molecule# 1001

1,1,2-trichloroethane

PointGroup: Cs

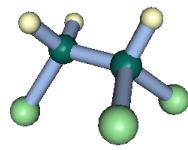
E= -1458.748855440 au

ZPE= 0.048395 au

LUMO_eps= -0.03917 au

HOMO_eps= -0.31347 au

Dipole= 2.696 debye



8

C	1.056688	-0.825383	0.000000
C	0.623146	0.625677	0.000000
Cl	-0.291928	-2.006932	0.000000
Cl	-0.291928	1.061629	1.479874
Cl	-0.291928	1.061629	-1.479874
H	1.650902	-1.016853	-0.889604
H	1.650902	-1.016853	0.889604
H	1.507532	1.254404	0.000000

Molecule# 1002

1,1,2-trifluoroethene

PointGroup: Cs

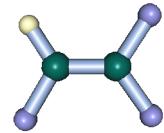
E= -376.442811541 au

ZPE= 0.029198 au

LUMO_eps= -0.01312 au

HOMO_eps= -0.27634 au

Dipole= 1.285 debye



6

C	0.000000	0.430631	0.000000
C	-0.704353	-0.686847	0.000000
F	1.314791	0.500587	0.000000
F	-0.554822	1.630861	0.000000
F	-0.092517	-1.882156	0.000000
H	-1.780948	-0.706341	0.000000

Molecule# 1003

1,1,2-trifluoropropene

PointGroup: Cs

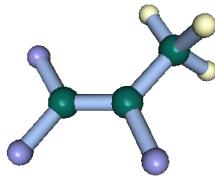
E= -415.781436877 au

ZPE= 0.056836 au

LUMO_eps= -0.01585 au

HOMO_eps= -0.26019 au

Dipole= 2.023 debye



9

C	-0.035450	-0.681860	0.000000
F	1.048578	-1.447157	0.000000
F	-1.137562	-1.409159	0.000000
C	0.000000	0.641679	0.000000
F	-1.187405	1.293847	0.000000
C	1.198490	1.512864	0.000000
H	2.107235	0.915995	0.000000
H	1.201017	2.155061	0.882809
H	1.201017	2.155061	-0.882809

Molecule# 1004

1,1,2-trimethylhydrazine

PointGroup: C1

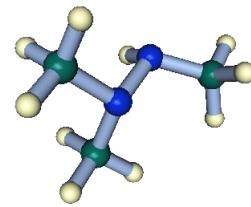
E= -229.886490050 au

ZPE= 0.136341 au

LUMO_eps= -0.01265 au

HOMO_eps= -0.23006 au

Dipole= 1.258 debye



15

C	1.979205	-0.084993	-0.208488
C	-1.523606	-0.931315	-0.078157
C	-0.762496	1.356133	0.045941
N	0.728676	-0.487073	0.418360
N	-0.413231	-0.017131	-0.292792
H	2.801931	-0.442661	0.411618
H	2.096531	0.998915	-0.340160
H	2.053124	-0.556251	-1.187265
H	-1.223290	-1.932786	-0.375989
H	-2.371774	-0.616432	-0.686760
H	-1.848711	-0.963839	0.974835
H	-1.044241	1.465794	1.107744
H	-1.603731	1.682831	-0.565341
H	0.077866	2.017471	-0.159362
H	0.695565	-0.162564	1.385928

Molecule# 1005

1,1,2,2-tetrabromocyclopentane

PointGroup: C2

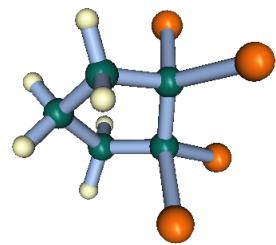
E= -10491.113913300 au

ZPE= 0.099507 au

LUMO_eps= -0.07121 au

HOMO_eps= -0.27686 au

Dipole= 2.740 debye



15

C	0.000000	0.000000	2.693335
C	0.538475	1.120980	1.766647
C	-0.538475	-1.120980	1.766647
C	0.000000	0.776480	0.375559
C	0.000000	-0.776480	0.375559
Br	0.983336	1.629747	-1.078597
Br	-1.889434	1.429343	0.276857
Br	1.889434	-1.429343	0.276857
Br	-0.983336	-1.629747	-1.078597
H	0.797053	-0.368652	3.334861
H	-0.797053	0.368652	3.334861
H	0.233979	2.118709	2.066640
H	1.625336	1.101079	1.726125
H	-0.233979	-2.118709	2.066640
H	-1.625336	-1.101079	1.726125

Molecule# 1006

1,1,2,2-tetrachlorocyclopentane

PointGroup: C2

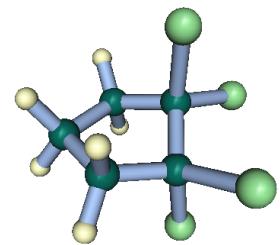
E= -2035.141320380 au

ZPE= 0.102136 au

LUMO_eps= -0.04031 au

HOMO_eps= -0.30368 au

Dipole= 3.057 debye



15

C	0.000000	0.000000	2.379326
C	-0.540152	1.120038	1.453423
C	0.540152	-1.120038	1.453423
C	0.000000	0.780705	0.063279
C	0.000000	-0.780705	0.063279
Cl	-0.918814	1.530370	-1.269894
Cl	1.722064	1.361119	-0.048861
Cl	-1.722064	-1.361119	-0.048861
Cl	0.918814	-1.530370	-1.269894
H	0.795834	0.369632	3.021692
H	-0.795834	-0.369632	3.021692
H	-1.626332	1.099741	1.409111
H	-0.232881	2.118369	1.749841
H	1.626332	-1.099741	1.409111
H	0.232881	-2.118369	1.749841

Molecule# 1007

1,1,2,3,3,3-hexafluoroprop-1-ene

PointGroup: C1

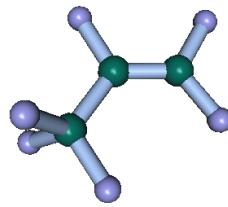
E= -713.613633510 au

ZPE= 0.033879 au

LUMO_eps= -0.03567 au

HOMO_eps= -0.30397 au

Dipole= 1.086 debye



9

C	0.245890	-0.471484	-0.000001
C	1.412981	0.161547	0.000001
C	-1.126370	0.134384	-0.000001
F	0.234429	-1.812633	0.000002
F	2.559922	-0.475620	0.000002
F	1.575610	1.460961	0.000000
F	-1.821022	-0.263524	1.082021
F	-1.082861	1.471534	-0.000098
F	-1.821079	-0.263683	-1.081926

Molecule# 1008

1,1,3-trifluoropropene

PointGroup: Cs

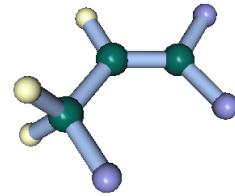
E= -415.780400731 au

ZPE= 0.057530 au

LUMO_eps= -0.01742 au

HOMO_eps= -0.27345 au

Dipole= 2.645 debye



9

C	0.000000	0.862132	0.000000
F	-1.305149	0.683741	0.000000
F	0.270153	2.162974	0.000000
C	0.934721	-0.068353	0.000000
H	1.955306	0.288216	0.000000
C	0.754530	-1.551413	0.000000
F	-0.579844	-1.931007	0.000000
H	1.221377	-1.991895	0.885372
H	1.221377	-1.991895	-0.885372

Molecule# 1009

1,1,3,3-tetrachloropropane

PointGroup: C2

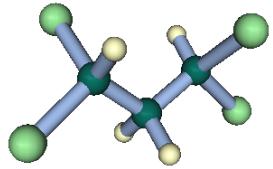
E= -1957.709919150 au

ZPE= 0.067597 au

LUMO_eps= -0.04366 au

HOMO_eps= -0.31775 au

Dipole= 0.164 debye



11

C	0.000000	0.000000	0.731800
C	0.000000	1.274009	-0.097804
C	0.000000	-1.274009	-0.097804
Cl	0.132799	2.700697	0.986148
Cl	-1.483724	1.397852	-1.115518
Cl	1.483724	-1.397852	-1.115518
Cl	-0.132799	-2.700697	0.986148
H	-0.881449	-0.008441	1.372394
H	0.881449	0.008441	1.372394
H	0.836615	1.328750	-0.781690
H	-0.836615	-1.328750	-0.781690

Molecule# 1010

1,1,3,3-tetrafluoropropane

PointGroup: Cs

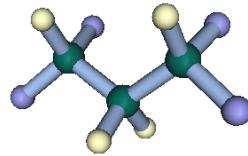
E= -516.311613505 au

ZPE= 0.073824 au

LUMO_eps= -0.01703 au

HOMO_eps= -0.36052 au

Dipole= 2.313 debye



11

C	0.448354	-0.545579	0.000000
C	-0.285414	-0.171763	1.270135
C	-0.285414	-0.171763	-1.270135
F	0.361469	-0.731547	2.340045
F	-0.285414	1.179129	1.461730
F	-0.285414	1.179129	-1.461730
F	0.361469	-0.731547	-2.340045
H	0.581940	-1.627632	0.000000
H	1.431669	-0.074796	0.000000
H	-1.323885	-0.509706	1.300971
H	-1.323885	-0.509706	-1.300971

Molecule# 1011

1,1,3,4-oxadiazol-2-yl-3H-imidazol-2-one

PointGroup: Cs

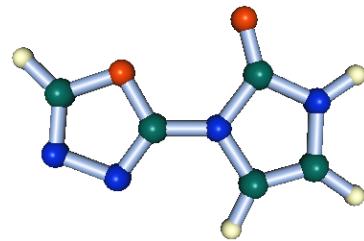
E= -562.568756174 au

ZPE= 0.102143 au

LUMO_eps= -0.03800 au

HOMO_eps= -0.23516 au

Dipole= 3.707 debye



15

C	-0.749149	-2.765389	0.000000
C	-0.579479	-0.671889	0.000000
C	0.123559	2.779879	0.000000
C	-0.748568	1.763546	0.000000
C	1.389116	0.865788	0.000000
N	-1.948842	-2.317880	0.000000
N	-1.848213	-0.922014	0.000000
N	1.407751	2.245729	0.000000
N	0.000000	0.571384	0.000000
O	2.321679	0.097408	0.000000
O	0.193548	-1.775534	0.000000
H	-0.403540	-3.783062	0.000000
H	-0.057518	3.838204	0.000000
H	-1.820876	1.742621	0.000000
H	2.272372	2.755109	0.000000

Molecule# 1012

1,1H-pyrrol-2-yl-3H-imidazol-2-one

PointGroup: Cs

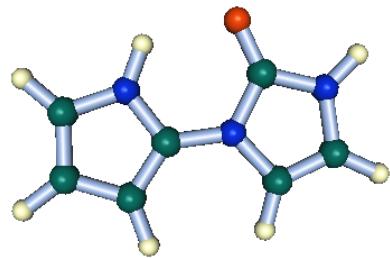
E= -510.631184859 au

ZPE= 0.138700 au

LUMO_eps= -0.01810 au

HOMO_eps= -0.19793 au

Dipole= 3.247 debye



18

C	2.000783	-2.375333	0.000000
C	1.952841	-0.953690	0.000000
C	0.709392	-2.839143	0.000000
C	0.619213	-0.612080	0.000000
C	-0.282242	2.841230	0.000000
C	0.654875	1.876810	0.000000
C	-1.378739	0.841614	0.000000
N	-0.129515	-1.752458	0.000000
N	-1.520850	2.212219	0.000000
N	0.000000	0.643566	0.000000
O	-2.261036	-0.010039	0.000000
H	2.889351	-2.982383	0.000000
H	2.791003	-0.279563	0.000000
H	0.317417	-3.839971	0.000000
H	-0.176176	3.909258	0.000000
H	1.724825	1.950503	0.000000
H	-1.139214	-1.728251	0.000000
H	-2.423096	2.650993	0.000000

Molecule# 1013

1,2-acetylenediol

PointGroup: C1

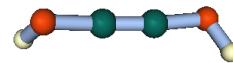
E= -227.843385572 au

ZPE= 0.036919 au

LUMO_eps= -0.02766 au

HOMO_eps= -0.24601 au

Dipole= 1.956 debye



6

O -1.911245 0.085603 -0.071095

O 1.911245 -0.085603 -0.071094

C -0.597007 -0.013624 0.006112

C 0.597007 0.013624 0.006111

H -2.328814 -0.541074 0.532088

H 2.328813 0.541078 0.532085

Molecule# 1014

1,2-butadiene

PointGroup: Cs

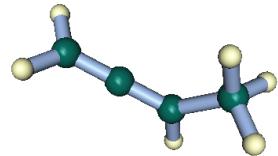
E= -156.039733573 au

ZPE= 0.083619 au

LUMO_eps= -0.01422 au

HOMO_eps= -0.25818 au

Dipole= 0.459 debye



10

C	-0.676877	1.824455	0.000000
C	0.000000	0.712806	0.000000
C	0.674729	-0.400337	0.000000
C	0.070788	-1.779546	0.000000
H	-0.970419	2.308430	0.924346
H	-0.970419	2.308430	-0.924346
H	1.759891	-0.339248	0.000000
H	-1.016629	-1.735258	0.000000
H	0.392869	-2.343309	-0.878652
H	0.392869	-2.343309	0.878652

Molecule# 1015

1,2-butanediamine

PointGroup: C1

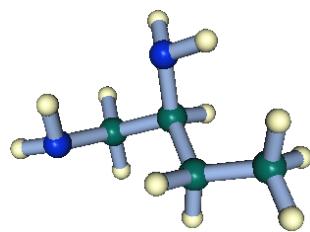
E= -269.261843647 au

ZPE= 0.166595 au

LUMO_eps= -0.01651 au

HOMO_eps= -0.23418 au

Dipole= 1.693 debye



18

N	1.990811	-0.622856	-0.629420
H	1.931431	0.145537	-1.286847
H	2.964238	-0.880555	-0.536839
C	-2.421072	-0.350244	-0.096681
H	-3.045807	-1.165912	-0.462671
H	-2.766459	-0.095407	0.908123
H	-2.614499	0.507889	-0.743569
N	0.014105	1.506798	-0.328520
H	0.497986	2.259825	0.146270
H	-0.921393	1.837328	-0.524861
C	-0.946476	-0.754688	-0.096316
H	-0.829081	-1.675676	0.479986
H	-0.616481	-0.980777	-1.110214
C	1.427116	-0.214502	0.656216
H	2.012213	0.572109	1.158562
H	1.424096	-1.077830	1.325625
C	-0.009887	0.295010	0.507813
H	-0.368749	0.512414	1.525817

Molecule# 1016

1,2-chloroethyl-1-nitrosourea

PointGroup: C1

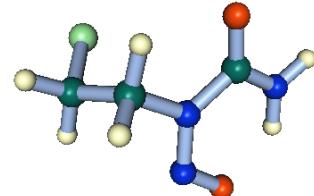
E= -892.986199488 au

ZPE= 0.108008 au

LUMO_eps= -0.09332 au

HOMO_eps= -0.26777 au

Dipole= 1.425 debye



15

C1	-2.331716	0.385323	-0.842661
O	0.800067	1.956894	0.684740
O	1.924475	-1.710939	-0.590900
N	0.559473	-0.319605	0.435360
N	0.933917	-1.565968	0.100956
N	2.266673	0.888042	-0.680548
C	1.219264	0.950722	0.158620
C	-0.659018	-0.298092	1.257074
C	-1.897922	-0.742235	0.503473
H	2.749788	1.749947	-0.864293
H	2.588978	-0.000540	-1.031486
H	-0.513599	-0.974263	2.100509
H	-0.765445	0.714099	1.630691
H	-2.748841	-0.765557	1.178688
H	-1.762439	-1.721470	0.055027

Molecule# 1017

1,2-diaminopropane

PointGroup: C1

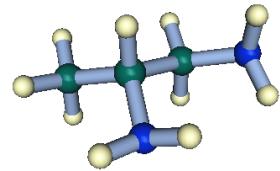
E= -229.935511682 au

ZPE= 0.137950 au

LUMO_eps= -0.01893 au

HOMO_eps= -0.23800 au

Dipole= 2.066 debye



15

N	0.515491	1.391494	-0.213362
H	-0.258480	1.947494	0.128733
H	1.364140	1.866364	0.068915
N	-2.061342	-0.127690	0.037236
H	-2.181732	0.757797	-0.436282
H	-2.220834	0.015135	1.026891
C	-0.749795	-0.711690	-0.229148
H	-0.747392	-1.729706	0.168410
H	-0.635640	-0.788418	-1.312659
C	1.758237	-0.700957	-0.022941
H	1.744056	-1.722779	0.358287
H	1.887491	-0.735988	-1.105935
H	2.629221	-0.200050	0.404284
C	0.469629	0.030604	0.335268
H	0.371697	0.035781	1.433164

Molecule# 1018

1,2-dibromoethane

PointGroup: C2h

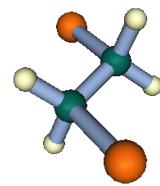
E= -5227.119613500 au

ZPE= 0.056688 au

LUMO_eps= -0.04925 au

HOMO_eps= -0.29291 au

Dipole= 0.000 debye



8

C	0.493728	0.567234	0.000000
C	-0.493728	-0.567234	0.000000
Br	-0.493728	2.283784	0.000000
Br	0.493728	-2.283784	0.000000
H	1.112645	0.580282	0.889576
H	1.112645	0.580282	-0.889576
H	-1.112645	-0.580282	-0.889576
H	-1.112645	-0.580282	0.889576

Molecule# 1019

1,2-dichloro-1-cyanoethane

PointGroup: C1

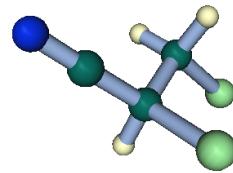
E= -1091.384213050 au

ZPE= 0.056198 au

LUMO_eps= -0.05942 au

HOMO_eps= -0.32760 au

Dipole= 1.924 debye



9

C1	0.551587	1.629115	0.087511
C1	-2.244644	-0.339481	-0.083117
N	2.790232	-1.254867	0.059102
C	0.482758	-0.120609	-0.375006
C	-0.599970	-0.872040	0.395411
C	1.784559	-0.732929	-0.133991
H	0.269104	-0.138557	-1.441420
H	-0.528062	-1.933131	0.170399
H	-0.494775	-0.714549	1.464113

Molecule# 1020

1,2-dichloro-1,1,2,2-tetrafluoroethane

PointGroup: C2h

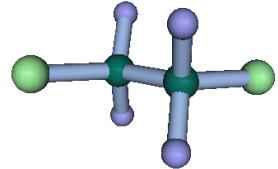
E= -1396.228328330 au

ZPE= 0.025008 au

LUMO_eps= -0.05043 au

HOMO_eps= -0.35225 au

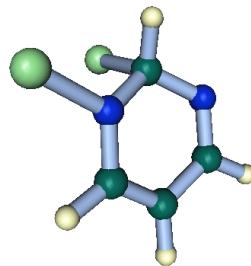
Dipole= 0.000 debye



8

C	-0.237982	0.743614	0.000000
C	0.237982	-0.743614	0.000000
Cl	-2.016512	0.831072	0.000000
Cl	2.016512	-0.831072	0.000000
F	0.237982	1.361871	1.086622
F	0.237982	1.361871	-1.086622
F	-0.237982	-1.361871	1.086622
F	-0.237982	-1.361871	-1.086622

Molecule# 1021
1,2-dichloro-1,2-dihydropyrimidine
PointGroup: C1
E= -1184.832359440 au
ZPE= 0.079799 au
LUMO_eps= -0.08210 au
HOMO_eps= -0.24798 au
Dipole= 4.319 debye



12

C1	0.166446	2.029748	-0.534405
C1	-2.226375	-0.504117	0.180096
N	-0.509875	-0.569838	0.156783
N	1.549944	0.221170	0.996445
C	0.208766	0.520260	0.714401
C	0.106052	-1.471911	-0.652182
C	1.460676	-1.542010	-0.638384
C	2.129257	-0.705879	0.304895
H	-0.325278	0.953353	1.547915
H	-0.533226	-2.118979	-1.232017
H	1.984941	-2.262604	-1.244494
H	3.183372	-0.869602	0.506885

Molecule# 1022

1,2-dichlorobutane

PointGroup: C1

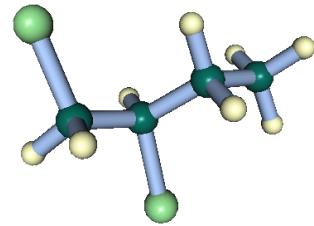
E= -1077.786920750 au

ZPE= 0.114175 au

LUMO_eps= -0.02099 au

HOMO_eps= -0.30684 au

Dipole= 0.808 debye



14

H	0.819970	0.970836	1.504408
H	-1.166548	-1.746969	-0.177938
H	-0.984908	-0.880520	1.362012
C	-1.009069	-0.777888	0.281092
H	0.177283	0.021144	-1.322049
Cl	1.582703	-1.367580	-0.036028
C	0.252711	-0.117091	-0.245865
C	0.632489	1.180766	0.448756
H	2.728827	1.294378	-0.120432
H	2.019134	2.837293	0.352290
H	1.638622	2.140940	-1.219876
C	1.825906	1.901249	-0.171533
H	-0.246766	1.827735	0.407093
Cl	-2.476694	0.215400	-0.120455

Molecule# 1023

1,2-dichloroethane

PointGroup: C2

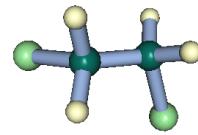
E= -999.125393823 au

ZPE= 0.057820 au

LUMO_eps= -0.02284 au

HOMO_eps= -0.30504 au

Dipole= 2.769 debye



8

C	-0.299342	0.692073	0.892875
C	0.299342	-0.692073	0.892875
Cl	0.299342	1.715125	-0.469310
Cl	-0.299342	-1.715125	-0.469310
H	-1.381552	0.661641	0.812196
H	-0.016551	1.207148	1.808816
H	0.016551	-1.207148	1.808816
H	1.381552	-0.661641	0.812196

Molecule# 1024

1,2-dichloroethyl hydroperoxide

PointGroup: C1

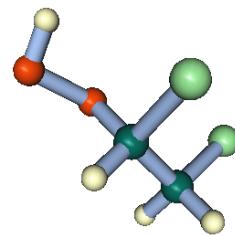
E= -1149.534563450 au

ZPE= 0.065269 au

LUMO_eps= -0.03260 au

HOMO_eps= -0.31128 au

Dipole= 1.813 debye



10

C1	-0.802776	1.542890	-0.140419
C1	2.113305	-0.235887	-0.445398
O	-0.818187	-1.131783	-0.204327
O	-2.257807	-1.225852	-0.211671
C	-0.450958	-0.091853	0.628640
C	1.015455	-0.237799	0.975858
H	-1.051458	-0.091718	1.536612
H	1.314562	0.581471	1.620958
H	1.157889	-1.186487	1.487459
H	-2.479028	-0.683324	-0.985157

Molecule# 1025

1,2-dichloropropane

PointGroup: C1

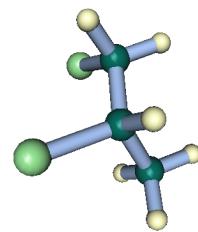
E= -1038.456421230 au

ZPE= 0.085780 au

LUMO_eps= -0.02009 au

HOMO_eps= -0.30234 au

Dipole= 2.882 debye



11

C	0.666782	1.690821	-0.460286
C	-0.725969	0.098901	0.986609
C	0.649984	0.536037	0.521680
Cl	-1.857919	-0.342878	-0.351048
Cl	1.569886	-0.883973	-0.164823
H	0.168266	1.420936	-1.388454
H	0.146881	2.547529	-0.025224
H	1.689864	1.985265	-0.683868
H	-0.661903	-0.769025	1.634334
H	-1.198048	0.919690	1.523433
H	1.206722	0.797530	1.421558

Molecule# 1026

1,2-dicyano-1,2-ethenedithiol

PointGroup: C1

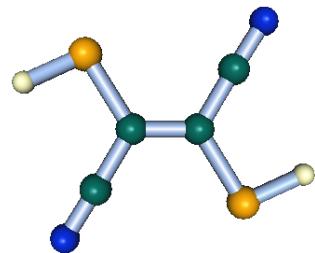
E= -1059.611811960 au

ZPE= 0.047805 au

LUMO_eps= -0.11612 au

HOMO_eps= -0.25977 au

Dipole= 0.187 debye



10

S	1.653853	-1.466360	-0.041522
S	-1.653853	1.466359	-0.041519
N	1.962540	2.243904	0.036069
N	-1.962540	-2.243904	0.036069
C	0.678815	0.016108	0.014810
C	-0.678816	-0.016108	0.014811
C	1.374141	1.251705	0.022854
C	-1.374142	-1.251705	0.022855
H	2.827783	-0.852149	0.185852
H	-2.827783	0.852148	0.185851

Molecule# 1027

1,2-dicyano-2-hydroxylamino-ethane

PointGroup: C1

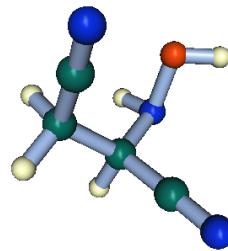
E= -394.960648160 au

ZPE= 0.094307 au

LUMO_eps= -0.04493 au

HOMO_eps= -0.29368 au

Dipole= 6.101 debye



13

O	0.313702	-1.614925	-0.926768
N	1.171613	-1.268187	0.163198
N	1.427390	2.027391	-0.681155
N	-2.527750	0.403730	-0.742264
C	0.711444	-0.025519	0.777150
C	-0.791840	0.053445	1.169705
C	1.112029	1.119852	-0.051970
C	-1.739571	0.231309	0.075617
H	0.885285	-1.552765	-1.700527
H	1.045190	-2.024365	0.828812
H	1.278390	0.046227	1.709846
H	-1.048671	-0.855680	1.716626
H	-0.920956	0.890916	1.857922

Molecule# 1028

1,2-dicyanobromoethene

PointGroup: C1

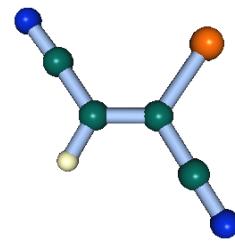
E= -2836.786662110 au

ZPE= 0.039801 au

LUMO_eps= -0.13028 au

HOMO_eps= -0.30900 au

Dipole= 0.240 debye



8

Br	0.277012	-1.240273	-0.000005
N	2.688866	1.669070	0.000004
N	-3.195621	0.568095	0.000005
C	0.327500	0.649473	0.000002
C	-0.772903	1.418364	0.000006
C	1.628930	1.216824	0.000003
C	-2.099383	0.924470	0.000006
H	-0.652998	2.494613	0.000011

Molecule# 1029

1,2-dicyanofluoroethane

PointGroup: C1

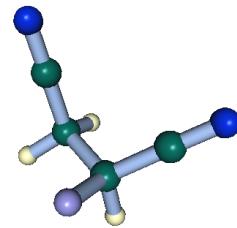
E= -363.663657196 au

ZPE= 0.065331 au

LUMO_eps= -0.04979 au

HOMO_eps= -0.35972 au

Dipole= 5.618 debye



10

F	0.548649	1.404763	-0.866830
N	1.973333	-1.532425	-0.071295
N	-2.338792	-0.929583	-0.574584
C	0.660912	0.696914	0.317359
C	-0.731990	0.476706	0.920774
C	1.389652	-0.554071	0.072761
C	-1.622829	-0.312424	0.077679
H	1.247307	1.305371	1.008994
H	-0.623459	-0.014179	1.889654
H	-1.177948	1.457246	1.092538

Molecule# 1030

1,2-diethoxyethane

PointGroup: C2

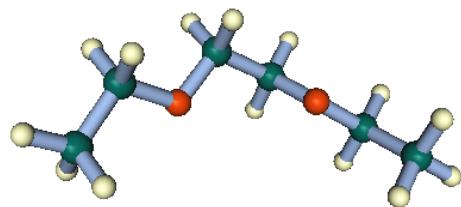
E= -387.651629093 au

ZPE= 0.196897 au

LUMO_eps= -0.00954 au

HOMO_eps= -0.25612 au

Dipole= 1.148 debye



22

C	-0.185454	3.476467	1.177678
C	0.185454	-3.476467	1.177678
C	0.448568	2.723875	0.026404
C	-0.448568	-2.723875	0.026404
C	0.330721	0.678899	-1.157349
C	-0.330721	-0.678899	-1.157349
O	-0.185454	1.462479	-0.100569
O	0.185454	-1.462479	-0.100569
H	0.289479	4.450910	1.299148
H	-1.249152	3.631512	0.997075
H	-0.073398	2.919207	2.107537
H	-0.289479	-4.450910	1.299148
H	1.249152	-3.631512	0.997075
H	0.073398	-2.919207	2.107537
H	1.523271	2.581941	0.202423
H	0.343221	3.289948	-0.909829
H	-1.523271	-2.581941	0.202423
H	-0.343221	-3.289948	-0.909829
H	0.140113	1.170529	-2.121857
H	1.415919	0.554537	-1.050343
H	-0.140113	-1.170529	-2.121857
H	-1.415919	-0.554537	-1.050343

Molecule# 1031
1,2-difluoro-3-nitrobenzene

PointGroup: C1

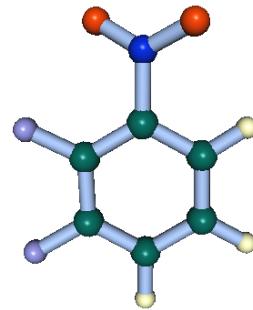
E= -635.451455630 au

ZPE= 0.086438 au

LUMO_eps= -0.11277 au

HOMO_eps= -0.29025 au

Dipole= 4.845 debye



14

F	-0.174377	-1.959003	-0.132114
F	-2.700777	-1.150004	-0.078605
O	2.821157	0.734982	-0.401394
O	2.306279	-1.197619	0.437397
N	2.021435	-0.091571	0.012142
C	0.601826	0.299791	0.013607
C	-0.410428	-0.657728	-0.033324
C	-1.733657	-0.226270	-0.015537
C	0.291444	1.653903	0.071365
C	-2.054339	1.114433	0.058602
C	-1.032431	2.057202	0.104097
H	1.101788	2.365330	0.093910
H	-3.095956	1.401601	0.074126
H	-1.273459	3.108243	0.162559

Molecule# 1032

1,2-difluoroethane

PointGroup: C2h

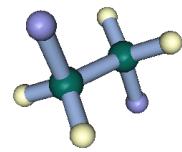
E= -278.408461645 au

ZPE= 0.060783 au

LUMO_eps= -0.00835 au

HOMO_eps= -0.34980 au

Dipole= 0.000 debye



8

C	0.425915	0.627157	0.000000
C	-0.425915	-0.627157	0.000000
F	-0.425915	1.731378	0.000000
F	0.425915	-1.731378	0.000000
H	1.051850	0.677105	0.891207
H	1.051850	0.677105	-0.891207
H	-1.051850	-0.677105	0.891207
H	-1.051850	-0.677105	-0.891207

Molecule# 1033

1,2-dihydro-3H-1,2,4-triazol-3-ylidenemethanone

PointGroup: C1

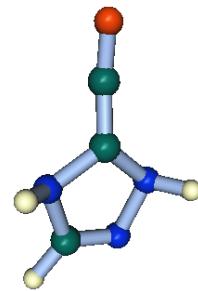
E= -355.628315506 au

ZPE= 0.067146 au

LUMO_eps= -0.07132 au

HOMO_eps= -0.19558 au

Dipole= 3.154 debye



10

O	2.804747	0.017257	-0.101685
N	-0.501813	-1.172528	0.046451
N	-0.518237	1.148566	0.064488
N	-1.829526	-0.691292	-0.149633
C	0.336696	0.001975	0.169153
C	-1.784183	0.580024	-0.127805
C	1.635206	0.015429	-0.087720
H	-0.507329	-1.788898	0.852503
H	-0.455507	1.869545	0.772931
H	-2.654421	1.203511	-0.262863

Molecule# 1034

1,2-diisocyanatoethane

PointGroup: C1

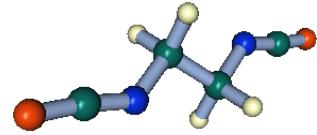
E= -414.945028289 au

ZPE= 0.083334 au

LUMO_eps= -0.03490 au

HOMO_eps= -0.30118 au

Dipole= 0.000 debye



12

O	-4.169729	-0.037851	-0.000189
O	4.169729	0.037850	-0.000331
N	-1.822306	0.260406	0.000120
N	1.822306	-0.260406	0.000229
C	-0.587346	-0.486761	0.000192
C	0.587346	0.486762	0.000114
C	-3.002288	0.047253	-0.000041
C	3.002288	-0.047254	-0.000081
H	-0.530798	-1.125725	-0.882692
H	-0.530812	-1.125555	0.883200
H	0.530823	1.125555	-0.882895
H	0.530787	1.125727	0.882997

Molecule# 1035

1,2-dimethoxyethane

PointGroup: C2

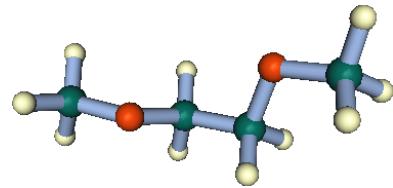
E= -308.984997502 au

ZPE= 0.140556 au

LUMO_eps= -0.00968 au

HOMO_eps= -0.25901 au

Dipole= 1.359 debye



16

C	0.170671	2.748478	-0.443046
C	-0.170671	-2.748478	-0.443046
C	-0.170671	0.735400	0.732131
C	0.170671	-0.735400	0.732131
O	0.508228	1.383432	-0.325029
O	-0.508228	-1.383432	-0.325029
H	0.742895	3.152831	-1.275405
H	0.423122	3.306090	0.467816
H	-0.898648	2.880525	-0.647014
H	0.898648	-2.880525	-0.647014
H	-0.742895	-3.152831	-1.275405
H	-0.423122	-3.306090	0.467816
H	0.125486	1.172411	1.696274
H	-1.256057	0.857539	0.624047
H	-0.125486	-1.172411	1.696274
H	1.256057	-0.857539	0.624047

Molecule# 1036

1,2-dimethylhydrazine

PointGroup: C2

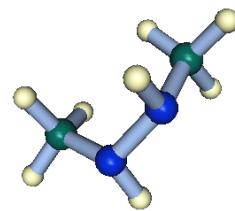
E= -190.561533832 au

ZPE= 0.109131 au

LUMO_eps= -0.01318 au

HOMO_eps= -0.22968 au

Dipole= 1.506 debye



12

C	0.414691	1.407380	0.525760
N	0.414691	0.576813	-0.674955
N	-0.414691	-0.576813	-0.674955
C	-0.414691	-1.407380	0.525760
H	-1.350955	-0.279245	-0.913971
H	-0.587418	1.808180	0.689219
H	0.736630	0.902508	1.444977
H	1.084191	2.249794	0.349899
H	1.350955	0.279245	-0.913971
H	-1.084191	-2.249794	0.349899
H	-0.736630	-0.902508	1.444977
H	0.587418	-1.808180	0.689219

Molecule# 1037

1,2-divinylbenzene

PointGroup: C2

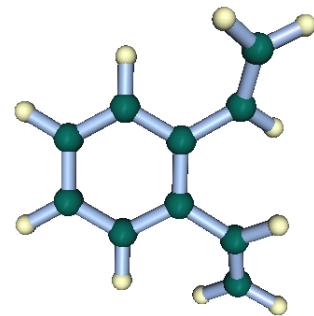
E= -387.186599623 au

ZPE= 0.166110 au

LUMO_eps= -0.05418 au

HOMO_eps= -0.23238 au

Dipole= 0.083 debye



20

C	-0.002677	0.695637	2.287492
C	0.002677	-0.695637	2.287492
C	-0.005281	1.380849	1.083628
C	0.005281	-1.380849	1.083628
C	0.002677	0.706828	-0.143419
C	-0.002677	-0.706828	-0.143419
C	0.504833	2.671718	-1.602985
C	-0.504833	-2.671718	-1.602985
C	-0.027936	1.466513	-1.404857
C	0.027936	-1.466513	-1.404857
H	-0.012494	1.242389	3.220751
H	0.012494	-1.242389	3.220751
H	-0.044540	2.461435	1.086304
H	0.044540	-2.461435	1.086304
H	0.415967	3.169418	-2.558579
H	1.054385	3.194867	-0.831116
H	-0.415967	-3.169418	-2.558579
H	-1.054385	-3.194867	-0.831116
H	-0.534592	0.991304	-2.236512
H	0.534592	-0.991304	-2.236512

Molecule# 1038

1,2-ethanediol

PointGroup: C1

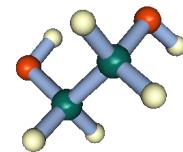
E= -230.356418248 au

ZPE= 0.085097 au

LUMO_eps= -0.02184 au

HOMO_eps= -0.27845 au

Dipole= 2.377 debye



10

C	0.680732	0.592289	-0.291181
C	-0.721940	0.567772	0.287742
O	1.404236	-0.594510	0.050668
O	-1.459811	-0.557597	-0.160898
H	1.214042	1.489687	0.038901
H	0.632713	0.600665	-1.379775
H	-1.271483	1.455526	-0.029664
H	-0.669565	0.583184	1.385698
H	1.668590	-0.545996	0.974636
H	-0.882437	-1.326578	-0.087321

Molecule# 1039

1,2-ethanediyl dicyanate

PointGroup: C2

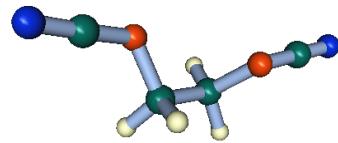
E= -414.848122287 au

ZPE= 0.082333 au

LUMO_eps= -0.03877 au

HOMO_eps= -0.32072 au

Dipole= 4.145 debye



12

O	-0.194628	1.442226	-0.211553
O	0.194628	-1.442226	-0.211553
N	0.795033	3.647186	-0.572454
N	-0.795033	-3.647186	-0.572454
C	0.339745	0.667888	0.903873
C	-0.339745	-0.667888	0.903873
C	0.339745	2.601889	-0.389104
C	-0.339745	-2.601889	-0.389104
H	1.417300	0.568273	0.779108
H	0.119945	1.195921	1.831875
H	-1.417300	-0.568273	0.779108
H	-0.119945	-1.195921	1.831875

Molecule# 1040

1,2-fluoroethyl-1-nitrosourea

PointGroup: C1

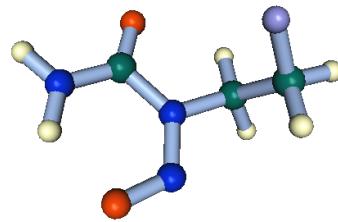
E= -532.628682037 au

ZPE= 0.109469 au

LUMO_eps= -0.09227 au

HOMO_eps= -0.26685 au

Dipole= 1.335 debye



15

F	2.238616	-0.469672	-1.083891
O	-0.514809	-2.003549	0.451487
O	-1.632764	1.813980	-0.275594
N	-0.198773	0.275717	0.380007
N	-0.548484	1.562718	0.217650
N	-2.134520	-0.747839	-0.527734
C	-0.963461	-0.934369	0.104720
C	1.144957	0.122000	0.957118
C	2.245900	0.443632	-0.031865
H	-2.462917	0.183522	-0.731508
H	-2.687718	-1.568038	-0.704569
H	1.225249	-0.904699	1.298472
H	1.231055	0.793777	1.810409
H	2.119544	1.439137	-0.458411
H	3.215888	0.378152	0.464183

Molecule# 1041

1,2-furylpyridin-2-one

PointGroup: C1

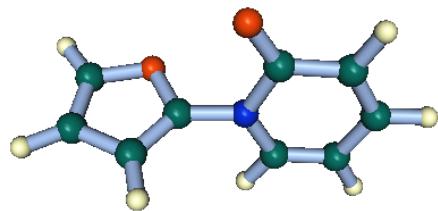
E= -552.542179449 au

ZPE= 0.143103 au

LUMO_eps= -0.06180 au

HOMO_eps= -0.23341 au

Dipole= 3.935 debye



19

C	-3.194575	-0.313665	0.532954
C	-1.888732	-0.508814	1.083438
C	-3.009799	0.096865	-0.744869
C	-1.019311	-0.203012	0.091580
C	3.135362	-0.257975	-0.067413
C	2.506179	0.937102	0.061393
C	2.396422	-1.469775	-0.153237
C	1.044926	-1.406409	-0.107584
C	1.064931	1.048883	0.123453
N	0.385002	-0.209485	0.027326
O	0.429863	2.079331	0.252424
O	-1.682395	0.164204	-1.036752
H	-4.138874	-0.452415	1.029472
H	-1.631730	-0.812260	2.082940
H	-3.678984	0.370087	-1.539794
H	4.216627	-0.293566	-0.105985
H	3.049817	1.867462	0.131301
H	2.886862	-2.424324	-0.258784
H	0.409095	-2.276074	-0.174091

Molecule# 1042

1,2-furylpyrrole

PointGroup: C1

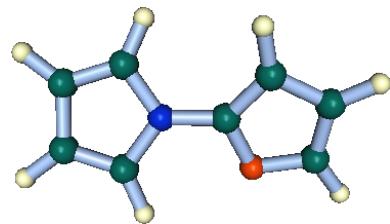
E= -439.156096335 au

ZPE= 0.132513 au

LUMO_eps= -0.02436 au

HOMO_eps= -0.21720 au

Dipole= 1.350 debye



17

C	-2.772926	-0.745430	0.127040
C	-2.835748	0.657366	-0.109605
C	2.860308	0.583052	0.103711
C	1.551119	1.154181	0.212862
C	-1.451987	-1.096859	0.185131
C	-1.550872	1.119466	-0.190721
C	2.691852	-0.736863	-0.133470
C	0.685887	0.123810	0.019734
N	-0.697666	0.046430	-0.010764
O	1.353226	-1.035205	-0.194701
H	-3.604798	-1.419043	0.239788
H	-3.724063	1.255180	-0.219283
H	3.800352	1.097381	0.201917
H	1.298133	2.176815	0.425961
H	-0.974196	-2.044614	0.349051
H	-1.163532	2.103939	-0.379320
H	3.360167	-1.565371	-0.273248

Molecule# 1043

1,2-naphthalenedione

PointGroup: C1

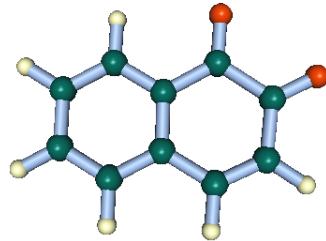
E= -535.297983691 au

ZPE= 0.132180 au

LUMO_eps= -0.13166 au

HOMO_eps= -0.25698 au

Dipole= 6.431 debye



18

O	1.361068	-2.102147	0.000000
C	1.045295	-0.935880	-0.000003
C	-0.368855	-0.479577	0.000039
C	-0.663338	0.897964	0.000004
C	-1.998519	1.302976	-0.000021
C	-3.022439	0.362805	-0.000027
C	-2.725364	-0.995943	-0.000004
C	-1.400135	-1.413451	0.000019
C	0.412017	1.881771	0.000016
C	1.715208	1.558479	0.000033
C	2.154699	0.161657	0.000003
O	3.320597	-0.165604	-0.000046
H	-2.234107	2.359259	-0.000035
H	-4.052746	0.691593	-0.000046
H	-3.523054	-1.725709	0.000000
H	-1.145325	-2.463972	0.000055
H	0.118437	2.925051	0.000016
H	2.492067	2.310977	0.000032

Molecule# 1044

1,2-oxazole-4-carbonitrile

PointGroup: Cs

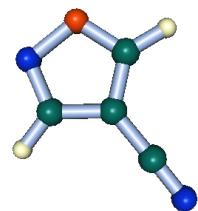
E= -338.400286113 au

ZPE= 0.056540 au

LUMO_eps= -0.07338 au

HOMO_eps= -0.30344 au

Dipole= 1.568 debye



9

O	0.710722	-1.733894	0.000000
N	-0.691138	-1.797404	0.000000
N	-0.085068	2.920338	0.000000
C	0.000000	0.355924	0.000000
C	1.091283	-0.460386	0.000000
C	-1.094603	-0.562112	0.000000
C	-0.038720	1.769277	0.000000
H	2.149576	-0.263840	0.000000
H	-2.149674	-0.341769	0.000000

Molecule# 1045

1,2-pentadiene

PointGroup: Cs

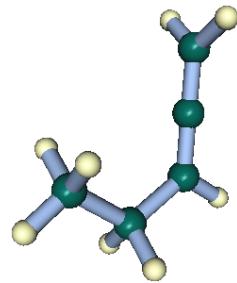
E= -195.367456103 au

ZPE= 0.112190 au

LUMO_eps= -0.01441 au

HOMO_eps= -0.25677 au

Dipole= 0.510 debye



13

C	-1.396817	0.429335	0.000000
C	-1.472698	-1.093148	0.000000
C	0.000000	1.004651	0.000000
C	1.112304	0.327742	0.000000
C	2.229478	-0.340821	0.000000
H	-1.928062	0.827718	0.870383
H	-1.928062	0.827718	-0.870383
H	-0.983848	-1.513104	-0.879616
H	-2.511270	-1.424852	0.000000
H	-0.983848	-1.513104	0.879616
H	0.069668	2.089604	0.000000
H	2.715910	-0.630267	-0.924292
H	2.715910	-0.630267	0.924292

Molecule# 1046

1,2-propadiene-1,3-dione

PointGroup: D(infinity)h

E= -264.828376754 au

ZPE= 0.021576 au

LUMO_eps= -0.07692 au

HOMO_eps= -0.30271 au

Dipole= 0.000 debye



5

C 0.000000 0.000000 0.000000

C 0.000000 0.000000 1.271509

C 0.000000 0.000000 -1.271509

O 0.000000 0.000000 2.431267

O 0.000000 0.000000 -2.431267

Molecule# 1047

1,2-thiazole-1-oxide

PointGroup: C1

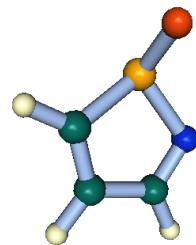
E= -644.333510796 au

ZPE= 0.057880 au

LUMO_eps= -0.10586 au

HOMO_eps= -0.26019 au

Dipole= 5.239 debye



9

C	-1.612388	0.682359	0.140260
C	-1.488887	-0.779323	0.122520
C	-0.420753	1.265282	-0.005680
N	-0.318061	-1.288315	-0.012961
O	1.964766	0.007831	0.533864
S	0.794812	-0.007586	-0.382382
H	-2.559721	1.190971	0.248025
H	-2.350133	-1.435001	0.211100
H	-0.166681	2.311049	-0.063797

Molecule# 1048

1,2-thiazole-3-carbonitrile

PointGroup: C1

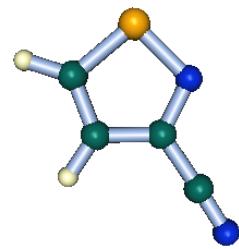
E= -661.414447658 au

ZPE= 0.053471 au

LUMO_eps= -0.08619 au

HOMO_eps= -0.29364 au

Dipole= 5.354 debye



9

S	-1.711330	-0.591498	0.000002
N	-0.125713	-1.050663	0.000000
N	3.206102	-0.162108	-0.000004
C	-0.041278	1.287387	0.000000
C	0.631726	0.033488	-0.000001
C	-1.390605	1.091295	0.000002
C	2.056708	-0.099158	-0.000002
H	0.453822	2.244922	0.000000
H	-2.174575	1.830378	0.000003

Molecule# 1049

1,2-thiazole-3(2H)-thione

PointGroup: C1

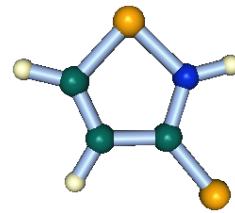
E= -967.367005037 au

ZPE= 0.057299 au

LUMO_eps= -0.07270 au

HOMO_eps= -0.21774 au

Dipole= 4.931 debye



9

S	-1.852923	-0.547135	0.000003
S	2.341496	-0.118506	0.000003
N	-0.197443	-0.956196	-0.000012
C	0.689320	0.084870	-0.000004
C	-0.074363	1.311044	-0.000004
C	-1.409363	1.123574	0.000003
H	0.409589	2.273247	-0.000007
H	0.109128	-1.916200	0.000016
H	-2.187332	1.869648	0.000005

Molecule# 1050

1,2-thiazole-4-carbonitrile

PointGroup: C1

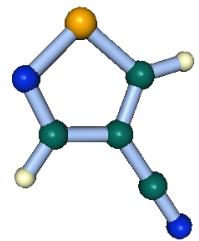
E= -661.417330959 au

ZPE= 0.053649 au

LUMO_eps= -0.08328 au

HOMO_eps= -0.29236 au

Dipole= 2.933 debye



9

S	1.790737	-0.475898	-0.000002
N	1.364374	1.134172	-0.000002
N	-3.240588	-0.146020	-0.000007
C	-0.672756	0.008613	0.000004
C	0.191251	-1.060988	0.000003
C	0.060358	1.235299	0.000002
C	-2.089661	-0.084352	0.000005
H	-0.056134	-2.109489	0.000004
H	-0.397308	2.215358	0.000003

Molecule# 1051

1,2-thienylpyridin-4-one

PointGroup: C1

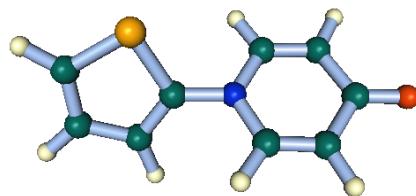
E= -875.516016318 au

ZPE= 0.139949 au

LUMO_eps= -0.05899 au

HOMO_eps= -0.23043 au

Dipole= 7.053 debye



19

C	-3.260747	0.996763	0.430923
C	-1.865684	1.229535	0.570709
C	-3.546891	-0.215226	-0.118964
C	-1.112417	0.187192	0.114195
C	2.381637	1.125229	-0.488236
C	2.306330	-1.101133	0.504790
C	1.033891	1.153086	-0.447360
C	0.961179	-1.008421	0.530032
C	3.145966	-0.022380	-0.008396
N	0.292939	0.105453	0.062562
O	4.374161	-0.076554	-0.036314
S	-2.114227	-1.095088	-0.513823
H	-4.018281	1.696745	0.749056
H	-1.438528	2.118035	1.010517
H	-4.511080	-0.656491	-0.304364
H	2.922894	1.963430	-0.901979
H	2.789940	-1.988514	0.885958
H	0.451171	1.981024	-0.821014
H	0.328052	-1.786428	0.929407

Molecule# 1052

1,2,3-dithiazolidin-4-imine

PointGroup: C1

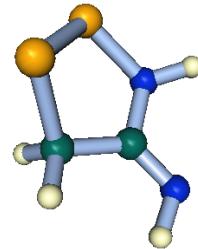
E= -984.619981726 au

ZPE= 0.068192 au

LUMO_eps= -0.06844 au

HOMO_eps= -0.22960 au

Dipole= 1.443 debye



10

S	-1.169858	-1.011282	0.175331
S	-1.142550	1.044339	-0.322638
N	0.518150	-1.217936	-0.077229
N	2.527323	-0.088722	-0.233399
C	1.295329	-0.062239	0.065703
C	0.478211	1.133537	0.539987
H	0.785257	-1.791625	-0.865407
H	2.962650	0.821413	-0.123246
H	0.970963	2.062828	0.267287
H	0.320110	1.097290	1.618539

Molecule# 1053

1,2,3-oxadiazole

PointGroup: Cs

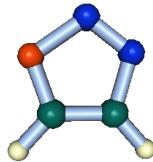
E= -262.163649858 au

ZPE= 0.045066 au

LUMO_eps= -0.06148 au

HOMO_eps= -0.29782 au

Dipole= 3.505 debye



7

O -1.090936 0.355540 0.000000

N -0.611357 -1.025671 0.000000

N 0.631549 -0.984727 0.000000

C 1.095265 0.310964 0.000000

C 0.000000 1.106756 0.000000

H 2.142317 0.547367 0.000000

H -0.127759 2.174789 0.000000

Molecule# 1054

1,2,3-oxathiazole

PointGroup: C1

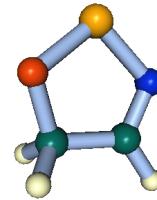
E= -606.238272674 au

ZPE= 0.052950 au

LUMO_eps= -0.04637 au

HOMO_eps= -0.22192 au

Dipole= 2.433 debye



8

S	1.186410	-0.064006	0.045138
O	-0.061150	-1.221903	-0.137878
N	0.175744	1.267799	-0.042280
C	-1.314499	-0.572652	0.090963
C	-1.045628	0.909737	-0.039631
H	-2.026854	-0.942923	-0.648855
H	-1.699331	-0.803961	1.095565
H	-1.836625	1.649104	-0.077924

Molecule# 1055

1,2,3-thiadiazole-2(3H)-carbonitrile

PointGroup: C1

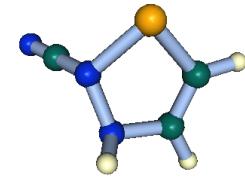
E= -678.591130487 au

ZPE= 0.063871 au

LUMO_eps= -0.07103 au

HOMO_eps= -0.24001 au

Dipole= 5.432 debye



10

S	0.596501	-1.254311	-0.215908
N	-0.521489	0.078464	-0.630668
N	0.161630	1.335417	-0.521980
N	-2.690102	0.007425	0.617646
C	1.600362	-0.083701	0.655744
C	1.269049	1.169256	0.363538
C	-1.667835	0.056671	0.083610
H	0.450648	1.618461	-1.455320
H	2.392643	-0.412715	1.306776
H	1.752966	2.060731	0.730728

Molecule# 1056

1,2,3-triazine-1,3,5(2H,4H)-triol

PointGroup: C1

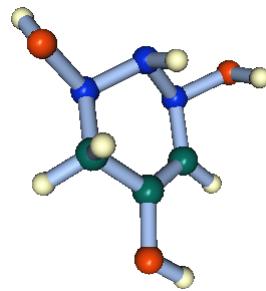
E= -508.451417911 au

ZPE= 0.121665 au

LUMO_eps= -0.03104 au

HOMO_eps= -0.22570 au

Dipole= 2.882 debye



16

O	0.569873	2.594176	0.155646
O	-2.539726	-0.757181	0.081104
O	2.008157	-1.846819	0.105094
N	0.242253	1.348825	-0.423189
N	-1.244557	-0.381906	-0.375129
N	-0.961120	0.888970	0.212235
C	1.064960	-0.864269	0.012715
C	1.310785	0.421165	-0.255557
C	-0.329937	-1.403053	0.142311
H	0.854272	2.424313	1.072480
H	-3.127779	-0.379891	-0.584305
H	2.891387	-1.470128	0.025779
H	-0.747833	0.743910	1.215313
H	2.292040	0.814411	-0.479160
H	-0.568583	-1.662971	1.182597
H	-0.430815	-2.305323	-0.461686

Molecule# 1057

1,2,3-triazine

PointGroup: C2v

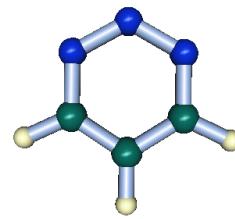
E= -280.397915348 au

ZPE= 0.063258 au

LUMO_eps= -0.08434 au

HOMO_eps= -0.26818 au

Dipole= 5.028 debye



9

N	0.000000	1.151590	0.730933
N	0.000000	0.000000	1.376561
N	0.000000	-1.151590	0.730933
C	0.000000	-1.164165	-0.603698
C	0.000000	0.000000	-1.346005
C	0.000000	1.164165	-0.603698
H	0.000000	-2.145712	-1.060908
H	0.000000	0.000000	-2.426768
H	0.000000	2.145712	-1.060908

Molecule# 1058

1,2,3-triazole

PointGroup: Cs

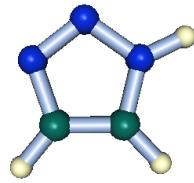
E= -242.316977901 au

ZPE= 0.058925 au

LUMO_eps= -0.02225 au

HOMO_eps= -0.27864 au

Dipole= 4.430 debye



8

N	0.000000	1.067552	0.000000
N	-1.127818	0.334603	0.000000
N	-0.769838	-0.912161	0.000000
C	0.589795	-0.989098	0.000000
C	1.100389	0.282255	0.000000
H	-0.062722	2.071574	0.000000
H	1.103956	-1.933077	0.000000
H	2.101258	0.672603	0.000000

Molecule# 1059

1,2,3-trichloropropane

PointGroup: Cs

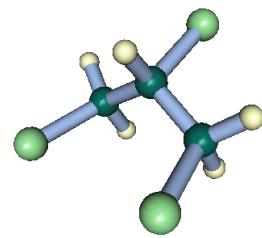
E= -1498.081326130 au

ZPE= 0.077051 au

LUMO_eps= -0.03992 au

HOMO_eps= -0.29764 au

Dipole= 1.571 debye



11

C	0.430741	0.570041	0.000000
C	-0.305104	0.279695	1.300643
C	-0.305104	0.279695	-1.300643
Cl	0.726567	2.382023	0.000000
Cl	-0.305104	-1.475215	-1.736081
Cl	-0.305104	-1.475215	1.736081
H	1.416453	0.115060	0.000000
H	0.183833	0.788707	-2.122928
H	0.183833	0.788707	2.122928
H	-1.342701	0.596935	-1.244192
H	-1.342701	0.596935	1.244192

Molecule# 1060

1,2,3-trifluorobenzene

PointGroup: C2v

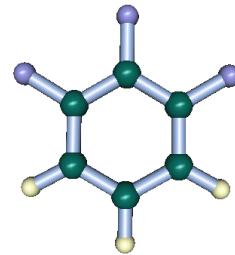
E= -530.152855425 au

ZPE= 0.076064 au

LUMO_eps= -0.03412 au

HOMO_eps= -0.27410 au

Dipole= 2.927 debye



12

C	0.000000	0.000000	-2.055605
C	0.000000	1.208669	-1.369465
C	0.000000	1.195102	0.013528
C	0.000000	0.000000	0.720519
C	0.000000	-1.195102	0.013528
C	0.000000	-1.208669	-1.369465
F	0.000000	-2.344755	0.704591
F	0.000000	0.000000	2.056059
F	0.000000	2.344755	0.704591
H	0.000000	0.000000	-3.135818
H	0.000000	2.157806	-1.884800
H	0.000000	-2.157806	-1.884800

Molecule# 1061

1,2,3-trimethylbenzene

PointGroup: Cs

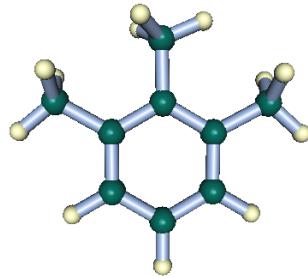
E= -350.325811212 au

ZPE= 0.182898 au

LUMO_eps= -0.01247 au

HOMO_eps= -0.23803 au

Dipole= 0.756 debye



21

C	-0.013713	-2.140034	0.000000
C	-1.206232	-1.434267	0.000000
C	1.188364	-1.448980	0.000000
C	-1.219337	-0.039134	0.000000
C	1.211026	-0.056326	0.000000
C	0.000000	0.658904	0.000000
C	-2.548821	0.677092	0.000000
C	2.533357	0.666411	0.000000
C	0.040515	2.167409	0.000000
H	-0.020953	-3.222033	0.000000
H	-2.147129	-1.970109	0.000000
H	2.124223	-1.993715	0.000000
H	-2.669919	1.314846	0.878141
H	-2.669919	1.314846	-0.878141
H	-3.368212	-0.040077	0.000000
H	2.643869	1.309810	-0.876251
H	2.643869	1.309810	0.876251
H	3.361993	-0.039937	0.000000
H	0.571159	2.550206	-0.875359
H	-0.951091	2.609692	0.000000
H	0.571159	2.550206	0.875359

Molecule# 1062

1,2,3-trioxolane

PointGroup: Cs

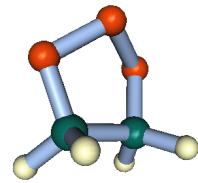
E= -304.219674727 au

ZPE= 0.066218 au

LUMO_eps= -0.01962 au

HOMO_eps= -0.27252 au

Dipole= 3.469 debye



9

O	-0.557524	-1.069370	0.000000
O	0.138457	-0.482273	1.115905
O	0.138457	-0.482273	-1.115905
C	0.138457	0.901420	0.775632
C	0.138457	0.901420	-0.775632
H	1.040255	1.327083	1.210950
H	1.040255	1.327083	-1.210950
H	-0.748557	1.400059	1.169152
H	-0.748557	1.400059	-1.169152

Molecule# 1063

1,2,3,4-oxatriazole

PointGroup: Cs

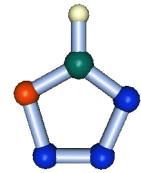
E= -278.197476050 au

ZPE= 0.033042 au

LUMO_eps= -0.07908 au

HOMO_eps= -0.34422 au

Dipole= 2.877 debye



6

C	0.000000	1.060596	0.000000
N	1.107973	0.392861	0.000000
N	0.687701	-0.924391	0.000000
N	-0.543555	-1.038784	0.000000
O	-1.082437	0.312079	0.000000
H	-0.105336	2.131991	0.000000

Molecule# 1064

1,2,3,4-tetrafluorobenzene

PointGroup: C2v

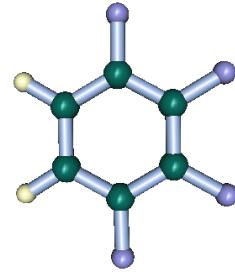
E= -629.420559277 au

ZPE= 0.067899 au

LUMO_eps= -0.04534 au

HOMO_eps= -0.27365 au

Dipole= 2.476 debye



12

C	0.000000	1.377987	-0.525257
C	0.000000	0.695340	-1.726214
C	0.000000	-0.695340	-1.726214
C	0.000000	-1.377987	-0.525257
C	0.000000	-0.694285	0.684098
C	0.000000	0.694285	0.684098
F	0.000000	2.719143	-0.501822
H	0.000000	1.255360	-2.649366
H	0.000000	-1.255360	-2.649366
F	0.000000	-2.719143	-0.501822
F	0.000000	-1.357117	1.841111
F	0.000000	1.357117	1.841111

Molecule# 1065

1,2,3,4-tetrahydronaphthalene

PointGroup: C2

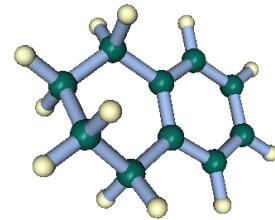
E= -388.443473422 au

ZPE= 0.193153 au

LUMO_eps= -0.01629 au

HOMO_eps= -0.23978 au

Dipole= 0.800 debye



22

C	0.001554	0.695598	2.566237
C	-0.001554	-0.695598	2.566237
C	0.001554	1.377725	1.359666
C	-0.001554	-1.377725	1.359666
C	-0.000611	0.700261	0.137630
C	0.000611	-0.700261	0.137630
C	-0.033424	1.492200	-1.154152
C	0.033424	-1.492200	-1.154152
C	0.363799	0.671723	-2.381520
C	-0.363799	-0.671723	-2.381520
H	0.004381	1.242851	3.499649
H	-0.004381	-1.242851	3.499649
H	0.004118	2.461556	1.357812
H	-0.004118	-2.461556	1.357812
H	-1.048027	1.879885	-1.300277
H	0.609583	2.369836	-1.057795
H	1.048027	-1.879885	-1.300277
H	-0.609583	-2.369836	-1.057795
H	0.142317	1.233423	-3.290989
H	1.444186	0.496649	-2.375566
H	-0.142317	-1.233423	-3.290989
H	-1.444186	-0.496649	-2.375566

Molecule# 1066

1,2,3,4-tetrazine

PointGroup: C2v

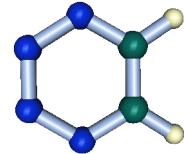
E= -296.407383574 au

ZPE= 0.050255 au

LUMO_eps= -0.11215 au

HOMO_eps= -0.27680 au

Dipole= 4.596 debye



8

N	0.000000	1.355099	-0.047558
N	0.000000	0.655407	-1.178699
N	0.000000	-0.655407	-1.178699
N	0.000000	-1.355099	-0.047558
C	0.000000	-0.693285	1.096489
C	0.000000	0.693285	1.096489
H	0.000000	-1.283068	2.004868
H	0.000000	1.283068	2.004868

Molecule# 1067

1,2,3,5-oxatriazole

PointGroup: Cs

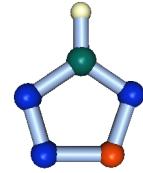
E= -278.180476224 au

ZPE= 0.033136 au

LUMO_eps= -0.09563 au

HOMO_eps= -0.34891 au

Dipole= 2.069 debye



6

O	-0.672368	-0.891320	0.000000
N	0.733709	-0.902550	0.000000
N	1.120509	0.284725	0.000000
C	0.000000	1.089677	0.000000
N	-1.090635	0.393352	0.000000
H	0.033864	2.163813	0.000000

Molecule# 1068

1,2,3,5-tetrazine

PointGroup: C2v

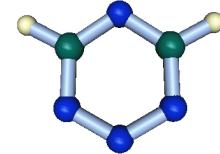
E= -296.439719769 au

ZPE= 0.051366 au

LUMO_eps= -0.11416 au

HOMO_eps= -0.27560 au

Dipole= 2.638 debye



8

N	0.000000	1.144299	-0.704266
N	0.000000	0.000000	-1.359116
N	0.000000	-1.144299	-0.704266
C	0.000000	-1.104612	0.629854
N	0.000000	0.000000	1.362678
C	0.000000	1.104612	0.629854
H	0.000000	-2.061100	1.138272
H	0.000000	2.061100	1.138272

Molecule# 1069

1,2,3,5-thatriazolidine

PointGroup: C1

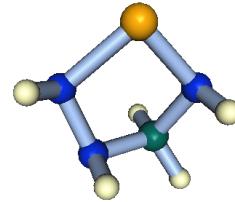
E= -603.596499610 au

ZPE= 0.078844 au

LUMO_eps= -0.03252 au

HOMO_eps= -0.21274 au

Dipole= 3.084 debye



10

S	1.269184	0.021994	-0.048659
N	-0.119168	1.321785	-0.175767
N	0.137736	-1.247091	0.185652
N	-1.310755	0.631314	0.167212
C	-1.144328	-0.729142	-0.328537
H	0.047793	2.004441	0.559957
H	0.046503	-1.444294	1.177121
H	-1.422604	0.577582	1.179868
H	-1.098328	-0.703317	-1.415165
H	-1.969031	-1.353519	0.008300

Molecule# 1070

1,2,3,6-tetrahydropyridine

PointGroup: C1

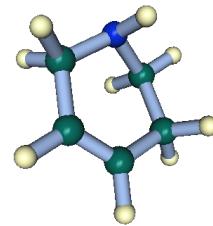
E= -250.769127360 au

ZPE= 0.134513 au

LUMO_eps= -0.01404 au

HOMO_eps= -0.22626 au

Dipole= 0.974 debye



15

H	-1.470270	2.051300	0.139796
C	-0.812779	1.192330	0.058323
H	0.914318	2.364351	-0.092773
C	0.501406	1.362711	-0.053276
H	2.325124	0.404708	0.529666
H	1.868711	0.112198	-1.129780
C	1.463386	0.206961	-0.115255
H	0.675255	-1.115005	1.396505
H	1.389091	-1.962725	0.036134
C	0.779659	-1.100064	0.308149
H	-2.309570	-0.197466	-0.590760
H	-1.867638	-0.356258	1.088810
C	-1.454743	-0.170688	0.089051
H	-0.487677	-1.340668	-1.269513
N	-0.556988	-1.272562	-0.261434

Molecule# 1071

1,2,4-dioxazolidine

PointGroup: C1

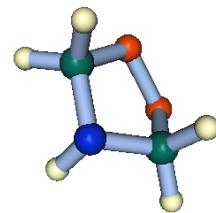
E= -284.420226066 au

ZPE= 0.080416 au

LUMO_eps= -0.01747 au

HOMO_eps= -0.25513 au

Dipole= 2.199 debye



10

O	-0.804673	-0.888677	-0.282832
O	0.593732	-1.074262	0.088267
N	0.083188	1.201711	-0.098487
C	-1.066719	0.402826	0.261301
C	1.178668	0.263372	0.057915
H	-1.160116	0.336299	1.347953
H	-1.985776	0.765925	-0.193125
H	1.887205	0.349580	-0.766514
H	1.686489	0.379914	1.015848
H	0.005718	1.462625	-1.073532

Molecule# 1072

1,2,4-oxadiazole

PointGroup: Cs

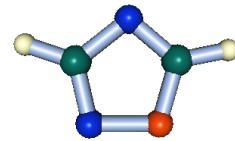
E= -262.186356381 au

ZPE= 0.046390 au

LUMO_eps= -0.05158 au

HOMO_eps= -0.31962 au

Dipole= 1.162 debye



7

C 0.672289 -0.872864 0.000000

C 0.000000 1.080516 0.000000

N 1.115151 0.428577 0.000000

N -0.618412 -1.018822 0.000000

O -1.086341 0.307970 0.000000

H 1.331150 -1.725351 0.000000

H -0.151329 2.147397 0.000000

Molecule# 1073

1,2,4-thiadiazole

PointGroup: Cs

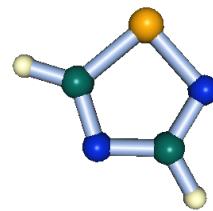
E= -585.196768765 au

ZPE= 0.043493 au

LUMO_eps= -0.06468 au

HOMO_eps= -0.29508 au

Dipole= 1.507 debye



7

C	-0.690377	-1.160681	0.000000
C	1.195972	-0.095042	0.000000
N	0.670277	-1.287237	0.000000
N	-1.238357	0.028231	0.000000
S	0.000000	1.143132	0.000000
H	-1.314687	-2.042848	0.000000
H	2.257676	0.100119	0.000000

Molecule# 1074

1,2,4-triazine

PointGroup: Cs

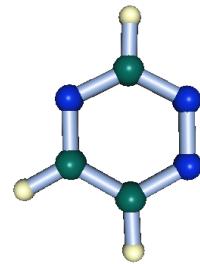
E= -280.423706033 au

ZPE= 0.064093 au

LUMO_eps= -0.09259 au

HOMO_eps= -0.25578 au

Dipole= 2.636 debye



9

C	0.000000	1.283548	0.000000
N	1.195886	0.688755	0.000000
N	-1.187170	0.683937	0.000000
C	1.154952	-0.633315	0.000000
C	-0.067010	-1.302568	0.000000
N	-1.219098	-0.643966	0.000000
H	-0.131661	-2.382786	0.000000
H	2.096736	-1.170292	0.000000
H	-0.020059	2.366010	0.000000

Molecule# 1075

1,2,4-triazole-5-mercaptomethyl-3-thione

PointGroup: C1

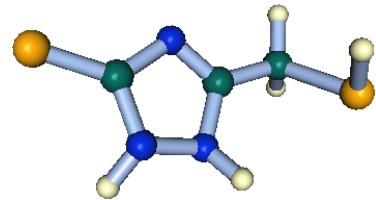
E= -1078.108368400 au

ZPE= 0.089085 au

LUMO_eps= -0.07263 au

HOMO_eps= -0.21709 au

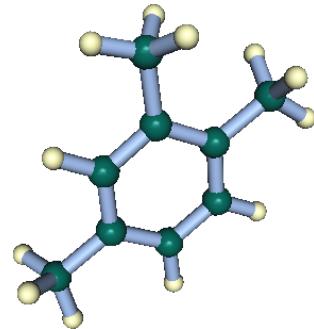
Dipole= 6.268 debye



13

S	3.158398	0.012249	-0.430328
S	-3.209591	-0.375034	-0.249597
N	0.242548	1.157410	0.432157
N	-1.076255	1.253277	-0.028584
N	-0.552113	-0.911454	0.160999
C	0.499106	-0.189314	0.400050
C	1.863333	-0.733224	0.644600
C	-1.610629	-0.027657	-0.042353
H	0.910796	1.791602	0.010985
H	2.185538	-0.503864	1.660042
H	1.837961	-1.811016	0.524244
H	-1.629039	2.025841	0.310848
H	2.703714	-0.491460	-1.593112

Molecule# 1076
 1,2,4-trimethylbenzene
 PointGroup: C1
 E= -350.328735811 au
 ZPE= 0.182558 au
 LUMO_eps= -0.01160 au
 HOMO_eps= -0.23261 au
 Dipole= 0.410 debye



21

C	1.195758	-1.298145	-0.004519
C	-0.164078	-1.590289	-0.001142
C	0.666857	1.027078	-0.003574
C	1.634761	0.020991	-0.004468
C	-1.127279	-0.586152	0.001431
C	-0.698001	0.753544	-0.000391
C	3.101945	0.363537	0.005491
C	-2.592222	-0.934876	0.003747
C	-1.694071	1.883282	-0.000809
H	1.916869	-2.105981	-0.008032
H	-0.483106	-2.625508	-0.001941
H	0.988228	2.062856	-0.006517
H	3.350936	1.071949	-0.786662
H	3.394831	0.823552	0.952224
H	3.716693	-0.524973	-0.134151
H	-3.103136	-0.529106	0.880359
H	-3.105416	-0.531909	-0.872848
H	-2.735435	-2.014351	0.005643
H	-1.191305	2.849145	-0.002610
H	-2.346579	1.844113	-0.876396
H	-2.344609	1.846392	0.876330

Molecule# 1077

1,2,4-trioxolane

PointGroup: C2

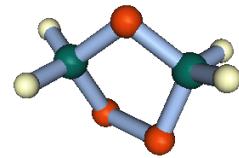
E= -304.294154696 au

ZPE= 0.067583 au

LUMO_eps= -0.01706 au

HOMO_eps= -0.28848 au

Dipole= 1.118 debye



9

O	0.000000	0.000000	1.185426
C	0.000000	1.126270	0.321884
C	0.000000	-1.126270	0.321884
O	-0.368242	-0.630282	-0.948481
O	0.368242	0.630282	-0.948481
H	-0.997388	1.574227	0.297170
H	0.997388	-1.574227	0.297170
H	0.765842	1.843110	0.617669
H	-0.765842	-1.843110	0.617669

Molecule# 1078

1,2,4,5-hexatetraene

PointGroup: Cs

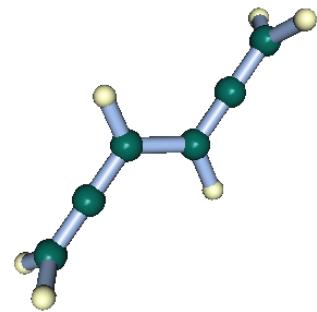
E= -232.219557372 au

ZPE= 0.093057 au

LUMO_eps= -0.02928 au

HOMO_eps= -0.23519 au

Dipole= 0.000 debye



12

C	0.604942	1.720376	0.000000
C	0.606915	3.019337	0.000000
C	0.604942	0.411180	0.000000
C	-0.604954	-0.411180	0.000000
C	-0.604953	-1.720376	0.000000
C	-0.606912	-3.019337	0.000000
H	0.608735	3.586335	0.924515
H	0.608735	3.586335	-0.924515
H	1.556375	-0.110823	0.000000
H	-1.556386	0.110823	0.000000
H	-0.608669	-3.586335	-0.924515
H	-0.608669	-3.586335	0.924515

Molecule# 1079

1,2,4,5-tetrafluorobenzene

PointGroup: D2h

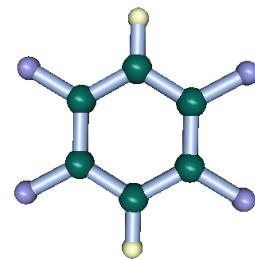
E= -629.425464044 au

ZPE= 0.067693 au

LUMO_eps= -0.05302 au

HOMO_eps= -0.26784 au

Dipole= 0.000 debye



12

C	0.000000	1.191371	0.693954
C	0.000000	0.000000	1.397434
C	0.000000	-1.191371	0.693954
C	0.000000	-1.191371	-0.693954
C	0.000000	0.000000	-1.397434
C	0.000000	1.191371	-0.693954
F	0.000000	2.357926	1.354335
H	0.000000	0.000000	2.477199
F	0.000000	-2.357926	1.354335
F	0.000000	-2.357926	-1.354335
H	0.000000	0.000000	-2.477199
F	0.000000	2.357926	-1.354335

Molecule# 1080

1,2,4,5-tetraoxane

PointGroup: C2

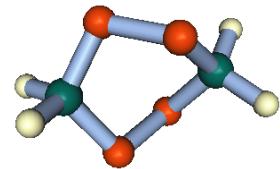
E= -379.451293229 au

ZPE= 0.071073 au

LUMO_eps= -0.03735 au

HOMO_eps= -0.28650 au

Dipole= 0.002 debye



10

O	0.667290	1.027732	-0.440985
O	1.225661	0.020424	0.440386
O	-1.225661	-0.020424	0.440386
O	-0.667290	-1.027732	-0.440985
C	-0.667290	1.205624	0.000454
C	0.667290	-1.205624	0.000454
H	-0.743907	1.858599	0.874591
H	-1.180482	1.619002	-0.872517
H	1.180482	-1.619002	-0.872517
H	0.743907	-1.858599	0.874591

Molecule# 1081

1,2,4,5-tetrazine

PointGroup: D2h

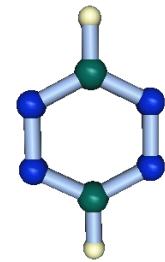
E= -296.428585760 au

ZPE= 0.051322 au

LUMO_eps= -0.12561 au

HOMO_eps= -0.26005 au

Dipole= 0.000 debye



8

N 0.000000 1.188502 0.658697

N 0.000000 1.188502 -0.658697

C 0.000000 0.000000 -1.262286

N 0.000000 -1.188502 -0.658697

N 0.000000 -1.188502 0.658697

C 0.000000 0.000000 1.262286

H 0.000000 0.000000 -2.343802

H 0.000000 0.000000 2.343802

Molecule# 1082

1,2,5-oxadiazole

PointGroup: C2v

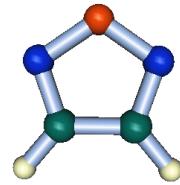
E= -262.146027961 au

ZPE= 0.045628 au

LUMO_eps= -0.06856 au

HOMO_eps= -0.33468 au

Dipole= 3.408 debye



7

O 0.000000 0.000000 1.125015

N 0.000000 1.129079 0.352670

C 0.000000 0.709443 -0.877819

C 0.000000 -0.709443 -0.877819

N 0.000000 -1.129079 0.352670

H 0.000000 1.401671 -1.701840

H 0.000000 -1.401671 -1.701840

Molecule# 1083

1,2,5-oxathiazolidine-4-carboxylic acid

PointGroup: C1

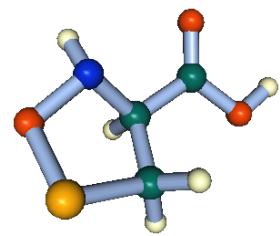
E= -796.055713058 au

ZPE= 0.091758 au

LUMO_eps= -0.04789 au

HOMO_eps= -0.22732 au

Dipole= 3.296 debye



13

S	2.173408	-0.484649	-0.218616
O	1.706873	1.062931	0.309144
O	-2.406268	1.061439	-0.306376
O	-2.347569	-1.153252	0.077835
N	0.354539	1.209545	-0.199575
C	-0.337365	0.073070	0.423591
C	-1.793433	0.075562	0.003121
C	0.479207	-1.171035	0.031849
H	-3.285795	-1.061746	-0.148192
H	0.051131	2.086883	0.215271
H	-0.334047	0.154184	1.518761
H	0.458740	-1.921418	0.816656
H	0.138929	-1.604861	-0.903801

Molecule# 1084

1,2,5-triazole

PointGroup: C2v

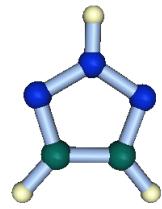
E= -242.323497971 au

ZPE= 0.059612 au

LUMO_eps= -0.02474 au

HOMO_eps= -0.28820 au

Dipole= 0.193 debye



8

N	0.000000	1.125330	0.353534
N	0.000000	0.000000	1.049856
N	0.000000	-1.125330	0.353534
C	0.000000	-0.700907	-0.908175
C	0.000000	0.700907	-0.908175
H	0.000000	0.000000	2.055597
H	0.000000	-1.396879	-1.727982
H	0.000000	1.396879	-1.727982

Molecule# 1085

1,2,6-oxathiazine

PointGroup: C1

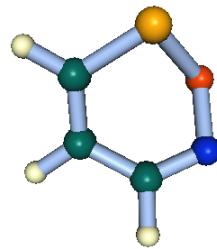
E= -644.303593032 au

ZPE= 0.057773 au

LUMO_eps= -0.08757 au

HOMO_eps= -0.23534 au

Dipole= 3.681 debye



9

S	-1.333869	-0.074841	-0.191279
O	-0.280808	-1.189269	0.481817
N	1.033450	-1.218918	-0.164297
C	-0.367982	1.345481	0.076452
C	1.577197	-0.062059	-0.172578
C	0.965100	1.208069	0.174489
H	-0.880250	2.298065	0.110510
H	2.586562	-0.065980	-0.571412
H	1.602013	2.063015	0.346729

Molecule# 1086

1,3-benzodithiole-2-thione

PointGroup: C2

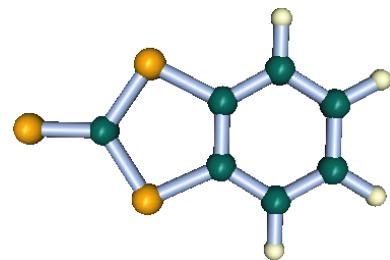
E= -1463.923513560 au

ZPE= 0.088978 au

LUMO_eps= -0.08200 au

HOMO_eps= -0.23233 au

Dipole= 4.826 debye



14

S	0.000000	0.000000	3.335105
C	0.000000	0.000000	1.696705
S	0.000000	1.461876	0.723589
C	0.000039	0.699784	-0.860302
C	0.000068	1.401474	-2.063160
C	0.000035	0.696981	-3.258264
C	-0.000035	-0.696981	-3.258264
C	-0.000068	-1.401474	-2.063160
C	-0.000039	-0.699784	-0.860302
S	0.000000	-1.461876	0.723589
H	0.000110	2.482729	-2.063133
H	0.000064	1.236910	-4.194881
H	-0.000064	-1.236910	-4.194881
H	-0.000110	-2.482729	-2.063133

Molecule# 1087

1,3-butadiene

PointGroup: C2h

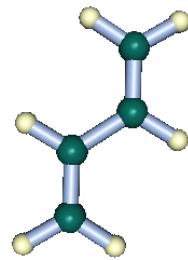
E= -156.057496422 au

ZPE= 0.084904 au

LUMO_eps= -0.04241 au

HOMO_eps= -0.24365 au

Dipole= 0.000 debye



10

C	0.599705	1.744134	0.000000
C	-0.599705	-1.744134	0.000000
C	0.599705	0.409791	0.000000
C	-0.599705	-0.409791	0.000000
H	1.519840	2.311174	0.000000
H	-0.324442	2.309081	0.000000
H	-1.519840	-2.311174	0.000000
H	0.324442	-2.309081	0.000000
H	1.546374	-0.121919	0.000000
H	-1.546374	0.121919	0.000000

Molecule# 1088

1,3-butanediol

PointGroup: C1

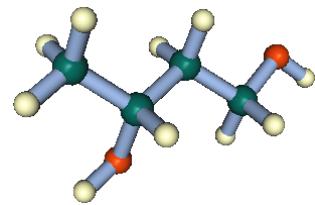
E= -309.015641262 au

ZPE= 0.140899 au

LUMO_eps= -0.01658 au

HOMO_eps= -0.27560 au

Dipole= 2.003 debye



16

O	1.184971	1.329150	-0.264204
H	2.036345	1.691201	-0.001541
O	-2.681176	-0.346785	-0.166650
H	-3.437773	0.227118	-0.020588
C	2.195242	-0.882182	-0.037797
H	2.250223	-1.017985	-1.118621
H	3.142448	-0.457668	0.302556
H	2.084428	-1.861246	0.430820
C	1.029926	0.029059	0.326369
H	0.993181	0.139993	1.418550
C	-0.305850	-0.521316	-0.153420
H	-0.443749	-1.523300	0.259028
H	-0.284509	-0.618015	-1.241427
C	-1.493637	0.335082	0.248850
H	-1.499349	0.479259	1.336354
H	-1.425692	1.317864	-0.222316

Molecule# 1089

1,3-cyclohexadiene

PointGroup: C2

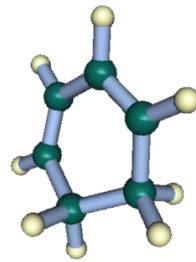
E= -233.507352345 au

ZPE= 0.122001 au

LUMO_eps= -0.03565 au

HOMO_eps= -0.21922 au

Dipole= 0.507 debye



14

H	1.227612	-0.261128	2.198784
C	0.724797	-0.096543	1.254344
H	-1.227612	0.261128	2.198784
C	-0.724797	0.096543	1.254344
H	-2.497556	0.149519	0.117407
C	-1.419944	0.043846	0.113143
H	2.497556	-0.149519	0.117407
C	1.419944	-0.043846	0.113143
H	-1.272086	0.182344	-2.028442
H	-0.737591	-1.338573	-1.350141
C	-0.724797	-0.251426	-1.190421
H	1.272086	-0.182344	-2.028442
H	0.737591	1.338573	-1.350141
C	0.724797	0.251426	-1.190421

Molecule# 1090

1,3-cyclopentadiene

PointGroup: C2v

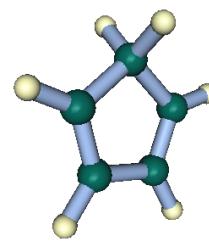
E= -194.176081755 au

ZPE= 0.092255 au

LUMO_eps= -0.02862 au

HOMO_eps= -0.22631 au

Dipole= 0.473 debye



11

C	-0.987747	-0.732496	0.000000
C	-0.987747	0.732496	0.000000
C	0.280659	-1.176401	0.000000
C	0.280659	1.176401	0.000000
C	1.213319	0.000000	0.000000
H	-1.877331	-1.345222	0.000000
H	-1.877331	1.345222	0.000000
H	0.605805	-2.205253	0.000000
H	0.605805	2.205253	0.000000
H	1.874095	0.000000	0.874476
H	1.874095	0.000000	-0.874476

Molecule# 1091

1,3-diazine

PointGroup: C2v

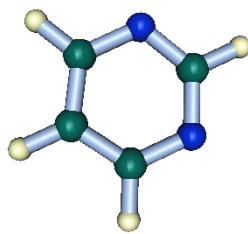
E= -264.419869899 au

ZPE= 0.076844 au

LUMO_eps= -0.05866 au

HOMO_eps= -0.26627 au

Dipole= 2.360 debye



10

C	0.000000	0.000000	-1.307744
N	0.000000	1.191556	-0.712170
N	0.000000	-1.191556	-0.712170
C	0.000000	-1.180628	0.620975
C	0.000000	1.180628	0.620975
C	0.000000	0.000000	1.349488
H	0.000000	0.000000	2.429940
H	0.000000	0.000000	-2.391534
H	0.000000	-2.145739	1.114908
H	0.000000	2.145739	1.114908

Molecule# 1092

1,3-dichlorobutane

PointGroup: C1

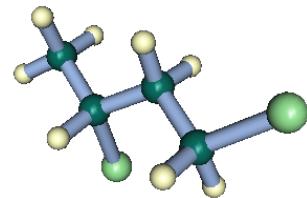
E= -1077.788260350 au

ZPE= 0.114264 au

LUMO_eps= -0.01839 au

HOMO_eps= -0.29836 au

Dipole= 2.470 debye



14

C	-2.173897	1.524699	-0.102751
H	-2.210085	1.552101	-1.191500
H	-3.180147	1.347902	0.271737
H	-1.838899	2.500384	0.255787
C	-1.216511	0.451803	0.380282
H	-1.222850	0.398251	1.467431
Cl	-1.855348	-1.193546	-0.136424
C	0.204566	0.645728	-0.135500
H	0.516270	1.656393	0.140769
H	0.207952	0.595476	-1.225135
C	1.199715	-0.350388	0.431283
H	1.239358	-0.310969	1.516948
H	0.984119	-1.365316	0.116205
Cl	2.880115	0.016766	-0.145466

Molecule# 1093

1,3-dichloronitropropane

PointGroup: C1

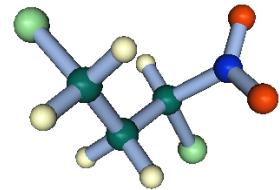
E= -1243.028251140 au

ZPE= 0.088869 au

LUMO_eps= -0.10702 au

HOMO_eps= -0.32034 au

Dipole= 3.018 debye



13

C1	1.969671	-1.392624	-0.227155
C1	-2.726372	-0.166639	-0.549480
O	1.299667	1.497740	1.060977
O	1.142038	1.750743	-1.088218
N	1.039851	1.108331	-0.061878
C	0.528061	-0.332445	-0.214217
C	-0.425033	-0.704823	0.900645
C	-1.706486	0.113665	0.924971
H	0.086211	-0.366790	-1.201970
H	-0.662786	-1.761718	0.786146
H	0.086276	-0.577124	1.855350
H	-2.317628	-0.174091	1.774333
H	-1.520016	1.182620	0.971618

Molecule# 1094

1,3-dichloropropane

PointGroup: C2

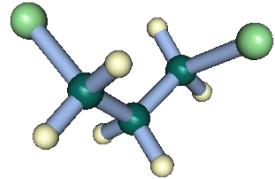
E= -1038.457653490 au

ZPE= 0.086561 au

LUMO_eps= -0.01633 au

HOMO_eps= -0.30237 au

Dipole= 2.302 debye



11

C	0.000000	0.000000	1.245285
C	0.000000	1.281625	0.433521
C	0.000000	-1.281625	0.433521
Cl	-1.529889	1.476800	-0.530841
Cl	1.529889	-1.476800	-0.530841
H	0.878901	0.017822	1.895082
H	-0.878901	-0.017822	1.895082
H	0.056209	2.153738	1.077110
H	0.813369	1.306239	-0.284878
H	-0.813369	-1.306239	-0.284878
H	-0.056209	-2.153738	1.077110

Molecule# 1095

1,3-diethylthiourea

PointGroup: C2

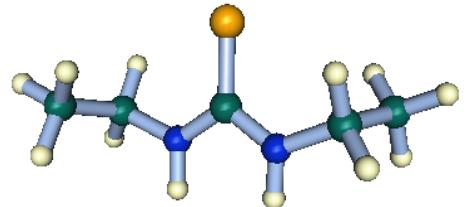
E= -705.624877907 au

ZPE= 0.173478 au

LUMO_eps= -0.02855 au

HOMO_eps= -0.20635 au

Dipole= 4.854 debye



20

C	0.000000	0.000000	-0.140930
S	0.000000	0.000000	1.541614
N	-0.517952	-1.016530	-0.880814
N	0.517952	1.016530	-0.880814
C	-1.052435	-2.261346	-0.344065
C	1.052435	2.261346	-0.344065
H	1.838995	2.593560	-1.024235
H	1.512770	2.026931	0.612762
C	0.000000	3.353187	-0.170351
H	-1.838995	-2.593560	-1.024235
H	-1.512770	-2.026931	0.612762
C	0.000000	-3.353187	-0.170351
H	0.475134	-3.601948	-1.121155
H	-0.461950	-4.260562	0.222206
H	0.769069	-3.029798	0.529468
H	0.461950	4.260562	0.222206
H	-0.769069	3.029798	0.529468
H	-0.475134	3.601948	-1.121155
H	-0.367821	-0.990573	-1.876978
H	0.367821	0.990573	-1.876978

Molecule# 1096

1,3-dihydro-2H-benzimidazole-2-thione

PointGroup: C2v

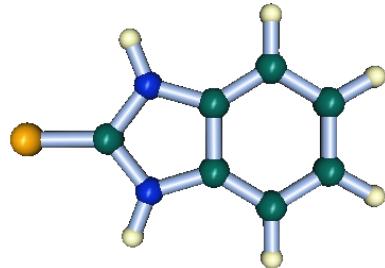
E= -778.251754098 au

ZPE= 0.121025 au

LUMO_eps= -0.04504 au

HOMO_eps= -0.21179 au

Dipole= 4.519 debye



16

N	0.000000	1.086138	0.759003
C	0.000000	0.000000	1.598098
S	0.000000	0.000000	3.259399
C	0.000000	0.701967	-0.573500
C	0.000000	1.422352	-1.756178
C	0.000000	0.697607	-2.946432
C	0.000000	-0.697607	-2.946432
C	0.000000	-1.422352	-1.756178
C	0.000000	-0.701967	-0.573500
N	0.000000	-1.086138	0.759003
H	0.000000	2.023318	1.120645
H	0.000000	2.503243	-1.758725
H	0.000000	1.228712	-3.887766
H	0.000000	-1.228712	-3.887766
H	0.000000	-2.503243	-1.758725
H	0.000000	-2.023318	1.120645

Molecule# 1097

1,3-dihydro-2H-imidazol-2-one

PointGroup: C2v

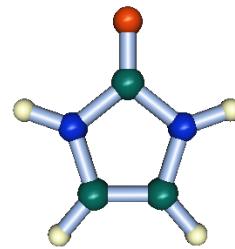
E= -301.582039808 au

ZPE= 0.075496 au

LUMO_eps= -0.01856 au

HOMO_eps= -0.21395 au

Dipole= 4.003 debye



10

C	0.000000	0.672790	-1.380599
C	0.000000	-0.672790	-1.380599
C	0.000000	0.000000	0.812326
N	0.000000	1.085426	-0.051191
N	0.000000	-1.085426	-0.051191
O	0.000000	0.000000	2.030042
H	0.000000	1.365081	-2.201042
H	0.000000	-1.365081	-2.201042
H	0.000000	2.030184	0.285825
H	0.000000	-2.030184	0.285825

Molecule# 1098

1,3-dihydro-2H-pyrrol-2-one

PointGroup: Cs

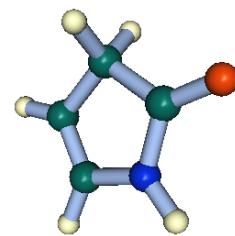
E= -285.514838440 au

ZPE= 0.086012 au

LUMO_eps= -0.02328 au

HOMO_eps= -0.23257 au

Dipole= 3.512 debye



11

C	0.607256	-1.472453	0.000000
C	-0.720908	-1.347453	0.000000
C	0.000000	0.838463	0.000000
C	1.215158	-0.096851	0.000000
N	-1.101042	0.002861	0.000000
O	-0.024582	2.048657	0.000000
H	1.152714	-2.400270	0.000000
H	-1.477373	-2.115225	0.000000
H	1.831991	0.113272	0.876531
H	1.831991	0.113272	-0.876531
H	-2.044414	0.349438	0.000000

Molecule# 1099

1,3-dimethylnaphthalene

PointGroup: Cs

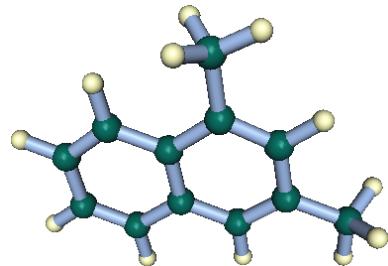
E= -464.691310745 au

ZPE= 0.202153 au

LUMO_eps= -0.04550 au

HOMO_eps= -0.21743 au

Dipole= 0.575 debye

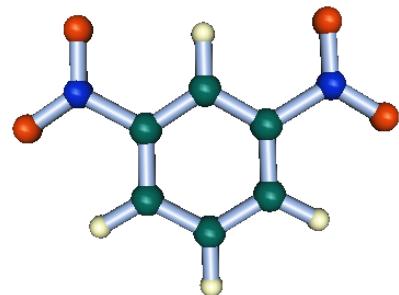


24

C	2.773055	1.261111	0.000000
C	1.856389	2.329988	0.000000
C	2.317617	-0.031831	0.000000
C	0.505981	2.084632	0.000000
C	0.453695	-1.652390	0.000000
C	-1.801003	-0.844292	0.000000
C	0.931909	-0.319067	0.000000
C	0.000000	0.762178	0.000000
C	-0.887961	-1.928786	0.000000
C	-1.398841	0.467661	0.000000
C	-1.410513	-3.339932	0.000000
C	-2.419621	1.574311	0.000000
H	3.835851	1.463645	0.000000
H	2.220247	3.348890	0.000000
H	3.018072	-0.857766	0.000000
H	-0.183202	2.916945	0.000000
H	1.175542	-2.460565	0.000000
H	-2.862447	-1.065376	0.000000
H	-2.031880	-3.530639	0.877960
H	-2.031880	-3.530639	-0.877960
H	-0.598144	-4.065331	0.000000
H	-2.318622	2.216328	0.878002
H	-2.318622	2.216328	-0.878002
H	-3.429158	1.166683	0.000000

Molecule# 1100
1,3-dinitrobenzene
PointGroup: C2v

E= -641.494303305 au
ZPE= 0.105103 au
LUMO_eps= -0.12852 au
HOMO_eps= -0.32044 au
Dipole= 4.332 debye



16

O	0.000000	3.490824	0.071542
N	0.000000	2.463811	-0.588557
O	0.000000	2.410623	-1.806860
C	0.000000	1.181426	0.151124
C	0.000000	0.000000	-0.570360
C	0.000000	-1.181426	0.151124
N	0.000000	-2.463811	-0.588557
O	0.000000	-3.490824	0.071542
O	0.000000	-2.410623	-1.806860
C	0.000000	-1.204752	1.538926
C	0.000000	0.000000	2.229613
C	0.000000	1.204752	1.538926
H	0.000000	0.000000	-1.647700
H	0.000000	-2.152894	2.053303
H	0.000000	0.000000	3.309868
H	0.000000	2.152894	2.053303

Molecule# 1101

1,3-dioxane

PointGroup: Cs

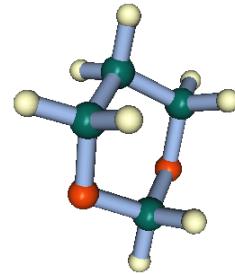
E= -307.789650762 au

ZPE= 0.122180 au

LUMO_eps= -0.01167 au

HOMO_eps= -0.27414 au

Dipole= 2.105 debye



14

H	0.551499	-2.301909	0.000000
H	1.666462	-0.888490	0.000000
C	0.613674	-1.217264	0.000000
O	-0.017447	-0.764404	1.171597
O	-0.017447	-0.764404	-1.171597
H	-0.553642	0.923256	-2.152989
H	1.017015	1.020150	-1.338331
C	-0.017447	0.661398	-1.242927
H	1.017015	1.020150	1.338331
H	-0.553642	0.923256	2.152989
C	-0.017447	0.661398	1.242927
H	-0.568831	2.344294	0.000000
H	-1.736457	1.016352	0.000000
C	-0.672158	1.256703	0.000000

Molecule# 1102

1,3-dioxetane

PointGroup: D2h

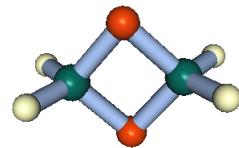
E= -229.098174557 au

ZPE= 0.062725 au

LUMO_eps= -0.00869 au

HOMO_eps= -0.26378 au

Dipole= 0.000 debye



8

C	-0.985328	0.000000	0.000000
C	0.985328	0.000000	0.000000
O	0.000000	1.035861	0.000000
O	0.000000	-1.035861	0.000000
H	-1.603663	0.000000	0.903194
H	1.603663	0.000000	0.903194
H	-1.603663	0.000000	-0.903194
H	1.603663	0.000000	-0.903194

Molecule# 1103

1,3-dioxolan-2-one

PointGroup: C2

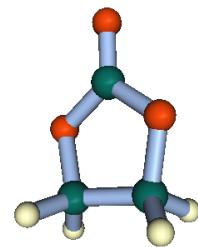
E= -342.537806687 au

ZPE= 0.074731 au

LUMO_eps= -0.02346 au

HOMO_eps= -0.30988 au

Dipole= 5.465 debye



10

C	0.000000	0.000000	0.851993
C	-0.168984	0.745968	-1.301801
C	0.168984	-0.745968	-1.301801
O	0.000000	0.000000	2.039757
O	0.000000	1.114456	0.074557
O	0.000000	-1.114456	0.074557
H	0.504009	1.345920	-1.908473
H	-1.201132	0.944052	-1.592185
H	-0.504009	-1.345920	-1.908473
H	1.201132	-0.944052	-1.592185

Molecule# 1104

1,3-dioxolane

PointGroup: C1

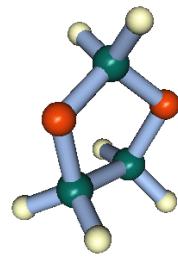
E= -268.454534630 au

ZPE= 0.092542 au

LUMO_eps= -0.01182 au

HOMO_eps= -0.26759 au

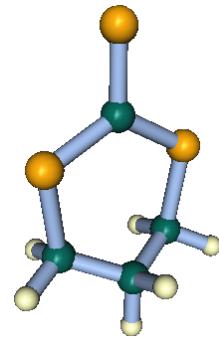
Dipole= 1.424 debye



11

H	-1.638593	-1.153756	0.688314
H	-1.454271	-0.881074	-1.060827
C	-1.031076	-0.669148	-0.077087
H	-0.970288	1.084448	1.225130
H	-1.528273	1.455561	-0.426021
C	-0.860191	0.833461	0.164191
O	0.306808	-1.179852	-0.027728
O	0.477289	1.074627	-0.266338
H	1.499157	0.001110	1.176675
H	2.050598	-0.197573	-0.525731
C	1.186084	-0.075466	0.125395

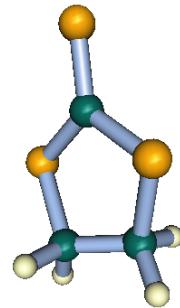
Molecule# 1105
 1,3-dithiane-2-thione
 PointGroup: Cs
 E= -1350.763265370 au
 ZPE= 0.093769 au
 LUMO_eps= -0.07580 au
 HOMO_eps= -0.22753 au
 Dipole= 5.953 debye



13

S	-0.195948	2.519947	0.000000
C	-0.116097	0.874513	0.000000
S	-0.033616	0.069956	1.548701
C	-0.033616	-1.749646	1.260469
C	0.684442	-2.198644	0.000000
C	-0.033616	-1.749646	-1.260469
S	-0.033616	0.069956	-1.548701
H	0.452909	-2.143490	2.151791
H	-1.066908	-2.096687	1.261615
H	1.716281	-1.844930	0.000000
H	0.715928	-3.291933	0.000000
H	0.452909	-2.143490	-2.151791
H	-1.066908	-2.096687	-1.261615

Molecule# 1106
1,3-dithiolane-2-thione
PointGroup: C2
E= -1311.441277110 au
ZPE= 0.065227 au
LUMO_eps= -0.07960 au
HOMO_eps= -0.23018 au
Dipole= 5.108 debye



10

H	0.649149	1.161865	-2.677287
H	-0.649149	-1.161865	-2.677287
S	0.000000	0.000000	2.320077
C	0.000000	0.000000	0.684261
S	-0.642955	-1.323450	-0.281165
S	0.642955	1.323450	-0.281165
H	1.004355	-1.158971	-2.032629
C	0.000000	-0.759876	-1.900808
H	-1.004355	1.158971	-2.032629
C	0.000000	0.759876	-1.900808

Molecule# 1107

1,3-dithiole-2-thione

PointGroup: C2v

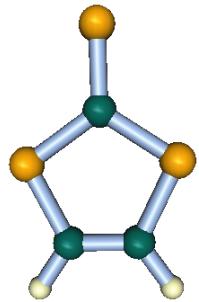
E= -1310.219077860 au

ZPE= 0.041543 au

LUMO_eps= -0.08067 au

HOMO_eps= -0.23035 au

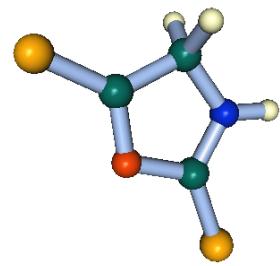
Dipole= 4.515 debye



8

S	0.000000	0.000000	2.271299
C	0.000000	0.000000	0.630759
S	0.000000	1.453602	-0.360432
C	0.000000	0.668708	-1.915944
C	0.000000	-0.668708	-1.915944
S	0.000000	-1.453602	-0.360432
H	0.000000	1.287666	-2.800087
H	0.000000	-1.287666	-2.800087

Molecule# 1108
1,3-oxazolidine-2,5-dithione
PointGroup: C1
E= -1042.629472590 au
ZPE= 0.062635 au
LUMO_eps= -0.09760 au
HOMO_eps= -0.24647 au
Dipole= 4.866 debye



10

S	-2.641922	-0.576015	0.000004
S	2.636269	-0.592371	-0.000006
O	0.011190	-0.739778	-0.000001
N	-0.727198	1.331855	0.000004
C	-1.137706	0.051692	0.000002
C	1.141741	0.018753	-0.000002
C	0.712543	1.468811	0.000000
H	-1.390465	2.086210	0.000006
H	1.091158	1.983830	0.885264
H	1.091154	1.983833	-0.885262

Molecule# 1109

1,3-pentadiyne

PointGroup: Cs

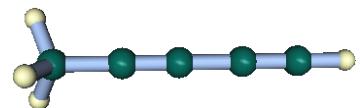
E= -192.888433049 au

ZPE= 0.065631 au

LUMO_eps= -0.02581 au

HOMO_eps= -0.25583 au

Dipole= 1.354 debye



9

C	0.000000	0.150318	0.000000
C	0.002169	-1.056593	0.000000
C	-0.002595	1.513662	0.000000
C	0.004244	-2.507221	0.000000
C	-0.005012	2.718859	0.000000
H	-0.007164	3.779665	0.000000
H	0.514494	-2.897262	0.882841
H	0.514494	-2.897262	-0.882841
H	-1.014660	-2.899289	0.000000

Molecule# 1110

1,3-propanediol

PointGroup: C1

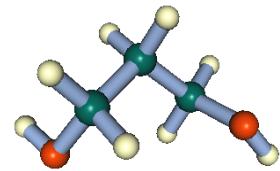
E= -269.682984945 au

ZPE= 0.113176 au

LUMO_eps= -0.01806 au

HOMO_eps= -0.27880 au

Dipole= 1.918 debye



13

C	0.008318	0.961105	-0.023694
C	-1.114125	0.158565	0.611742
C	1.116320	0.099589	-0.621439
O	-1.812567	-0.530130	-0.430109
O	1.810846	-0.677414	0.357585
H	-0.412195	1.593028	-0.810995
H	0.431966	1.633237	0.729520
H	-0.700353	-0.553181	1.331700
H	-1.795932	0.830612	1.143845
H	1.818672	0.728131	-1.178324
H	0.691233	-0.621872	-1.316811
H	-2.402771	-1.178879	-0.038359
H	2.320068	-0.086283	0.919958

Molecule# 1111

1,3-propanedithiol

PointGroup: C2v

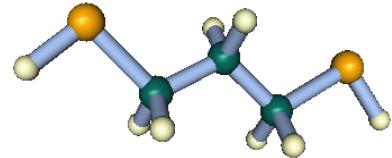
E= -915.633774367 au

ZPE= 0.102773 au

LUMO_eps= -0.02376 au

HOMO_eps= -0.24487 au

Dipole= 2.649 debye



13

C	0.000000	0.000000	0.156756
C	0.000000	1.260347	-0.704215
C	0.000000	-1.260347	-0.704215
H	0.877590	0.000000	0.806673
H	-0.877590	0.000000	0.806673
S	0.000000	2.743925	0.388305
S	0.000000	-2.743925	0.388305
H	0.000000	3.667139	-0.589694
H	0.000000	-3.667139	-0.589694
H	0.885217	1.290973	-1.337416
H	-0.885217	1.290973	-1.337416
H	-0.885217	-1.290973	-1.337416
H	0.885217	-1.290973	-1.337416

Molecule# 1112

1,3-pyridinylethanone

PointGroup: Cs

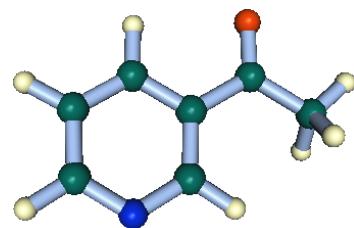
E= -401.079499787 au

ZPE= 0.125716 au

LUMO_eps= -0.08110 au

HOMO_eps= -0.26595 au

Dipole= 0.953 debye



16

C	1.696861	-1.488658	0.000000
C	1.351488	-0.149893	0.000000
C	0.678555	-2.438597	0.000000
C	-0.937596	-0.833228	0.000000
C	0.000000	0.201553	0.000000
C	-0.380417	1.650164	0.000000
C	-1.846581	2.020736	0.000000
N	-0.617071	-2.126889	0.000000
O	0.479637	2.507928	0.000000
H	2.731891	-1.800787	0.000000
H	2.096554	0.633301	0.000000
H	0.915030	-3.496491	0.000000
H	-1.998650	-0.616441	0.000000
H	-2.350642	1.614767	0.878826
H	-2.350642	1.614767	-0.878826
H	-1.935004	3.103219	0.000000

Molecule# 1113
1,3-thiazol-2-yl thiocyanate

PointGroup: C1

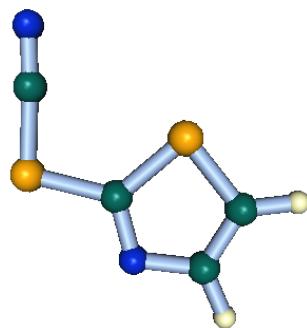
E= -1059.630692160 au

ZPE= 0.054527 au

LUMO_eps= -0.06315 au

HOMO_eps= -0.26095 au

Dipole= 3.374 debye



10

S	-0.684744	1.213061	-0.000080
S	1.377318	-1.154886	0.000075
N	-1.268379	-1.298952	0.000129
N	2.990519	1.193133	-0.000175
C	-0.269821	-0.479529	0.000045
C	-2.349814	0.743056	-0.000014
C	-2.455845	-0.611093	0.000096
C	2.305403	0.262740	-0.000076
H	-3.132667	1.481541	-0.000061
H	-3.383034	-1.162635	0.000156

Molecule# 1114

1,3-thiazol-5-ylacetylenethiol

PointGroup: C1

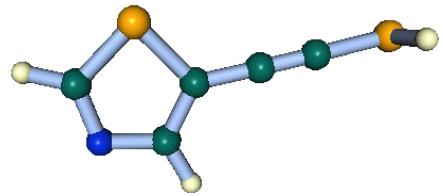
E= -1043.551104450 au

ZPE= 0.064178 au

LUMO_eps= -0.07168 au

HOMO_eps= -0.25033 au

Dipole= 1.474 debye



11

S	1.614785	-1.191862	0.001186
S	-3.692874	-0.024363	-0.096618
N	2.742645	1.118425	-0.006729
C	0.591906	0.228939	0.007977
C	1.399557	1.341512	0.002099
C	3.000380	-0.156035	-0.008147
C	-0.807791	0.156773	0.016980
C	-2.014959	0.076694	0.041513
H	1.022687	2.352845	0.003954
H	3.998149	-0.568105	-0.014777
H	-3.984497	-0.041414	1.222310

Molecule# 1115

1,3-thiazolidine-2-thione

PointGroup: C1

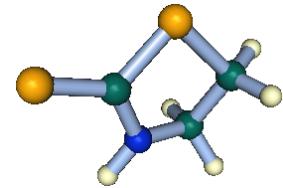
E= -968.600170436 au

ZPE= 0.081395 au

LUMO_eps= -0.04507 au

HOMO_eps= -0.22108 au

Dipole= 5.751 debye



11

S	2.227257	0.061467	0.015437
C	0.580287	0.139250	0.025344
N	-0.170607	1.260373	0.108482
C	-1.590238	1.151842	-0.196876
C	-1.989229	-0.260741	0.225693
S	-0.486681	-1.273692	-0.086772
H	0.312643	2.142650	0.044203
H	-1.765588	1.297506	-1.267875
H	-2.152266	1.906954	0.352089
H	-2.821611	-0.645528	-0.356536
H	-2.233067	-0.310700	1.285146

Molecule# 1116

1,3,2-dithiazole

PointGroup: Cs

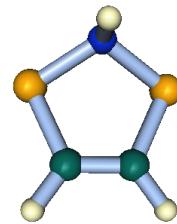
E= -929.212547355 au

ZPE= 0.050402 au

LUMO_eps= -0.04724 au

HOMO_eps= -0.21542 au

Dipole= 2.151 debye



8

S	0.104910	-0.330209	1.416746
S	0.104910	-0.330209	-1.416746
N	-0.487995	-1.151970	0.000000
C	0.104910	1.282613	0.665107
C	0.104910	1.282613	-0.665107
H	0.150997	2.157376	1.295596
H	0.150997	2.157376	-1.295596
H	-1.502056	-1.075624	0.000000

Molecule# 1117

1,3,2-oxathiazole

PointGroup: C1

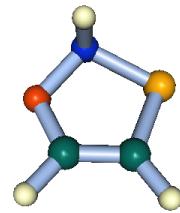
E= -606.189255627 au

ZPE= 0.053029 au

LUMO_eps= -0.03958 au

HOMO_eps= -0.21873 au

Dipole= 2.442 debye



8

S	-1.224006	0.049081	-0.107328
O	1.242809	-0.702537	-0.222880
N	-0.052232	-1.238625	0.159007
C	0.065658	1.249525	0.142810
C	1.244683	0.655383	0.012729
H	-0.124065	2.299324	0.277492
H	2.227513	1.098553	0.002818
H	0.041759	-1.321948	1.173704

Molecule# 1118

1,3,4-oxadiazole

PointGroup: C2v

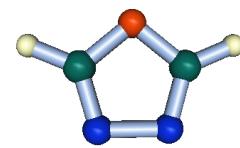
E= -262.195184150 au

ZPE= 0.046253 au

LUMO_eps= -0.03757 au

HOMO_eps= -0.30332 au

Dipole= 3.182 debye



7

O 0.000000 0.000000 1.123780

C 0.000000 1.052759 0.266386

N 0.000000 0.701433 -0.967868

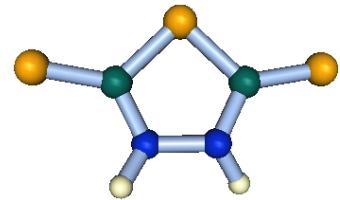
N 0.000000 -0.701433 -0.967868

C 0.000000 -1.052759 0.266386

H 0.000000 2.044558 0.681643

H 0.000000 -2.044558 0.681643

Molecule# 1119
1,3,4-thiadiazolidine-2,5-dithione
PointGroup: C2
E= -1381.628890000 au
ZPE= 0.047898 au
LUMO_eps= -0.07562 au
HOMO_eps= -0.24424 au
Dipole= 3.520 debye



9
C 0.000000 1.290037 -0.095700
S 0.000000 0.000000 1.123017
C 0.000000 -1.290037 -0.095700
S 0.098380 -2.902976 0.183152
S -0.098380 2.902976 0.183152
N 0.082142 0.693918 -1.317219
N -0.082142 -0.693918 -1.317219
H -0.281158 1.189103 -2.119842
H 0.281158 -1.189103 -2.119842

Molecule# 1120

1,3,4-triazole

PointGroup: C2v

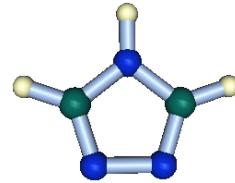
E= -242.333782560 au

ZPE= 0.058943 au

LUMO_eps= -0.02917 au

HOMO_eps= -0.27075 au

Dipole= 5.676 debye



8

N 0.000000 0.691069 -0.992631

N 0.000000 -0.691069 -0.992631

C 0.000000 -1.080094 0.251566

N 0.000000 0.000000 1.085367

C 0.000000 1.080094 0.251566

H 0.000000 -2.100069 0.594993

H 0.000000 0.000000 2.090477

H 0.000000 2.100069 0.594993

Molecule# 1121

1,3,5-triazine

PointGroup: C3h

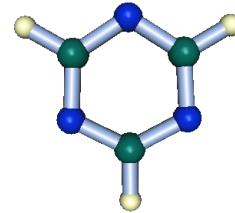
E= -280.466241040 au

ZPE= 0.065142 au

LUMO_eps= -0.07102 au

HOMO_eps= -0.28986 au

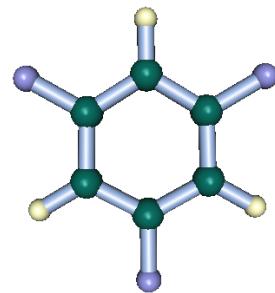
Dipole= 0.000 debye



9

C	0.000000	1.292045	0.000000
N	1.184015	0.683592	0.000000
N	-1.184015	0.683592	0.000000
C	1.118944	-0.646022	0.000000
C	-1.118944	-0.646022	0.000000
N	0.000000	-1.367183	0.000000
H	0.000000	2.376108	0.000000
H	-2.057770	-1.188054	0.000000
H	2.057770	-1.188054	0.000000

Molecule# 1122
1,3,5-trifluorobenzene
PointGroup: D3h
E= -530.164519595 au
ZPE= 0.075735 au
LUMO_eps= -0.03432 au
HOMO_eps= -0.27732 au
Dipole= 0.000 debye



12

C	0.000000	1.361787	0.000000
C	-1.217446	0.702893	0.000000
C	1.217446	0.702893	0.000000
C	-1.179342	-0.680894	0.000000
C	1.179342	-0.680894	0.000000
C	0.000000	-1.405786	0.000000
F	-2.344663	-1.353692	0.000000
F	2.344663	-1.353692	0.000000
H	-2.151626	1.242242	0.000000
H	2.151626	1.242242	0.000000
F	0.000000	2.707384	0.000000
H	0.000000	-2.484484	0.000000

Molecule# 1123

1,3,5-trioxane

PointGroup: C3

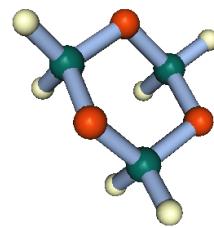
E= -343.707293428 au

ZPE= 0.098658 au

LUMO_eps= -0.01102 au

HOMO_eps= -0.29176 au

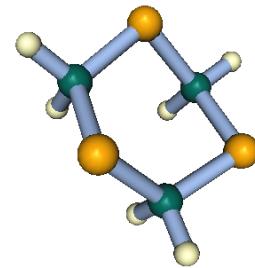
Dipole= 2.022 debye



12

C	0.000000	1.334824	0.178381
C	1.155992	-0.667412	0.178381
C	-1.155992	-0.667412	0.178381
O	1.164984	0.672604	-0.261238
O	-1.164984	0.672604	-0.261238
O	0.000000	-1.345208	-0.261238
H	0.000000	1.389553	1.278381
H	0.000000	2.328144	-0.258762
H	2.016232	-1.164072	-0.258762
H	1.203388	-0.694777	1.278381
H	-1.203388	-0.694777	1.278381
H	-2.016232	-1.164072	-0.258762

Molecule# 1124
 1,3,5-trithiane
 PointGroup: C3v
 E= -1312.642007460 au
 ZPE= 0.086893 au
 LUMO_eps= -0.01882 au
 HOMO_eps= -0.23605 au
 Dipole= 2.080 debye



12
 C 0.000000 1.600757 0.401027
 C 1.386296 -0.800378 0.401027
 C -1.386296 -0.800378 0.401027
 S 1.549588 0.894655 -0.250561
 S -1.549588 0.894655 -0.250561
 S 0.000000 -1.789310 -0.250561
 H 0.000000 1.541440 1.489315
 H 0.000000 2.649012 0.113501
 H 2.294111 -1.324506 0.113501
 H 1.334926 -0.770720 1.489315
 H -1.334926 -0.770720 1.489315
 H -2.294111 -1.324506 0.113501

Molecule# 1125

1,4-butanediol

PointGroup: C2h

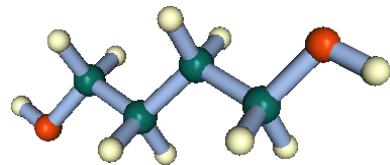
E= -309.010929728 au

ZPE= 0.141345 au

LUMO_eps= -0.01405 au

HOMO_eps= -0.28055 au

Dipole= 0.000 debye



16

O	1.498061	2.666221	0.000000
O	-1.498061	-2.666221	0.000000
C	1.498061	1.237514	0.000000
C	-1.498061	-1.237514	0.000000
C	0.056538	0.762057	0.000000
C	-0.056538	-0.762057	0.000000
H	2.406126	2.980641	0.000000
H	-2.406126	-2.980641	0.000000
H	-0.445072	1.179692	0.876807
H	-0.445072	1.179692	-0.876807
H	0.445072	-1.179692	0.876807
H	0.445072	-1.179692	-0.876807
H	-2.018661	-0.854825	-0.885586
H	-2.018661	-0.854825	0.885586
H	2.018661	0.854825	-0.885586
H	2.018661	0.854825	0.885586

Molecule# 1126

1,4-butanedithiol

PointGroup: C2h

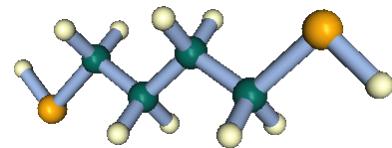
E= -954.962597196 au

ZPE= 0.131136 au

LUMO_eps= -0.01997 au

HOMO_eps= -0.24489 au

Dipole= 0.000 debye



16

S	1.472597	3.116152	0.000000
S	-1.472597	-3.116152	0.000000
C	1.472597	1.273536	0.000000
C	-1.472597	-1.273536	0.000000
C	0.034763	0.765028	0.000000
C	-0.034763	-0.765028	0.000000
H	2.807152	3.283532	0.000000
H	-2.807152	-3.283532	0.000000
H	-0.487695	1.156420	0.876726
H	-0.487695	1.156420	-0.876726
H	0.487695	-1.156420	0.876726
H	0.487695	-1.156420	-0.876726
H	-2.001588	-0.922653	-0.884650
H	-2.001588	-0.922653	0.884650
H	2.001588	0.922653	-0.884650
H	2.001588	0.922653	0.884650

Molecule# 1127

1,4-cyclohexadiene

PointGroup: D2h

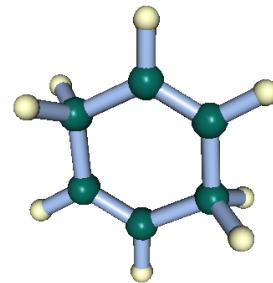
E= -233.507433239 au

ZPE= 0.121802 au

LUMO_eps= -0.01229 au

HOMO_eps= -0.23757 au

Dipole= 0.000 debye



14

C	1.494187	0.000000	0.000000
C	-1.494187	0.000000	0.000000
C	-0.664224	1.251037	0.000000
C	0.664224	1.251037	0.000000
C	-0.664224	-1.251037	0.000000
C	0.664224	-1.251037	0.000000
H	1.198840	-2.194197	0.000000
H	-1.198840	-2.194197	0.000000
H	1.198840	2.194197	0.000000
H	-1.198840	2.194197	0.000000
H	2.167593	0.000000	0.866807
H	-2.167593	0.000000	0.866807
H	2.167593	0.000000	-0.866807
H	-2.167593	0.000000	-0.866807

Molecule# 1128

1,4-diazabicyclo[2.2.2]octane

PointGroup: C2

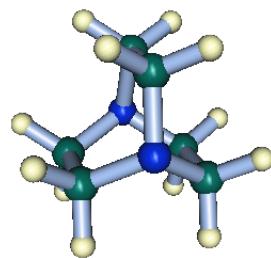
E= -345.452682378 au

ZPE= 0.182646 au

LUMO_eps= -0.01286 au

HOMO_eps= -0.19263 au

Dipole= 0.002 debye



20

N	0.000164	1.282141	0.000519
N	-0.000164	-1.282141	0.000519
C	0.000164	0.780285	1.382256
C	-1.196693	0.781006	-0.691218
C	1.196818	0.780687	-0.691334
C	-0.000164	-0.780285	1.382256
C	1.196693	-0.781006	-0.691218
C	-1.196818	-0.780687	-0.691334
H	-0.879522	1.179699	1.890037
H	0.880122	1.179356	1.889830
H	-1.194813	1.179661	-1.707165
H	-2.076388	1.180253	-0.183417
H	2.076725	1.179835	-0.183814
H	1.194755	1.179230	-1.707324
H	0.879522	-1.179699	1.890037
H	-0.880122	-1.179356	1.889830
H	1.194813	-1.179661	-1.707165
H	2.076388	-1.180253	-0.183417
H	-2.076725	-1.179835	-0.183814
H	-1.194755	-1.179230	-1.707324

Molecule# 1129

1,4-dichlorobutane

PointGroup: C2

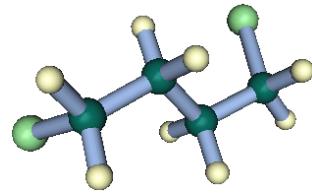
E= -1077.785225070 au

ZPE= 0.114869 au

LUMO_eps= -0.01874 au

HOMO_eps= -0.29890 au

Dipole= 3.204 debye



14

C	-0.721870	0.249030	0.685981
C	0.721870	-0.249030	0.685981
C	-1.761587	-0.853628	0.754122
C	1.761587	0.853628	0.754122
Cl	-1.761587	-1.906934	-0.730679
Cl	1.761587	1.906934	-0.730679
H	-0.904673	0.868385	-0.192246
H	-0.885885	0.888194	1.561267
H	0.904673	-0.868385	-0.192246
H	0.885885	-0.888194	1.561267
H	-1.591489	-1.527110	1.590678
H	-2.766336	-0.447769	0.821230
H	1.591489	1.527110	1.590678
H	2.766336	0.447769	0.821230

Molecule# 1130

1,4-dimethylcyclohexane

PointGroup: C2h

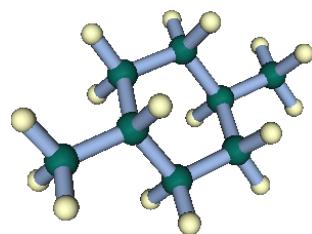
E= -314.625790858 au

ZPE= 0.224695 au

LUMO_eps= -0.00912 au

HOMO_eps= -0.29248 au

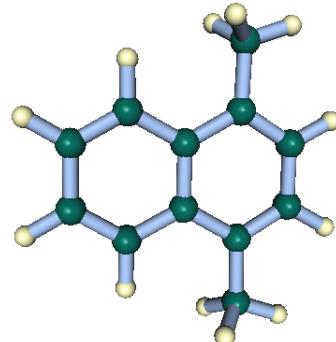
Dipole= 0.000 debye



24

C	-0.128603	0.754635	1.257237
C	0.128603	-0.754635	1.257237
C	-0.128603	0.754635	-1.257237
C	0.128603	-0.754635	-1.257237
C	0.420511	1.441390	0.000000
C	-0.420511	-1.441390	0.000000
C	0.128603	2.941424	0.000000
C	-0.128603	-2.941424	0.000000
H	-1.207697	0.938689	1.316247
H	0.309333	1.209266	2.149736
H	1.207697	-0.938689	1.316247
H	-0.309333	-1.209266	2.149736
H	0.309333	1.209266	-2.149736
H	-1.207697	0.938689	-1.316247
H	-0.309333	-1.209266	-2.149736
H	1.207697	-0.938689	-1.316247
H	1.509662	1.308301	0.000000
H	-1.509662	-1.308301	0.000000
H	0.549005	3.428483	-0.881999
H	-0.948008	3.128721	0.000000
H	0.549005	3.428483	0.881999
H	0.948008	-3.128721	0.000000
H	-0.549005	-3.428483	0.881999
H	-0.549005	-3.428483	-0.881999

Molecule# 1131
 1,4-dimethylnaphthalene
 PointGroup: C2v
 E= -464.689433431 au
 ZPE= 0.202616 au
 LUMO_eps= -0.04855 au
 HOMO_eps= -0.21629 au
 Dipole= 0.099 debye



24

C	-2.671994	-0.703009	0.000000
C	-2.671994	0.703009	0.000000
C	-1.484704	-1.389843	0.000000
C	-1.484704	1.389843	0.000000
C	2.165927	-0.704380	0.000000
C	2.165927	0.704380	0.000000
C	-0.238733	-0.715972	0.000000
C	-0.238733	0.715972	0.000000
C	1.000485	-1.427436	0.000000
C	1.000485	1.427436	0.000000
C	1.037034	-2.932491	0.000000
C	1.037034	2.932491	0.000000
H	-3.609860	-1.242469	0.000000
H	-3.609860	1.242469	0.000000
H	-1.499421	-2.470177	0.000000
H	-1.499421	2.470177	0.000000
H	3.114870	-1.226313	0.000000
H	3.114870	1.226313	0.000000
H	2.065976	-3.288434	0.000000
H	0.540170	-3.350821	0.878303
H	0.540170	-3.350821	-0.878303
H	0.540170	3.350821	0.878303
H	2.065976	3.288434	0.000000
H	0.540170	3.350821	-0.878303

Molecule# 1132

1,4-dimethylnorborane

PointGroup: C2v

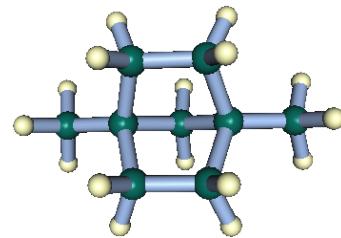
E= -352.727305046 au

ZPE= 0.231031 au

LUMO_eps= -0.01220 au

HOMO_eps= -0.28550 au

Dipole= 0.034 debye



25

C	0.000000	0.000000	1.162215
C	0.000000	1.146150	0.130119
C	0.000000	-1.146150	0.130119
C	1.246419	0.777460	-0.711377
C	-1.246419	0.777460	-0.711377
C	-1.246419	-0.777460	-0.711377
C	1.246419	-0.777460	-0.711377
H	-0.887511	0.000000	1.799660
H	0.887511	0.000000	1.799660
C	0.000000	2.567261	0.662990
C	0.000000	-2.567261	0.662990
H	2.149630	1.169313	-0.239900
H	-2.149630	-1.169313	-0.239900
H	2.149630	-1.169313	-0.239900
H	-2.149630	1.169313	-0.239900
H	1.195920	-1.204338	-1.714197
H	-1.195920	1.204338	-1.714197
H	1.195920	1.204338	-1.714197
H	-1.195920	-1.204338	-1.714197
H	0.882939	-2.760591	1.276063
H	0.000000	-3.294790	-0.152370
H	-0.882939	-2.760591	1.276063
H	-0.882939	2.760591	1.276063
H	0.000000	3.294790	-0.152370
H	0.882939	2.760591	1.276063

Molecule# 1133

1,4-dimethylpiperazine

PointGroup: C2h

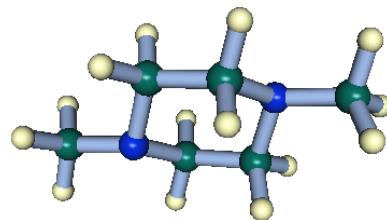
E= -346.681686610 au

ZPE= 0.201902 au

LUMO_eps= -0.00952 au

HOMO_eps= -0.22024 au

Dipole= 0.000 debye



22

C	-0.156412	0.744515	1.198880
C	0.156412	-0.744515	1.198880
C	-0.156412	0.744515	-1.198880
C	0.156412	-0.744515	-1.198880
C	0.156412	2.817089	0.000000
C	-0.156412	-2.817089	0.000000
N	0.372203	1.382577	0.000000
N	-0.372203	-1.382577	0.000000
H	-1.249175	0.882535	1.278396
H	0.300386	1.211676	2.073396
H	1.249175	-0.882535	1.278396
H	-0.300386	-1.211676	2.073396
H	0.300386	1.211676	-2.073396
H	-1.249175	0.882535	-1.278396
H	-0.300386	-1.211676	-2.073396
H	1.249175	-0.882535	-1.278396
H	0.618271	3.260208	0.882966
H	-0.912825	3.090807	0.000000
H	0.618271	3.260208	-0.882966
H	0.912825	-3.090807	0.000000
H	-0.618271	-3.260208	-0.882966
H	-0.618271	-3.260208	0.882966

Molecule# 1134

1,4-dioxane

PointGroup: C2h

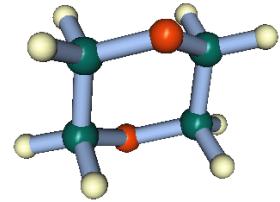
E= -307.781807831 au

ZPE= 0.121913 au

LUMO_eps= -0.00854 au

HOMO_eps= -0.24983 au

Dipole= 0.000 debye



14

C	0.225402	0.725379	1.173820
C	-0.225402	-0.725379	1.173820
C	0.225402	0.725379	-1.173820
C	-0.225402	-0.725379	-1.173820
O	-0.225402	1.393629	0.000000
O	0.225402	-1.393629	0.000000
H	-0.194991	1.264433	2.022632
H	1.320586	0.773781	1.230887
H	0.194991	-1.264433	2.022632
H	-1.320586	-0.773781	1.230887
H	1.320586	0.773781	-1.230887
H	-0.194991	1.264433	-2.022632
H	-1.320586	-0.773781	-1.230887
H	0.194991	-1.264433	-2.022632

Molecule# 1135

1,4-dithiane

PointGroup: C2h

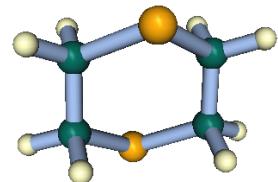
E= -953.754024604 au

ZPE= 0.114715 au

LUMO_eps= -0.01194 au

HOMO_eps= -0.22743 au

Dipole= 0.000 debye



14

C	0.285090	0.705076	1.402750
C	-0.285090	-0.705076	1.402750
C	0.285090	0.705076	-1.402750
C	-0.285090	-0.705076	-1.402750
S	-0.285090	1.732970	0.000000
S	0.285090	-1.732970	0.000000
H	-0.049188	1.244965	2.289919
H	1.374611	0.679803	1.411268
H	0.049188	-1.244965	2.289919
H	-1.374611	-0.679803	1.411268
H	1.374611	0.679803	-1.411268
H	-0.049188	1.244965	-2.289919
H	-1.374611	-0.679803	-1.411268
H	0.049188	-1.244965	-2.289919

Molecule# 1136

1,4-naphthalenedione

PointGroup: C1

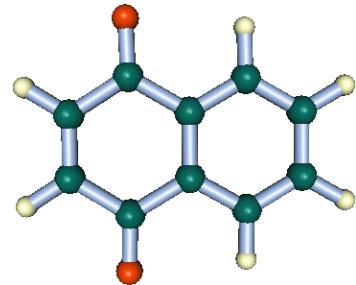
E= -535.309619100 au

ZPE= 0.132541 au

LUMO_eps= -0.12923 au

HOMO_eps= -0.27713 au

Dipole= 1.444 debye



18

O	-1.061346	-2.675415	0.000027
C	-1.022143	-1.457090	0.000009
C	0.261151	-0.701650	-0.000016
C	0.261151	0.701650	0.000016
C	-1.022143	1.457090	-0.000009
O	-1.061346	2.675415	-0.000027
C	-2.274483	0.667940	-0.000007
C	-2.274483	-0.667940	0.000007
C	1.470163	1.394082	0.000035
C	2.669385	0.696780	0.000020
C	2.669385	-0.696780	-0.000020
C	1.470163	-1.394082	-0.000035
H	-3.189344	1.246182	0.000000
H	-3.189344	-1.246182	-0.000001
H	1.449164	2.474559	0.000078
H	3.606515	1.236642	0.000045
H	3.606515	-1.236642	-0.000045
H	1.449163	-2.474559	-0.000077

Molecule# 1137

1,4-pentadiene

PointGroup: Cs

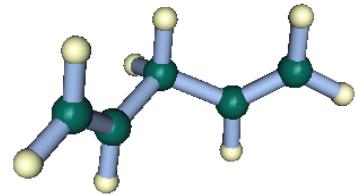
E= -195.377432871 au

ZPE= 0.112982 au

LUMO_eps= -0.01497 au

HOMO_eps= -0.26627 au

Dipole= 0.305 debye



13

C	-0.175224	0.514096	2.220039
C	-0.175224	0.514096	-2.220039
C	-0.175224	-0.393919	1.253232
C	-0.175224	-0.393919	-1.253232
C	0.654344	-0.322824	0.000000
H	-0.793280	0.403263	3.100778
H	0.443638	1.401787	2.165483
H	-0.793280	0.403263	-3.100778
H	0.443638	1.401787	-2.165483
H	-0.815578	-1.266462	1.348079
H	-0.815578	-1.266462	-1.348079
H	1.352792	-1.169518	0.000000
H	1.256964	0.587167	0.000000

Molecule# 1138

1,4-pyridylethanone

PointGroup: Cs

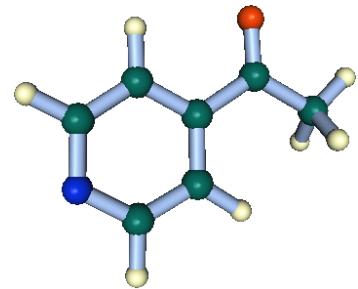
E= -401.077779855 au

ZPE= 0.125585 au

LUMO_eps= -0.08914 au

HOMO_eps= -0.27089 au

Dipole= 2.485 debye



16

C	-1.004320	-0.762666	0.000000
C	1.322736	-0.237243	0.000000
C	-0.645498	-2.106337	0.000000
C	1.576680	-1.600517	0.000000
C	0.000000	0.203071	0.000000
C	-0.278823	1.682041	0.000000
C	-1.715873	2.149965	0.000000
N	0.617007	-2.529678	0.000000
O	0.639000	2.474708	0.000000
H	-2.050239	-0.492383	0.000000
H	2.126827	0.484057	0.000000
H	-1.409956	-2.874662	0.000000
H	2.596289	-1.967379	0.000000
H	-2.245005	1.777376	0.878947
H	-2.245005	1.777376	-0.878947
H	-1.733368	3.235824	0.000000

Molecule# 1139

1,5-heptadiyne

PointGroup: C1

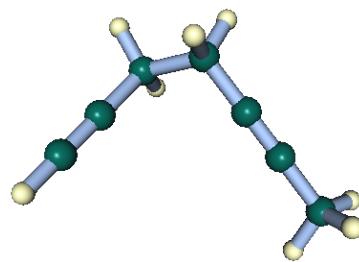
E= -271.536844176 au

ZPE= 0.122356 au

LUMO_eps= -0.01408 au

HOMO_eps= -0.25701 au

Dipole= 0.699 debye



15

C	-2.375167	1.623271	-0.199143
C	-2.007050	0.527064	0.118833
C	1.874986	-0.008026	-0.044601
C	0.850272	-0.614152	-0.202794
C	3.114009	0.734257	0.139370
C	-1.564604	-0.810976	0.487974
C	-0.398446	-1.345731	-0.378509
H	-2.697409	2.595513	-0.476233
H	3.585287	0.955741	-0.819838
H	2.929194	1.683095	0.646012
H	3.828780	0.168899	0.739903
H	-2.406200	-1.502168	0.396639
H	-1.262452	-0.817791	1.537388
H	-0.697428	-1.320675	-1.428857
H	-0.243770	-2.396855	-0.121794

Molecule# 1140

1,5-hexadiene

PointGroup: C2

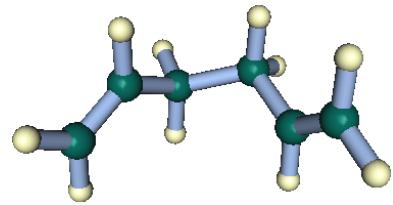
E= -234.705388931 au

ZPE= 0.141327 au

LUMO_eps= -0.01188 au

HOMO_eps= -0.26170 au

Dipole= 0.536 debye



16

C	0.143509	2.259213	-0.972760
C	-0.143509	-2.259213	-0.972760
C	-0.493542	1.494787	-0.095250
C	0.493542	-1.494787	-0.095250
C	0.143509	0.758656	1.044302
C	-0.143509	-0.758656	1.044302
H	-0.382876	2.769274	-1.768280
H	1.216623	2.403065	-0.926974
H	0.382876	-2.769274	-1.768280
H	-1.216623	-2.403065	-0.926974
H	-1.570475	1.377799	-0.187498
H	1.570475	-1.377799	-0.187498
H	-0.232692	1.168727	1.987200
H	1.222919	0.929600	1.037802
H	-1.222919	-0.929600	1.037802
H	0.232692	-1.168727	1.987200

Molecule# 1141

1,6-dimethylnaphthalene

PointGroup: Ci

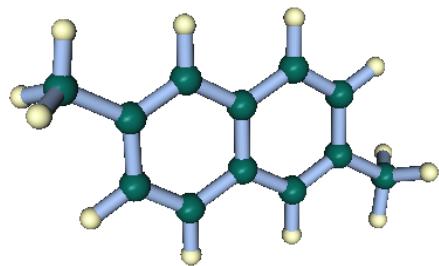
E= -464.692588569 au

ZPE= 0.201760 au

LUMO_eps= -0.04312 au

HOMO_eps= -0.21778 au

Dipole= 0.000 debye



24

C	-0.072264	1.827345	-0.349034
C	0.072264	-1.827345	0.349034
C	-1.374617	2.108960	-0.034074
C	1.374617	-2.108960	0.034074
C	1.779072	0.182743	-0.544682
C	-1.779072	-0.182743	0.544682
C	0.438570	0.512106	-0.228855
C	-0.438570	-0.512106	0.228855
C	-2.259063	1.098577	0.422509
C	2.259063	-1.098577	-0.422509
C	-3.684425	1.447260	0.756865
C	3.684425	-1.447260	-0.756865
H	0.585539	2.614560	-0.696015
H	-0.585539	-2.614560	0.696015
H	-1.742638	3.122803	-0.134031
H	1.742638	-3.122803	0.134031
H	2.435555	0.972293	-0.891642
H	-2.435555	-0.972293	0.891642
H	-4.237087	0.574737	1.102510
H	-3.731712	2.207391	1.539862
H	-4.206005	1.852269	-0.113324
H	4.206005	-1.852269	0.113324
H	3.731712	-2.207391	-1.539862
H	4.237087	-0.574737	-1.102510

Molecule# 1142

1H-1,2,4-triazole

PointGroup: Cs

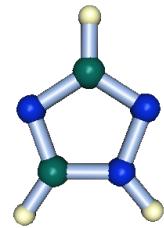
E= -242.343781966 au

ZPE= 0.059724 au

LUMO_eps= -0.02037 au

HOMO_eps= -0.28540 au

Dipole= 2.820 debye



8

N	0.687175	-0.997210	0.000000
C	-0.670085	-0.896250	0.000000
H	-1.325913	-1.750118	0.000000
N	-1.137377	0.337628	0.000000
N	0.000000	1.069665	0.000000
H	-0.046582	2.073946	0.000000
C	1.075604	0.260484	0.000000
H	2.090800	0.620191	0.000000

Molecule# 1143

1H-benzimidazole

PointGroup: Cs

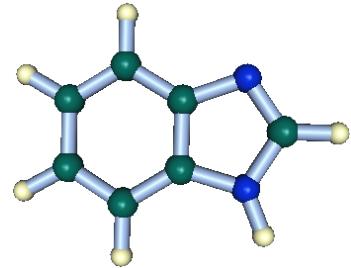
E= -380.005636204 au

ZPE= 0.118151 au

LUMO_eps= -0.03194 au

HOMO_eps= -0.23697 au

Dipole= 3.459 debye



15

C	2.223779	-0.070950	0.000000
C	1.362423	1.015554	0.000000
C	0.000000	0.733827	0.000000
C	-0.501452	-0.584713	0.000000
N	-1.888696	-0.569217	0.000000
C	-2.211130	0.692186	0.000000
N	-1.126415	1.533371	0.000000
C	0.383372	-1.663536	0.000000
C	1.741213	-1.390393	0.000000
H	3.291494	0.100590	0.000000
H	1.739293	2.029395	0.000000
H	-3.218802	1.076717	0.000000
H	-1.153964	2.537179	0.000000
H	0.008732	-2.677482	0.000000
H	2.449793	-2.207335	0.000000

Molecule# 1144

1H-imidazole

PointGroup: Cs

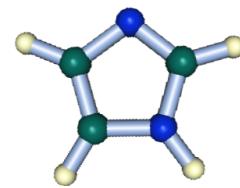
E= -226.305303188 au

ZPE= 0.071065 au

LUMO_eps= -0.02090 au

HOMO_eps= -0.24093 au

Dipole= 3.716 debye



9

C	0.635171	-0.982628	0.000000
C	1.116435	0.296921	0.000000
C	-1.089077	0.282717	0.000000
N	-0.739829	-0.979874	0.000000
N	0.000000	1.101780	0.000000
H	1.196253	-1.901176	0.000000
H	2.113523	0.697918	0.000000
H	-2.097453	0.661493	0.000000
H	-0.008690	2.106362	0.000000

Molecule# 1145

1H-indene

PointGroup: Cs

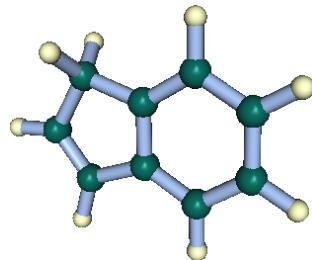
E= -347.886773442 au

ZPE= 0.140214 au

LUMO_eps= -0.03364 au

HOMO_eps= -0.22497 au

Dipole= 0.737 debye



17

C	-1.855229	-1.337950	0.000000
C	-0.499088	-1.653073	0.000000
C	0.428036	-0.615933	0.000000
C	0.000000	0.724298	0.000000
C	1.213119	1.619187	0.000000
C	1.890304	-0.626401	0.000000
C	2.352575	0.633211	0.000000
C	-1.348795	1.031328	0.000000
C	-2.277760	-0.010338	0.000000
H	-2.590250	-2.131799	0.000000
H	-0.176462	-2.686234	0.000000
H	1.242418	2.275992	0.875487
H	1.242418	2.275992	-0.875487
H	2.494096	-1.522542	0.000000
H	3.391246	0.927949	0.000000
H	-1.686610	2.060169	0.000000
H	-3.335828	0.214508	0.000000

Molecule# 1146

1H-indole

PointGroup: Cs

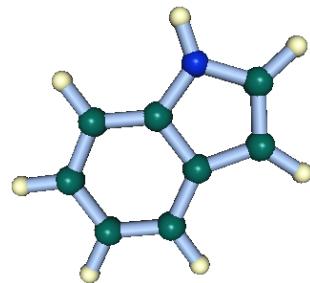
E= -363.951603135 au

ZPE= 0.129528 au

LUMO_eps= -0.02277 au

HOMO_eps= -0.21329 au

Dipole= 2.110 debye



16

C	1.780721	-1.390068	0.000000
C	2.244479	-0.063173	0.000000
C	0.427376	-1.674703	0.000000
C	1.363098	1.004249	0.000000
C	-1.922320	-0.531592	0.000000
C	-2.246341	0.794059	0.000000
C	-0.491170	-0.616487	0.000000
C	0.000000	0.713959	0.000000
N	-1.093515	1.551035	0.000000
H	2.498544	-2.199111	0.000000
H	3.309164	0.126774	0.000000
H	0.081991	-2.700230	0.000000
H	1.723021	2.024849	0.000000
H	-2.621351	-1.350213	0.000000
H	-3.211971	1.269781	0.000000
H	-1.059845	2.553449	0.000000

Molecule# 1147

1H-pyrazin-2-one

PointGroup: Cs

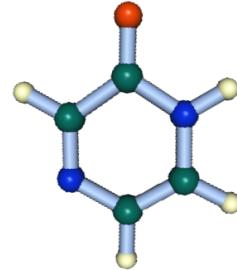
E= -339.680247074 au

ZPE= 0.081462 au

LUMO_eps= -0.07970 au

HOMO_eps= -0.24877 au

Dipole= 4.150 debye



11

C	0.100732	-1.751447	0.000000
C	-1.100249	-1.123375	0.000000
C	1.230486	0.248996	0.000000
C	0.000000	1.043061	0.000000
N	1.273925	-1.045277	0.000000
N	-1.140617	0.238051	0.000000
O	-0.072478	2.260456	0.000000
H	0.169795	-2.828181	0.000000
H	-2.046117	-1.644386	0.000000
H	2.160066	0.806767	0.000000
H	-2.022892	0.729333	0.000000

Molecule# 1148

1H-pyrazole-1-OS-thioperroxol

PointGroup: C1

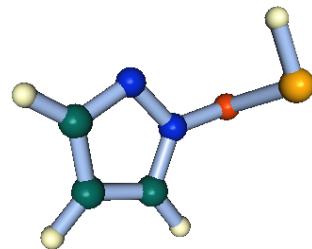
E= -699.676752725 au

ZPE= 0.073034 au

LUMO_eps= -0.07233 au

HOMO_eps= -0.26629 au

Dipole= 1.443 debye



11

S	2.234917	-0.046861	-0.380987
O	1.029141	0.354103	0.770290
N	-0.255522	0.153491	0.329665
N	-0.759156	-1.072879	0.283649
C	-1.110151	1.132332	-0.046094
C	-2.009920	-0.883942	-0.135575
C	-2.285470	0.479908	-0.353541
H	2.229010	-1.378082	-0.153039
H	-0.817337	2.166144	-0.049950
H	-2.661697	-1.731812	-0.260982
H	-3.205769	0.926620	-0.684484

Molecule# 1149

1H-pyrazole

PointGroup: Cs

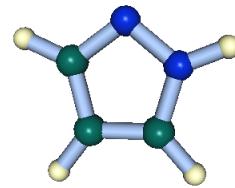
E= -226.288457122 au

ZPE= 0.071138 au

LUMO_eps= -0.01483 au

HOMO_eps= -0.25891 au

Dipole= 2.282 debye



9

C	0.662598	-0.995432	0.000000
C	-0.743268	-0.890370	0.000000
C	1.107645	0.307032	0.000000
N	-1.142688	0.375589	0.000000
N	0.000000	1.085189	0.000000
H	1.262650	-1.887482	0.000000
H	-1.475618	-1.680369	0.000000
H	2.098322	0.726839	0.000000
H	-0.048386	2.088195	0.000000

Molecule# 1150

1H-pyrimidin-4-one

PointGroup: Cs

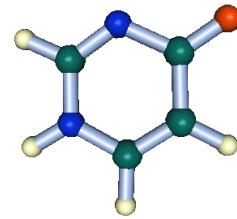
E= -339.680253235 au

ZPE= 0.081483 au

LUMO_eps= -0.04880 au

HOMO_eps= -0.25076 au

Dipole= 7.856 debye



11

C	1.223728	0.268149	0.000000
C	1.156706	-1.073788	0.000000
C	-1.203480	-0.921610	0.000000
C	0.000000	1.076085	0.000000
N	-1.223091	0.359317	0.000000
N	-0.072567	-1.688836	0.000000
O	0.011892	2.291393	0.000000
H	2.174691	0.778052	0.000000
H	2.019381	-1.723884	0.000000
H	-2.135162	-1.480194	0.000000
H	-0.146168	-2.691497	0.000000

Molecule# 1151

1H-pyrrol-3-ylhydrazine

PointGroup: C1

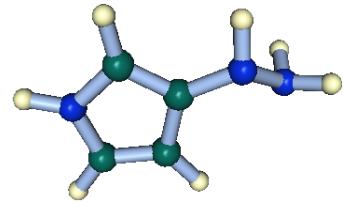
E= -320.962194396 au

ZPE= 0.116116 au

LUMO_eps= -0.01596 au

HOMO_eps= -0.18890 au

Dipole= 2.239 debye



14

C	-0.375827	1.083218	-0.143727
C	-1.730720	0.914545	0.013207
C	-0.800510	-1.127958	0.050865
C	0.213730	-0.211135	-0.126043
N	-1.984695	-0.422966	0.119352
N	2.473612	0.408232	0.261342
N	1.571203	-0.508797	-0.347613
H	0.147064	2.015954	-0.252645
H	-2.523634	1.639838	0.060015
H	-0.779966	-2.201879	0.108656
H	-2.889932	-0.832811	0.250080
H	3.335494	0.406023	-0.266084
H	2.672619	0.160352	1.227596
H	1.777472	-1.474780	-0.124995

Molecule# 1152

1H-pyrrole-3-carboxamide

PointGroup: C1

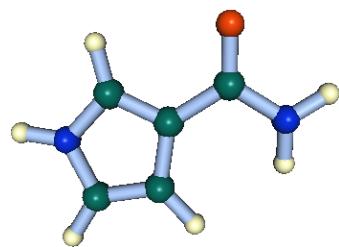
E= -379.030702312 au

ZPE= 0.109304 au

LUMO_eps= -0.02122 au

HOMO_eps= -0.23432 au

Dipole= 4.175 debye



14

C	-0.828503	1.164117	-0.040476
C	-2.134122	0.751924	-0.019718
C	-0.858343	-1.090763	0.034212
C	-0.008337	-0.005922	-0.006066
C	1.460971	-0.144754	-0.008282
N	-2.135628	-0.622343	0.026759
N	2.177223	1.021662	0.019301
O	2.017893	-1.232462	-0.050329
H	-0.508559	2.191256	-0.090948
H	-3.051869	1.312081	-0.038511
H	-0.625407	-2.139469	0.067307
H	-2.958272	-1.197272	0.051277
H	1.744712	1.904010	0.219798
H	3.175101	0.946245	0.113271

Molecule# 1153

1H-tetrazol-5-amine

PointGroup: C1

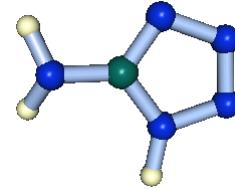
E= -313.736986270 au

ZPE= 0.063546 au

LUMO_eps= -0.03826 au

HOMO_eps= -0.26833 au

Dipole= 6.237 debye



9

C	-0.621011	-0.043215	-0.003296
H	0.001740	2.009175	-0.056030
N	0.197961	1.024633	-0.005588
N	1.486430	0.574685	0.004451
N	1.411372	-0.699900	0.008559
N	0.119936	-1.131006	0.009304
H	-2.446118	0.747717	0.423321
H	-2.419586	-0.896323	0.073092
N	-1.988552	0.002833	-0.076813

Molecule# 1154

1H-tetrazole

PointGroup: Cs

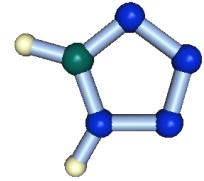
E= -258.350522055 au

ZPE= 0.046771 au

LUMO_eps= -0.03805 au

HOMO_eps= -0.30655 au

Dipole= 5.345 debye



7

C	1.064770	0.234648	0.000000
N	0.637569	-1.003032	0.000000
N	-0.722757	-0.922964	0.000000
N	-1.117376	0.298568	0.000000
N	0.000000	1.052457	0.000000
H	2.089591	0.560077	0.000000
H	-0.060257	2.056832	0.000000

Molecule# 1155

1H,3H,7H-xanthine

PointGroup: Cs

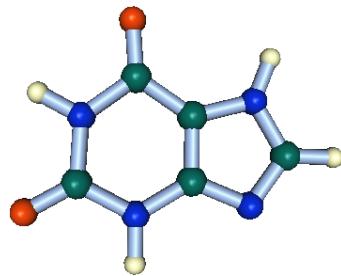
E= -562.660590518 au

ZPE= 0.104991 au

LUMO_eps= -0.05901 au

HOMO_eps= -0.24977 au

Dipole= 4.330 debye



15

C	-1.932966	1.927138	0.000000
C	0.000000	0.897330	0.000000
C	-1.047973	0.007447	0.000000
C	1.374607	0.492230	0.000000
C	0.451293	-1.869624	0.000000
N	-2.246899	0.640758	0.000000
N	-0.597110	2.140003	0.000000
N	-0.830130	-1.346171	0.000000
N	1.466665	-0.911751	0.000000
O	2.362098	1.204052	0.000000
O	0.680205	-3.060162	0.000000
H	-2.646470	2.733790	0.000000
H	-0.115294	3.023307	0.000000
H	-1.595394	-2.001005	0.000000
H	2.401286	-1.294218	0.000000

Molecule# 1156

1H,3H,8H-alloxanthine

PointGroup: Cs

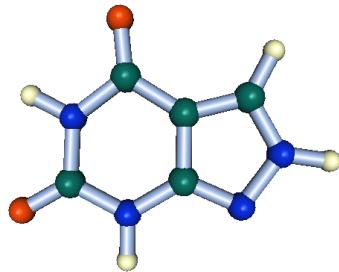
E= -562.639769046 au

ZPE= 0.104991 au

LUMO_eps= -0.05804 au

HOMO_eps= -0.26169 au

Dipole= 4.840 debye



15

C	-0.513595	-1.847902	0.000000
N	0.778933	-1.359597	0.000000
C	1.042726	-0.011300	0.000000
C	0.000000	0.939529	0.000000
C	0.650742	2.159172	0.000000
N	1.962308	1.874826	0.000000
N	2.241607	0.540130	0.000000
N	-1.509334	-0.870626	0.000000
C	-1.390022	0.528250	0.000000
O	-0.770109	-3.032395	0.000000
H	2.729469	2.523638	0.000000
O	-2.370508	1.243288	0.000000
H	0.271382	3.165642	0.000000
H	-2.450739	-1.235751	0.000000
H	1.521119	-2.040297	0.000000

Molecule# 1157

1H,3H,9H-alloxanthine

PointGroup: Cs

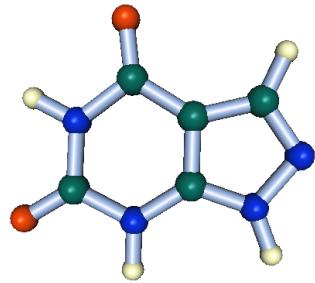
E= -562.633106152 au

ZPE= 0.104511 au

LUMO_eps= -0.04317 au

HOMO_eps= -0.26086 au

Dipole= 4.266 debye



15

C	-0.531875	-1.845904	0.000000
N	0.771404	-1.348773	0.000000
C	1.003562	-0.002016	0.000000
C	0.000000	0.950259	0.000000
C	0.690256	2.188187	0.000000
N	1.994421	2.015793	0.000000
N	2.175035	0.654328	0.000000
N	-1.513744	-0.871250	0.000000
C	-1.384929	0.539209	0.000000
O	-0.763178	-3.034653	0.000000
O	-2.371414	1.243358	0.000000
H	-2.459834	-1.224597	0.000000
H	1.502564	-2.040445	0.000000
H	3.109527	0.285765	0.000000
H	0.272581	3.180547	0.000000

Molecule# 1158

1H,3H,9H-xanthine

PointGroup: Cs

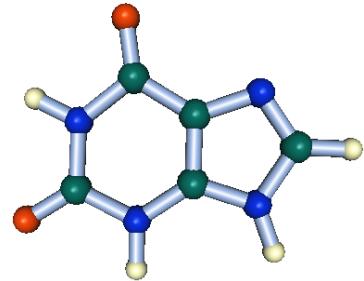
E= -562.646064705 au

ZPE= 0.104205 au

LUMO_eps= -0.04339 au

HOMO_eps= -0.24691 au

Dipole= 7.322 debye



15

C	-0.494582	-1.855654	0.000000
N	0.801387	-1.341554	0.000000
C	1.003289	0.010465	0.000000
C	0.000000	0.951847	0.000000
N	0.543549	2.219652	0.000000
C	1.828513	2.045590	0.000000
N	2.176164	0.698429	0.000000
N	-1.483837	-0.891134	0.000000
C	-1.384973	0.528592	0.000000
O	-0.710820	-3.048700	0.000000
H	2.579315	2.817576	0.000000
O	-2.386498	1.205693	0.000000
H	-2.426033	-1.254649	0.000000
H	1.543280	-2.021140	0.000000
H	3.107654	0.319474	0.000000

Molecule# 1159

1H,7H-hypoxanthine

PointGroup: Cs

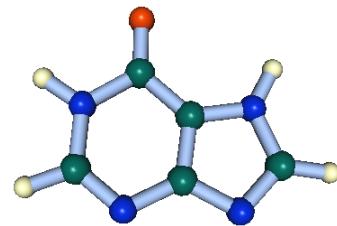
E= -487.372642498 au

ZPE= 0.100189 au

LUMO_eps= -0.04995 au

HOMO_eps= -0.24836 au

Dipole= 1.515 debye



14

C	-2.032028	1.358919	0.000000
C	0.000000	0.554262	0.000000
C	-0.943969	-0.466855	0.000000
C	0.643023	-2.033412	0.000000
C	1.406961	0.316403	0.000000
N	-2.208454	0.057574	0.000000
N	-0.625765	-1.795763	0.000000
N	-0.718202	1.721541	0.000000
N	1.625317	-1.077018	0.000000
O	2.326607	1.119304	0.000000
H	-2.822899	2.090916	0.000000
H	0.998377	-3.056608	0.000000
H	-0.336554	2.652448	0.000000
H	2.594034	-1.361433	0.000000

Molecule# 1160

1H,8H-allopurinol

PointGroup: Cs

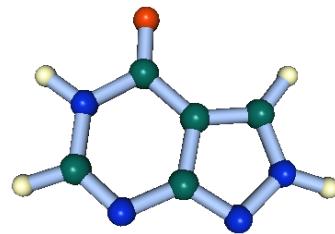
E= -487.349128288 au

ZPE= 0.100187 au

LUMO_eps= -0.05583 au

HOMO_eps= -0.25334 au

Dipole= 0.836 debye



14

C	0.728933	-1.997108	0.000000
N	-0.543008	-1.810437	0.000000
C	-0.914571	-0.487179	0.000000
C	0.000000	0.605212	0.000000
C	-0.793070	1.736321	0.000000
N	-2.058612	1.279355	0.000000
N	-2.176192	-0.065847	0.000000
N	1.685510	-1.008834	0.000000
C	1.424753	0.375734	0.000000
H	1.120457	-3.007750	0.000000
O	2.329973	1.187587	0.000000
H	-0.552002	2.784573	0.000000
H	2.661361	-1.265449	0.000000
H	-2.899755	1.830394	0.000000

Molecule# 1161

1H,9H-allopurinol

PointGroup: Cs

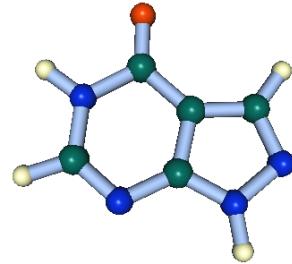
E= -487.354635732 au

ZPE= 0.100139 au

LUMO_eps= -0.05636 au

HOMO_eps= -0.25466 au

Dipole= 3.722 debye



14

C	0.743618	-1.988841	0.000000
N	-0.536382	-1.791562	0.000000
C	-0.865081	-0.470779	0.000000
C	0.000000	0.626262	0.000000
C	-0.849694	1.757502	0.000000
N	-2.119175	1.395232	0.000000
N	-2.113501	0.036902	0.000000
N	1.682928	-1.003258	0.000000
C	1.418760	0.396955	0.000000
H	1.125544	-3.002395	0.000000
O	2.336731	1.192002	0.000000
H	-0.582351	2.800421	0.000000
H	2.661588	-1.251117	0.000000
H	-2.981334	-0.470717	0.000000

Molecule# 1162

1H,9H-hypoxanthine

PointGroup: Cs

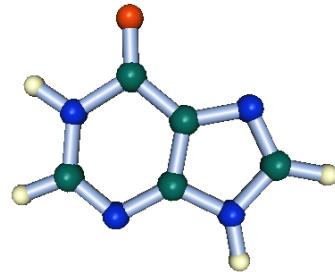
E= -487.371150726 au

ZPE= 0.100051 au

LUMO_eps= -0.04811 au

HOMO_eps= -0.24197 au

Dipole= 5.257 debye



14

C	0.682278	-2.011975	0.000000
N	-0.594186	-1.780881	0.000000
C	-0.879403	-0.454202	0.000000
C	0.000000	0.622440	0.000000
N	-0.689283	1.811813	0.000000
C	-1.948126	1.467994	0.000000
N	-2.127037	0.103915	0.000000
N	1.638326	-1.045896	0.000000
C	1.418524	0.367369	0.000000
H	1.040118	-3.033903	0.000000
H	-2.782873	2.149310	0.000000
H	-2.996743	-0.401694	0.000000
O	2.361664	1.128525	0.000000
H	2.611808	-1.314335	0.000000

Molecule# 1163

1R-1,2,2-trifluoroethoxybenzene

PointGroup: C1

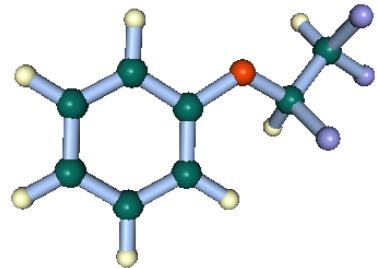
E= -684.072012050 au

ZPE= 0.138223 au

LUMO_eps= -0.03242 au

HOMO_eps= -0.25594 au

Dipole= 3.398 debye



19

C	3.765859	0.209204	-0.140016
C	2.871247	1.268614	-0.080295
C	3.285014	-1.096397	-0.096293
C	1.501209	1.040638	0.021750
C	1.922891	-1.340443	-0.004248
C	1.037573	-0.269346	0.047854
C	-1.259747	0.330131	-0.172330
C	-2.570202	-0.417612	-0.421522
O	-0.303784	-0.607745	0.144654
F	-1.447135	1.227529	0.863041
F	-3.502465	0.470307	-0.869796
F	-3.033392	-0.973051	0.723910
H	4.827889	0.396517	-0.213025
H	3.234180	2.287210	-0.099256
H	3.972559	-1.930152	-0.137897
H	0.820685	1.874043	0.108414
H	1.531930	-2.347555	0.026613
H	-0.988788	0.912792	-1.057218
H	-2.444324	-1.202689	-1.168659

Molecule# 1164
1R-2S-1,2-dimethylcyclohexane

PointGroup: C1

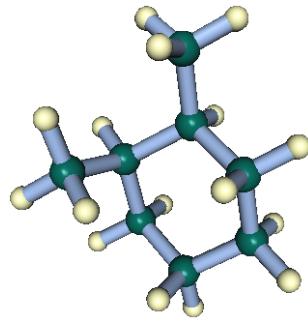
E= -314.620112683 au

ZPE= 0.225225 au

LUMO_eps= -0.01201 au

HOMO_eps= -0.29080 au

Dipole= 0.130 debye



24

C	-1.970214	0.143052	0.172978
C	-1.480744	-1.307690	0.157221
C	-1.121757	1.024428	-0.749887
C	0.015884	-1.401750	0.468056
C	0.383838	0.959334	-0.431292
C	0.859319	-0.515324	-0.460979
C	0.725765	1.702133	0.867397
C	2.355971	-0.676582	-0.191592
H	-3.018288	0.190873	-0.131201
H	-1.932318	0.529274	1.195719
H	-2.052364	-1.909311	0.867681
H	-1.667570	-1.737320	-0.832885
H	-1.274482	0.696175	-1.783249
H	-1.464303	2.061271	-0.701898
H	0.192158	-1.114610	1.509552
H	0.350636	-2.438687	0.380000
H	0.910384	1.478545	-1.239286
H	0.676087	-0.866606	-1.483879
H	0.286020	1.232479	1.747768
H	1.802459	1.755395	1.027304
H	0.352228	2.726827	0.824022
H	2.609678	-0.437246	0.842406
H	2.671869	-1.705362	-0.374491
H	2.949430	-0.027309	-0.838979

Molecule# 1165

2-(2-oxoethylideneamino)oxyethenone

PointGroup: C1

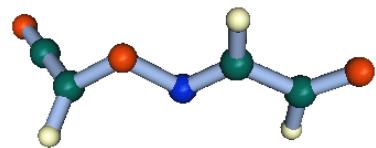
E= -434.684823245 au

ZPE= 0.067287 au

LUMO_eps= -0.10224 au

HOMO_eps= -0.26383 au

Dipole= 2.340 debye

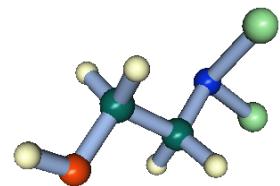


11

O	-0.632058	0.672130	-0.429729
O	-3.588830	-0.935067	-0.145234
O	3.802898	-0.381162	-0.172489
N	0.433297	0.185855	0.340131
C	-1.809404	0.727301	0.307417
C	1.516191	0.170796	-0.329905
C	-2.745700	-0.171725	0.074575
C	2.724311	-0.315122	0.366593
H	-1.953915	1.509033	1.036401
H	1.584308	0.490399	-1.366547
H	2.568061	-0.615137	1.416763

Molecule# 1166
2-(dichloroamino)ethanol
PointGroup: C1

E= -1129.663173220 au
ZPE= 0.077255 au
LUMO_eps= -0.08896 au
HOMO_eps= -0.27331 au
Dipole= 2.111 debye



11
Cl -1.849785 -1.123139 -0.022675
Cl -0.868753 1.577128 -0.107884
O 3.067182 -0.524320 -0.216469
N -0.501598 -0.072327 0.461280
C 0.718626 -0.556060 -0.215103
C 1.945213 0.179416 0.310336
H 0.651673 -0.480227 -1.301963
H 0.800148 -1.607945 0.057284
H 1.941056 0.161427 1.404237
H 1.942057 1.219714 -0.021165
H 3.870903 -0.050056 0.012492

Molecule# 1167

2-(ethylsulfanyl)propane

PointGroup: Cs

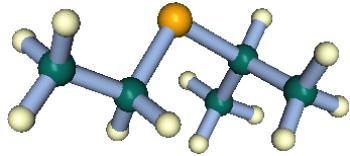
E= -596.069153390 au

ZPE= 0.160532 au

LUMO_eps= -0.01379 au

HOMO_eps= -0.22029 au

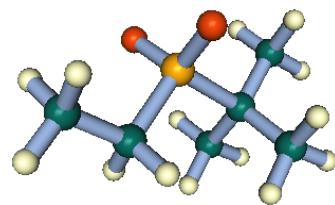
Dipole= 1.657 debye



18

C	2.666741	0.979974	0.000000
C	1.486493	0.014956	0.000000
C	-1.390067	-1.170055	1.269098
C	-1.390067	-1.170055	-1.269098
S	-0.074320	0.976753	0.000000
C	-1.390067	-0.320258	0.000000
H	3.605889	0.424701	0.000000
H	-2.287687	0.301951	0.000000
H	-1.434533	-0.547568	2.161409
H	-1.434533	-0.547568	-2.161409
H	2.652471	1.620505	0.882058
H	2.652471	1.620505	-0.882058
H	1.518737	-0.621415	-0.883489
H	1.518737	-0.621415	0.883489
H	-2.253602	-1.839615	1.272426
H	-2.253602	-1.839615	-1.272426
H	-0.496721	-1.792940	1.332175
H	-0.496721	-1.792940	-1.332175

Molecule# 1168
 2-(ethylsulphonyl)-2-methylpropane
 PointGroup: C1
 E= -785.874161846 au
 ZPE= 0.197330 au
 LUMO_eps= -0.02085 au
 HOMO_eps= -0.28046 au
 Dipole= 4.527 debye



23

C	2.997773	0.483515	0.000057
C	1.557720	0.984322	0.000121
S	0.416742	-0.436191	-0.000065
O	0.613609	-1.153289	1.261894
O	0.613589	-1.152943	-1.262224
C	-1.319656	0.252037	0.000043
C	-1.530669	1.078796	-1.268848
C	-2.218473	-0.990363	-0.000134
C	-1.530653	1.078424	1.269179
H	3.200853	-0.118000	0.883955
H	3.200858	-0.117760	-0.884004
H	3.675634	1.337082	0.000174
H	1.333115	1.569196	-0.889556
H	1.333115	1.568964	0.889950
H	-1.294421	0.500665	-2.160245
H	-2.578720	1.378917	-1.323741
H	-0.931778	1.989640	-1.272598
H	-2.047743	-1.601398	0.884308
H	-3.260021	-0.665474	-0.000085
H	-2.047745	-1.601141	-0.884754
H	-0.931790	1.989286	1.273173
H	-2.578712	1.378497	1.324194
H	-1.294359	0.500043	2.160402

Molecule# 1169

2-(isopropylsulfanyl)propane

PointGroup: C1

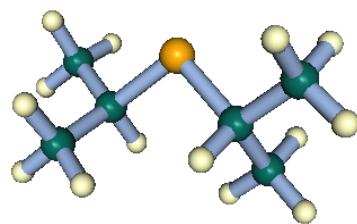
E= -635.398986616 au

ZPE= 0.188460 au

LUMO_eps= -0.01375 au

HOMO_eps= -0.22082 au

Dipole= 1.669 debye



21

C	1.734839	-1.077796	-1.065905
C	2.632719	0.591958	0.605922
C	-1.734840	-1.077794	1.065906
C	-2.632718	0.591958	-0.605923
C	1.441089	-0.271419	0.195238
C	-1.441089	-0.271419	-0.195238
S	0.000000	0.866458	0.000000
H	2.591479	-1.736141	-0.899071
H	0.892872	-1.704377	-1.358644
H	1.969701	-0.415640	-1.900083
H	3.513715	-0.035344	0.754087
H	2.435115	1.129802	1.532456
H	2.869539	1.323680	-0.168464
H	-2.591478	-1.736141	0.899071
H	-0.892872	-1.704375	1.358647
H	-1.969704	-0.415638	1.900082
H	-3.513714	-0.035344	-0.754090
H	-2.435113	1.129802	-1.532458
H	-2.869540	1.323680	0.168462
H	1.204385	-0.950113	1.015660
H	-1.204384	-0.950114	-1.015659

Molecule# 1170

2-(methylsulfanyl)propane

PointGroup: C1

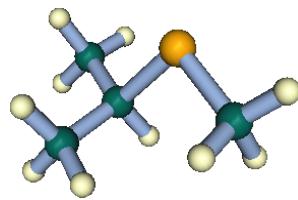
E= -556.742120448 au

ZPE= 0.131803 au

LUMO_eps= -0.01263 au

HOMO_eps= -0.22226 au

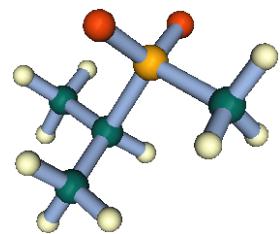
Dipole= 1.659 debye



15

C	2.099858	0.369973	0.299455
S	0.769670	-0.705032	-0.323442
C	-0.727952	0.124983	0.364432
C	-0.985167	1.492597	-0.260375
C	-1.906973	-0.823775	0.163596
H	3.037274	-0.105810	0.018885
H	2.064635	1.361496	-0.147229
H	2.058488	0.449131	1.385117
H	-0.544665	0.242009	1.434900
H	-0.145508	2.172003	-0.117608
H	-1.738088	-1.779969	0.657497
H	-1.166779	1.398813	-1.331795
H	-1.863937	1.955096	0.196475
H	-2.816392	-0.380971	0.573674
H	-2.078342	-1.013952	-0.897490

Molecule# 1171
 2-(methylsulphonyl)propane
 PointGroup: C1
 E= -707.217593333 au
 ZPE= 0.141278 au
 LUMO_eps= -0.02272 au
 HOMO_eps= -0.29018 au
 Dipole= 4.708 debye



17

C	1.914502	-1.078827	-0.104407
C	1.061527	0.128342	-0.489304
C	1.601028	1.440504	0.068529
S	-0.649449	-0.198934	0.095737
C	-1.646361	1.149604	-0.566671
O	-1.109835	-1.428241	-0.547411
O	-0.671628	-0.094970	1.553917
H	1.500968	-2.001807	-0.504676
H	2.919668	-0.945747	-0.505540
H	1.988659	-1.170348	0.978888
H	0.955561	0.177066	-1.574814
H	2.625979	1.581977	-0.276903
H	1.023346	2.303886	-0.259803
H	1.607003	1.421611	1.157570
H	-1.554403	1.165975	-1.649467
H	-2.667243	0.908253	-0.279320
H	-1.340836	2.090018	-0.118649

Molecule# 1172

2-[(difluoroamino)methyl]acrylonitrile

PointGroup: C1

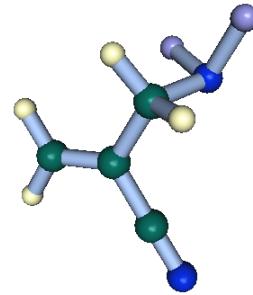
E= -464.027992531 au

ZPE= 0.078892 au

LUMO_eps= -0.08762 au

HOMO_eps= -0.31086 au

Dipole= 4.424 debye



12

F	-1.560515	0.669193	1.027935
F	-2.395956	-0.758181	-0.402751
N	-1.190368	-0.448376	0.254141
N	2.540504	-1.531236	0.370739
C	-0.339313	0.108786	-0.819505
C	1.022612	0.458263	-0.274893
C	1.448448	1.716095	-0.160431
C	1.869720	-0.636358	0.095191
H	-0.826459	0.978775	-1.258076
H	-0.271637	-0.689646	-1.557439
H	0.810176	2.542787	-0.438338
H	2.436402	1.945546	0.210865

Molecule# 1173

2-2'-disulfanediyl diacetonitrile

PointGroup: C2

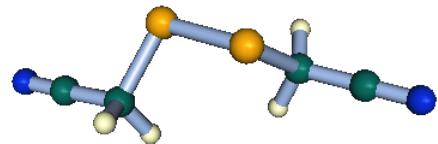
E= -1060.845926800 au

ZPE= 0.075081 au

LUMO_eps= -0.07583 au

HOMO_eps= -0.29103 au

Dipole= 0.892 debye



12

S	0.406791	0.942610	0.784578
S	-0.406791	-0.942610	0.784578
N	0.183607	4.290300	-0.635604
N	-0.183607	-4.290300	-0.635604
C	-0.625549	1.822703	-0.494613
C	0.625549	-1.822703	-0.494613
C	-0.183607	3.202009	-0.580957
C	0.183607	-3.202009	-0.580957
H	-0.505885	1.334775	-1.459501
H	-1.669096	1.778086	-0.191095
H	0.505885	-1.334775	-1.459501
H	1.669096	-1.778086	-0.191095

Molecule# 1174

2-5-diethynyl-1-3-4-oxadiazole

PointGroup: C1

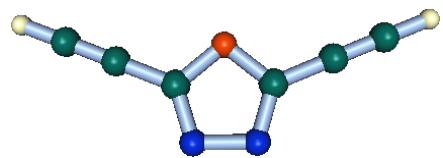
E= -414.534963373 au

ZPE= 0.064090 au

LUMO_eps= -0.08599 au

HOMO_eps= -0.27448 au

Dipole= 3.357 debye



11

O	0.000000	0.687878	0.000070
N	-0.688992	-1.412640	-0.000142
N	0.688992	-1.412640	-0.000140
C	-1.060811	-0.167259	-0.000017
C	1.060811	-0.167259	-0.000015
C	-2.366481	0.358061	0.000033
C	2.366481	0.358061	0.000038
C	-3.480741	0.800640	0.000075
C	3.480741	0.800640	0.000084
H	-4.469667	1.188310	0.000112
H	4.469667	1.188310	0.000122

Molecule# 1175

2-amino-2-cyanoethanethioamide

PointGroup: C1

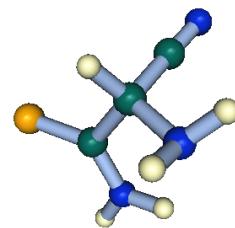
E= -679.897914593 au

ZPE= 0.088401 au

LUMO_eps= -0.06564 au

HOMO_eps= -0.23407 au

Dipole= 5.467 debye



12

S	-1.950591	-0.686147	-0.303940
N	1.432922	1.428952	-0.545421
N	-0.711841	1.245188	1.046284
N	2.117170	-1.659656	0.627854
C	0.684478	0.164121	-0.583266
C	-0.693718	0.297052	0.111210
C	1.467167	-0.871492	0.100755
H	0.479303	-0.201586	-1.591769
H	1.137544	2.029439	-1.305751
H	2.426777	1.267897	-0.644579
H	-1.552470	1.410472	1.572884
H	0.102983	1.832653	1.159037

Molecule# 1176

2-amino-2-iminoethanethioamide

PointGroup: C1

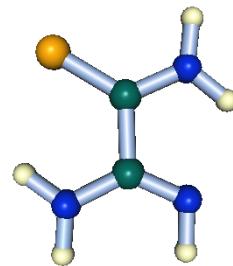
E= -641.812784982 au

ZPE= 0.083203 au

LUMO_eps= -0.07693 au

HOMO_eps= -0.23142 au

Dipole= 2.243 debye



11

S	-1.746638	-0.491801	-0.024174
N	1.069100	-1.539005	0.070067
N	-0.321863	1.747667	0.040754
N	2.022193	0.634247	-0.054121
C	1.041264	-0.187875	-0.000463
C	-0.357714	0.420697	0.009753
H	0.188021	-2.026997	0.000787
H	1.927591	-2.037227	-0.074943
H	0.590765	2.186653	0.033004
H	-1.174968	2.277579	0.029518
H	2.927486	0.171511	-0.054209

Molecule# 1177

2-amino-2-nitroso-3-sulfanylpropanoic acid

PointGroup: C1

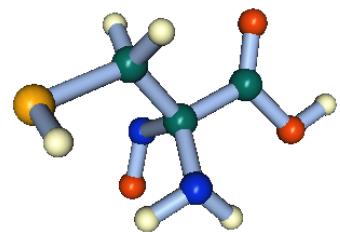
E= -851.437100760 au

ZPE= 0.103025 au

LUMO_eps= -0.11447 au

HOMO_eps= -0.24020 au

Dipole= 2.338 debye



15

S	2.590627	-0.398383	0.022037
O	-1.809480	-1.599735	-0.671452
O	-2.549580	0.115934	0.577774
O	-0.025063	2.199939	-0.680860
N	-0.181727	1.093324	-1.068444
N	-0.043483	0.595039	1.433653
C	-0.211472	0.021895	0.148750
C	-1.585305	-0.610668	-0.028144
C	0.874555	-0.989357	-0.229063
H	2.628680	-0.584070	1.353771
H	-3.394862	-0.321472	0.396688
H	-0.824033	1.185978	1.685952
H	0.803667	1.150378	1.462821
H	0.792491	-1.224457	-1.287032
H	0.726816	-1.911112	0.325783

Molecule# 1178

2-amino-3,3-difluoropropanoic acid

PointGroup: C1

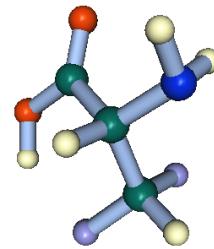
E= -522.436679380 au

ZPE= 0.092937 au

LUMO_eps= -0.03135 au

HOMO_eps= -0.28648 au

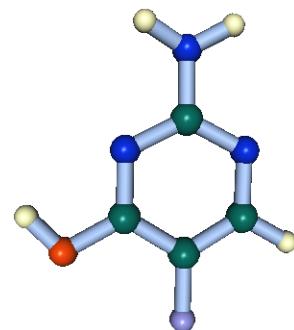
Dipole= 3.276 debye



13

F	-1.745208	-0.927739	-0.493927
F	-1.346524	0.380082	1.235265
O	2.196225	-0.085244	0.474269
O	0.848450	-1.764507	-0.054074
N	0.475358	1.931411	-0.401493
C	0.139589	0.538365	-0.608811
C	-1.288396	0.325650	-0.123236
C	1.157136	-0.455672	0.009476
H	-0.057623	-1.892498	-0.368997
H	1.337386	2.150616	-0.884107
H	0.664237	2.091296	0.582030
H	0.119355	0.341464	-1.684857
H	-1.972645	1.066109	-0.531789

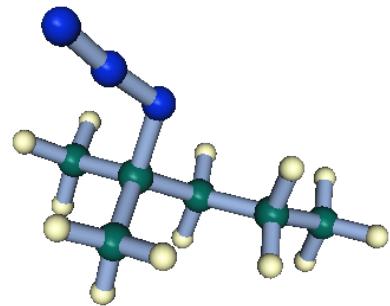
Molecule# 1179
 2-amino-4-hydroxy-5-fluoropyrimidine
 PointGroup: C1
 E= -494.358120461 au
 ZPE= 0.090268 au
 LUMO_eps= -0.04650 au
 HOMO_eps= -0.23862 au
 Dipole= 2.616 debye



13

F	-2.432062	-0.840581	-0.001430
O	-1.549974	1.772119	0.004185
N	0.623463	1.045644	-0.000115
N	1.145451	-1.283249	0.004540
N	2.809376	0.312221	-0.053279
C	-0.665617	0.765530	-0.000417
C	-1.116639	-0.556241	-0.001881
C	1.480636	0.009952	-0.004752
C	-0.163020	-1.546056	0.003960
H	-1.037104	2.592592	0.000511
H	3.451036	-0.430928	0.156545
H	3.081893	1.251498	0.171878
H	-0.467661	-2.586310	0.010977

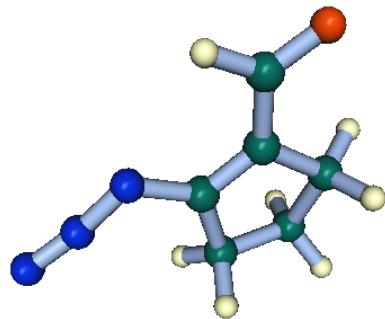
Molecule# 1180
 2-azido-2-methylpentane
 PointGroup: C1
 E= -400.821848514 au
 ZPE= 0.190898 au
 LUMO_eps= -0.03336 au
 HOMO_eps= -0.25841 au
 Dipole= 2.609 debye



22

N	0.859731	-0.762092	-0.403390
N	2.049387	-0.946307	-0.188347
N	3.137721	-1.220267	-0.036056
C	0.291648	0.571345	0.012070
C	-1.196524	0.509338	-0.367515
C	0.982348	1.682950	-0.785949
C	0.502842	0.782356	1.515246
C	-2.032716	-0.571619	0.318400
C	-3.460252	-0.628326	-0.225082
H	-1.253030	0.365417	-1.449882
H	-1.630745	1.492153	-0.162114
H	0.564501	2.654726	-0.520022
H	2.052937	1.712880	-0.577082
H	0.845343	1.530789	-1.856315
H	0.024062	1.708878	1.835252
H	1.564949	0.858780	1.752680
H	0.084771	-0.038464	2.094828
H	-1.547898	-1.539559	0.179221
H	-2.067572	-0.392248	1.395396
H	-3.978282	0.323071	-0.084883
H	-3.466515	-0.852334	-1.293656
H	-4.044468	-1.399694	0.278104

Molecule# 1181
 2-azidocyclopentene-1-carbaldehyde
 PointGroup: C1
 E= -472.424321694 au
 ZPE= 0.129318 au
 LUMO_eps= -0.08025 au
 HOMO_eps= -0.24902 au
 Dipole= 3.931 debye



17

O	-2.841359	-1.632448	-0.003270
N	1.285402	-0.975322	-0.019771
N	2.484031	-0.680505	-0.010863
N	3.605627	-0.567935	-0.006143
C	0.339502	0.047766	0.013908
C	-0.993794	-0.172117	0.008810
C	0.682021	1.512322	0.110918
C	-1.750128	1.127746	0.107057
C	-0.671031	2.199116	-0.176680
C	-1.636105	-1.476759	-0.036351
H	1.467801	1.806010	-0.588127
H	1.055913	1.737532	1.115662
H	-2.583844	1.169965	-0.593065
H	-2.183781	1.237766	1.105376
H	-0.710080	2.486415	-1.227487
H	-0.808422	3.103763	0.412368
H	-0.954916	-2.343981	-0.107093

Molecule# 1182

2-azidothiophene

PointGroup: C1

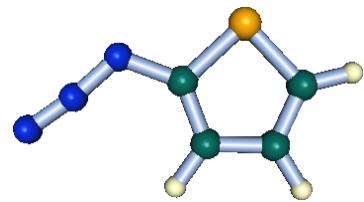
E= -716.742973144 au

ZPE= 0.069669 au

LUMO_eps= -0.05469 au

HOMO_eps= -0.22932 au

Dipole= 1.737 debye



11

S	-1.312415	-1.115521	-0.000006
N	1.348922	-0.797364	0.000029
N	2.371560	-0.112910	-0.000008
N	3.375724	0.402319	-0.000020
C	0.117911	-0.130110	0.000011
C	-0.182896	1.205002	0.000013
C	-2.320123	0.290783	-0.000010
C	-1.585097	1.436766	0.000000
H	0.562508	1.986411	0.000024
H	-3.390599	0.180287	-0.000019
H	-2.025487	2.422671	0.000000

Molecule# 1183

2-bromo-1-hydroxy-1,3-diazole

PointGroup: C1

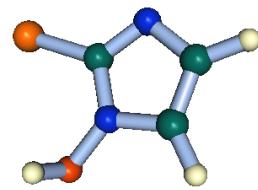
E= -2875.114708120 au

ZPE= 0.064220 au

LUMO_eps= -0.03337 au

HOMO_eps= -0.24642 au

Dipole= 3.247 debye



10

Br	1.609682	-0.108887	-0.000424
O	-0.796097	2.027941	-0.108472
N	-1.114546	0.693819	0.008470
N	-0.885405	-1.493997	0.003875
C	-2.394034	0.187966	0.004912
C	-0.248703	-0.359225	-0.009483
C	-2.223542	-1.167075	0.006904
H	-3.252412	0.833543	-0.006403
H	-2.981114	-1.931316	0.009792
H	-0.539240	2.316544	0.778826

Molecule# 1184

2-bromo-1,1,1,2-tetrafluoroethane

PointGroup: C1

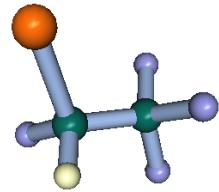
E= -3050.603485470 au

ZPE= 0.034796 au

LUMO_eps= -0.05243 au

HOMO_eps= -0.31854 au

Dipole= 1.411 debye



8

C	0.111194	0.620791	-0.476624
C	1.296892	-0.232668	-0.001488
F	0.216553	1.856288	0.076347
F	2.441146	0.372868	-0.365963
F	1.266078	-1.439625	-0.582574
F	1.315089	-0.391303	1.322830
Br	-1.592251	-0.188959	0.010656
H	0.130479	0.700778	-1.560048

Molecule# 1185

2-bromo-2-chloro-1,1,1-trifluoroethane

PointGroup: C1

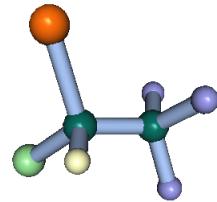
E= -3410.956066030 au

ZPE= 0.033165 au

LUMO_eps= -0.06357 au

HOMO_eps= -0.31456 au

Dipole= 1.316 debye



8

C	0.114916	0.364072	-0.514219
C	1.223710	-0.565104	0.000141
F	2.418094	-0.132455	-0.439100
F	1.268902	-0.633076	1.331926
F	1.043171	-1.805349	-0.482264
Cl	0.394145	2.031249	0.030712
Br	-1.641135	-0.301211	0.013267
H	0.135967	0.355260	-1.597038

Molecule# 1186

2-bromo-2-methylpropane

PointGroup: C3v

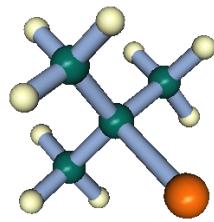
E= -2732.153552190 au

ZPE= 0.121334 au

LUMO_eps= -0.02479 au

HOMO_eps= -0.27417 au

Dipole= 2.531 debye



14

C	0.000000	1.456592	-1.294738
C	1.261445	-0.728296	-1.294738
C	-1.261445	-0.728296	-1.294738
C	0.000000	0.000000	-0.855241
Br	0.000000	0.000000	1.177386
H	-0.883594	1.980671	-0.934701
H	0.883594	1.980671	-0.934701
H	0.000000	1.497716	-2.387858
H	2.157108	-0.225121	-0.934701
H	1.273514	-1.755550	-0.934701
H	1.297060	-0.748858	-2.387858
H	-2.157108	-0.225121	-0.934701
H	-1.273514	-1.755550	-0.934701
H	-1.297060	-0.748858	-2.387858

Molecule# 1187

2-bromo-3-butynamide

PointGroup: C1

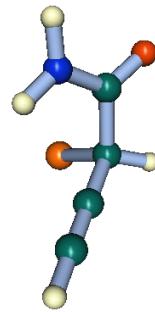
E= -2859.092625150 au

ZPE= 0.073381 au

LUMO_eps= -0.07676 au

HOMO_eps= -0.27669 au

Dipole= 3.970 debye



11

Br	1.462125	-0.223304	0.131859
O	-1.550818	-1.806817	-0.771136
N	-1.927978	-0.517930	1.058103
C	-0.330036	0.244951	-0.636531
C	-1.337872	-0.803882	-0.124226
C	-0.646468	1.619403	-0.345895
C	-0.942772	2.755741	-0.100889
H	-2.571762	-1.184705	1.446730
H	-1.756710	0.344991	1.542373
H	-0.205109	0.071387	-1.699781
H	-1.195516	3.766746	0.103231

Molecule# 1188

2-bromo-3-hydroxy-1-propen-1-one

PointGroup: C1

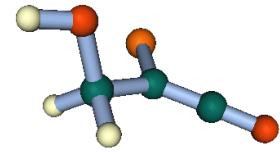
E= -2840.855636570 au

ZPE= 0.056571 au

LUMO_eps= -0.08854 au

HOMO_eps= -0.24557 au

Dipole= 2.720 debye



9

Br	1.331781	-0.104442	-0.016627
O	-1.343384	2.469502	-0.177094
O	-1.595812	-1.835253	-0.575224
C	-0.549120	0.161855	0.215110
C	-0.972544	1.384167	-0.004358
C	-1.438830	-0.981513	0.556754
H	-1.922598	-2.690484	-0.278819
H	-2.407475	-0.581724	0.878095
H	-1.005715	-1.533357	1.396182

Molecule# 1189

2-bromo-N-cyanoacetamide

PointGroup: C1

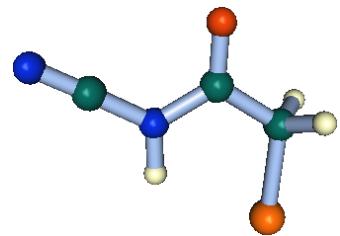
E= -2875.179662420 au

ZPE= 0.062863 au

LUMO_eps= -0.05739 au

HOMO_eps= -0.30979 au

Dipole= 4.992 debye



10

Br	-1.822464	-0.386598	0.000000
O	1.646268	1.822022	0.000000
N	1.283970	-0.432569	-0.000001
N	3.675928	-1.135774	0.000000
C	0.879378	0.894432	0.000000
C	-0.615995	1.166915	0.000000
C	2.575324	-0.795297	0.000000
H	0.577496	-1.156929	0.000000
H	-0.856462	1.746884	0.884894
H	-0.856466	1.746887	-0.884891

Molecule# 1190

2-bromo-N-hydroxyacetamide

PointGroup: C1

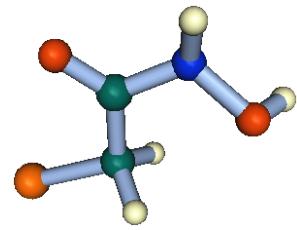
E= -2858.113725980 au

ZPE= 0.068498 au

LUMO_eps= -0.04282 au

HOMO_eps= -0.28589 au

Dipole= 4.395 debye



10

Br	-1.716813	-0.126699	-0.010487
O	2.843398	-1.026778	0.176526
O	0.746263	1.739763	0.072081
N	2.421968	0.266322	-0.204683
C	0.162775	-0.622427	0.035584
C	1.086074	0.585257	-0.006498
H	0.346574	-1.282717	-0.805941
H	0.329741	-1.183726	0.950373
H	3.064690	0.974427	0.128766
H	3.183300	-1.418629	-0.636734

Molecule# 1191

2-bromoacrylic acid

PointGroup: C1

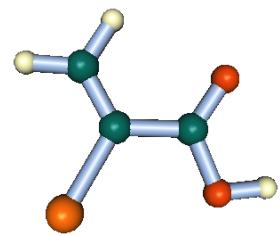
E= -2840.898108810 au

ZPE= 0.057304 au

LUMO_eps= -0.08046 au

HOMO_eps= -0.27777 au

Dipole= 0.254 debye



9

Br	1.392704	-0.180081	-0.000001
O	-2.669326	0.199942	-0.000004
O	-1.268206	-1.552003	0.000004
C	-1.546092	-0.237750	0.000000
C	-0.332369	0.636802	0.000001
C	-0.463930	1.956714	0.000003
H	-2.119249	-2.014336	0.000003
H	0.387981	2.618788	0.000005
H	-1.458758	2.380273	0.000003

Molecule# 1192

2-bromochloroethene

PointGroup: Cs

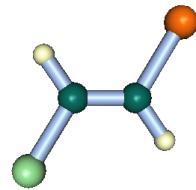
E= -3111.882339760 au

ZPE= 0.033085 au

LUMO_eps= -0.03838 au

HOMO_eps= -0.26386 au

Dipole= 0.091 debye



6

Br	-1.518775	-0.624968	0.000000
Cl	2.621245	1.066465	0.000000
C	0.000000	0.510460	0.000000
C	1.227543	0.024346	0.000000
H	-0.236417	1.562080	0.000000
H	1.467110	-1.026952	0.000000

Molecule# 1193

2-bromoethanone

PointGroup: C1

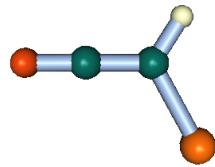
E= -2726.280204500 au

ZPE= 0.023383 au

LUMO_eps= -0.09401 au

HOMO_eps= -0.24890 au

Dipole= 1.250 debye



5

Br 1.040669 -0.116643 0.000000

O -2.722493 -0.455318 0.000003

C -0.611053 0.823474 -0.000013

C -1.731631 0.147662 -0.000002

H -0.587373 1.898233 0.000043

Molecule# 1194

2-bromoethenimine

PointGroup: C1

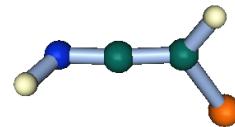
E= -2706.390652890 au

ZPE= 0.035143 au

LUMO_eps= -0.06918 au

HOMO_eps= -0.24444 au

Dipole= 1.783 debye



6

Br	1.062465	-0.122998	0.000390
N	-2.784157	-0.413339	-0.127960
C	-0.591979	0.821230	0.011881
C	-1.727585	0.179592	0.007361
H	-3.258320	-0.701178	0.727135
H	-0.521463	1.894559	0.039491

Molecule# 1195

2-bromoethylisocyanate

PointGroup: C1

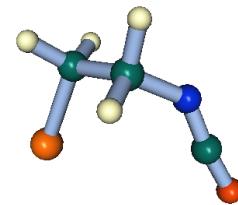
E= -2821.031069280 au

ZPE= 0.070204 au

LUMO_eps= -0.03582 au

HOMO_eps= -0.29184 au

Dipole= 3.648 debye



10

Br	-1.348575	-0.496729	0.033420
O	2.744713	-1.356928	-0.005847
N	1.761073	0.788135	-0.179037
C	0.676014	1.566183	0.358859
C	-0.650037	1.308808	-0.332914
C	2.204873	-0.321207	-0.046476
H	0.918673	2.620383	0.205614
H	0.579485	1.404172	1.433564
H	-0.560282	1.378536	-1.411868
H	-1.408068	1.998180	0.026210

Molecule# 1196

2-bromoethylisothiocyanate

PointGroup: C1

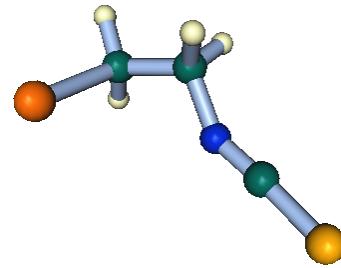
E= -3143.990980630 au

ZPE= 0.067465 au

LUMO_eps= -0.04684 au

HOMO_eps= -0.25831 au

Dipole= 3.564 debye



10

Br	-2.001735	-0.544799	0.029212
S	3.643384	-0.549890	0.002998
N	1.131283	0.598370	-0.187268
C	0.107233	1.427445	0.365759
C	-1.231365	1.231791	-0.317835
C	2.213269	0.123905	-0.062989
H	0.018284	1.238446	1.437381
H	0.395384	2.476224	0.232945
H	-1.146128	1.315303	-1.396130
H	-1.954745	1.948795	0.056670

Molecule# 1197

2-bromofluoroethene

PointGroup: C1

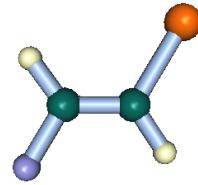
E= -2751.523420130 au

ZPE= 0.034604 au

LUMO_eps= -0.02888 au

HOMO_eps= -0.26530 au

Dipole= 0.189 debye



6

Br	-1.189259	-0.038129	0.000000
F	2.886841	0.037952	0.000000
C	0.621468	0.510920	0.000000
C	1.605812	-0.367832	0.000000
H	0.779348	1.577216	0.000000
H	1.499472	-1.442800	0.000000

Molecule# 1198

2-bromopropane

PointGroup: Cs

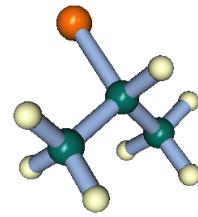
E= -2692.823997750 au

ZPE= 0.093632 au

LUMO_eps= -0.02026 au

HOMO_eps= -0.27701 au

Dipole= 2.419 debye



11

C	0.065066	-1.568074	1.270934
C	0.065066	-1.568074	-1.270934
C	-0.446164	-0.919782	0.000000
Br	0.065066	1.019211	0.000000
H	-0.321839	-1.071682	2.158578
H	-0.256927	-2.612906	1.294570
H	1.154020	-1.547578	1.310964
H	-0.321839	-1.071682	-2.158578
H	-0.256927	-2.612906	-1.294570
H	1.154020	-1.547578	-1.310964
H	-1.531606	-0.872470	0.000000

Molecule# 1199

2-bromothiazole

PointGroup: C1

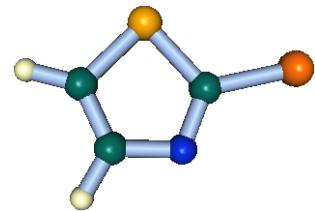
E= -3142.771216000 au

ZPE= 0.045047 au

LUMO_eps= -0.05221 au

HOMO_eps= -0.25920 au

Dipole= 2.304 debye



8

Br	-1.713736	0.021348	0.000003
S	1.193634	-1.194360	-0.000004
N	0.771555	1.345276	-0.000005
C	0.164507	0.211741	-0.000018
C	2.558028	-0.131730	0.000012
C	2.133775	1.158702	0.000000
H	3.565356	-0.510519	0.000023
H	2.778493	2.023897	0.000005

Molecule# 1200

2-butanamine

PointGroup: C1

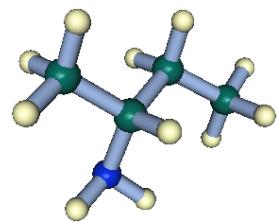
E= -213.893144716 au

ZPE= 0.148570 au

LUMO_eps= -0.01385 au

HOMO_eps= -0.24369 au

Dipole= 1.178 debye



16

N	0.585676	1.381629	-0.230174
H	-0.201181	1.952915	0.050435
H	1.420699	1.844860	0.107244
C	1.770975	-0.732575	-0.002480
H	1.914810	-0.792002	-1.082494
H	2.641620	-0.231533	0.426249
H	1.738854	-1.745293	0.401057
C	0.486227	0.022813	0.322074
H	0.370190	0.037096	1.417614
C	-0.738648	-0.689705	-0.258545
H	-0.627441	-0.732000	-1.345347
H	-0.732698	-1.721265	0.103456
C	-2.075899	-0.042076	0.099323
H	-2.909692	-0.633466	-0.280918
H	-2.171947	0.956485	-0.330085
H	-2.198874	0.042059	1.181772

Molecule# 1201

2-butanethiol

PointGroup: C1

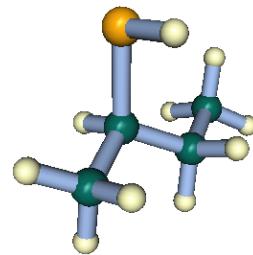
E= -556.743258899 au

ZPE= 0.130820 au

LUMO_eps= -0.01442 au

HOMO_eps= -0.24058 au

Dipole= 1.718 debye



15

S	1.003766	-1.201120	-0.007299
H	1.244543	-0.995639	1.301926
C	1.183258	1.587414	-0.017139
H	1.384325	1.633112	1.054995
H	0.747685	2.544290	-0.314961
C	0.224532	0.446006	-0.342190
H	0.071406	0.407063	-1.423635
C	-1.135558	0.616531	0.342215
H	-1.467515	1.642836	0.153798
H	-0.998475	0.536154	1.424474
C	-2.218912	-0.353099	-0.120370
H	-2.402233	-0.253586	-1.192432
H	-1.934408	-1.386199	0.075183
H	-3.159570	-0.156548	0.395174
H	2.134068	1.465332	-0.532831

Molecule# 1202

2-butanol

PointGroup: C1

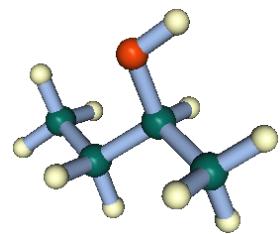
E= -233.770810550 au

ZPE= 0.135764 au

LUMO_eps= -0.01503 au

HOMO_eps= -0.27884 au

Dipole= 1.552 debye



15

C	2.068952	-0.029590	0.114749
C	-1.781327	-0.695111	0.003653
C	0.738327	-0.671951	-0.270753
C	-0.478716	0.030019	0.319827
O	-0.490635	1.363576	-0.211065
H	2.209786	-0.036654	1.197896
H	2.114065	1.005156	-0.221346
H	2.905645	-0.568790	-0.331134
H	-1.921866	-0.773729	-1.075400
H	-1.779793	-1.700291	0.428681
H	-2.637934	-0.160756	0.420748
H	0.719889	-1.714419	0.057213
H	0.628666	-0.681241	-1.358792
H	-0.354839	0.083409	1.410162
H	-1.241958	1.838511	0.155634

Molecule# 1203

2-butanone

PointGroup: C1

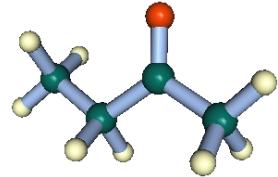
E= -232.564589619 au

ZPE= 0.111768 au

LUMO_eps= -0.02563 au

HOMO_eps= -0.25645 au

Dipole= 2.935 debye



13

C	-1.883170	-0.506701	0.017217
H	-2.671790	0.234445	-0.081330
H	-2.008340	-1.043418	0.960588
H	-1.965083	-1.246251	-0.781367
C	2.019993	-0.020927	0.024676
H	2.107093	0.570058	0.935544
H	2.127700	0.662992	-0.815819
C	0.683365	-0.747236	-0.030294
H	0.608044	-1.363355	-0.932946
H	0.580955	-1.453175	0.800501
C	-0.528385	0.169660	-0.010123
O	-0.421739	1.375414	-0.011414
H	2.844518	-0.733384	-0.002718

Molecule# 1204

2-butenedioic acid

PointGroup: C2h

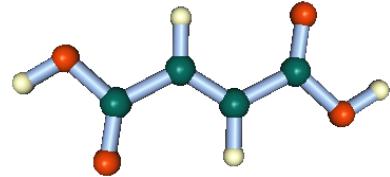
E= -455.928792272 au

ZPE= 0.082505 au

LUMO_eps= -0.10872 au

HOMO_eps= -0.30680 au

Dipole= 0.000 debye



12

C	0.031152	1.911320	0.000000
C	0.450591	0.488912	0.000000
C	-0.450591	-0.488912	0.000000
C	-0.031152	-1.911320	0.000000
O	1.105518	-2.312587	0.000000
O	-1.105518	2.312587	0.000000
O	1.105518	2.733674	0.000000
O	-1.105518	-2.733674	0.000000
H	1.509349	0.269845	0.000000
H	-1.509349	-0.269845	0.000000
H	0.771942	3.643174	0.000000
H	-0.771942	-3.643174	0.000000

Molecule# 1205

2-butoxyethanol

PointGroup: C1

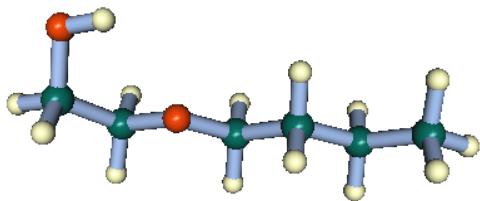
E= -387.662015839 au

ZPE= 0.198075 au

LUMO_eps= -0.01297 au

HOMO_eps= -0.27302 au

Dipole= 2.452 debye



22

C	4.089165	0.588477	0.122469
C	2.923903	-0.328181	-0.246075
C	1.567017	0.231891	0.182347
C	0.411798	-0.680523	-0.186833
C	-3.172463	-0.056120	0.344075
C	-1.956993	-0.859646	-0.067429
O	-3.273599	1.167332	-0.370804
O	-0.806302	-0.090619	0.241637
H	3.988063	1.565495	-0.353995
H	4.136511	0.751152	1.200924
H	5.043295	0.163461	-0.191317
H	2.923021	-0.497172	-1.326931
H	3.074567	-1.308953	0.214777
H	1.555650	0.393751	1.263323
H	1.405218	1.208369	-0.282062
H	0.381813	-0.843154	-1.272776
H	0.532797	-1.663858	0.288024
H	-3.138051	0.127329	1.424009
H	-4.077395	-0.622897	0.124143
H	-1.992298	-1.069512	-1.143946
H	-1.937954	-1.816743	0.471425
H	-2.430595	1.623640	-0.273584

Molecule# 1206

2-butyne

PointGroup: D3

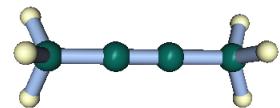
E= -156.043088061 au

ZPE= 0.083863 au

LUMO_eps= -0.01136 au

HOMO_eps= -0.25467 au

Dipole= 0.000 debye



10

C	0.000000	0.000000	0.600514
C	0.000000	0.000000	-0.600514
C	0.000000	0.000000	2.057156
C	0.000000	0.000000	-2.057156
H	0.037656	1.017156	2.451360
H	-0.899710	-0.475967	2.451360
H	0.862055	-0.541189	2.451360
H	0.899710	-0.475967	-2.451360
H	-0.037656	1.017156	-2.451360
H	-0.862055	-0.541189	-2.451360

Molecule# 1207
2-butynedinitrile
PointGroup: D(infinity)h
E= -261.910692066 au
ZPE= 0.026700 au
LUMO_eps= -0.12681 au
HOMO_eps= -0.34007 au
Dipole= 0.000 debye



6
C 0.000000 0.000000 0.603507
C 0.000000 0.000000 -0.603507
C 0.000000 0.000000 1.966164
C 0.000000 0.000000 -1.966164
N 0.000000 0.000000 3.122257
N 0.000000 0.000000 -3.122257

Molecule# 1208

2-butynedioic acid

PointGroup: C2

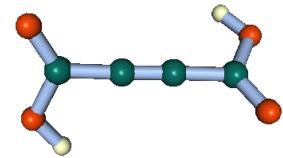
E= -454.647647471 au

ZPE= 0.058211 au

LUMO_eps= -0.10652 au

HOMO_eps= -0.32387 au

Dipole= 2.471 debye



10

O	0.456164	2.811298	0.519791
O	-0.456164	-2.811298	0.519791
O	-1.460125	2.429632	-0.552434
O	1.460125	-2.429632	-0.552434
C	-0.456164	2.004868	-0.060552
C	0.456164	-2.004868	-0.060552
C	-0.123481	0.588917	-0.035196
C	0.123481	-0.588917	-0.035196
H	1.213127	2.300420	0.835627
H	-1.213127	-2.300420	0.835627

Molecule# 1209

2-chloro-1-butene

PointGroup: Cs

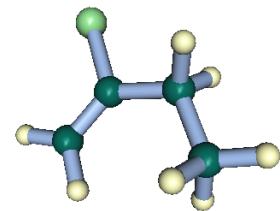
E= -616.921268152 au

ZPE= 0.099217 au

LUMO_eps= -0.01510 au

HOMO_eps= -0.26217 au

Dipole= 1.904 debye



12

C	2.147973	-1.066945	0.000000
H	2.507268	-2.095782	0.000000
H	2.554206	-0.572788	0.882885
H	2.554206	-0.572788	-0.882885
C	0.621595	-1.051458	0.000000
H	0.241625	-1.595107	-0.869387
H	0.241625	-1.595107	0.869387
C	0.604486	1.490130	0.000000
H	1.683307	1.546561	0.000000
C	0.000000	0.312724	0.000000
Cl	-1.769241	0.256602	0.000000
H	0.050536	2.416069	0.000000

Molecule# 1210

2-chloro-1,1,1-trifluoroethane

PointGroup: Cs

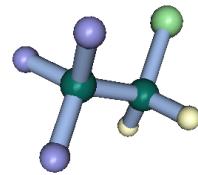
E= -837.342654324 au

ZPE= 0.043413 au

LUMO_eps= -0.02304 au

HOMO_eps= -0.32836 au

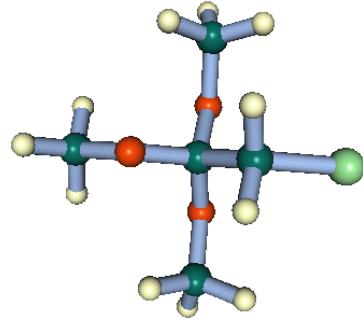
Dipole= 1.937 debye



8

C	-0.858750	0.493126	0.000000
C	0.656851	0.425801	0.000000
F	1.143435	-0.195496	1.084579
F	1.143435	1.687623	0.000000
F	1.143435	-0.195496	-1.084579
Cl	-1.605455	-1.130914	0.000000
H	-1.184311	1.021148	0.890634
H	-1.184311	1.021148	-0.890634

Molecule# 1211
 2-chloro-1,1,1-trimethoxyethane
 PointGroup: C1
 E= -883.196592497 au
 ZPE= 0.163884 au
 LUMO_eps= -0.01389 au
 HOMO_eps= -0.28730 au
 Dipole= 2.590 debye



20

C	0.266243	-2.381801	-0.314834
C	2.705992	0.000050	0.290476
C	0.265910	2.381868	-0.314817
C	-0.892239	-0.000056	0.940151
C	0.318956	0.000034	-0.011152
O	0.356269	-1.082293	-0.886845
O	1.407928	0.000118	0.889584
O	0.356106	1.082375	-0.886837
Cl	-2.460390	-0.000138	0.062875
H	0.547176	-3.074651	-1.104011
H	-0.754234	-2.608050	0.002453
H	0.948511	-2.502078	0.529039
H	2.859400	-0.886862	-0.324693
H	3.413060	0.000864	1.115990
H	2.858879	0.886125	-0.326020
H	0.948187	2.502235	0.529035
H	-0.754592	2.607970	0.002494
H	0.546724	3.074761	-1.104000
H	-0.869091	0.879866	1.572354
H	-0.868985	-0.879996	1.572325

Molecule# 1212

2-chloro-2-methylpropane

PointGroup: C3v

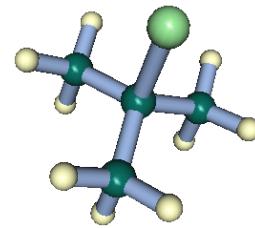
E= -618.159465754 au

ZPE= 0.121829 au

LUMO_eps= -0.01580 au

HOMO_eps= -0.29353 au

Dipole= 2.407 debye



14

C	0.000000	1.456520	-0.815071
C	1.261383	-0.728260	-0.815071
C	-1.261383	-0.728260	-0.815071
C	0.000000	0.000000	-0.370596
Cl	0.000000	0.000000	1.489306
H	-0.883600	1.977898	-0.450456
H	0.883600	1.977898	-0.450456
H	0.000000	1.501962	-1.906872
H	2.154710	-0.223729	-0.450456
H	1.271110	-1.754169	-0.450456
H	1.300737	-0.750981	-1.906872
H	-2.154710	-0.223729	-0.450456
H	-1.271110	-1.754169	-0.450456
H	-1.300737	-0.750981	-1.906872

Molecule# 1213

2-chloro-3-cyano-5-fluoropyridine

PointGroup: C1

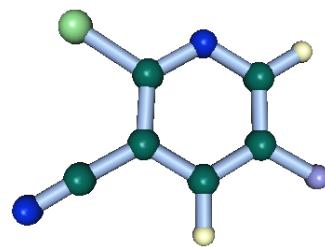
E= -899.550078210 au

ZPE= 0.069094 au

LUMO_eps= -0.10221 au

HOMO_eps= -0.29043 au

Dipole= 3.408 debye



12

C1	-2.197577	-1.227671	-0.000015
F	3.325479	0.455112	0.000010
N	0.390768	-1.596694	-0.000015
N	-2.115599	2.508502	0.000021
C	-0.276396	0.703136	0.000006
C	-0.547172	-0.677505	-0.000008
C	2.027709	0.116243	0.000004
C	1.061483	1.100236	0.000013
C	1.668300	-1.221079	-0.000009
C	-1.309558	1.686129	0.000014
H	1.333645	2.145419	0.000023
H	2.423474	-1.996630	-0.000016

Molecule# 1214

2-chloro-3-nitrosoturan

PointGroup: C1

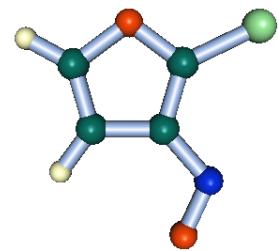
E= -819.076438773 au

ZPE= 0.057344 au

LUMO_eps= -0.11150 au

HOMO_eps= -0.23815 au

Dipole= 3.529 debye



10

C1	1.926269	-1.029667	0.000000
O	1.000529	1.396322	0.000001
O	-2.545474	-1.255419	-0.000001
N	-1.326289	-1.296988	-0.000001
C	-0.699105	-0.046948	0.000000
C	0.667284	0.101086	0.000000
C	-1.242421	1.285636	0.000000
C	-0.184456	2.114819	0.000001
H	-2.285347	1.546278	0.000000
H	-0.065452	3.182198	0.000001

Molecule# 1215

2-chloro-3-propenedisulfide

PointGroup: C1

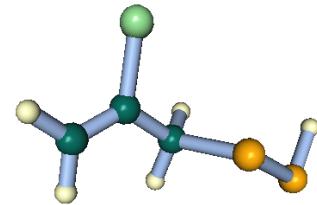
E= -1374.042049220 au

ZPE= 0.072051 au

LUMO_eps= -0.05677 au

HOMO_eps= -0.25469 au

Dipole= 1.572 debye



11

C1	-2.213770	-1.116422	0.019613
S	1.043133	0.085348	-0.719629
S	2.876136	-0.099112	0.233234
C	-1.513151	0.487919	0.204363
C	-0.101760	0.501799	0.686458
C	-2.230617	1.563308	-0.088361
H	2.830146	-1.417869	0.524098
H	0.054997	-0.235049	1.469729
H	0.155816	1.491757	1.054508
H	-3.249590	1.496805	-0.437101
H	-1.792416	2.545606	0.022903

Molecule# 1216

2-chloro-4-oxo-3-butenoyl chloride

PointGroup: C1

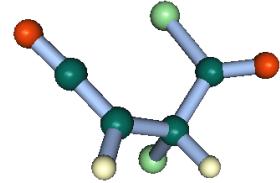
E= -1224.625270300 au

ZPE= 0.052568 au

LUMO_eps= -0.08519 au

HOMO_eps= -0.27824 au

Dipole= 2.688 debye



10

C1	1.196824	-1.594182	-0.748571
C1	-0.018487	1.607823	-0.809981
O	1.639322	1.360355	1.198885
O	-2.947869	-0.058570	-0.171301
C	0.488767	-0.684550	0.702596
C	0.860125	0.779605	0.528686
C	-0.940974	-0.958589	0.955829
C	-1.982431	-0.450327	0.322211
H	1.078224	-1.040998	1.539221
H	-1.194497	-1.722002	1.679561

Molecule# 1217

2-chloro-5-cyanothiophene

PointGroup: C1

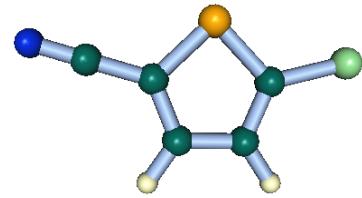
E= -1104.998531620 au

ZPE= 0.056012 au

LUMO_eps= -0.08356 au

HOMO_eps= -0.26487 au

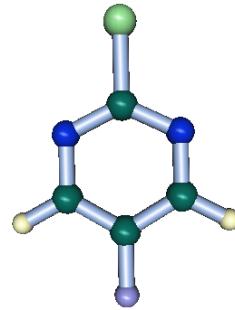
Dipole= 3.897 debye



10

C1	2.782522	-0.268531	0.000000
S	-0.110760	-1.024111	-0.000001
N	-3.828995	-0.415531	-0.000002
C	-0.790124	1.468188	0.000000
C	0.622911	1.455790	0.000000
C	-1.342826	0.212106	0.000000
C	1.123743	0.185775	0.000000
C	-2.711030	-0.129258	-0.000001
H	-1.387679	2.366653	0.000000
H	1.243873	2.337262	0.000002

Molecule# 1218
2-chloro-5-fluoropyrimidine
PointGroup: C2v
E= -823.323511811 au
ZPE= 0.058767 au
LUMO_eps= -0.08508 au
HOMO_eps= -0.28810 au
Dipole= 2.289 debye



10

C1	0.000000	0.000000	2.618722
F	0.000000	0.000000	-3.087327
N	0.000000	1.187499	0.290904
N	0.000000	-1.187499	0.290904
C	0.000000	0.000000	0.875246
C	0.000000	0.000000	-1.745780
C	0.000000	1.189332	-1.040282
C	0.000000	-1.189332	-1.040282
H	0.000000	2.145496	-1.549203
H	0.000000	-2.145496	-1.549203

Molecule# 1219

2-chloro-5-fluorothiophene

PointGroup: C1

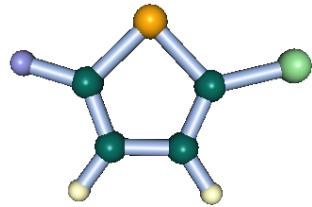
E= -1111.991161400 au

ZPE= 0.049248 au

LUMO_eps= -0.04095 au

HOMO_eps= -0.24270 au

Dipole= 1.135 debye



9

C1	-2.515817	-0.128816	0.000007
S	0.326747	-1.096199	-0.000007
F	2.880120	-0.361130	-0.000011
C	-0.231182	1.433389	0.000009
C	1.195500	1.353571	0.000004
C	-0.825108	0.213609	0.000004
C	1.617947	0.069156	-0.000005
H	-0.784651	2.359095	0.000016
H	1.861563	2.201781	0.000006

Molecule# 1220

2-chloro-5-isocyanatothiophene

PointGroup: C1

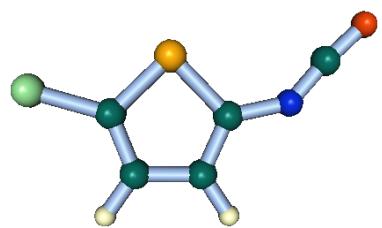
E= -1180.268507720 au

ZPE= 0.060647 au

LUMO_eps= -0.05720 au

HOMO_eps= -0.23741 au

Dipole= 1.781 debye



11

C1	3.117903	-0.625315	0.000000
S	0.125551	-0.848541	0.000000
O	-4.150489	-0.844343	-0.000002
N	-2.237269	0.548089	0.000001
C	-0.101979	1.727519	0.000002
C	-0.867078	0.598532	0.000001
C	1.293679	1.456131	0.000001
C	1.565665	0.124962	0.000000
C	-3.170305	-0.208471	0.000000
H	-0.528661	2.718444	0.000002
H	2.060415	2.214641	0.000002

Molecule# 1221

2-chloroallylisothiocyanate

PointGroup: C1

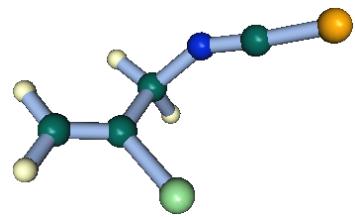
E= -1068.089074980 au

ZPE= 0.072563 au

LUMO_eps= -0.04770 au

HOMO_eps= -0.25654 au

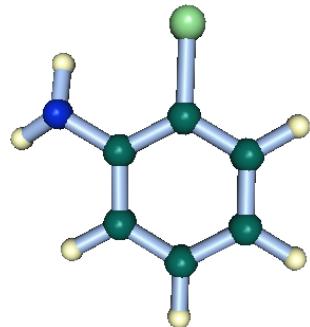
Dipole= 3.704 debye



11

C1	-1.347415	1.412561	0.204092
S	2.973465	0.301056	-0.225140
N	0.624438	-1.122322	0.123077
C	-1.679642	-0.291748	-0.037658
C	-0.706921	-1.216488	0.644751
C	1.609055	-0.467672	-0.001390
C	-2.720952	-0.690146	-0.750013
H	-0.681309	-1.001003	1.716381
H	-1.057855	-2.239216	0.515322
H	-2.900921	-1.746442	-0.895230
H	-3.409606	0.008805	-1.199480

Molecule# 1222
 2-chloroaniline
 PointGroup: C1
 E= -747.350798436 au
 ZPE= 0.107465 au
 LUMO_eps= -0.02489 au
 HOMO_eps= -0.22043 au
 Dipole= 1.822 debye



14

C	2.353096	0.002148	0.005068
C	1.834314	-1.289002	0.004046
C	1.509217	1.100037	-0.001011
C	0.457168	-1.465035	0.000236
C	0.115237	0.948254	-0.007408
C	-0.381938	-0.362325	-0.004647
N	-0.722435	2.046777	-0.068656
Cl	-2.123824	-0.611727	0.002158
H	3.423493	0.156593	0.009813
H	2.488997	-2.148477	0.007665
H	1.921615	2.101235	-0.007590
H	0.024888	-2.455106	0.003520
H	-0.338871	2.918571	0.253707
H	-1.680635	1.894648	0.199077

Molecule# 1223

2-chlorobutane

PointGroup: C1

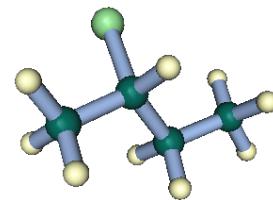
E= -618.157057917 au

ZPE= 0.122583 au

LUMO_eps= -0.01311 au

HOMO_eps= -0.29461 au

Dipole= 2.307 debye



14

C	-2.206969	-0.247941	0.120536
C	1.308098	1.482588	-0.007133
C	-1.084035	0.682292	-0.327997
C	0.256250	0.451574	0.355516
Cl	0.901845	-1.220351	-0.068863
H	-3.140782	0.008425	-0.380359
H	-2.375597	-0.171892	1.196607
H	-1.974733	-1.286618	-0.109767
H	0.967730	2.473657	0.301639
H	2.253331	1.274190	0.490384
H	1.481667	1.499431	-1.083110
H	-1.364879	1.719380	-0.116341
H	-0.943092	0.614242	-1.409190
H	0.124917	0.404075	1.435284

Molecule# 1224

2-chloroethenimine

PointGroup: C1

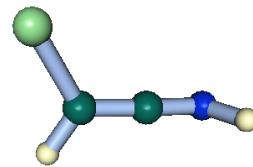
E= -592.393731363 au

ZPE= 0.035688 au

LUMO_eps= -0.06113 au

HOMO_eps= -0.24629 au

Dipole= 1.890 debye



6

C1	1.481060	-0.246052	0.000891
N	-2.257610	-0.337290	-0.128337
C	0.026216	0.722480	0.011202
C	-1.156808	0.167770	0.008826
H	-2.756780	-0.587380	0.724562
H	0.165580	1.789797	0.038481

Molecule# 1225

2-chloroethylisothiocyanate

PointGroup: C1

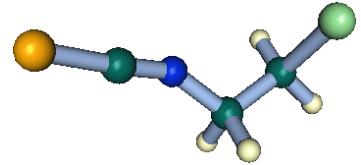
E= -1029.995761650 au

ZPE= 0.068102 au

LUMO_eps= -0.04434 au

HOMO_eps= -0.25816 au

Dipole= 3.662 debye



10

C1	-2.404059	-0.918678	0.064286
S	3.086866	-0.390320	0.010773
N	0.477949	0.509740	-0.210547
C	-0.645305	1.190578	0.353524
C	-1.953863	0.791832	-0.301178
C	1.598040	0.139991	-0.071736
H	-0.688979	1.001710	1.427947
H	-0.514156	2.267281	0.204283
H	-1.896342	0.876305	-1.382173
H	-2.760260	1.414766	0.074888

Molecule# 1226

2-chlorophenol

PointGroup: Cs

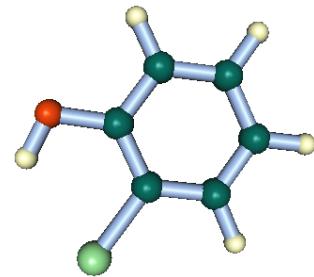
E= -767.224120028 au

ZPE= 0.095270 au

LUMO_eps= -0.03207 au

HOMO_eps= -0.24266 au

Dipole= 0.968 debye



13

C	1.592286	-1.728677	0.000000
C	2.181509	-0.467693	0.000000
C	0.212578	-1.863151	0.000000
C	1.379088	0.665360	0.000000
C	-0.604239	-0.733979	0.000000
C	0.000000	0.525088	0.000000
O	-1.948598	-0.906903	0.000000
Cl	-1.036509	1.945558	0.000000
H	2.211530	-2.615032	0.000000
H	3.256995	-0.363392	0.000000
H	-0.258879	-2.835831	0.000000
H	1.812238	1.655014	0.000000
H	-2.379775	-0.041703	0.000000

Molecule# 1227

2-chloropropane

PointGroup: Cs

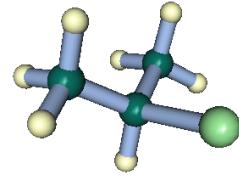
E= -578.829403920 au

ZPE= 0.094245 au

LUMO_eps= -0.01423 au

HOMO_eps= -0.29611 au

Dipole= 2.340 debye



11

C	-0.574621	-0.905235	1.270480
C	-0.574621	-0.905235	-1.270480
C	-0.574621	-0.076502	0.000000
Cl	0.896612	1.024877	0.000000
H	-0.565593	-0.272482	2.155996
H	-1.473445	-1.525794	1.299465
H	0.295393	-1.561000	1.305554
H	-0.565593	-0.272482	-2.155996
H	-1.473445	-1.525794	-1.299465
H	0.295393	-1.561000	-1.305554
H	-1.411924	0.617470	0.000000

Molecule# 1228

2-chloropyridine

PointGroup: Cs

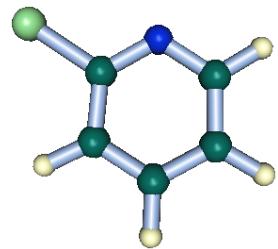
E= -708.011078235 au

ZPE= 0.078971 au

LUMO_eps= -0.05322 au

HOMO_eps= -0.27097 au

Dipole= 3.415 debye



11

C	1.117724	-1.621803	0.000000
C	-0.134070	-2.228093	0.000000
C	1.198783	-0.239009	0.000000
C	-1.256435	-1.414617	0.000000
C	0.000000	0.468958	0.000000
N	-1.193392	-0.079209	0.000000
Cl	0.066001	2.226123	0.000000
H	2.020758	-2.217277	0.000000
H	-0.237807	-3.303639	0.000000
H	2.145204	0.279330	0.000000
H	-2.252452	-1.840652	0.000000

Molecule# 1229

2-cyano-3-iminoacrylamide

PointGroup: C1

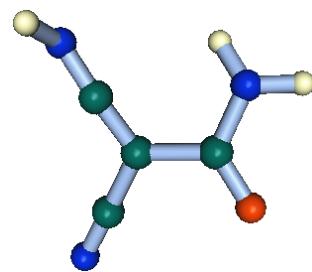
E= -393.814127565 au

ZPE= 0.070682 au

LUMO_eps= -0.07669 au

HOMO_eps= -0.28239 au

Dipole= 7.298 debye



11

O	1.200695	-1.750566	0.240229
N	2.095132	0.298369	-0.157996
N	-2.390612	-1.479398	-0.111412
N	-0.628948	2.555406	-0.003648
C	-0.321090	0.047446	-0.017924
C	1.054680	-0.568996	0.024318
C	-1.457343	-0.805306	-0.066056
C	-0.506482	1.358873	0.056891
H	1.962629	1.187336	-0.607887
H	3.009679	-0.117160	-0.220990
H	-0.725463	3.121623	0.835062

Molecule# 1230

2-deoxypentofuranose

PointGroup: C1

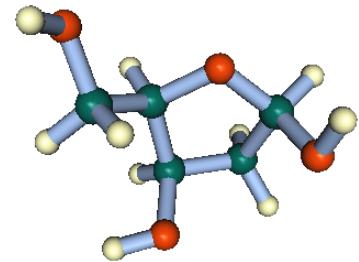
E= -497.622980298 au

ZPE= 0.157591 au

LUMO_eps= -0.02225 au

HOMO_eps= -0.26965 au

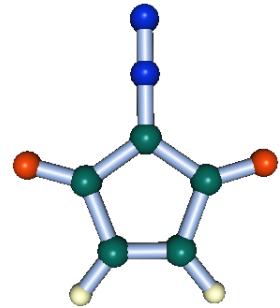
Dipole= 1.719 debye



19

C	-1.668271	0.461239	-0.765783
C	-0.367440	1.210024	-0.479394
C	0.689515	0.089265	-0.593294
C	-1.400343	-0.953458	-0.265482
C	1.856173	0.212999	0.364984
O	-0.004904	-1.155032	-0.396645
O	-0.459865	1.805275	0.814836
O	-1.823763	-1.057773	1.077424
O	2.879640	-0.684977	-0.054645
H	-2.518456	0.921796	-0.270321
H	-1.851125	0.435667	-1.839895
H	-0.178406	1.985616	-1.225571
H	1.093392	0.077484	-1.611423
H	-1.886026	-1.728437	-0.864473
H	1.515337	-0.010936	1.377193
H	2.231369	1.245733	0.342390
H	0.267278	2.422971	0.931773
H	-1.567425	-1.926770	1.403733
H	3.507392	-0.803481	0.662654

Molecule# 1231
2-diazo-4-cyclopentene-1,3-dione
PointGroup: Cs
E= -451.782003302 au
ZPE= 0.065603 au
LUMO_eps= -0.11629 au
HOMO_eps= -0.27830 au
Dipole= 2.048 debye



11

O	-2.366456	-0.102241	0.000000
O	2.366456	-0.102242	0.000000
N	0.000000	1.711499	0.000000
N	0.000000	2.831814	0.000000
C	0.000000	0.410913	0.000000
C	-1.204476	-0.433611	0.000000
C	1.204475	-0.433612	0.000000
C	-0.666466	-1.837920	0.000000
C	0.666466	-1.837921	0.000000
H	-1.332425	-2.687206	0.000000
H	1.332424	-2.687207	0.000000

Molecule# 1232

2-ethoxyethanol

PointGroup: C1

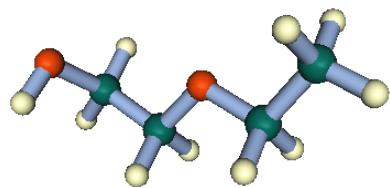
E= -309.001662493 au

ZPE= 0.140689 au

LUMO_eps= -0.01623 au

HOMO_eps= -0.26642 au

Dipole= 2.692 debye



16

C	-2.749765	-0.583904	-0.153459
C	-1.683862	0.394741	0.292969
C	1.943584	0.269479	-0.404816
C	0.638750	0.818274	0.137976
O	2.366200	-0.943905	0.203717
O	-0.429726	-0.030575	-0.214940
H	-3.725084	-0.279288	0.228236
H	-2.802470	-0.625322	-1.241261
H	-2.530599	-1.585069	0.216980
H	-1.640996	0.446136	1.389514
H	-1.909147	1.406285	-0.072242
H	2.712674	1.045372	-0.307406
H	1.826768	0.042599	-1.464123
H	0.481049	1.826798	-0.273000
H	0.701134	0.920416	1.233025
H	2.502636	-0.793628	1.144037

Molecule# 1233

2-ethyl-1,3-butadiene

PointGroup: C1

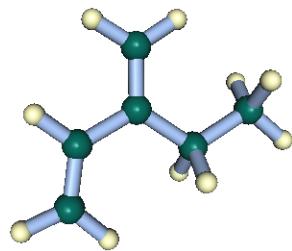
E= -234.715488588 au

ZPE= 0.141864 au

LUMO_eps= -0.03813 au

HOMO_eps= -0.23918 au

Dipole= 0.408 debye



16

C	-0.431809	1.690207	-0.000125
C	0.097948	0.460822	-0.000034
C	1.557665	0.319248	-0.000030
C	2.248973	-0.821807	0.000057
C	-0.736939	-0.798581	0.000064
H	0.202753	2.566781	-0.000196
H	-1.497262	1.864489	-0.000133
H	2.107527	1.255021	-0.000107
H	1.772778	-1.792680	0.000137
H	3.330020	-0.814825	0.000051
C	-2.250834	-0.611254	0.000050
H	-0.448920	-1.398382	-0.868916
H	-0.448919	-1.398250	0.869134
H	-2.589661	-0.066300	0.881969
H	-2.748682	-1.581216	0.000132
H	-2.589661	-0.066449	-0.881960

Molecule# 1234

2-ethylacrolein

PointGroup: C1

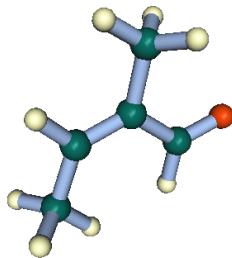
E= -270.656906803 au

ZPE= 0.117322 au

LUMO_eps= -0.06853 au

HOMO_eps= -0.25962 au

Dipole= 3.695 debye



14

C	2.315360	-0.488363	0.000127
C	1.228339	0.539082	0.000162
C	-0.105961	0.377961	0.000037
C	-1.055394	1.543354	0.000099
C	-0.727198	-0.958438	-0.000171
O	-1.927501	-1.139157	-0.000289
H	2.957003	-0.350602	0.874410
H	1.962408	-1.515125	-0.000023
H	2.957142	-0.350395	-0.874021
H	1.592453	1.563287	0.000311
H	-1.709375	1.509936	0.872664
H	-1.709240	1.510139	-0.872576
H	-0.516479	2.489320	0.000251
H	-0.044780	-1.824879	-0.000220

Molecule# 1235

2-ethylpyrazine

PointGroup: C1

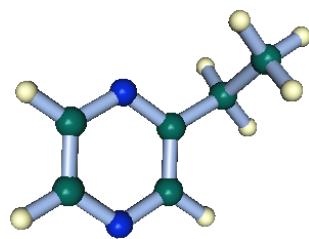
E= -343.076886725 au

ZPE= 0.132657 au

LUMO_eps= -0.06262 au

HOMO_eps= -0.25567 au

Dipole= 0.710 debye



16

C	2.233334	-0.116230	0.218263
C	1.430378	-1.225938	-0.017669
C	0.433277	1.226506	-0.053715
C	-0.386763	0.119094	-0.289925
C	-2.716909	-0.220171	0.627717
C	-1.861257	0.258329	-0.552378
N	1.734306	1.117813	0.199732
N	0.129285	-1.113947	-0.269666
H	3.291804	-0.223926	0.422137
H	1.847245	-2.226480	-0.005825
H	0.020691	2.228991	-0.073988
H	-2.497551	-1.261629	0.860291
H	-3.777994	-0.138114	0.391141
H	-2.522970	0.375105	1.521205
H	-2.091480	1.300250	-0.781301
H	-2.107242	-0.330802	-1.437880

Molecule# 1236

2-ethylpyridine

PointGroup: C1

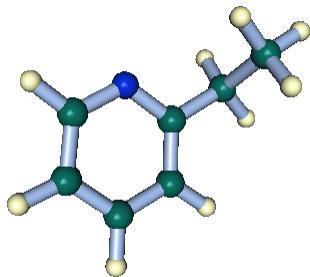
E= -327.038897374 au

ZPE= 0.144546 au

LUMO_eps= -0.03714 au

HOMO_eps= -0.25970 au

Dipole= 1.813 debye



17

C	1.751556	1.082901	0.182606
C	2.271460	-0.203318	0.214278
C	0.398740	1.250753	-0.075620
C	1.403367	-1.263547	-0.016890
C	-0.401322	0.128061	-0.295305
C	-2.726106	-0.194903	0.645780
C	-1.881035	0.248415	-0.555272
N	0.103790	-1.111829	-0.264838
H	2.388226	1.940873	0.354047
H	3.319053	-0.385161	0.408951
H	-0.037426	2.240056	-0.109962
H	1.770415	-2.283998	-0.005475
H	-2.495860	-1.225772	0.912489
H	-3.789953	-0.129702	0.414763
H	-2.530642	0.432256	1.517119
H	-2.122699	1.279481	-0.819168
H	-2.127609	-0.375408	-1.416356

Molecule# 1237

2-ethynyl-5-nitrothiophene

PointGroup: C1

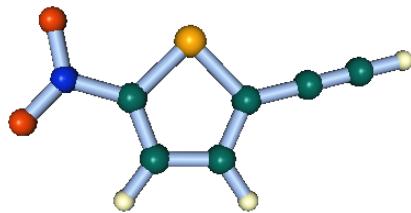
E= -833.850966443 au

ZPE= 0.078252 au

LUMO_eps= -0.12064 au

HOMO_eps= -0.26711 au

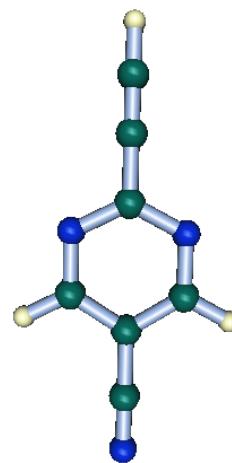
Dipole= 4.988 debye



13

S	-0.341510	-0.991986	-0.000006
O	2.519011	-1.365713	-0.000008
O	3.108200	0.731357	0.000007
N	2.272192	-0.162941	0.000001
C	0.889034	0.218887	0.000002
C	0.400378	1.497039	0.000009
C	-1.005032	1.513710	0.000008
C	-1.562355	0.249687	0.000001
C	-2.927020	-0.091395	-0.000003
C	-4.090699	-0.393484	-0.000005
H	1.038617	2.365715	0.000015
H	-1.603763	2.410935	0.000014
H	-5.119557	-0.656096	-0.000007

Molecule# 1238
 2-ethynylpyrimidine-5-carbonitrile
 PointGroup: C2v
 E= -432.858411075 au
 ZPE= 0.083890 au
 LUMO_eps= -0.10868 au
 HOMO_eps= -0.29125 au
 Dipole= 2.631 debye



13

C	0.000000	0.000000	-3.930784
C	0.000000	0.000000	-2.731540
C	0.000000	0.000000	2.793427
C	0.000000	1.188249	0.632112
C	0.000000	-1.188249	0.632112
C	0.000000	0.000000	-1.302335
C	0.000000	0.000000	1.369921
N	0.000000	0.000000	3.945700
N	0.000000	1.194481	-0.690626
N	0.000000	-1.194481	-0.690626
H	0.000000	0.000000	-4.992828
H	0.000000	2.149383	1.132106
H	0.000000	-2.149383	1.132106

Molecule# 1239

2-fluoro-1H-triazine

PointGroup: C1

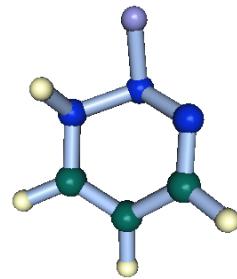
E= -380.803414330 au

ZPE= 0.076969 au

LUMO_eps= -0.07006 au

HOMO_eps= -0.23421 au

Dipole= 4.168 debye



11

F	-2.150096	-0.001053	0.020213
N	-0.814685	0.069525	-0.443341
N	-0.277930	1.215684	0.168577
N	-0.249750	-1.157396	0.094708
C	1.005130	1.204416	0.110976
C	1.127688	-1.139416	0.040064
C	1.779078	0.018424	-0.196713
H	-0.688110	-1.456788	0.966414
H	1.504722	2.099325	0.462256
H	1.610499	-2.086619	0.240445
H	2.848926	0.058329	-0.316594

Molecule# 1240

2-fluoro-2-nitro-3H-furan

PointGroup: C1

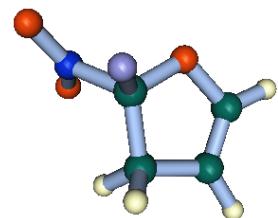
E= -535.176575524 au

ZPE= 0.086622 au

LUMO_eps= -0.09400 au

HOMO_eps= -0.27145 au

Dipole= 4.357 debye



13

F	-0.375818	1.697446	0.222764
O	0.626983	0.220870	-1.127340
O	-2.388585	0.216606	-0.155235
O	-1.228699	-1.610380	0.030610
N	-1.359931	-0.402241	-0.018206
C	-0.021614	0.404745	0.085285
C	0.896960	-0.092476	1.209348
C	1.920548	-0.209156	-0.846755
C	2.155262	-0.394312	0.440990
H	0.482254	-0.975565	1.692874
H	1.010076	0.694126	1.955231
H	2.540130	-0.330936	-1.718095
H	3.084893	-0.718520	0.875072

Molecule# 1241

2-fluoroethenimine

PointGroup: C1

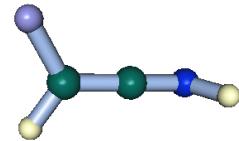
E= -232.027624120 au

ZPE= 0.037077 au

LUMO_eps= -0.06106 au

HOMO_eps= -0.24848 au

Dipole= 1.953 debye



6

F	1.606461	-0.410727	0.002376
N	-1.822683	-0.186473	-0.129924
C	0.603795	0.505949	0.008579
C	-0.650353	0.130122	0.010605
H	-2.343052	-0.348985	0.733356
H	0.923032	1.534412	0.039623

Molecule# 1242

2-fluorophenol

PointGroup: Cs

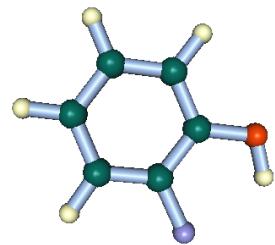
E= -406.866490830 au

ZPE= 0.096635 au

LUMO_eps= -0.02529 au

HOMO_eps= -0.24168 au

Dipole= 0.818 debye



13

C	-1.104968	-1.663429	0.000000
C	-1.932817	-0.545821	0.000000
C	0.277669	-1.523878	0.000000
C	-1.373010	0.728438	0.000000
C	0.848168	-0.256096	0.000000
C	0.000000	0.846928	0.000000
O	2.201785	-0.118858	0.000000
F	0.585079	2.077027	0.000000
H	-1.536548	-2.654610	0.000000
H	-3.007204	-0.659939	0.000000
H	0.930968	-2.385091	0.000000
H	-1.982396	1.621014	0.000000
H	2.424943	0.819401	0.000000

Molecule# 1243

2-fluoropyridine

PointGroup: Cs

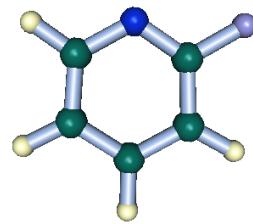
E= -347.661779582 au

ZPE= 0.080626 au

LUMO_eps= -0.05145 au

HOMO_eps= -0.27553 au

Dipole= 3.374 debye



11

C	0.000000	0.890610	0.000000
C	1.213082	0.212929	0.000000
C	1.150826	-1.170346	0.000000
C	-0.094041	-1.795003	0.000000
C	-1.228714	-0.999639	0.000000
N	-1.183800	0.338362	0.000000
F	0.025740	2.234588	0.000000
H	2.146052	0.755943	0.000000
H	2.060970	-1.754404	0.000000
H	-0.181364	-2.871685	0.000000
H	-2.217635	-1.440986	0.000000

Molecule# 1244

2-formyl-3-oxoacrylonitrile

PointGroup: C1

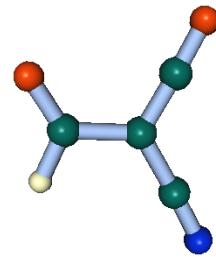
E= -358.301006162 au

ZPE= 0.041809 au

LUMO_eps= -0.11126 au

HOMO_eps= -0.30169 au

Dipole= 1.175 debye



8

O	-1.068209	2.068569	-0.000013
O	-1.835661	-1.349617	0.000009
N	2.746608	-0.160912	0.000000
C	0.178758	-0.075978	0.000000
C	-0.472691	1.094157	-0.000007
C	-0.632050	-1.322264	0.000009
C	1.595368	-0.094455	0.000000
H	-0.011614	-2.233995	0.000017

Molecule# 1245

2-furylmethanol

PointGroup: C1

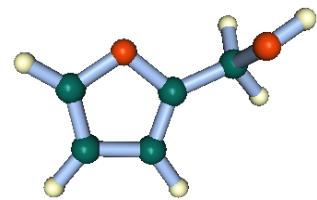
E= -344.688677085 au

ZPE= 0.102400 au

LUMO_eps= -0.02342 au

HOMO_eps= -0.23627 au

Dipole= 1.565 debye



13

O	2.347421	-0.187082	-0.656389
C	1.620033	0.221901	0.509756
C	0.166572	0.196034	0.229739
C	-0.747500	1.169251	-0.020672
C	-2.002371	0.514222	-0.220304
C	-1.758701	-0.811172	-0.075955
O	-0.446384	-1.026217	0.202246
H	3.264764	-0.337168	-0.408291
H	1.894901	1.240412	0.798884
H	1.842877	-0.446236	1.347719
H	-0.548601	2.226247	-0.064386
H	-2.952138	0.969176	-0.441152
H	-2.378300	-1.687460	-0.135014

Molecule# 1246

2-hexanone

PointGroup: C1

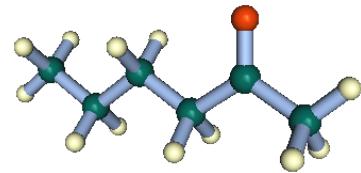
E= -311.220449577 au

ZPE= 0.168525 au

LUMO_eps= -0.02504 au

HOMO_eps= -0.25518 au

Dipole= 2.889 debye



19

C	1.713767	0.184314	-0.006094
C	2.992613	-0.627337	0.018624
C	-3.398174	0.257813	0.014447
C	0.415711	-0.605242	-0.018955
C	-2.129427	-0.592675	-0.013892
C	-0.849467	0.243536	0.010725
O	1.732799	1.394734	-0.012565
H	3.048893	-1.205545	0.943733
H	3.010172	-1.344276	-0.804455
H	3.853628	0.032351	-0.047922
H	-3.440169	0.930013	-0.844742
H	-4.294888	-0.362918	-0.005028
H	-3.439164	0.873178	0.915292
H	0.440487	-1.300663	0.827754
H	0.432242	-1.246871	-0.907744
H	-2.134229	-1.223254	-0.908517
H	-2.132488	-1.278680	0.838933
H	-0.837342	0.875293	0.901856
H	-0.839678	0.931040	-0.837776

Molecule# 1247

2-hexyne

PointGroup: Cs

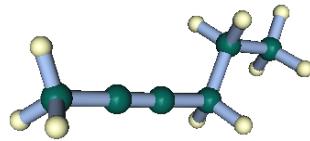
E= -234.699213520 au

ZPE= 0.140992 au

LUMO_eps= -0.01129 au

HOMO_eps= -0.25287 au

Dipole= 0.167 debye



16

C	1.212934	-2.830317	0.000000
C	-1.715980	2.860634	0.000000
C	0.924480	-0.299270	0.000000
C	0.000000	0.830193	0.000000
C	0.223042	-1.668570	0.000000
C	-0.778310	1.745812	0.000000
H	0.694512	-3.789693	0.000000
H	-2.748510	2.506561	0.000000
H	1.857339	-2.802347	0.881179
H	1.857339	-2.802347	-0.881179
H	-0.428117	-1.730803	-0.874251
H	-0.428117	-1.730803	0.874251
H	1.579877	-0.230796	-0.873928
H	1.579877	-0.230796	0.873928
H	-1.580599	3.490066	0.881436
H	-1.580599	3.490066	-0.881436

Molecule# 1248

2-hydroxy-3-sulfanylpropanethial

PointGroup: C1

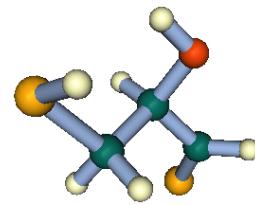
E= -989.650946333 au

ZPE= 0.086376 au

LUMO_eps= -0.10252 au

HOMO_eps= -0.24106 au

Dipole= 1.874 debye



12

O	-0.433596	1.791440	-0.034122
C	0.092369	0.494830	-0.264861
C	-0.760877	-0.602898	0.406048
S	-2.513763	-0.566762	-0.143480
S	2.654148	-0.553579	-0.123783
C	1.477017	0.465249	0.314637
H	-1.327788	1.811360	-0.398006
H	0.147240	0.280150	-1.336058
H	-0.734102	-0.508767	1.489120
H	-0.369979	-1.580613	0.134186
H	-2.975713	0.256316	0.814023
H	1.631903	1.192396	1.110975

Molecule# 1249

2-hydroxyethenethione

PointGroup: C1

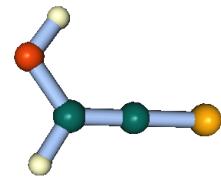
E= -550.858519443 au

ZPE= 0.035362 au

LUMO_eps= -0.10808 au

HOMO_eps= -0.21649 au

Dipole= 0.476 debye



6

S -1.667961 -0.117975 -0.000019

O 2.177698 -0.373093 0.000025

C -0.141968 0.236010 -0.000001

C 1.136462 0.528571 0.000012

H 1.833657 -1.273070 0.000026

H 1.465171 1.557929 0.000014

Molecule# 1250

2-hydroxypropanenitrile

PointGroup: C1

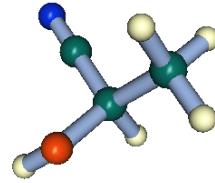
E= -247.379028422 au

ZPE= 0.078412 au

LUMO_eps= -0.02896 au

HOMO_eps= -0.32229 au

Dipole= 3.106 debye



10

C	1.176464	-1.121040	-0.130625
C	0.378337	0.070180	0.381926
O	0.913379	1.242348	-0.219964
H	0.423642	2.014994	0.081178
H	0.813225	-2.045334	0.315541
H	1.091458	-1.191726	-1.213368
H	2.223270	-0.983889	0.134284
C	-1.060337	-0.071096	0.078798
H	0.468455	0.125994	1.472411
N	-2.184838	-0.161013	-0.144418

Molecule# 1251

2-imidazolidinethione

PointGroup: C2

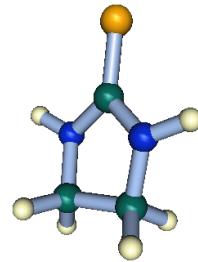
E= -625.756617297 au

ZPE= 0.097436 au

LUMO_eps= -0.02426 au

HOMO_eps= -0.21098 au

Dipole= 5.750 debye



12

S	0.000000	0.000000	2.086086
C	0.000000	0.000000	0.422971
N	0.000000	1.095429	-0.390077
C	-0.231274	0.733283	-1.785169
C	0.231274	-0.733283	-1.785169
N	0.000000	-1.095429	-0.390077
H	-0.275915	1.980156	-0.001574
H	0.347846	1.354361	-2.465670
H	-1.290782	0.811565	-2.048808
H	1.290782	-0.811565	-2.048808
H	-0.347846	-1.354361	-2.465670
H	0.275915	-1.980156	-0.001574

Molecule# 1252

2-isobutylpyrazine

PointGroup: C1

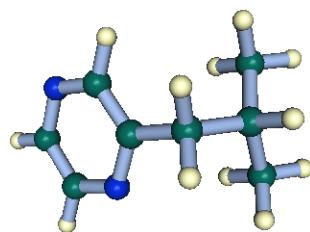
E= -421.730702923 au

ZPE= 0.189023 au

LUMO_eps= -0.06092 au

HOMO_eps= -0.25386 au

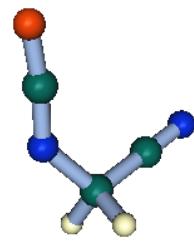
Dipole= 0.832 debye



22

C	2.780946	0.034090	-0.496412
C	2.081979	1.196215	-0.197941
C	1.046417	-1.191362	0.282233
C	0.324882	-0.029326	0.581800
C	-2.293729	1.300701	-0.581142
C	-2.259009	-1.219791	-0.767466
C	-1.051716	-0.083716	1.186804
C	-2.235332	-0.022090	0.185648
N	2.262542	-1.168677	-0.252894
N	0.864183	1.170413	0.338964
H	3.772639	0.071644	-0.930765
H	2.515504	2.170975	-0.390188
H	0.623598	-2.167465	0.490849
H	-1.429831	1.424092	-1.234865
H	-2.314015	2.154514	0.096934
H	-3.190666	1.339309	-1.201754
H	-3.158002	-1.199555	-1.385241
H	-1.400440	-1.213979	-1.441787
H	-2.251536	-2.166685	-0.224003
H	-1.144990	-1.004046	1.767797
H	-1.141864	0.752268	1.881855
H	-3.134101	-0.081540	0.807527

Molecule# 1253
2-isocyanatoacetonitrile
PointGroup: C1
E= -300.336145176 au
ZPE= 0.049808 au
LUMO_eps= -0.04013 au
HOMO_eps= -0.31892 au
Dipole= 3.596 debye



8
0 2.314952 -0.784408 0.074091
N 0.623911 0.847435 -0.202435
N -2.202485 -1.136869 -0.048234
C -0.767680 1.044455 0.111907
C 1.438243 -0.023374 -0.027656
C -1.574416 -0.177183 0.019351
H -1.175339 1.782439 -0.578436
H -0.871142 1.455478 1.118785

Molecule# 1254

2-isocyanatoethanedithioicacid

PointGroup: C1

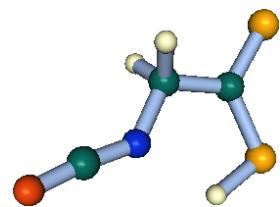
E= -1042.627266150 au

ZPE= 0.057885 au

LUMO_eps= -0.09596 au

HOMO_eps= -0.24502 au

Dipole= 1.162 debye



10

S	2.378504	-0.996830	-0.060055
S	1.032305	1.615124	-0.000766
O	-3.857822	-0.222967	-0.090876
N	-1.504533	-0.005601	0.047838
C	0.996939	-0.123544	0.017628
C	-0.336437	-0.850557	0.141815
C	-2.693129	-0.177700	-0.020459
H	-0.301843	1.818938	0.055450
H	-0.325396	-1.359868	1.107578
H	-0.355645	-1.618027	-0.631648

Molecule# 1255

2-isopropoxypropane

PointGroup: C2

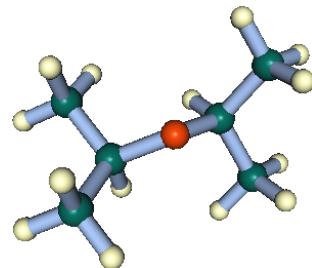
E= -312.420364573 au

ZPE= 0.191424 au

LUMO_eps= -0.01203 au

HOMO_eps= -0.25482 au

Dipole= 1.241 debye



21

C	0.000000	2.369897	0.648656
C	1.795861	1.149187	-0.648464
C	0.000000	-2.369897	0.648656
C	-1.795861	-1.149187	-0.648464
C	0.328511	1.169473	-0.225250
C	-0.328511	-1.169473	-0.225250
O	0.000000	0.000000	0.530194
H	0.237389	3.300652	0.131809
H	-1.057482	2.376595	0.910750
H	0.579665	2.331751	1.572195
H	2.036399	2.028649	-1.248423
H	2.027144	0.266481	-1.245332
H	2.440231	1.144037	0.231844
H	-0.237389	-3.300652	0.131809
H	1.057482	-2.376595	0.910750
H	-0.579665	-2.331751	1.572195
H	-2.036399	-2.028649	-1.248423
H	-2.027144	-0.266481	-1.245332
H	-2.440231	-1.144037	0.231844
H	-0.300157	1.205375	-1.123271
H	0.300157	-1.205375	-1.123271

Molecule# 1256

2-isothiocyanato-1,3-thiazole

PointGroup: C1

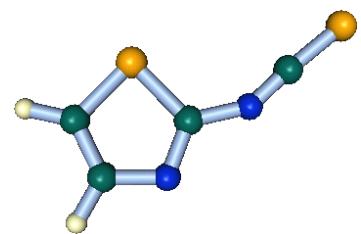
E= -1059.655952360 au

ZPE= 0.056032 au

LUMO_eps= -0.07789 au

HOMO_eps= -0.24787 au

Dipole= 2.757 debye



10

S	-1.176502	1.188742	0.000000
S	3.433639	0.144524	0.000000
N	-1.439432	-1.384848	0.000000
N	0.798861	-0.695105	0.000000
C	-0.535866	-0.452056	0.000000
C	-2.765808	0.515362	0.000000
C	-2.694196	-0.843269	0.000000
C	1.922253	-0.288941	0.000000
H	-3.639896	1.143256	0.000000
H	-3.548597	-1.502417	0.000000

Molecule# 1257

2-isothiocyanatoacetamide

PointGroup: C1

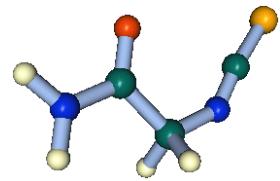
E= -699.802887912 au

ZPE= 0.074818 au

LUMO_eps= -0.03719 au

HOMO_eps= -0.24773 au

Dipole= 6.349 debye



11

S	2.745348	-0.356309	0.000063
O	-0.994220	-1.299184	0.000009
N	-3.011806	-0.267700	-0.000097
N	0.394126	1.102920	-0.000391
C	-1.019553	1.122041	0.000287
C	-1.651289	-0.284113	0.000026
C	1.362947	0.407332	-0.000131
H	-1.377130	1.669767	-0.876347
H	-1.376320	1.668960	0.877770
H	-3.544575	0.582927	-0.000097
H	-3.502658	-1.145330	-0.000094

Molecule# 1258

2-methoxy-1-propene

PointGroup: C1

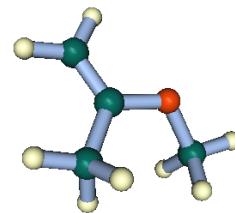
E= -232.525360175 au

ZPE= 0.112269 au

LUMO_eps= -0.01356 au

HOMO_eps= -0.22951 au

Dipole= 1.882 debye



13

C	1.837929	-0.075225	0.168133
H	1.826268	0.039396	1.255725
H	2.650139	-0.742755	-0.108297
H	2.008448	0.898348	-0.296127
O	0.647190	-0.693975	-0.300207
C	-0.598702	1.412224	-0.036759
H	-0.014163	1.839066	0.780446
H	-0.198576	1.814610	-0.970439
H	-1.625342	1.752574	0.072846
C	-0.558029	-0.087441	-0.037725
C	-1.627694	-0.863197	0.124504
H	-2.606952	-0.428216	0.248327
H	-1.538361	-1.939393	0.110257

Molecule# 1259

2-methoxy-2-methylpropane

PointGroup: Cs

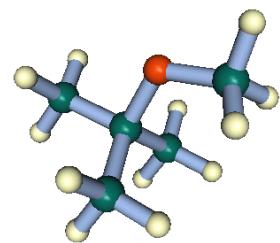
E= -273.084672576 au

ZPE= 0.162926 au

LUMO_eps= -0.01248 au

HOMO_eps= -0.25826 au

Dipole= 1.259 debye



18

C -0.634025 0.771526 1.262380

C 1.518392 1.037638 0.000000

C -0.634025 0.771526 -1.262380

C -0.634025 -1.948562 0.000000

C 0.140834 0.377397 0.000000

O 0.443226 -1.034249 0.000000

H -0.101780 0.437781 2.153609

H -0.741929 1.855478 1.313981

H -1.636409 0.343353 1.277197

H 2.081691 0.735411 -0.882718

H 2.081691 0.735411 0.882718

H 1.426783 2.124044 0.000000

H -1.636409 0.343353 -1.277197

H -0.741929 1.855478 -1.313981

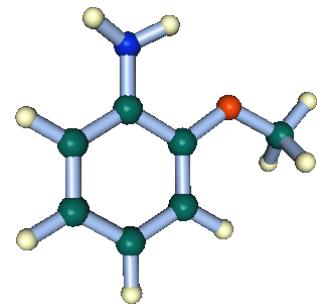
H -0.101780 0.437781 -2.153609

H -1.264755 -1.854556 -0.889485

H -1.264755 -1.854556 0.889485

H -0.189132 -2.942139 0.000000

Molecule# 1260
 2-methoxyaniline
 PointGroup: C1
 E= -402.285061030 au
 ZPE= 0.149514 au
 LUMO_eps= -0.01293 au
 HOMO_eps= -0.20003 au
 Dipole= 1.557 debye



18

C	-2.271210	-0.667396	0.006455
C	-1.340708	-1.693820	0.003564
C	-1.847275	0.658049	-0.000251
C	0.022067	-1.392654	-0.001131
C	-0.492758	0.980526	-0.008667
C	0.445302	-0.071805	-0.005646
C	2.767671	-0.660845	0.004342
N	-0.043263	2.295390	-0.074695
O	1.756422	0.332204	0.000731
H	-3.329530	-0.889156	0.012129
H	-1.659536	-2.726611	0.006451
H	-2.575105	1.460127	-0.006553
H	0.743830	-2.195462	0.001739
H	2.710088	-1.289626	-0.887662
H	2.704278	-1.291535	0.894876
H	3.714636	-0.127595	0.007528
H	-0.670523	2.990656	0.293401
H	0.914787	2.431518	0.203116

Molecule# 1261

2-methoxyethanamine

PointGroup: C1

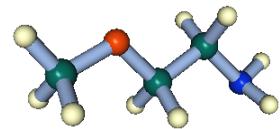
E= -249.794849715 au

ZPE= 0.125357 au

LUMO_eps= -0.01378 au

HOMO_eps= -0.24940 au

Dipole= 0.855 debye



14

C	2.394338	-0.198378	0.010397
C	-1.213963	0.512011	-0.011820
C	0.040704	-0.342423	0.060690
N	-2.400419	-0.343513	0.068122
O	1.170345	0.499841	-0.068361
H	3.193257	0.531998	-0.100922
H	2.481000	-0.946782	-0.786913
H	2.505379	-0.705551	0.976378
H	-1.223477	1.192544	0.840371
H	-1.165713	1.129196	-0.917074
H	0.034198	-1.091761	-0.745001
H	0.066402	-0.885403	1.013302
H	-2.543778	-0.851532	-0.796036
H	-3.233572	0.205897	0.230329

Molecule# 1262

2-methoxyethanol

PointGroup: C1

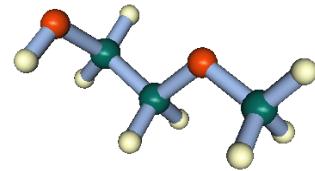
E= -269.668292942 au

ZPE= 0.112406 au

LUMO_eps= -0.01673 au

HOMO_eps= -0.26898 au

Dipole= 2.782 debye



13

C	-2.240901	-0.228900	0.078947
C	1.357635	0.506201	-0.241163
C	-0.057727	0.632576	0.286522
O	1.985166	-0.733246	0.058970
O	-0.911332	-0.260311	-0.393888
H	-2.296798	-0.511289	1.137407
H	-2.810353	-0.945359	-0.509172
H	-2.687110	0.766333	-0.039775
H	1.946368	1.347748	0.143838
H	1.344535	0.574466	-1.328580
H	-0.397375	1.669916	0.147193
H	-0.075546	0.427374	1.368715
H	2.031563	-0.840001	1.013883

Molecule# 1263

2-methoxyphenol

PointGroup: Cs

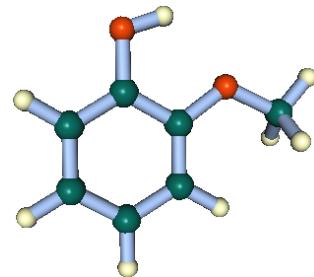
E= -422.159393855 au

ZPE= 0.137290 au

LUMO_eps= -0.01505 au

HOMO_eps= -0.21883 au

Dipole= 2.684 debye



17

C	-0.983062	-2.154025	0.000000
C	-1.860094	-1.080555	0.000000
C	0.392477	-1.934250	0.000000
C	-1.369349	0.225898	0.000000
C	0.887643	-0.641461	0.000000
C	0.000000	0.446658	0.000000
C	-0.195214	2.837494	0.000000
O	2.233459	-0.428850	0.000000
O	0.616159	1.672471	0.000000
H	-1.361602	-3.166654	0.000000
H	-2.928255	-1.246184	0.000000
H	1.093761	-2.757095	0.000000
H	-2.058350	1.057052	0.000000
H	-0.824743	2.879274	0.891811
H	-0.824743	2.879274	-0.891811
H	0.488417	3.681876	0.000000
H	2.384168	0.524940	0.000000

Molecule# 1264

2-methoxypropane

PointGroup: C1

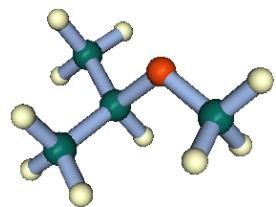
E= -233.756914632 au

ZPE= 0.135404 au

LUMO_eps= -0.01066 au

HOMO_eps= -0.26064 au

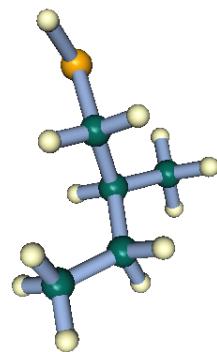
Dipole= 1.246 debye



15

C	-0.678099	1.442161	-0.097723
C	-1.602385	-0.909150	-0.006698
C	1.963999	-0.107579	0.092089
C	-0.421488	-0.006587	0.311499
O	0.708102	-0.560944	-0.366728
H	-1.546873	1.837096	0.431111
H	0.169074	2.086994	0.135299
H	-0.870837	1.501789	-1.170041
H	-2.500908	-0.561297	0.503988
H	-1.397458	-1.932194	0.306542
H	-1.795646	-0.912336	-1.080473
H	2.130121	0.953843	-0.119355
H	2.722137	-0.686882	-0.431688
H	2.076887	-0.270336	1.171121
H	-0.223479	-0.042199	1.392313

Molecule# 1265
 2-methyl-1-butanethiol
 PointGroup: C1
 E= -596.067925283 au
 ZPE= 0.159159 au
 LUMO_eps= -0.01639 au
 HOMO_eps= -0.23880 au
 Dipole= 1.715 debye



18
 C 0.033256 1.911012 -0.006826
 H -0.986044 2.108323 -0.337943
 H 0.093132 2.170909 1.052977
 H 0.697112 2.582639 -0.552731
 S -2.221681 -0.406315 -0.170182
 H -2.696542 -1.507291 0.437978
 C -0.500845 -0.518317 0.493893
 H -0.520646 -0.291581 1.560399
 H -0.169368 -1.544432 0.361547
 C 0.437737 0.451031 -0.231891
 H 0.370711 0.237349 -1.303989
 C 2.508461 -1.112816 -0.216529
 H 3.564281 -1.156476 0.053666
 H 2.018303 -1.959968 0.264207
 H 2.437887 -1.258057 -1.296481
 C 1.899038 0.226212 0.199414
 H 2.499117 1.032331 -0.230492
 H 1.973065 0.344573 1.285406

Molecule# 1266

2-methyl-1-butanol

PointGroup: C1

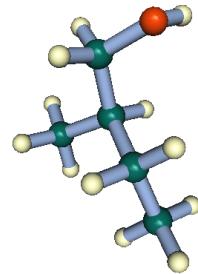
E= -273.093124947 au

ZPE= 0.164489 au

LUMO_eps= -0.01423 au

HOMO_eps= -0.27771 au

Dipole= 1.590 debye



18

C	-2.236267	-0.829238	-0.168845
C	-0.460692	1.802331	-0.023240
C	-0.836105	-0.683283	0.427209
C	1.500792	0.264459	0.201369
C	0.043139	0.374428	-0.255318
O	2.109917	-0.991421	-0.095886
H	-2.822588	0.085548	-0.074475
H	-2.186814	-1.082790	-1.230252
H	-2.790772	-1.623663	0.332395
H	-0.462102	2.045466	1.042320
H	-1.476626	1.936066	-0.392815
H	0.171194	2.533818	-0.530269
H	-0.321864	-1.644079	0.373767
H	-0.914617	-0.436619	1.491531
H	1.558959	0.362361	1.287435
H	2.087287	1.082323	-0.232344
H	0.027882	0.181040	-1.336643
H	2.185520	-1.080283	-1.050612

Molecule# 1267

2-methyl-1-buten-3-yne

PointGroup: Cs

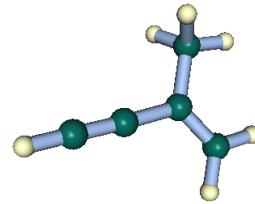
E= -194.132457528 au

ZPE= 0.089015 au

LUMO_eps= -0.03919 au

HOMO_eps= -0.25010 au

Dipole= 0.542 debye



11

C	-1.467731	0.790367	0.000000
H	-1.610102	1.869749	0.000000
H	-1.963613	0.371038	0.877295
H	-1.963613	0.371038	-0.877295
C	0.530643	-2.135031	0.000000
H	0.736992	-3.175778	0.000000
C	0.314957	-0.952176	0.000000
C	0.000000	0.441174	0.000000
C	0.966097	1.364809	0.000000
H	2.010863	1.089814	0.000000
H	0.725678	2.419275	0.000000

Molecule# 1268

2-methyl-1-butene

PointGroup: C1

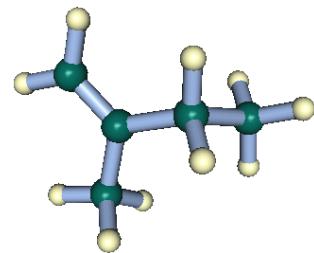
E= -196.617720948 au

ZPE= 0.136097 au

LUMO_eps= -0.01257 au

HOMO_eps= -0.25128 au

Dipole= 0.570 debye



15

C	0.997463	1.325679	0.022163
H	0.373584	1.884891	-0.678759
H	2.034359	1.430874	-0.293345
H	0.884792	1.810232	0.996291
C	-1.914097	0.084632	-0.392799
H	-1.882388	1.165754	-0.529981
H	-2.902148	-0.167486	-0.005719
H	-1.807245	-0.381100	-1.373424
C	-0.819378	-0.403315	0.566621
H	-0.933041	-1.477083	0.723891
H	-0.969525	0.073773	1.541238
C	0.586621	-0.119984	0.095100
C	1.423162	-1.102883	-0.231347
H	1.127074	-2.142429	-0.169432
H	2.431914	-0.902201	-0.569192

Molecule# 1269

2-methyl-1-propanamine

PointGroup: C1

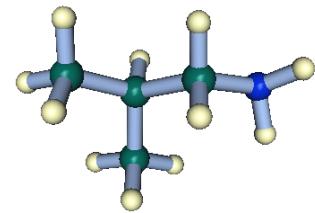
E= -213.890613321 au

ZPE= 0.148741 au

LUMO_eps= -0.01333 au

HOMO_eps= -0.24357 au

Dipole= 1.066 debye



16

N	-2.017293	-0.027830	-0.195165
H	-2.820908	-0.592269	0.048212
H	-2.147266	0.872192	0.248999
C	-0.776018	-0.669821	0.249843
H	-0.672045	-0.698833	1.345476
H	-0.809076	-1.707432	-0.088935
C	1.722505	-0.804982	0.017003
H	1.877218	-0.832599	1.098733
H	1.649672	-1.835748	-0.334919
H	2.613446	-0.362479	-0.430967
C	0.606424	1.454776	0.111148
H	1.501894	1.911846	-0.313053
H	-0.244796	2.059218	-0.204351
H	0.687235	1.520067	1.200032
C	0.469897	-0.001587	-0.340529
H	0.348831	-0.009471	-1.427859

Molecule# 1270

2-methyl-1-propanethiol

PointGroup: C1

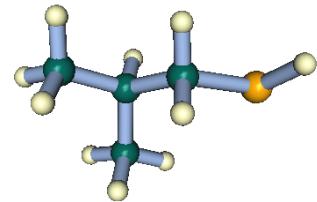
E= -556.741718590 au

ZPE= 0.130713 au

LUMO_eps= -0.01738 au

HOMO_eps= -0.23939 au

Dipole= 1.612 debye



15

C	1.015957	1.451343	0.163935
H	0.123868	2.040690	-0.046686
H	1.188253	1.483529	1.242634
H	1.861449	1.938979	-0.323138
S	-1.912944	0.066947	-0.125366
H	-2.706994	-0.873776	0.415091
C	2.163432	-0.784591	-0.063963
H	2.089609	-1.805448	-0.442007
H	3.013177	-0.307136	-0.553827
H	2.384593	-0.837208	1.004776
C	-0.305593	-0.718329	0.333908
H	-0.334382	-1.754724	0.003227
H	-0.203516	-0.701401	1.419378
C	0.875283	0.005676	-0.319616
H	0.696575	0.020737	-1.399165

Molecule# 1271

2-methyl-1-propanol

PointGroup: C1

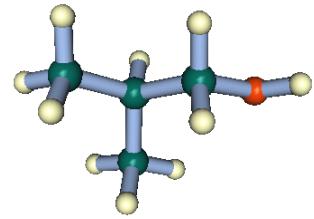
E= -233.766687867 au

ZPE= 0.135870 au

LUMO_eps= -0.01387 au

HOMO_eps= -0.28031 au

Dipole= 1.407 debye



15

C	0.590555	1.457337	0.129753
C	1.694739	-0.815651	0.002549
C	-0.789368	-0.654893	0.262196
C	0.447978	0.006154	-0.333326
O	-1.954191	0.041487	-0.185733
H	1.450174	1.933176	-0.344932
H	0.740265	1.505313	1.211861
H	-0.298201	2.037207	-0.113238
H	2.583805	-0.370690	-0.445730
H	1.613928	-1.840373	-0.364710
H	1.858337	-0.858604	1.082387
H	-0.832465	-1.704406	-0.050526
H	-0.727572	-0.631330	1.357984
H	0.314167	0.004019	-1.419727
H	-2.732335	-0.363889	0.205458

Molecule# 1272

2-methyl-1-propene

PointGroup: C2v

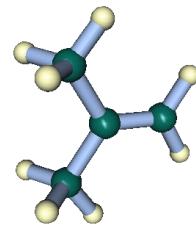
E= -157.291338993 au

ZPE= 0.107372 au

LUMO_eps= -0.01150 au

HOMO_eps= -0.25161 au

Dipole= 0.573 debye



12

C	0.000000	0.000000	1.454540
C	0.000000	0.000000	0.123825
C	0.000000	1.272551	-0.676777
C	0.000000	-1.272551	-0.676777
H	0.000000	-0.922142	2.021334
H	0.000000	0.922142	2.021334
H	0.876282	1.321528	-1.329331
H	-0.876282	1.321528	-1.329331
H	0.000000	2.153807	-0.037106
H	-0.876282	-1.321528	-1.329331
H	0.876282	-1.321528	-1.329331
H	0.000000	-2.153807	-0.037106

Molecule# 1273

2-methyl-1,2-propanediamine

PointGroup: Cs

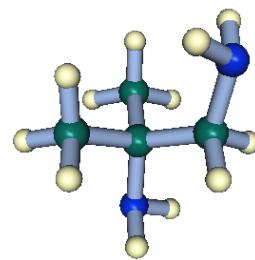
E= -269.263825240 au

ZPE= 0.165451 au

LUMO_eps= -0.01761 au

HOMO_eps= -0.22745 au

Dipole= 0.325 debye



18

C	-0.376341	0.220360	0.000000
H	1.502631	0.816125	0.875477
H	1.502631	0.816125	-0.875477
N	1.913976	-1.014914	0.000000
H	1.709887	-1.574258	0.817358
H	1.709887	-1.574258	-0.817358
N	-0.906035	1.595947	0.000000
H	-0.583445	2.106254	-0.814987
H	-0.583445	2.106254	0.814987
C	1.179166	0.245313	0.000000
C	-0.906035	-0.473601	-1.257115
C	-0.906035	-0.473601	1.257115
H	-0.558883	0.037001	-2.158942
H	-0.558883	0.037001	2.158942
H	-0.574785	-1.511227	1.310395
H	-0.574785	-1.511227	-1.310395
H	-1.995459	-0.462925	-1.263115
H	-1.995459	-0.462925	1.263115

Molecule# 1274

2-methyl-1,3-butadiene

PointGroup: Cs

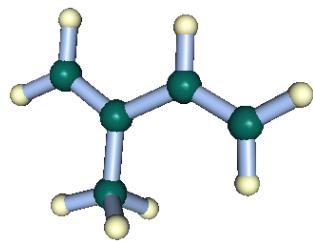
E= -195.389365429 au

ZPE= 0.113161 au

LUMO_eps= -0.03997 au

HOMO_eps= -0.23982 au

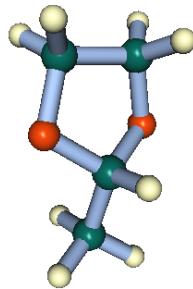
Dipole= 0.290 debye



13

C	-0.370784	-1.943846	0.000000
C	-0.590876	1.724659	0.000000
C	-0.821447	-0.687962	0.000000
C	0.000000	0.523640	0.000000
C	1.497508	0.383184	0.000000
H	-1.054523	-2.781159	0.000000
H	0.684570	-2.180530	0.000000
H	-0.016812	2.641330	0.000000
H	-1.668879	1.820992	0.000000
H	-1.893631	-0.520009	0.000000
H	1.840844	-0.168419	0.877918
H	1.981179	1.358162	0.000000
H	1.840844	-0.168419	-0.877918

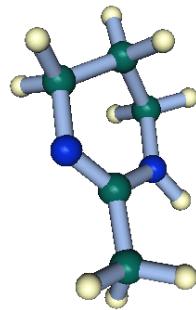
Molecule# 1275
 2-methyl-1,3-dioxolane
 PointGroup: C1
 E= -307.792644914 au
 ZPE= 0.120119 au
 LUMO_eps= -0.01004 au
 HOMO_eps= -0.26758 au
 Dipole= 1.175 debye



14

C	-2.091969	0.010752	-0.180597
H	-2.635094	-0.893942	0.090351
H	-2.624543	0.872125	0.220077
H	-2.045431	0.092193	-1.265498
C	-0.698672	-0.035879	0.388299
H	-0.716959	-0.130269	1.485995
O	0.030683	1.138373	0.045279
O	0.034322	-1.115337	-0.154500
C	1.399093	-0.761458	0.034643
H	1.998042	-1.291310	-0.702163
H	1.730930	-1.043846	1.039807
C	1.397982	0.765704	-0.146745
H	1.700345	1.065105	-1.151226
H	2.034073	1.270939	0.582825

Molecule# 1276
 2-methyl-1,4,5,6-tetrahydropyrimidine
 PointGroup: C1
 E= -306.170495836 au
 ZPE= 0.150027 au
 LUMO_eps= -0.01809 au
 HOMO_eps= -0.22064 au
 Dipole= 3.122 debye



17

C	0.941514	-0.098483	-0.014842
C	-1.781018	-0.019406	0.390258
C	-1.091888	-1.260357	-0.181491
C	-1.137073	1.235394	-0.190517
C	2.440033	-0.025730	0.105285
N	0.363471	-1.238193	-0.066973
N	0.305683	1.121283	-0.051204
H	-2.849215	-0.030386	0.168731
H	-1.669794	-0.010999	1.476831
H	-1.454663	-2.156545	0.325164
H	-1.359693	-1.380641	-1.237877
H	-1.420985	1.347734	-1.243241
H	-1.475506	2.129505	0.335358
H	2.734140	0.509347	1.011023
H	2.874653	0.500871	-0.747674
H	2.842634	-1.033035	0.140948
H	0.864952	1.954010	-0.054174

Molecule# 1277

2-methyl-1H-imidazole

PointGroup: Cs

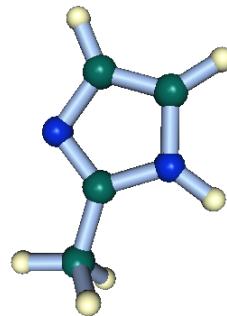
E= -265.641641590 au

ZPE= 0.098455 au

LUMO_eps= -0.02062 au

HOMO_eps= -0.22913 au

Dipole= 3.588 debye



12

C	-0.211213	2.098944	0.000000
H	-0.763664	2.429115	0.882489
H	0.758858	2.588726	0.000000
H	-0.763664	2.429115	-0.882489
N	-1.022980	-0.282177	0.000000
H	-2.004898	-0.069530	0.000000
C	0.000000	0.624449	0.000000
N	1.160665	0.009381	0.000000
C	0.880939	-1.338149	0.000000
H	1.664738	-2.075911	0.000000
C	-0.467672	-1.544500	0.000000
H	-1.067486	-2.436412	0.000000

Molecule# 1278

2-methyl-2-(methylsulfanyl)propane

PointGroup: Cs

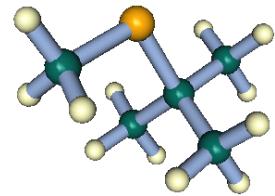
E= -596.069263039 au

ZPE= 0.159591 au

LUMO_eps= -0.01427 au

HOMO_eps= -0.22148 au

Dipole= 1.621 debye



18

S	-0.692409	-1.055906	0.000000
C	-0.026867	0.686541	0.000000
C	-1.284091	1.562967	0.000000
C	0.800267	-2.097232	0.000000
H	0.440552	-3.124595	0.000000
H	-0.998307	2.616921	0.000000
C	0.800267	0.953171	1.259728
C	0.800267	0.953171	-1.259728
H	1.404795	-1.943574	0.891889
H	1.404795	-1.943574	-0.891889
H	0.214552	0.768111	-2.159589
H	0.214552	0.768111	2.159589
H	1.131617	1.995073	1.274003
H	1.131617	1.995073	-1.274003
H	1.692762	0.328379	1.299095
H	1.692762	0.328379	-1.299095
H	-1.895101	1.377247	-0.883681
H	-1.895101	1.377247	0.883681

Molecule# 1279

2-methyl-2-butanethiol

PointGroup: C1

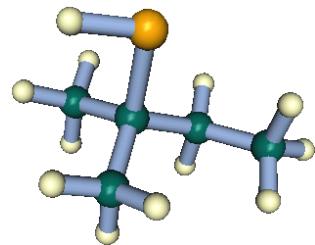
E= -596.069390796 au

ZPE= 0.158423 au

LUMO_eps= -0.01696 au

HOMO_eps= -0.23808 au

Dipole= 1.704 debye



18

H	-2.241590	-1.215243	-0.387645
H	-0.912425	-2.289504	-0.826315
H	-1.300954	-0.896147	-1.846390
C	-1.239595	-1.246048	-0.816810
C	-0.259075	-0.399357	-0.001092
H	1.407768	-1.489975	-0.756299
H	1.007906	-0.079353	-1.707859
C	1.124715	-0.435306	-0.681589
H	2.022628	1.398388	0.091245
H	3.169518	0.252206	-0.593787
H	2.473612	-0.046308	0.992131
C	2.255992	0.338004	-0.004285
H	0.185174	-1.926656	1.466143
H	-1.196829	-0.915576	1.889107
H	0.434562	-0.280652	2.066600
C	-0.201951	-0.903990	1.442827
H	-2.042025	1.174320	0.484066
S	-0.817991	1.387168	-0.031582

Molecule# 1280

2-methyl-2-butanol

PointGroup: C1

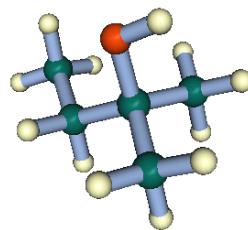
E= -273.100268978 au

ZPE= 0.163381 au

LUMO_eps= -0.01647 au

HOMO_eps= -0.27689 au

Dipole= 1.521 debye



18

C	-2.165229	-0.019777	-0.016641
C	0.534517	1.417395	-0.549756
C	1.641044	-0.836748	-0.424661
C	-0.864975	-0.710060	-0.425335
C	0.429999	-0.005131	0.007651
O	0.376349	0.043462	1.448394
H	-3.021673	-0.639001	-0.286612
H	-2.292415	0.942994	-0.512746
H	-2.195466	0.147199	1.059086
H	0.507717	1.416045	-1.640747
H	-0.278903	2.041128	-0.183517
H	1.476800	1.877169	-0.242684
H	1.695208	-0.921627	-1.511210
H	2.569524	-0.374559	-0.081065
H	1.582438	-1.839278	-0.001025
H	-0.835262	-0.834371	-1.510827
H	-0.842950	-1.714358	0.004098
H	1.172045	0.476886	1.772546

Molecule# 1281

2-methyl-2-butene

PointGroup: Cs

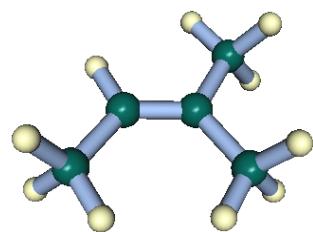
E= -196.620997039 au

ZPE= 0.135374 au

LUMO_eps= -0.01124 au

HOMO_eps= -0.23630 au

Dipole= 0.208 debye



15

C	-0.735351	-0.665405	0.000000
C	0.000000	0.449055	0.000000
C	-0.272212	-2.090707	0.000000
C	-0.654331	1.805181	0.000000
C	1.503840	0.487539	0.000000
H	-1.815046	-0.542325	0.000000
H	0.811162	-2.190686	0.000000
H	-0.654737	-2.622552	0.875627
H	-0.654737	-2.622552	-0.875627
H	-1.741078	1.730857	0.000000
H	-0.352201	2.386480	0.876320
H	-0.352201	2.386480	-0.876320
H	1.872880	1.029375	-0.875759
H	1.872880	1.029375	0.875759
H	1.961399	-0.498430	0.000000

Molecule# 1282

2-methyl-2-propanamine

PointGroup: Cs

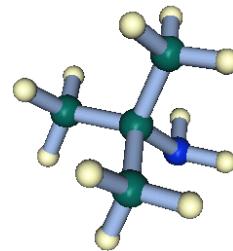
E= -213.895462123 au

ZPE= 0.147546 au

LUMO_eps= -0.01643 au

HOMO_eps= -0.24413 au

Dipole= 1.186 debye



16

N	0.544724	1.387269	0.000000
H	0.216989	1.895686	0.813925
H	0.216989	1.895686	-0.813925
C	-1.527556	-0.018978	0.000000
H	-1.923151	0.487103	0.883105
H	-1.923151	0.487103	-0.883105
H	-1.910040	-1.041945	0.000000
C	0.544724	-0.686055	1.255867
H	1.634333	-0.676871	1.262856
H	0.196491	-0.179088	2.158818
H	0.203288	-1.720826	1.303577
C	0.011620	0.010930	0.000000
C	0.544724	-0.686055	-1.255867
H	1.634333	-0.676871	-1.262856
H	0.203288	-1.720826	-1.303577
H	0.196491	-0.179088	-2.158818

Molecule# 1283

2-methyl-2-propanethiol

PointGroup: Cs

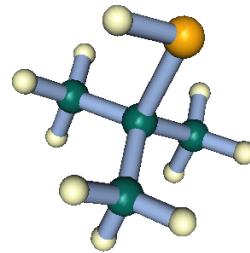
E= -556.744275416 au

ZPE= 0.130052 au

LUMO_eps= -0.01800 au

HOMO_eps= -0.23963 au

Dipole= 1.748 debye



15

C	0.836982	-0.734002	1.259163
C	0.836982	-0.734002	-1.259163
C	0.836982	1.444049	0.000000
C	0.356343	-0.010366	0.000000
S	-1.509289	0.094963	0.000000
H	0.477461	-1.763198	1.286405
H	1.929912	-0.761420	1.279568
H	0.489091	-0.229768	2.159568
H	0.489091	-0.229768	-2.159568
H	0.477461	-1.763198	-1.286405
H	1.929912	-0.761420	-1.279568
H	0.487296	1.977794	0.883980
H	1.928534	1.468659	0.000000
H	0.487296	1.977794	-0.883980
H	-1.751158	-1.228962	0.000000

Molecule# 1284

2-methyl-2H-tetrazole

PointGroup: Cs

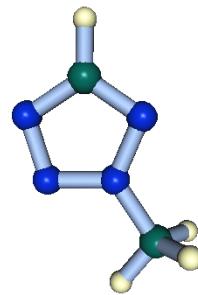
E= -297.684032886 au

ZPE= 0.075063 au

LUMO_eps= -0.04036 au

HOMO_eps= -0.30356 au

Dipole= 2.907 debye



10

H	1.261590	-2.270226	0.000000
C	0.638250	-1.394165	0.000000
N	1.115640	-0.158335	0.000000
N	-0.709343	-1.427292	0.000000
N	-1.101004	-0.179300	0.000000
N	0.000000	0.555258	0.000000
H	0.482613	2.378013	0.888585
H	-1.062032	2.314158	0.000000
H	0.482613	2.378013	-0.888585
C	-0.021889	2.005452	0.000000

Molecule# 1285

2-methyl-3-pentanol

PointGroup: C1

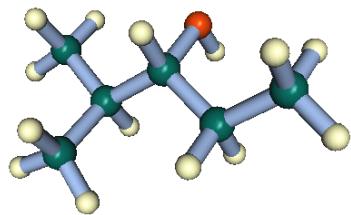
E= -312.423748935 au

ZPE= 0.192032 au

LUMO_eps= -0.01366 au

HOMO_eps= -0.27465 au

Dipole= 1.631 debye



21

C	-2.743598	0.279380	0.263321
C	1.527637	1.583398	0.042847
C	2.226050	-0.822775	0.228502
C	-1.371578	0.649289	-0.298578
C	1.159473	0.137171	-0.308936
C	-0.242383	-0.258067	0.197134
O	-0.529559	-1.629626	-0.112600
H	-3.515575	0.944672	-0.125339
H	-2.752787	0.361074	1.352137
H	-3.015995	-0.743733	0.008715
H	0.893332	2.312783	-0.458542
H	1.450647	1.753470	1.119924
H	2.558304	1.792091	-0.246918
H	3.203847	-0.588092	-0.194843
H	1.989120	-1.858593	-0.004759
H	2.306790	-0.736724	1.315244
H	-1.393282	0.611750	-1.394424
H	-1.144600	1.683054	-0.034580
H	1.140378	0.049342	-1.403355
H	-0.228904	-0.235027	1.291831
H	-0.588412	-1.719433	-1.070029

Molecule# 1286

2-methyl-4,5-dihydro-1,3-oxazole

PointGroup: Cs

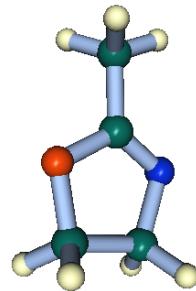
E= -286.715850448 au

ZPE= 0.109031 au

LUMO_eps= -0.01193 au

HOMO_eps= -0.25340 au

Dipole= 1.316 debye



13

C	0.336343	2.129295	0.000000
C	0.540978	-1.506450	0.000000
C	-0.989729	-1.289163	0.000000
N	-1.159293	0.170312	0.000000
O	1.078204	-0.160300	0.000000
C	0.000000	0.680984	0.000000
H	0.910587	-2.017738	0.887540
H	0.910587	-2.017738	-0.887540
H	-1.473240	-1.716662	0.879292
H	-1.473240	-1.716662	-0.879292
H	0.932661	2.376888	0.879004
H	0.932661	2.376888	-0.879004
H	-0.576148	2.717242	0.000000

Molecule# 1287

2-methylbutane

PointGroup: Cs

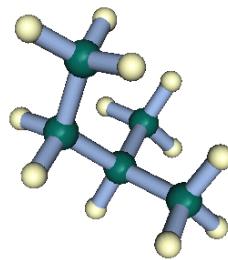
E= -197.846871396 au

ZPE= 0.159461 au

LUMO_eps= -0.01196 au

HOMO_eps= -0.31579 au

Dipole= 0.155 debye



17

C	0.350820	-1.850666	0.000000
C	0.350820	1.050444	1.263414
C	0.350820	1.050444	-1.263414
C	-0.805408	-0.847966	0.000000
C	-0.414139	0.642850	0.000000
H	-0.031506	-2.872394	0.000000
H	0.984723	-1.741982	0.880927
H	0.984723	-1.741982	-0.880927
H	1.332012	0.574521	1.311117
H	-0.197555	0.775240	2.166524
H	0.512150	2.129575	1.288536
H	1.332012	0.574521	-1.311117
H	0.512150	2.129575	-1.288536
H	-0.197555	0.775240	-2.166524
H	-1.436172	-1.037018	-0.873465
H	-1.436172	-1.037018	0.873465
H	-1.356290	1.201080	0.000000

Molecule# 1288

2-methylbutanenitrile

PointGroup: C1

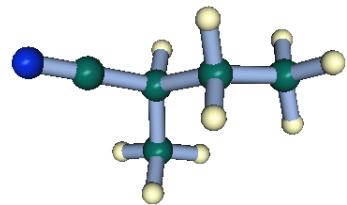
E= -250.792272078 au

ZPE= 0.130596 au

LUMO_eps= -0.02062 au

HOMO_eps= -0.32722 au

Dipole= 4.293 debye



15

C	-1.519478	-0.306091	0.116403
N	-2.579509	-0.707080	-0.081472
C	-0.053322	1.653906	-0.147603
H	-0.178135	1.700270	-1.229566
H	-0.816479	2.281556	0.309582
H	0.921467	2.065882	0.106210
C	2.314757	-0.422465	0.087354
H	2.455299	-0.421432	1.170184
H	2.992332	-1.166370	-0.331717
H	2.625607	0.550800	-0.292013
C	0.870992	-0.753554	-0.283413
H	0.745929	-0.734085	-1.368367
H	0.638768	-1.770647	0.035713
C	-0.164996	0.202947	0.349922
H	-0.015943	0.195124	1.434302

Molecule# 1289

2-methylfuran

PointGroup: Cs

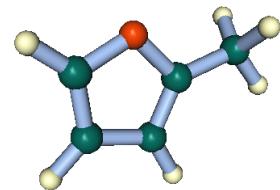
E= -269.448442119 au

ZPE= 0.097364 au

LUMO_eps= -0.00901 au

HOMO_eps= -0.22606 au

Dipole= 0.665 debye



12

O	1.035246	-0.245795	0.000000
C	0.000000	0.646987	0.000000
C	0.492364	-1.497390	0.000000
C	-1.179136	-0.026476	0.000000
C	-0.858244	-1.422573	0.000000
C	0.358496	2.086650	0.000000
H	1.190884	-2.314077	0.000000
H	-2.160525	0.415739	0.000000
H	-1.544479	-2.251632	0.000000
H	-0.545250	2.693073	0.000000
H	0.948262	2.350033	0.880725
H	0.948262	2.350033	-0.880725

Molecule# 1290

2-methylhexane

PointGroup: Cs

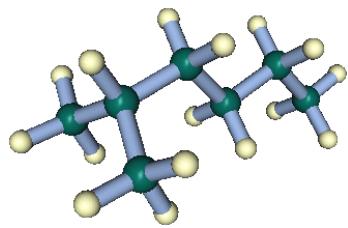
E= -276.502738984 au

ZPE= 0.216088 au

LUMO_eps= -0.01159 au

HOMO_eps= -0.30617 au

Dipole= 0.154 debye



23

C	-0.868384	3.234895	0.000000
C	-0.219571	-2.152365	1.263450
C	-0.219571	-2.152365	-1.263450
C	0.268040	2.213869	0.000000
C	-0.219571	0.763488	0.000000
C	0.930524	-0.247686	0.000000
C	0.542679	-1.739197	0.000000
H	-0.486911	4.257021	0.000000
H	-1.503449	3.118553	-0.880742
H	-1.503449	3.118553	0.880742
H	-1.205277	-1.685922	1.310069
H	-0.370188	-3.233066	1.289312
H	0.325690	-1.871056	2.166571
H	-1.205277	-1.685922	-1.310069
H	-0.370188	-3.233066	-1.289312
H	0.325690	-1.871056	-2.166571
H	0.905576	2.378650	0.873933
H	0.905576	2.378650	-0.873933
H	-0.856827	0.606146	0.874834
H	-0.856827	0.606146	-0.874834
H	1.561967	-0.056811	-0.873944
H	1.561967	-0.056811	0.873944
H	1.487050	-2.293848	0.000000

Molecule# 1291

2-methylpentan-2-ol

PointGroup: C1

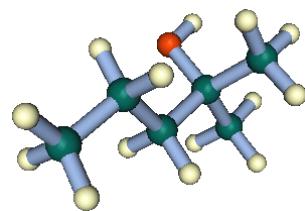
E= -312.428053825 au

ZPE= 0.191667 au

LUMO_eps= -0.01624 au

HOMO_eps= -0.27645 au

Dipole= 1.516 debye



21

C	3.005568	-0.234641	-0.075870
C	-1.946912	-1.107066	-0.387839
C	-1.238412	1.280682	-0.728586
C	1.632830	0.413030	0.105069
C	0.492710	-0.535387	-0.269388
C	-0.931821	-0.029161	0.003653
O	-0.996264	0.187836	1.428670
H	3.165367	-0.547167	-1.110366
H	3.109196	-1.119822	0.554911
H	3.807682	0.455938	0.188183
H	-2.963517	-0.784311	-0.150713
H	-1.747156	-2.030635	0.155349
H	-1.906985	-1.318328	-1.457633
H	-0.578207	2.078717	-0.394031
H	-2.268050	1.591351	-0.535843
H	-1.124654	1.164869	-1.807771
H	1.507934	0.728735	1.141736
H	1.583749	1.318038	-0.504908
H	0.564713	-0.793340	-1.330153
H	0.615355	-1.469442	0.286075
H	-1.879090	0.497967	1.653569

Molecule# 1292

2-methylpentane

PointGroup: C1

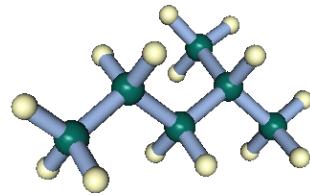
E= -237.176390093 au

ZPE= 0.187767 au

LUMO_eps= -0.01022 au

HOMO_eps= -0.31266 au

Dipole= 0.146 debye



20

C	2.838715	-0.210284	0.151499
C	-1.452331	1.374908	0.194977
C	-2.150229	-1.037838	0.031809
C	1.495560	0.356257	-0.307569
C	0.304604	-0.477105	0.169426
C	-1.071855	-0.012797	-0.331369
H	2.897031	-0.252318	1.241150
H	2.988894	-1.224454	-0.224592
H	3.671051	0.400513	-0.201048
H	-0.743775	2.142198	-0.116896
H	-1.487672	1.377435	1.287781
H	-2.438033	1.672153	-0.167266
H	-2.241995	-1.138272	1.116369
H	-3.126439	-0.741164	-0.355760
H	-1.914534	-2.023603	-0.373148
H	1.400426	1.383805	0.050622
H	1.479386	0.411612	-1.400581
H	0.457236	-1.513257	-0.149856
H	0.293963	-0.498723	1.265583
H	-1.022318	0.045239	-1.424998

Molecule# 1293

2-methylpentene

PointGroup: C1

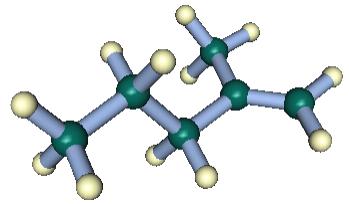
E= -235.945840899 au

ZPE= 0.164446 au

LUMO_eps= -0.01161 au

HOMO_eps= -0.25032 au

Dipole= 0.597 debye



18

C	-1.943932	-1.168905	-0.210590
C	-1.162345	-0.135589	0.096240
C	-1.665731	1.281359	0.033583
C	2.748156	-0.046354	0.013425
C	0.268935	-0.331004	0.532941
C	1.316548	0.202314	-0.457619
H	-1.582768	-2.188058	-0.155400
H	-2.970744	-1.031650	-0.524857
H	-1.553525	1.775593	1.002859
H	-1.100728	1.876555	-0.687415
H	-2.716479	1.319449	-0.249678
H	2.941697	-1.113171	0.142398
H	2.938946	0.440991	0.971889
H	3.474380	0.337828	-0.704090
H	0.450856	-1.395047	0.699684
H	0.420342	0.167127	1.497865
H	1.169178	1.273433	-0.612395
H	1.159056	-0.273982	-1.428743

Molecule# 1294

2-methylpiperidine

PointGroup: C1

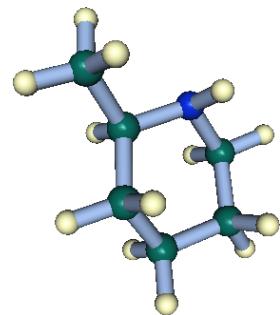
E= -291.332492352 au

ZPE= 0.185944 au

LUMO_eps= -0.01091 au

HOMO_eps= -0.21993 au

Dipole= 1.085 debye



20

C	-1.876724	-0.056528	0.292117
C	-1.220756	1.238754	-0.193233
C	0.269212	1.266716	0.162963
C	0.993150	0.003566	-0.331778
N	0.336494	-1.236054	0.101240
C	-1.093530	-1.276574	-0.206570
C	2.458080	-0.022920	0.084158
H	-2.914516	-0.113656	-0.046636
H	-1.900320	-0.067386	1.387040
H	-1.331150	1.311007	-1.280554
H	-1.729106	2.108897	0.227207
H	0.744092	2.156300	-0.259637
H	0.385539	1.333833	1.250920
H	0.947191	0.002171	-1.427861
H	0.478094	-1.362314	1.097987
H	-1.506343	-2.198011	0.207370
H	-1.194856	-1.349044	-1.294590
H	2.954195	-0.908747	-0.311642
H	2.551510	-0.040360	1.173496
H	2.983619	0.861609	-0.277729

Molecule# 1295

2-methylpropan-2-ol

PointGroup: Cs

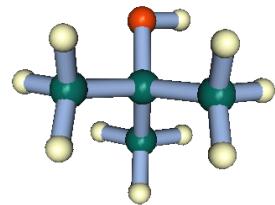
E= -233.774440750 au

ZPE= 0.134845 au

LUMO_eps= -0.01706 au

HOMO_eps= -0.27797 au

Dipole= 1.609 debye



15

C	-0.486076	-0.705434	1.261168
C	-0.486076	-0.705434	-1.261168
C	1.521674	0.142791	0.000000
C	0.001813	0.012259	0.000000
O	-0.486076	1.369657	0.000000
H	-1.577070	-0.763138	1.276432
H	-0.099320	-1.724561	1.310729
H	-0.160405	-0.167882	2.151574
H	-0.160405	-0.167882	-2.151574
H	-1.577070	-0.763138	-1.276432
H	-0.099320	-1.724561	-1.310729
H	1.854033	0.688346	0.883017
H	1.994672	-0.839511	0.000000
H	1.854033	0.688346	-0.883017
H	-1.448562	1.351622	0.000000

Molecule# 1296

2-methylpropanal

PointGroup: C1

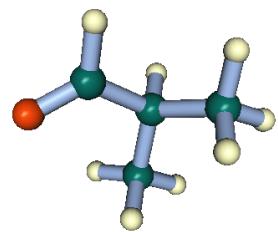
E= -232.553241485 au

ZPE= 0.111981 au

LUMO_eps= -0.03937 au

HOMO_eps= -0.26311 au

Dipole= 2.867 debye



13

C	0.937510	-0.611839	-0.203807
C	-1.492937	-0.871125	0.255516
C	-0.484063	1.465272	0.040969
C	-0.424750	0.011005	-0.411659
O	1.895644	-0.059648	0.273304
H	1.010074	-1.671441	-0.531638
H	-1.421772	-1.909325	-0.072827
H	-2.490925	-0.510468	0.007755
H	-1.387988	-0.851504	1.341538
H	-1.458920	1.896200	-0.188710
H	0.282990	2.063378	-0.448681
H	-0.321324	1.543319	1.116354
H	-0.591848	-0.042855	-1.496335

Molecule# 1297

2-methylpropanamide

PointGroup: C1

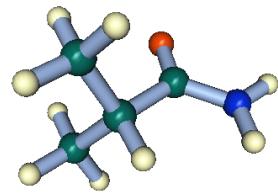
E= -287.963922234 au

ZPE= 0.130008 au

LUMO_eps= -0.02264 au

HOMO_eps= -0.25884 au

Dipole= 3.683 debye



15

C	1.353431	1.270810	0.013760
H	0.841398	2.180726	-0.302096
H	1.417446	1.279075	1.101271
H	2.364879	1.292140	-0.393745
C	1.362786	-1.262502	-0.056829
H	0.858541	-2.157090	-0.424699
H	1.425064	-1.331889	1.028585
C	0.615424	0.013505	-0.461515
H	0.538032	0.043857	-1.552099
N	-1.818851	0.026866	-0.759937
H	-2.762329	0.014931	-0.411347
H	-1.665858	0.059091	-1.750368
C	-0.791440	-0.007396	0.135988
O	-0.987670	-0.050347	1.337337
H	2.374939	-1.252626	-0.463060

Molecule# 1298

2-methylpropanenitrile

PointGroup: Cs

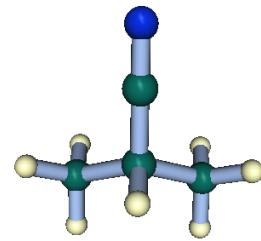
E= -211.465277096 au

ZPE= 0.102158 au

LUMO_eps= -0.02206 au

HOMO_eps= -0.33108 au

Dipole= 4.180 debye



12

N	-0.400750	-2.173012	0.000000
C	-0.026829	-1.085083	0.000000
H	1.527406	0.267302	0.000000
C	0.434603	0.306529	0.000000
H	0.322951	0.513931	2.170270
H	0.322951	0.513931	-2.170270
H	-1.114559	1.081957	-1.317044
H	-1.114559	1.081957	1.317044
C	-0.026829	1.027994	-1.276481
C	-0.026829	1.027994	1.276481
H	0.368182	2.043699	-1.284867
H	0.368182	2.043699	1.284867

Molecule# 1299

2-methylpyrazine

PointGroup: Cs

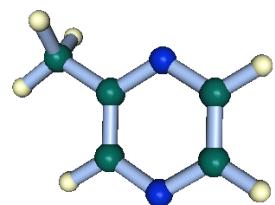
E= -303.749133624 au

ZPE= 0.103888 au

LUMO_eps= -0.06342 au

HOMO_eps= -0.25666 au

Dipole= 0.636 debye



13

C	-0.001868	-1.820771	0.000000
C	-1.182467	-1.087059	0.000000
C	1.179811	0.108531	0.000000
C	0.000000	0.858405	0.000000
C	0.008652	2.358272	0.000000
N	1.186439	-1.221482	0.000000
N	-1.186506	0.242772	0.000000
H	-0.015053	-2.903968	0.000000
H	-2.145893	-1.583765	0.000000
H	2.144697	0.602719	0.000000
H	-0.515539	2.739063	0.877425
H	1.023030	2.753583	0.000000
H	-0.515539	2.739063	-0.877425

Molecule# 1300

2-methylpyridine

PointGroup: Cs

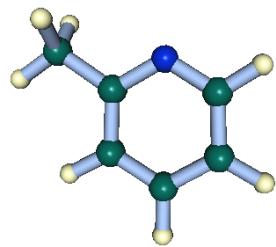
E= -287.711184349 au

ZPE= 0.115759 au

LUMO_eps= -0.03765 au

HOMO_eps= -0.26016 au

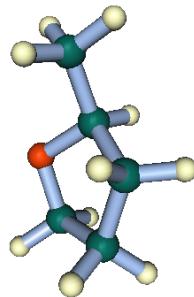
Dipole= 1.884 debye



14

N	1.184590	0.251105	0.000000
C	0.000000	0.875562	0.000000
C	-1.202367	0.166726	0.000000
C	-1.174475	-1.220655	0.000000
C	0.054155	-1.864985	0.000000
C	1.201261	-1.080306	0.000000
C	0.032915	2.378142	0.000000
H	-2.143876	0.698947	0.000000
H	-2.096226	-1.787364	0.000000
H	0.127330	-2.943410	0.000000
H	2.181582	-1.544032	0.000000
H	-0.968801	2.804749	0.000000
H	0.569466	2.743239	0.876757
H	0.569466	2.743239	-0.876757

Molecule# 1301
 2-methyltetrahydrofuran
 PointGroup: C1
 E= -271.875741472 au
 ZPE= 0.144295 au
 LUMO_eps= -0.01103 au
 HOMO_eps= -0.25971 au
 Dipole= 1.528 debye



16

C	-1.545200	0.674146	-0.126359
C	-0.105076	1.223728	0.005730
C	-1.368914	-0.846757	0.057412
C	0.732800	-0.011059	0.378649
C	2.152046	-0.027585	-0.146353
O	0.009355	-1.112893	-0.176593
H	-2.218989	1.088613	0.622495
H	-1.962003	0.904798	-1.105364
H	0.242266	1.630722	-0.944467
H	-0.020334	2.011011	0.754025
H	-1.637823	-1.149102	1.077531
H	-1.947361	-1.446214	-0.643058
H	0.744850	-0.121334	1.473448
H	2.155499	0.063414	-1.233368
H	2.721516	0.803002	0.273159
H	2.653606	-0.956606	0.123859

Molecule# 1302

2-methylthiophene

PointGroup: Cs

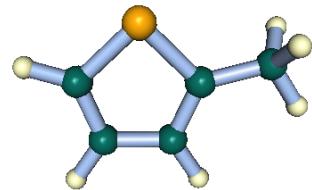
E= -592.432460336 au

ZPE= 0.094139 au

LUMO_eps= -0.02230 au

HOMO_eps= -0.23368 au

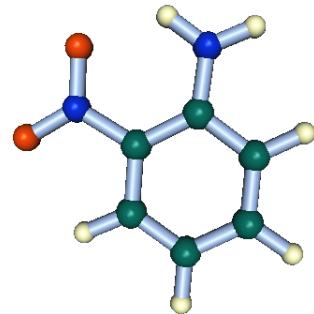
Dipole= 0.714 debye



12

C	-1.431534	-1.031992	0.000000
C	-1.295454	0.385519	0.000000
C	-0.233038	-1.675211	0.000000
C	0.000000	0.813659	0.000000
C	0.515874	2.217453	0.000000
S	1.080231	-0.550999	0.000000
H	-2.381672	-1.545414	0.000000
H	-2.133617	1.068000	0.000000
H	-0.039022	-2.734092	0.000000
H	-0.319300	2.917141	0.000000
H	1.127412	2.426894	0.879789
H	1.127412	2.426894	-0.879789

Molecule# 1303
 2-nitroaniline
 PointGroup: Cs
 E= -492.304836702 au
 ZPE= 0.119371 au
 LUMO_eps= -0.09561 au
 HOMO_eps= -0.23653 au
 Dipole= 4.877 debye



16

C	2.063464	-1.503763	0.000000
C	2.365819	-0.135580	0.000000
C	0.760060	-1.938693	0.000000
C	1.333452	0.772214	0.000000
C	-0.327896	-1.035393	0.000000
C	0.000000	0.344759	0.000000
N	-1.591077	-1.520223	0.000000
N	-1.021402	1.372732	0.000000
O	-0.674531	2.546284	0.000000
O	-2.211698	1.027891	0.000000
H	2.862699	-2.232880	0.000000
H	3.391203	0.202815	0.000000
H	0.541477	-2.998734	0.000000
H	1.518872	1.834417	0.000000
H	-1.742811	-2.511061	0.000000
H	-2.363649	-0.876785	0.000000

Molecule# 1304

2-nitrobutane

PointGroup: C1

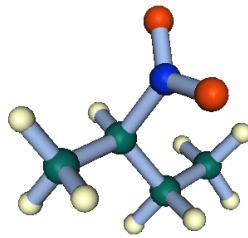
E= -363.106739533 au

ZPE= 0.134655 au

LUMO_eps= -0.07701 au

HOMO_eps= -0.30384 au

Dipole= 3.915 debye



16

C	0.729471	1.904216	-0.107889
C	-0.016491	0.615252	-0.425867
N	0.850921	-0.558678	0.026714
O	1.306585	-1.287691	-0.838614
O	1.039827	-0.688006	1.224692
C	-1.386010	0.520666	0.241641
C	-2.166261	-0.746449	-0.100809
H	0.857898	2.020360	0.966917
H	1.709251	1.922511	-0.584185
H	0.153750	2.749659	-0.483645
H	-0.096788	0.467156	-1.500194
H	-1.947266	1.400933	-0.080637
H	-1.253956	0.607897	1.320918
H	-2.318382	-0.842024	-1.177079
H	-1.649746	-1.642316	0.245321
H	-3.146754	-0.729962	0.374509

Molecule# 1305

2-nitrophenol

PointGroup: C1

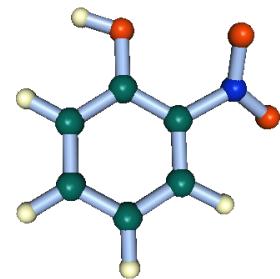
E= -512.162898537 au

ZPE= 0.106956 au

LUMO_eps= -0.09366 au

HOMO_eps= -0.26414 au

Dipole= 5.809 debye



15

C	-1.835597	-1.471168	0.106759
C	-2.531726	-0.267314	0.040621
C	-0.452973	-1.452868	0.080538
C	-1.850063	0.934346	-0.048731
C	0.235671	-0.246214	0.013147
C	-0.453434	0.973310	-0.060215
N	1.703827	-0.306080	0.022093
O	2.221476	-1.316606	-0.438893
O	2.315378	0.632295	0.504570
O	0.220545	2.138083	-0.177817
H	-2.364482	-2.410267	0.175643
H	-3.612989	-0.262929	0.054068
H	0.123142	-2.364653	0.116206
H	-2.397052	1.867174	-0.114478
H	-0.405869	2.862503	-0.281682

Molecule# 1306

2-nitropropane

PointGroup: Cs

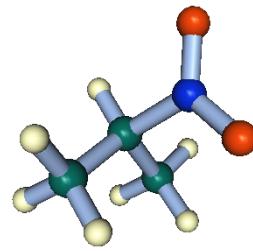
E= -323.778639601 au

ZPE= 0.106224 au

LUMO_eps= -0.07764 au

HOMO_eps= -0.30550 au

Dipole= 3.931 debye



13

C	-0.019580	1.273801	1.273937
C	-0.019580	1.273801	-1.273937
C	0.466570	0.597774	0.000000
N	-0.019580	-0.850943	0.000000
O	0.828786	-1.727382	0.000000
O	-1.224451	-1.038289	0.000000
H	0.370883	2.290811	1.305811
H	-1.106994	1.317390	1.296364
H	0.330843	0.747565	2.161338
H	0.330843	0.747565	-2.161338
H	0.370883	2.290811	-1.305811
H	-1.106994	1.317390	-1.296364
H	1.548465	0.498180	0.000000

Molecule# 1307

2-nitropropanedithioic acid

PointGroup: C1

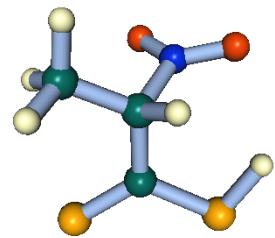
E= -1118.992211440 au

ZPE= 0.085047 au

LUMO_eps= -0.11700 au

HOMO_eps= -0.25549 au

Dipole= 2.781 debye



13

S	-1.970085	-1.004828	0.404057
S	-1.139601	1.747515	-0.120095
O	2.148970	1.195734	-0.147249
O	1.936106	-0.474436	1.215650
N	1.643397	0.143182	0.214618
C	0.530339	-0.432912	-0.684238
C	-0.823235	0.025273	-0.124545
C	0.716287	-1.928719	-0.821212
H	0.055105	2.176069	-0.582816
H	0.695123	0.073347	-1.632561
H	0.587915	-2.431303	0.132211
H	-0.020664	-2.316756	-1.520848
H	1.712761	-2.138853	-1.208928

Molecule# 1308

2-nitroso-3-pyridinol

PointGroup: Cs

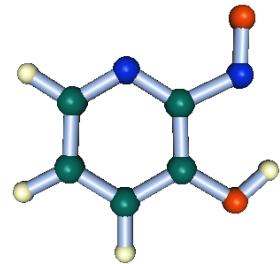
E= -452.970949028 au

ZPE= 0.089942 au

LUMO_eps= -0.12588 au

HOMO_eps= -0.24006 au

Dipole= 4.198 debye



13

O	2.164676	-0.539196	0.000000
O	0.084580	2.775541	0.000000
N	-1.331579	0.475000	0.000000
N	0.726390	1.750983	0.000000
C	0.000000	0.522358	0.000000
C	0.824411	-0.616949	0.000000
C	0.204822	-1.870177	0.000000
C	-1.905774	-0.710961	0.000000
C	-1.171952	-1.910799	0.000000
H	2.405510	0.402858	0.000000
H	0.809768	-2.765739	0.000000
H	-2.988888	-0.732364	0.000000
H	-1.693161	-2.858226	0.000000

Molecule# 1309

2-oxo-1-piperidinocarbaldehyde

PointGroup: C1

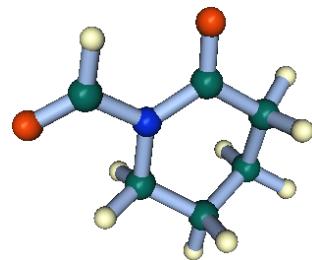
E= -439.449018860 au

ZPE= 0.149354 au

LUMO_eps= -0.05006 au

HOMO_eps= -0.26634 au

Dipole= 4.562 debye



18

C	-0.186018	1.136555	-0.016276
C	2.009439	0.143910	-0.020263
C	-1.688458	0.930915	-0.085110
C	-2.193334	-0.451194	0.319463
C	-1.329801	-1.518012	-0.342061
C	0.110985	-1.389348	0.120028
N	0.625043	-0.010474	-0.004995
O	0.292401	2.250735	-0.012180
O	2.774688	-0.789444	0.046595
H	2.318270	1.188945	-0.103512
H	-2.134838	1.730283	0.504410
H	-1.958505	1.134988	-1.126204
H	-2.147779	-0.565223	1.406075
H	-3.240882	-0.559386	0.036482
H	-1.680512	-2.521239	-0.096983
H	-1.383960	-1.417352	-1.429648
H	0.200795	-1.695360	1.165693
H	0.778519	-2.029625	-0.451356

Molecule# 1310

2-pentanol

PointGroup: C1

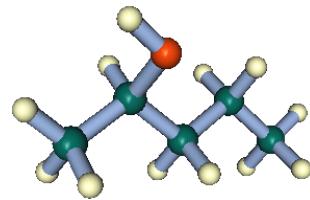
E= -273.098789669 au

ZPE= 0.164221 au

LUMO_eps= -0.01484 au

HOMO_eps= -0.27830 au

Dipole= 1.539 debye



18

C	-2.811044	-0.221945	-0.162139
C	2.221288	-0.900163	-0.048109
C	-1.473342	0.339233	0.316846
C	-0.280858	-0.504253	-0.134238
C	1.071410	0.028960	0.322589
O	1.239016	1.319777	-0.283419
H	-3.644676	0.394864	0.176352
H	-2.975117	-1.234898	0.212481
H	-2.852626	-0.264029	-1.252522
H	2.257486	-1.050421	-1.128043
H	3.179284	-0.482509	0.270000
H	2.107939	-1.872159	0.434921
H	-1.347052	1.358855	-0.049391
H	-1.474885	0.402013	1.409571
H	-0.391242	-1.525089	0.243683
H	-0.268458	-0.572453	-1.226633
H	1.048581	0.150408	1.414128
H	2.083920	1.686207	-0.006882

Molecule# 1311

2-pentanone

PointGroup: C1

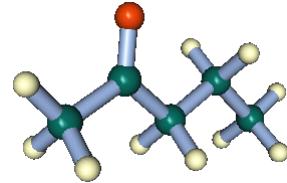
E= -271.892368574 au

ZPE= 0.140145 au

LUMO_eps= -0.02529 au

HOMO_eps= -0.25552 au

Dipole= 2.828 debye



16

C	1.137455	0.146005	-0.002101
C	2.339985	-0.775148	0.003438
C	-2.754057	-0.294448	-0.000481
C	-0.225440	-0.525525	-0.005704
C	-1.410723	0.432588	0.006368
O	1.262714	1.350118	-0.002835
H	2.311679	-1.443961	-0.859263
H	2.326989	-1.406936	0.894211
H	3.256222	-0.191143	-0.015540
H	-2.862511	-0.940914	0.873136
H	-2.864356	-0.920583	-0.888559
H	-3.583566	0.413374	0.008555
H	-0.263760	-1.203516	0.854803
H	-0.266645	-1.183799	-0.881400
H	-1.338759	1.077971	0.883375
H	-1.340329	1.097732	-0.855756

Molecule# 1312

2-phenylethanol

PointGroup: C1

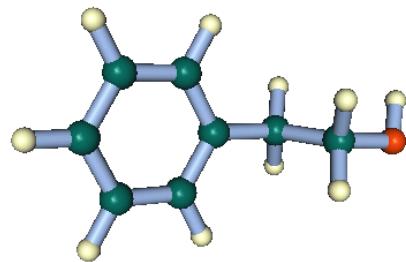
E= -386.239765262 au

ZPE= 0.161443 au

LUMO_eps= -0.02046 au

HOMO_eps= -0.25242 au

Dipole= 1.513 debye



19

C	2.814804	-0.001719	-0.301389
C	2.134649	-1.200607	-0.119441
C	2.136199	1.201043	-0.142617
C	0.785938	-1.194095	0.216238
C	0.787279	1.201961	0.193344
C	0.091182	0.006113	0.377674
C	-1.382308	0.006570	0.699381
C	-2.252301	-0.022112	-0.563342
O	-3.645434	-0.085015	-0.273276
H	3.864982	-0.004812	-0.560108
H	2.655224	-2.142017	-0.234918
H	2.657691	2.139541	-0.276374
H	0.266470	-2.133322	0.361844
H	0.269747	2.144962	0.321584
H	-1.634273	0.897699	1.281212
H	-1.639570	-0.859511	1.311331
H	-2.033440	-0.917594	-1.144566
H	-2.023001	0.842586	-1.195287
H	-3.913002	0.729665	0.162405

Molecule# 1313

2-propanamine

PointGroup: Cs

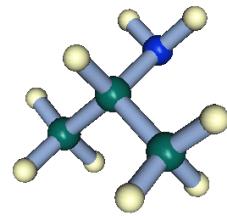
E= -174.566119025 au

ZPE= 0.120174 au

LUMO_eps= -0.01514 au

HOMO_eps= -0.24417 au

Dipole= 1.258 debye



13

C	0.291567	0.213459	0.000000
N	-0.907457	1.063947	0.000000
H	1.214879	0.812042	0.000000
C	0.291567	-0.643023	1.262440
C	0.291567	-0.643023	-1.262440
H	-0.926663	1.665263	-0.815022
H	-0.926663	1.665263	0.815022
H	-0.596181	-1.276761	1.290536
H	-0.596181	-1.276761	-1.290536
H	1.176573	-1.279494	1.299902
H	1.176573	-1.279494	-1.299902
H	0.290826	-0.021081	2.160146
H	0.290826	-0.021081	-2.160146

Molecule# 1314

2-propanethiol

PointGroup: Cs

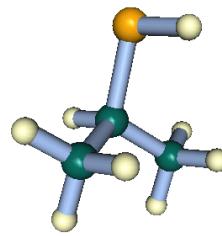
E= -517.415919250 au

ZPE= 0.102468 au

LUMO_eps= -0.01625 au

HOMO_eps= -0.24083 au

Dipole= 1.738 debye



12

C	0.054241	1.100477	1.268813
C	0.054241	1.100477	-1.268813
C	-0.409424	0.392082	0.000000
S	0.054241	-1.399668	0.000000
H	-0.309019	2.131146	1.280502
H	-0.310858	0.595967	2.161592
H	1.144294	1.131346	1.319556
H	-0.309019	2.131146	-1.280502
H	-0.310858	0.595967	-2.161592
H	1.144294	1.131346	-1.319556
H	-1.500071	0.339611	0.000000
H	1.389046	-1.220063	0.000000

Molecule# 1315

2-propanimine

PointGroup: Cs

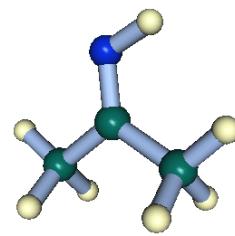
E= -173.347983914 au

ZPE= 0.096294 au

LUMO_eps= -0.01663 au

HOMO_eps= -0.26416 au

Dipole= 2.487 debye



11

C	0.000000	0.160391	0.000000
C	1.341166	-0.522197	0.000000
C	-1.204165	-0.750105	0.000000
N	-0.046207	1.430440	0.000000
H	2.139324	0.215075	0.000000
H	1.444083	-1.166052	0.876901
H	1.444083	-1.166052	-0.876901
H	-2.134256	-0.183538	0.000000
H	-1.190635	-1.402345	0.876352
H	-1.190635	-1.402345	-0.876352
H	-1.010521	1.763644	0.000000

Molecule# 1316

2-propanol

PointGroup: Cs

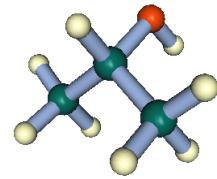
E= -194.442803397 au

ZPE= 0.107316 au

LUMO_eps= -0.01475 au

HOMO_eps= -0.27990 au

Dipole= 1.675 debye



12

C	0.287231	-0.610477	1.268740
C	0.287231	-0.610477	-1.268740
C	0.287231	0.234800	0.000000
O	-0.802494	1.166277	0.000000
H	1.168231	-1.253175	1.311423
H	0.281273	0.027361	2.152009
H	-0.596203	-1.253979	1.303814
H	1.168231	-1.253175	-1.311423
H	0.281273	0.027361	-2.152009
H	-0.596203	-1.253979	-1.303814
H	1.172769	0.873582	0.000000
H	-1.629582	0.672719	0.000000

Molecule# 1317

2-propene-1-ol

PointGroup: C1

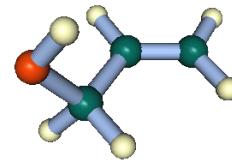
E= -193.202138429 au

ZPE= 0.084895 au

LUMO_eps= -0.02023 au

HOMO_eps= -0.27658 au

Dipole= 1.582 debye



10

C	1.798671	0.026140	-0.256881
C	0.665074	-0.290241	0.357148
C	-0.599255	0.505881	0.255208
O	-1.694874	-0.274273	-0.232077
H	2.690246	-0.577939	-0.155580
H	1.876485	0.910633	-0.878456
H	0.608435	-1.184136	0.970445
H	-0.440048	1.391472	-0.369265
H	-0.916428	0.847380	1.242042
H	-1.446641	-0.643903	-1.085425

Molecule# 1318

2-propenoylazide

PointGroup: C1

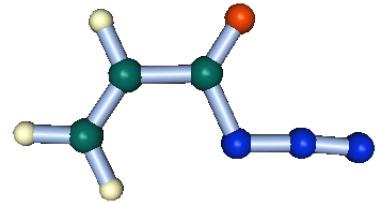
E= -355.660238006 au

ZPE= 0.065396 au

LUMO_eps= -0.08909 au

HOMO_eps= -0.29379 au

Dipole= 3.004 debye



10

O	0.112000	1.645041	0.000178
N	0.429060	-0.659026	-0.000089
N	1.652969	-0.464671	-0.000125
N	2.770025	-0.386800	-0.000154
C	-1.813590	0.267150	0.000107
C	-0.363056	0.533548	0.000075
C	-2.364559	-0.942577	-0.000011
H	-2.413662	1.167111	0.000239
H	-1.760433	-1.838905	-0.000143
H	-3.439057	-1.063786	0.000022

Molecule# 1319

2-propoxyethanol

PointGroup: C1

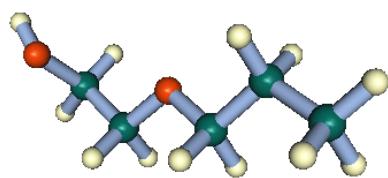
E= -348.329789802 au

ZPE= 0.168917 au

LUMO_eps= -0.01304 au

HOMO_eps= -0.26061 au

Dipole= 1.357 debye



19

C	-3.551731	-0.145916	0.178332
C	-2.160631	-0.497409	-0.345698
C	-1.084795	0.418115	0.210133
C	2.554528	0.252331	-0.341891
C	1.246011	0.820604	0.153652
O	2.871763	-0.915524	0.411744
O	0.173609	0.025383	-0.308235
H	-3.834247	0.874037	-0.090442
H	-4.305646	-0.815827	-0.235313
H	-3.600044	-0.226907	1.266045
H	-2.141876	-0.436709	-1.436016
H	-1.907786	-1.527183	-0.084984
H	-1.294438	1.463084	-0.062635
H	-1.068300	0.365578	1.307923
H	3.334739	1.012724	-0.218945
H	2.461235	0.020138	-1.407091
H	1.140374	1.851849	-0.212086
H	1.258753	0.851169	1.250942
H	3.573974	-1.397171	-0.032650

Molecule# 1320

2-propyn-1-ol

PointGroup: Cs

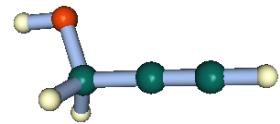
E= -191.942121706 au

ZPE= 0.060645 au

LUMO_eps= -0.02526 au

HOMO_eps= -0.27674 au

Dipole= 1.871 debye



8

C	-0.657272	-0.503422	0.000000
C	0.000000	0.795889	0.000000
C	0.514208	1.878089	0.000000
O	0.326252	-1.539360	0.000000
H	-1.299934	-0.577228	0.884602
H	-1.299934	-0.577228	-0.884602
H	0.977878	2.832712	0.000000
H	-0.129644	-2.386711	0.000000

Molecule# 1321

2-propyn-1-yl diazoacetate

PointGroup: C1

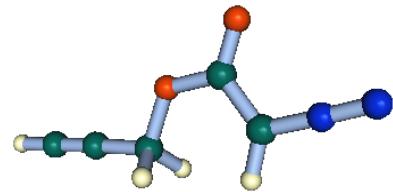
E= -452.927883586 au

ZPE= 0.085156 au

LUMO_eps= -0.08697 au

HOMO_eps= -0.26854 au

Dipole= 4.888 debye



13

O	-0.777836	0.622205	-0.000066
O	1.157333	1.699452	-0.000071
N	2.577306	-0.606933	0.000088
N	3.695819	-0.545596	0.000118
C	-1.504219	-0.618985	-0.000007
C	0.582712	0.639548	-0.000031
C	1.267948	-0.648464	0.000052
C	-2.928155	-0.331723	-0.000031
C	-4.108010	-0.128816	-0.000050
H	-1.247335	-1.201991	-0.888800
H	-1.247348	-1.201899	0.888849
H	0.837583	-1.633315	0.000081
H	-5.152401	0.062286	-0.000066

Molecule# 1322

2-pyridinol

PointGroup: Cs

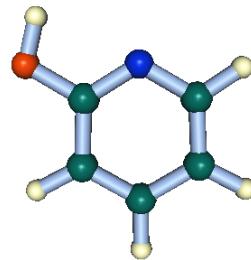
E= -323.645550291 au

ZPE= 0.093305 au

LUMO_eps= -0.04060 au

HOMO_eps= -0.24975 au

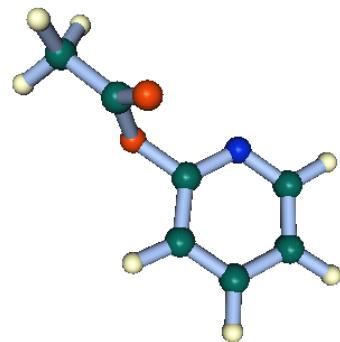
Dipole= 1.334 debye



12

N	-1.176140	0.295001	0.000000
C	0.000000	0.900809	0.000000
C	1.223975	0.226351	0.000000
C	1.190077	-1.154667	0.000000
C	-0.039417	-1.813282	0.000000
C	-1.189267	-1.042689	0.000000
O	0.005822	2.254025	0.000000
H	2.149101	0.783058	0.000000
H	2.113772	-1.717700	0.000000
H	-0.101257	-2.891524	0.000000
H	-2.168354	-1.506394	0.000000
H	-0.919060	2.536214	0.000000

Molecule# 1323
 2-pyridinyl acetate
 PointGroup: C1
 E= -476.348014092 au
 ZPE= 0.129791 au
 LUMO_eps= -0.04610 au
 HOMO_eps= -0.27304 au
 Dipole= 2.389 debye



17

C	-2.338453	1.106760	0.151750
C	-2.887654	-0.169877	0.191707
C	-0.990243	1.249733	-0.135297
C	-2.057419	-1.252130	-0.061697
C	-0.261460	0.091175	-0.369070
C	2.022769	-0.010003	0.246139
C	3.397877	-0.012120	-0.356274
N	-0.757678	-1.126595	-0.342613
O	1.751515	-0.164505	1.402471
O	1.078492	0.204899	-0.727454
H	-2.950154	1.977738	0.343578
H	-3.933897	-0.324461	0.412893
H	-0.509700	2.215713	-0.177084
H	-2.444289	-2.263759	-0.042752
H	3.510688	-0.894802	-0.986722
H	4.140400	-0.030768	0.435030
H	3.538129	0.862122	-0.990340

Molecule# 1324

2-sulfanyl-2,3-dihydro-1,2,3-oxadiazole

PointGroup: C1

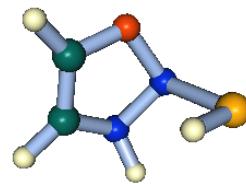
E= -661.527109167 au

ZPE= 0.065982 au

LUMO_eps= -0.04319 au

HOMO_eps= -0.21523 au

Dipole= 3.550 debye



10

S	-1.764262	-0.028731	0.281446
O	0.586821	-1.114709	-0.509303
N	-0.251683	0.006912	-0.828675
N	0.614061	1.105043	-0.503142
C	1.485936	-0.681423	0.451316
C	1.501411	0.645466	0.492509
H	-1.126094	0.003515	1.472452
H	0.064649	1.928199	-0.298450
H	2.039233	-1.439683	0.972831
H	2.095103	1.317395	1.084212

Molecule# 1325

2-sulfanyl-2,3-dihydro-1,2,3-thiadiazole

PointGroup: C1

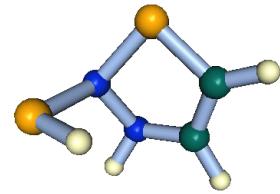
E= -984.545022057 au

ZPE= 0.063756 au

LUMO_eps= -0.05089 au

HOMO_eps= -0.20784 au

Dipole= 2.945 debye



10

S	-0.810277	-1.201087	-0.200139
S	1.913381	-0.044710	0.323269
N	0.443660	-0.088164	-0.739013
N	-0.252291	1.168391	-0.769326
C	-1.623704	0.083578	0.709655
C	-1.186766	1.266178	0.270196
H	1.326453	0.217777	1.515056
H	0.406206	1.926467	-0.878431
H	-2.353808	-0.114528	1.473493
H	-1.505287	2.242921	0.599065

Molecule# 1326

2-sulfanyl-2,3-dihydro-1,2,3-triazine-4(1H)-thione

PointGroup: C1

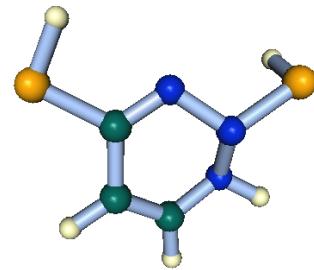
E= -1078.021092010 au

ZPE= 0.084216 au

LUMO_eps= -0.06327 au

HOMO_eps= -0.20801 au

Dipole= 2.577 debye



13

S	2.547758	-0.919099	-0.053026
S	-2.705184	-0.795536	0.103404
N	1.128924	-0.011693	-0.377571
N	-0.064029	-0.748349	-0.053981
N	1.139175	1.250598	0.371535
C	-1.124329	-0.028818	-0.115379
C	-1.120311	1.420199	-0.258114
C	0.038662	2.018372	0.067171
H	2.381553	-1.155465	1.277531
H	-2.221852	-2.049836	0.167875
H	2.042552	1.684451	0.251989
H	-2.024383	1.975775	-0.440590
H	0.148326	3.086836	0.195205

Molecule# 1327

2-sulfylformaldehyde-3-methylbutene

PointGroup: C1

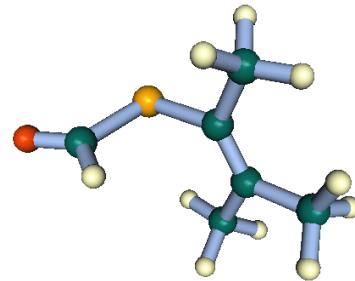
E= -708.211849291 au

ZPE= 0.145626 au

LUMO_eps= -0.04013 au

HOMO_eps= -0.25535 au

Dipole= 4.555 debye



18

C	-1.966141	-0.243997	0.652074
C	1.427449	-0.406198	-0.004522
C	0.548506	0.597372	-0.160463
C	1.159927	-1.840030	-0.373853
C	2.811134	-0.200827	0.559532
C	0.786607	2.053943	0.137899
O	-3.126754	-0.539822	0.672071
S	-1.103623	0.293545	-0.820783
H	-1.304658	-0.279475	1.536228
H	1.992891	-2.231161	-0.963195
H	1.099429	-2.460899	0.524518
H	0.242889	-1.970157	-0.939207
H	2.984133	0.790914	0.963815
H	3.562165	-0.391258	-0.212287
H	2.996780	-0.925244	1.356070
H	0.160197	2.390423	0.967818
H	1.822753	2.273115	0.382174
H	0.510533	2.664030	-0.723971

Molecule# 1328

2-thioformyl-3-thioxopropanoic acid

PointGroup: C1

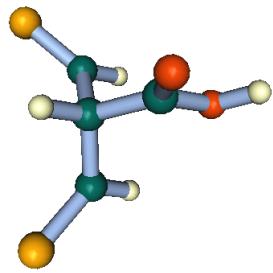
E= -1101.810283740 au

ZPE= 0.076273 au

LUMO_eps= -0.12492 au

HOMO_eps= -0.24759 au

Dipole= 3.080 debye



12

S	2.376125	-1.341871	-0.155715
S	-2.376123	-1.341874	-0.155714
O	-0.000002	2.271956	-1.220927
O	-0.000002	2.134769	1.026292
C	0.000000	0.080610	-0.199333
C	0.000000	1.613145	-0.221280
C	1.234770	-0.423018	0.519041
C	-1.234769	-0.423020	0.519042
H	-0.000002	3.100348	0.941425
H	0.000000	-0.255540	-1.230687
H	1.305553	-0.122487	1.562193
H	-1.305552	-0.122490	1.562194

Molecule# 1329

2-thioxo-1,3-thiazolidin-4-one

PointGroup: Cs

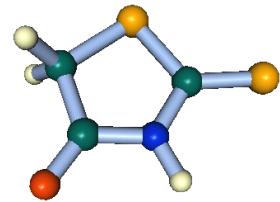
E= -1042.663027770 au

ZPE= 0.062305 au

LUMO_eps= -0.08545 au

HOMO_eps= -0.24809 au

Dipole= 2.050 debye



10

O	1.710629	-2.268770	0.000000
C	0.839149	-1.437452	0.000000
N	1.061346	-0.070202	0.000000
C	0.000000	0.800619	0.000000
S	0.108303	2.432861	0.000000
C	-0.653681	-1.727173	0.000000
S	-1.508948	-0.111223	0.000000
H	2.004537	0.291896	0.000000
H	-0.910734	-2.306252	0.884785
H	-0.910734	-2.306252	-0.884785

Molecule# 1330

2-thioxo-1,3-thiazolidin-5-one

PointGroup: C1

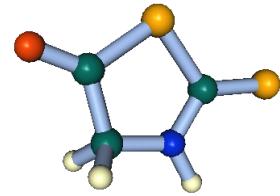
E= -1042.649114670 au

ZPE= 0.061905 au

LUMO_eps= -0.07313 au

HOMO_eps= -0.24025 au

Dipole= 3.739 debye



10

S	0.301124	-1.194128	-0.000003
S	-2.516695	-0.103145	-0.000004
O	2.855536	-0.380914	0.000003
N	-0.251435	1.319996	0.000004
C	-0.891421	0.133788	-0.000001
C	1.703099	-0.063528	0.000002
C	1.190060	1.371895	0.000006
H	-0.815242	2.155712	0.000006
H	1.584859	1.877534	-0.885017
H	1.584856	1.877528	0.885033

Molecule# 1331

2-thioxo-2,3-dihydro-1,3-thiazole-5-carbonitrile

PointGroup: C1

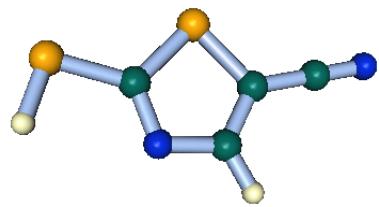
E= -1059.644979380 au

ZPE= 0.052788 au

LUMO_eps= -0.08625 au

HOMO_eps= -0.25941 au

Dipole= 3.918 debye



10

S	-0.132326	-1.067056	-0.000002
S	2.794229	-0.264794	-0.000005
N	0.642381	1.397235	0.000001
N	-3.851613	-0.306271	0.000006
C	-1.339600	0.198368	0.000002
C	1.094765	0.176601	-0.000002
C	-0.717729	1.417421	0.000003
C	-2.720759	-0.076305	0.000004
H	3.213634	1.014221	-0.000004
H	-1.239521	2.362120	0.000006

Molecule# 1332

2-thioxothioacetamide

PointGroup: C1

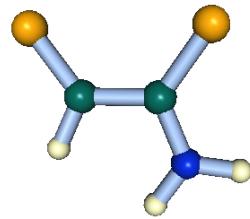
E= -929.242602727 au

ZPE= 0.050419 au

LUMO_eps= -0.13558 au

HOMO_eps= -0.23158 au

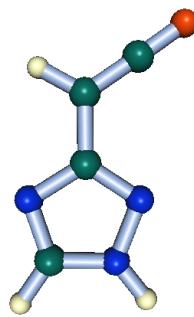
Dipole= 4.577 debye



8

S	-1.212773	-1.207584	0.003315
S	2.042508	-0.178536	-0.008928
N	-1.534033	1.415066	-0.011441
C	-0.689942	0.359550	0.002786
C	0.740967	0.774182	0.022682
H	-1.200704	2.364588	-0.016085
H	-2.525891	1.249315	-0.027968
H	0.882911	1.856177	0.061139

Molecule# 1333
 2,1H-1,2,4-triazol-3-yl-ethenone
 PointGroup: C1
 E= -393.813158108 au
 ZPE= 0.073645 au
 LUMO_eps= -0.05327 au
 HOMO_eps= -0.23292 au
 Dipole= 2.949 debye



11

O	3.181131	-0.527751	-0.000030
N	-0.504861	-0.979797	0.000012
N	-1.316186	1.134512	0.000007
N	-1.860177	-0.974625	0.000024
C	-0.220224	0.316198	0.000000
C	-2.321692	0.286099	0.000022
C	1.127446	0.850818	-0.000016
C	2.212545	0.104559	-0.000024
H	-2.366760	-1.842693	0.000036
H	-3.369334	0.536264	0.000030
H	1.267161	1.921766	-0.000023

Molecule# 1334

2,1H-pyridinone

PointGroup: Cs

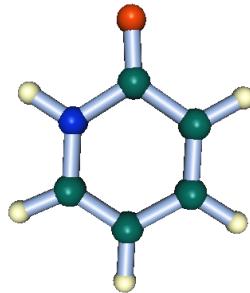
E= -323.646432376 au

ZPE= 0.093534 au

LUMO_eps= -0.05791 au

HOMO_eps= -0.23279 au

Dipole= 4.377 debye



12

C	1.261707	-1.038161	0.000000
C	1.243130	0.321689	0.000000
C	0.059615	-1.797793	0.000000
C	-1.119466	-1.125244	0.000000
C	0.000000	1.062865	0.000000
N	-1.136850	0.234049	0.000000
O	-0.131026	2.279065	0.000000
H	2.211330	-1.558148	0.000000
H	2.150199	0.907306	0.000000
H	0.072270	-2.875784	0.000000
H	-2.082206	-1.615153	0.000000
H	-2.015349	0.730776	0.000000

Molecule# 1335

2,1H-pyrrol-2-yl-1H-pyrrole

PointGroup: C2

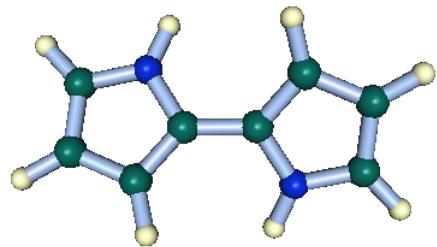
E= -419.310989853 au

ZPE= 0.145562 au

LUMO_eps= -0.01538 au

HOMO_eps= -0.18979 au

Dipole= 0.681 debye



18

C	-0.367218	2.951058	0.128332
C	0.367218	-2.951058	0.128332
C	-0.964817	1.668994	0.237015
C	0.964817	-1.668994	0.237015
C	0.964817	2.761561	-0.145704
C	-0.964817	-2.761561	-0.145704
C	0.021536	0.722146	0.022813
C	-0.021536	-0.722146	0.022813
N	1.189772	1.410224	-0.205634
N	-1.189772	-1.410224	-0.205634
H	-0.856131	3.902314	0.249268
H	0.856131	-3.902314	0.249268
H	-1.992085	1.462515	0.486567
H	1.992085	-1.462515	0.486567
H	1.761222	3.466788	-0.303118
H	-1.761222	-3.466788	-0.303118
H	2.062056	0.976796	-0.448014
H	-2.062056	-0.976796	-0.448014

Molecule# 1336

2,2'-(methylimino)diacetylenol

PointGroup: C1

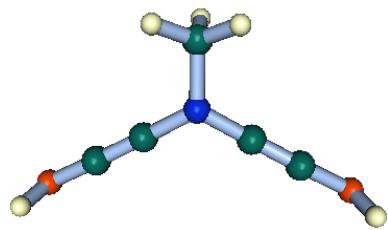
E= -398.695047896 au

ZPE= 0.091461 au

LUMO_eps= -0.02616 au

HOMO_eps= -0.20163 au

Dipole= 2.610 debye



13

O	3.378898	-1.121353	0.151039
O	-3.378897	-1.121355	0.151039
N	0.000000	0.726298	-0.101503
C	1.173373	0.061418	-0.031423
C	-1.173373	0.061419	-0.031423
C	2.234557	-0.498966	-0.039656
C	-2.234557	-0.498966	-0.039656
C	0.000000	2.188036	0.049856
H	3.788790	-1.339293	-0.695372
H	-3.788797	-1.339280	-0.695372
H	-0.000002	2.478463	1.103218
H	0.888064	2.590021	-0.432378
H	-0.888061	2.590022	-0.432382

Molecule# 1337

2,2'-bifuran

PointGroup: C2h

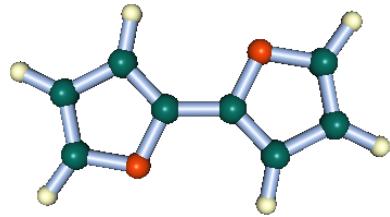
E= -459.032707773 au

ZPE= 0.120399 au

LUMO_eps= -0.04052 au

HOMO_eps= -0.20724 au

Dipole= 0.000 debye



16

C	-0.340935	2.925198	0.000000
C	0.340935	-2.925198	0.000000
C	-0.990750	1.654854	0.000000
C	0.990750	-1.654854	0.000000
C	0.990750	2.673861	0.000000
C	-0.990750	-2.673861	0.000000
C	0.001025	0.717171	0.000000
C	-0.001025	-0.717171	0.000000
O	1.221122	1.331017	0.000000
O	-1.221122	-1.331017	0.000000
H	-0.806983	3.895142	0.000000
H	0.806983	-3.895142	0.000000
H	-2.047458	1.455961	0.000000
H	2.047458	-1.455961	0.000000
H	1.864288	3.299524	0.000000
H	-1.864288	-3.299524	0.000000

Molecule# 1338

2,2'-iminodiacetylenol

PointGroup: C1

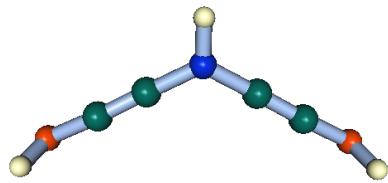
E= -359.374576435 au

ZPE= 0.063707 au

LUMO_eps= -0.02713 au

HOMO_eps= -0.20890 au

Dipole= 2.704 debye



10

O	-3.400108	-0.733442	-0.118928
O	3.400112	-0.733432	-0.118929
N	0.000000	1.083109	0.012803
C	-1.191775	0.449091	-0.005616
C	1.191770	0.449084	-0.005610
C	-2.247386	-0.118373	0.033472
C	2.247401	-0.118342	0.033478
H	-3.781620	-0.952804	0.740381
H	3.781529	-0.952982	0.740374
H	0.000002	2.090260	-0.001864

Molecule# 1339

2,2'-oxodiethenone

PointGroup: C2

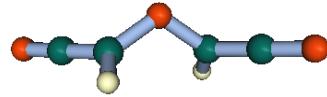
E= -379.323782261 au

ZPE= 0.050938 au

LUMO_eps= -0.09339 au

HOMO_eps= -0.24547 au

Dipole= 1.250 debye



9

O	0.000000	0.000000	0.648088
O	0.000000	3.317523	-0.078152
O	0.000000	-3.317523	-0.078152
C	-0.698728	0.939522	-0.114391
C	0.698728	-0.939522	-0.114391
C	-0.313392	2.199290	-0.102139
C	0.313392	-2.199290	-0.102139
H	-1.576390	0.640518	-0.667959
H	1.576390	-0.640518	-0.667959

Molecule# 1340

2,2-dichloroethanimidamide

PointGroup: C1

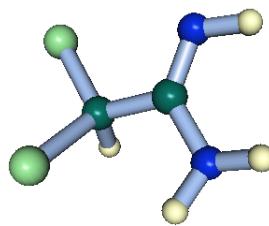
E= -1108.655389200 au

ZPE= 0.067986 au

LUMO_eps= -0.04439 au

HOMO_eps= -0.27556 au

Dipole= 3.722 debye



10

C1	-0.526261	1.700246	-0.274259
C1	-1.582683	-1.029630	0.088524
N	2.158124	0.361415	0.398415
N	1.210052	-1.612358	-0.532489
C	-0.238755	0.057016	0.456190
C	1.125544	-0.473565	0.016892
H	-0.244149	0.225219	1.527203
H	1.958781	1.347469	0.456439
H	3.066064	0.149391	0.018031
H	2.173371	-1.866660	-0.744155

Molecule# 1341

2,2-dichloropropane

PointGroup: C2v

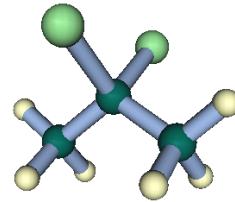
E= -1038.457578180 au

ZPE= 0.084593 au

LUMO_eps= -0.02270 au

HOMO_eps= -0.30224 au

Dipole= 2.421 debye



11

C	0.000000	0.000000	0.352403
Cl	1.474178	0.000000	-0.722182
Cl	-1.474178	0.000000	-0.722182
C	0.000000	1.271429	1.177208
C	0.000000	-1.271429	1.177208
H	0.000000	2.149972	0.537521
H	0.000000	-2.149972	0.537521
H	-0.887342	1.294212	1.809560
H	0.887342	1.294212	1.809560
H	0.887342	-1.294212	1.809560
H	-0.887342	-1.294212	1.809560

Molecule# 1342

2,2-dicyanoacetamide

PointGroup: C1

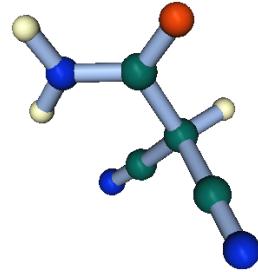
E= -393.826646209 au

ZPE= 0.071307 au

LUMO_eps= -0.04719 au

HOMO_eps= -0.31365 au

Dipole= 3.521 debye



11

O	-2.033653	0.612083	-0.561323
N	-1.365160	-1.096229	0.782146
N	1.209013	2.325640	0.584750
N	1.852388	-1.914574	-0.073469
C	0.319024	0.144506	-0.545846
C	-1.174935	-0.099455	-0.102612
C	0.820959	1.367480	0.085232
C	1.211308	-0.986418	-0.292477
H	0.261923	0.314072	-1.623641
H	-0.620032	-1.690702	1.101554
H	-2.304488	-1.280568	1.092902

Molecule# 1343

2,2-dicyanoethanedithioicacid

PointGroup: C1

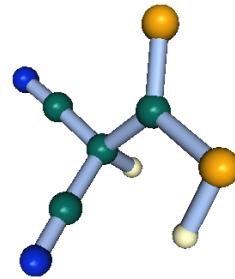
E= -1059.601401110 au

ZPE= 0.050975 au

LUMO_eps= -0.12437 au

HOMO_eps= -0.27159 au

Dipole= 3.901 debye



10

S	2.003409	0.770859	0.144997
S	0.824434	-1.874911	-0.296043
N	-2.788831	-1.286739	0.056249
N	-1.196262	2.646561	-0.557680
C	-0.747144	0.287249	0.481702
C	0.630661	-0.307408	0.072187
C	-1.869388	-0.620646	0.224187
C	-1.016190	1.603166	-0.112117
H	-0.695773	0.434643	1.567730
H	1.358300	1.937262	0.363284

Molecule# 1344

2,2-difluoro-1,3-dithiolane

PointGroup: C1

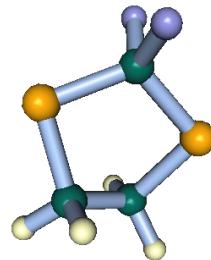
E= -1112.978523800 au

ZPE= 0.069617 au

LUMO_eps= -0.03963 au

HOMO_eps= -0.25818 au

Dipole= 3.845 debye



11

S	-0.180530	-1.510125	0.096697
S	-0.180530	1.510125	-0.096698
F	1.690299	-0.019073	-1.077617
F	1.690298	0.019073	1.077618
C	0.856748	0.000000	0.000000
C	-1.750263	-0.681445	-0.334640
C	-1.750262	0.681445	0.334641
H	-2.551770	-1.315256	0.043945
H	-1.841107	-0.594140	-1.415457
H	-2.551770	1.315257	-0.043944
H	-1.841105	0.594141	1.415458

Molecule# 1345

2,2-difluoro-2-isocyanatoethane

PointGroup: C1

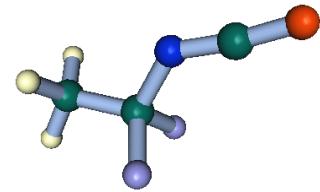
E= -445.976800271 au

ZPE= 0.063098 au

LUMO_eps= -0.02963 au

HOMO_eps= -0.33109 au

Dipole= 2.360 debye



10

F	-0.777482	-0.846334	1.091554
F	-0.777487	-0.846342	-1.091545
O	2.802791	0.007738	-0.000006
N	0.529576	0.669815	-0.000003
C	-0.715131	-0.014559	0.000002
C	-1.891632	0.924090	0.000000
C	1.670848	0.263476	-0.000005
H	-2.809445	0.341143	0.000005
H	-1.854854	1.552140	-0.887058
H	-1.854850	1.552146	0.887056

Molecule# 1346

2,2-dimethyl-1-propanethiol

PointGroup: Cs

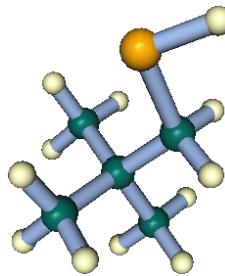
E= -596.068469363 au

ZPE= 0.158156 au

LUMO_eps= -0.01881 au

HOMO_eps= -0.23825 au

Dipole= 1.592 debye



18

C	0.674889	0.424910	0.000000
C	1.189289	1.875357	0.000000
H	2.280421	1.893123	0.000000
S	-1.677881	-1.162383	0.000000
H	-2.940602	-0.701861	0.000000
C	-0.864560	0.499457	0.000000
C	1.189289	-0.290385	1.258329
C	1.189289	-0.290385	-1.258329
H	-1.202991	1.037483	0.884380
H	-1.202991	1.037483	-0.884380
H	2.280323	-0.281639	1.280304
H	2.280323	-0.281639	-1.280304
H	0.862904	-1.329613	1.294987
H	0.862904	-1.329613	-1.294987
H	0.831671	0.202325	2.164531
H	0.831671	0.202325	-2.164531
H	0.846646	2.418019	-0.883096
H	0.846646	2.418019	0.883096

Molecule# 1347

2,2-dimethylbutane

PointGroup: Cs

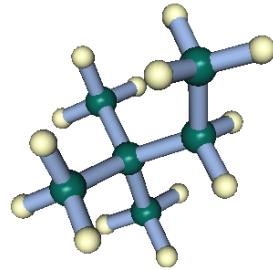
E= -237.175178103 au

ZPE= 0.187068 au

LUMO_eps= -0.01256 au

HOMO_eps= -0.31104 au

Dipole= 0.060 debye



20

C	-1.909658	-1.067465	0.000000
C	0.899358	-0.498996	1.255256
C	0.899358	1.663266	0.000000
C	0.899358	-0.498996	-1.255256
C	-1.169008	0.270451	0.000000
C	0.377490	0.217634	0.000000
H	-1.674987	-1.665724	0.881080
H	-2.987965	-0.901561	0.000000
H	-1.674987	-1.665724	-0.881080
H	0.598153	-1.546802	1.280112
H	0.527055	-0.021077	2.164092
H	1.990351	-0.471536	1.288745
H	0.553781	2.206619	-0.882017
H	0.553781	2.206619	0.882017
H	1.990950	1.686803	0.000000
H	0.598153	-1.546802	-1.280112
H	1.990351	-0.471536	-1.288745
H	0.527055	-0.021077	-2.164092
H	-1.486539	0.848219	0.873569
H	-1.486539	0.848219	-0.873569

Molecule# 1348

2,2-dimethylpropane

PointGroup: Td

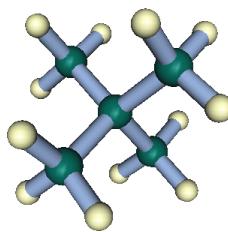
E= -197.850498021 au

ZPE= 0.159266 au

LUMO_eps= -0.01333 au

HOMO_eps= -0.32298 au

Dipole= 0.000 debye



17

C	0.000000	0.000000	0.000000
C	0.886726	0.886726	0.886726
C	-0.886726	-0.886726	0.886726
C	0.886726	-0.886726	-0.886726
C	-0.886726	0.886726	-0.886726
H	-1.529798	0.282357	-1.529798
H	1.529798	1.529798	0.282357
H	1.529798	-0.282357	-1.529798
H	1.529798	0.282357	1.529798
H	-1.529798	-0.282357	1.529798
H	1.529798	-1.529798	-0.282357
H	-0.282357	1.529798	-1.529798
H	0.282357	1.529798	1.529798
H	0.282357	-1.529798	-1.529798
H	-0.282357	-1.529798	1.529798
H	-1.529798	1.529798	-0.282357
H	-1.529798	-1.529798	0.282357

Molecule# 1349

2,2-furylcyclopropyl-3H-imidazole

PointGroup: C1

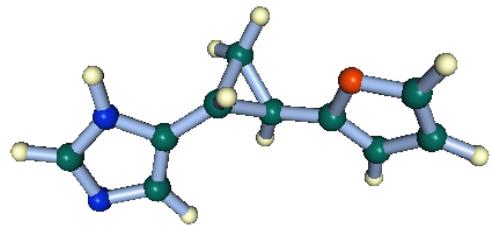
E= -571.962646386 au

ZPE= 0.183949 au

LUMO_eps= -0.01850 au

HOMO_eps= -0.22446 au

Dipole= 3.393 debye



23

C	4.003632	0.781182	-0.318561
C	2.827443	1.218501	0.371503
C	-2.371864	1.192790	-0.026218
C	3.730184	-0.458141	-0.785971
C	-4.074244	-0.047206	-0.382089
C	-1.871478	-0.079363	-0.130780
C	1.920234	0.210847	0.273998
C	0.008227	-1.281057	1.209323
C	-0.510143	-0.639727	-0.057973
C	0.549025	0.058342	0.769007
N	-3.738614	1.201606	-0.180938
N	-2.984446	-0.866017	-0.361682
O	2.461749	-0.825836	-0.433788
H	4.925307	1.321844	-0.446217
H	2.677596	2.159109	0.872631
H	-1.821739	2.102483	0.144386
H	4.287911	-1.179392	-1.354371
H	-5.072787	-0.417046	-0.546593
H	-0.640952	-1.290605	2.073149
H	0.657884	-2.137778	1.105053
H	-0.139037	-1.085527	-0.973867
H	0.211409	0.911932	1.338833
H	-2.984259	-1.864464	-0.477790

Molecule# 1350

2,2-nitrosoamino-3-sulfanylpropanoic acid

PointGroup: C1

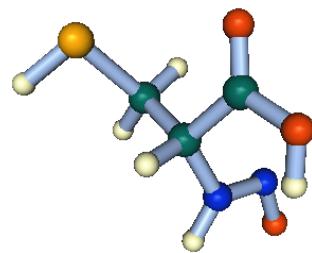
E= -851.435574369 au

ZPE= 0.103491 au

LUMO_eps= -0.09011 au

HOMO_eps= -0.26220 au

Dipole= 5.117 debye



15

S	-2.712144	-0.669688	0.037222
O	0.933735	2.198989	0.455731
O	-0.813211	1.753882	-0.838351
O	3.132632	-1.292925	-0.368579
N	1.364274	-0.584057	0.618722
N	2.135784	-0.617460	-0.478845
C	0.002543	-0.066606	0.511530
C	-0.932563	-0.985226	-0.286130
C	-0.000890	1.370282	-0.050456
H	-0.365039	0.012010	1.536683
H	-0.768377	-0.838439	-1.350349
H	-0.717791	-2.023048	-0.047362
H	1.618464	-1.240568	1.355307
H	-2.888807	-1.681239	0.906858
H	1.575667	1.706649	0.984110

Molecule# 1351

2,2,2-trifluoroethanol

PointGroup: C1

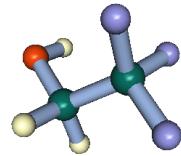
E= -452.961300802 au

ZPE= 0.057122 au

LUMO_eps= -0.02094 au

HOMO_eps= -0.32073 au

Dipole= 1.834 debye



9

C	0.903475	0.760982	-0.089733
C	-0.418912	0.014271	0.005675
O	2.010756	-0.082096	0.112517
F	-0.478794	-0.982705	-0.908971
F	-1.449314	0.849658	-0.237742
F	-0.616843	-0.540066	1.211194
H	0.924062	1.263938	-1.060758
H	0.919466	1.514977	0.695005
H	2.067608	-0.715645	-0.610367

Molecule# 1352

2,2,3,3-tetrabromobutane

PointGroup: C2h

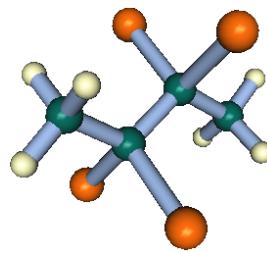
E= -10453.003325500 au

ZPE= 0.091089 au

LUMO_eps= -0.07549 au

HOMO_eps= -0.27288 au

Dipole= 0.000 debye



14

C	1.170094	1.608024	0.000000
C	-1.170094	-1.608024	0.000000
C	-0.094898	0.771068	0.000000
C	0.094898	-0.771068	0.000000
Br	-1.170094	1.298432	1.597049
Br	-1.170094	1.298432	-1.597049
Br	1.170094	-1.298432	-1.597049
Br	1.170094	-1.298432	1.597049
H	1.761250	1.388621	0.886339
H	1.761250	1.388621	-0.886339
H	0.910325	2.662377	0.000000
H	-0.910325	-2.662377	0.000000
H	-1.761250	-1.388621	-0.886339
H	-1.761250	-1.388621	0.886339

Molecule# 1353

2,2,3,3-tetrachlorobutane

PointGroup: C2h

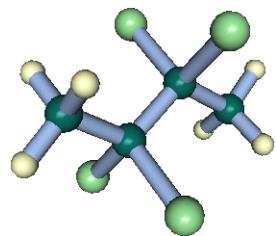
E= -1997.030959590 au

ZPE= 0.093723 au

LUMO_eps= -0.04187 au

HOMO_eps= -0.30182 au

Dipole= 0.000 debye



14

C	1.119788	1.638607	0.000000
C	-1.119788	-1.638607	0.000000
C	-0.125681	0.772915	0.000000
C	0.125681	-0.772915	0.000000
Cl	-1.119788	1.196241	1.462338
Cl	-1.119788	1.196241	-1.462338
Cl	1.119788	-1.196241	-1.462338
Cl	1.119788	-1.196241	1.462338
H	1.713774	1.435038	0.887218
H	1.713774	1.435038	-0.887218
H	0.825079	2.684199	0.000000
H	-0.825079	-2.684199	0.000000
H	-1.713774	-1.435038	-0.887218
H	-1.713774	-1.435038	0.887218

Molecule# 1354

2,2,3,3-tetrafluorobutane

PointGroup: C2

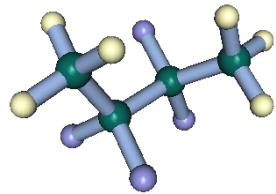
E= -555.650550604 au

ZPE= 0.099698 au

LUMO_eps= -0.01674 au

HOMO_eps= -0.34450 au

Dipole= 3.407 debye



14

C	0.328548	1.572029	1.131282
C	-0.328548	-1.572029	1.131282
C	-0.204552	0.748232	-0.013408
C	0.204552	-0.748232	-0.013408
F	-1.578360	0.789917	-0.017302
F	0.204552	1.293625	-1.195961
F	-0.204552	-1.293625	-1.195961
F	1.578360	-0.789917	-0.017302
H	-0.001444	2.599626	0.991670
H	-0.053588	1.204459	2.080962
H	1.415266	1.540080	1.139481
H	-1.415266	-1.540080	1.139481
H	0.001444	-2.599626	0.991670
H	0.053588	-1.204459	2.080962

Molecule# 1355

2,2,4-trimethylpentane

PointGroup: C1

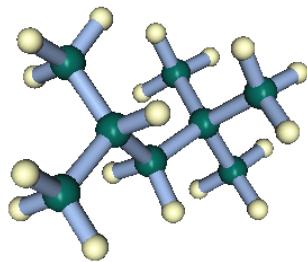
E= -315.825992083 au

ZPE= 0.243429 au

LUMO_eps= -0.01350 au

HOMO_eps= -0.30219 au

Dipole= 0.125 debye



26

C	-1.846468	1.363840	-0.077215
C	-2.662406	-1.005759	-0.096294
C	2.238415	-1.049347	-0.534903
C	1.347049	0.062739	1.517236
C	1.470851	1.310380	-0.660535
C	-0.206189	-0.619162	-0.388682
C	-1.491679	-0.085189	0.274492
C	1.189357	-0.053191	-0.006364
H	-1.878530	1.507566	-1.160137
H	-2.830639	1.621044	0.318884
H	-1.136791	2.079950	0.332372
H	-2.842778	-0.992361	-1.174393
H	-3.583115	-0.688469	0.396236
H	-2.465759	-2.039230	0.193579
H	2.126690	-2.027904	-0.064042
H	3.250825	-0.693599	-0.333918
H	2.141559	-1.185634	-1.614225
H	2.366909	0.355952	1.774490
H	0.675201	0.809842	1.941318
H	1.141903	-0.890029	2.010264
H	0.817786	2.095891	-0.286579
H	2.499514	1.619425	-0.462797
H	1.343993	1.257474	-1.743806
H	-0.175142	-1.692454	-0.177183
H	-0.319174	-0.537597	-1.476057
H	-1.366031	-0.145726	1.359582

Molecule# 1356

2,2,5-trimethylhexane

PointGroup: Cs

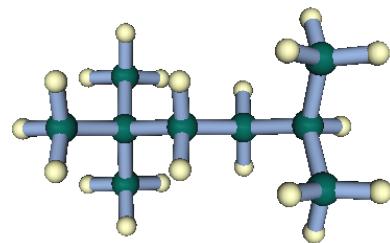
E= -355.156227875 au

ZPE= 0.271721 au

LUMO_eps= -0.01391 au

HOMO_eps= -0.30127 au

Dipole= 0.162 debye



29

C	0.261359	2.728775	1.263761
C	0.261359	2.728775	-1.263761
C	0.261359	-2.190212	-1.255251
C	0.261359	-2.190212	1.255251
C	-1.897219	-2.110279	0.000000
C	0.930924	0.602207	0.000000
C	-0.435871	-0.089408	0.000000
C	0.902632	2.145688	0.000000
C	-0.433736	-1.639048	0.000000
H	0.722844	2.323751	2.166617
H	-0.807615	2.513614	1.310589
H	0.375647	3.813898	1.290358
H	-0.807615	2.513614	-1.310589
H	0.375647	3.813898	-1.290358
H	0.722844	2.323751	-2.166617
H	-0.197356	-1.795095	-2.164364
H	1.321852	-1.937870	-1.278005
H	0.183154	-3.278767	-1.290423
H	1.321852	-1.937870	1.278005
H	-0.197356	-1.795095	2.164364
H	0.183154	-3.278767	1.290423
H	-2.428479	-1.746411	-0.882025
H	-2.428479	-1.746411	0.882025
H	-1.958193	-3.200485	0.000000
H	1.502655	0.279924	-0.874023
H	1.502655	0.279924	0.874023
H	-1.005955	0.238235	-0.873903
H	-1.005955	0.238235	0.873903
H	1.951716	2.460219	0.000000

Molecule# 1357

2,3-butanedione

PointGroup: C2h

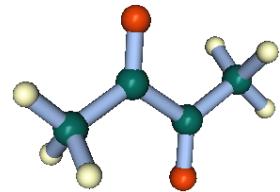
E= -306.599149877 au

ZPE= 0.092810 au

LUMO_eps= -0.09891 au

HOMO_eps= -0.25670 au

Dipole= 0.000 debye



12

C	1.188334	-1.577198	0.000000
H	1.793080	-1.322397	0.871672
H	0.948796	-2.636600	0.000000
H	1.793080	-1.322397	-0.871672
C	-1.188334	1.577198	0.000000
H	-1.793080	1.322397	0.871672
H	-0.948796	2.636600	0.000000
H	-1.793080	1.322397	-0.871672
C	0.078985	0.772271	0.000000
O	1.188334	1.252788	0.000000
C	-0.078985	-0.772271	0.000000
O	-1.188334	-1.252788	0.000000

Molecule# 1358

2,3-diamino-1,3-butadiene-1,4-dione

PointGroup: C2

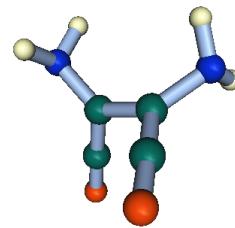
E= -414.862445434 au

ZPE= 0.081721 au

LUMO_eps= -0.05550 au

HOMO_eps= -0.23444 au

Dipole= 3.135 debye



12

O	0.662791	2.150274	-1.440821
O	-0.662791	-2.150274	-1.440821
N	-1.126502	1.290107	1.322386
N	1.126502	-1.290107	1.322386
C	-0.235728	0.702221	0.369706
C	0.235728	-0.702221	0.369706
C	0.235728	1.488873	-0.589450
C	-0.235728	-1.488873	-0.589450
H	-0.752204	1.293584	2.261984
H	-2.038657	0.851873	1.326339
H	0.752204	-1.293584	2.261984
H	2.038657	-0.851873	1.326339

Molecule# 1359

2,3-diazabutadiene

PointGroup: C2h

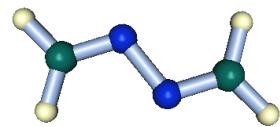
E= -188.123207085 au

ZPE= 0.061057 au

LUMO_eps= -0.06274 au

HOMO_eps= -0.25438 au

Dipole= 0.000 debye



8

C	0.655134	1.533738	0.000000
N	0.655134	0.265229	0.000000
N	-0.655134	-0.265229	0.000000
C	-0.655134	-1.533738	0.000000
H	-0.265958	2.114793	0.000000
H	1.612147	2.041686	0.000000
H	0.265958	-2.114793	0.000000
H	-1.612147	-2.041686	0.000000

Molecule# 1360

2,3-dichloro-1,3-cyclohexadien-5-yne

PointGroup: Cs

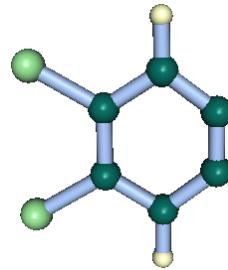
E= -1150.251190690 au

ZPE= 0.056185 au

LUMO_eps= -0.10943 au

HOMO_eps= -0.26949 au

Dipole= 0.776 debye



10

C1	1.404145	1.587201	0.000000
C1	1.404145	-1.587200	0.000000
C	-0.099467	0.708116	0.000000
C	-0.099467	-0.708116	0.000000
C	-1.288023	1.457987	0.000000
C	-1.288023	-1.457988	0.000000
C	-2.378023	0.619733	0.000000
C	-2.378023	-0.619734	0.000000
H	-1.277395	2.536568	0.000000
H	-1.277395	-2.536568	0.000000

Molecule# 1361

2,3-dihydro-1,2-thiazole-1-oxide

PointGroup: C1

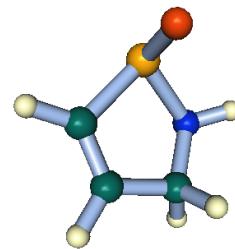
E= -645.558883773 au

ZPE= 0.081484 au

LUMO_eps= -0.04063 au

HOMO_eps= -0.24820 au

Dipole= 3.857 debye



11

C	-1.470654	0.825217	0.180286
C	-1.553390	-0.662462	0.294602
C	-0.306511	1.283031	-0.252180
N	-0.356943	-1.153514	-0.388425
O	1.719592	0.003041	0.864117
S	0.944753	-0.019129	-0.414780
H	-2.309000	1.451695	0.454288
H	-1.613318	-0.957897	1.349242
H	-2.442883	-1.050971	-0.208260
H	0.004141	2.307754	-0.379815
H	-0.029788	-2.068961	-0.109186

Molecule# 1362

2,3-dihydro-1,2,3-thiadiazole

PointGroup: C1

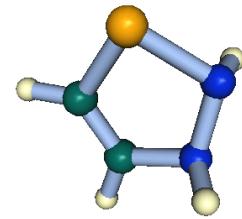
E= -586.341382712 au

ZPE= 0.066308 au

LUMO_eps= -0.03080 au

HOMO_eps= -0.21087 au

Dipole= 1.719 debye



9

S	-1.237044	0.001448	-0.107671
N	0.008561	-1.244800	0.162871
N	1.291262	-0.667661	-0.105066
C	-0.008423	1.263519	0.104972
C	1.217607	0.751160	0.046079
H	-0.002263	-1.404163	1.165699
H	1.571441	-0.928185	-1.047847
H	-0.273152	2.302314	0.208260
H	2.142819	1.306025	0.085693

Molecule# 1363

2,3-dihydro-1,3-oxazole

PointGroup: Cs

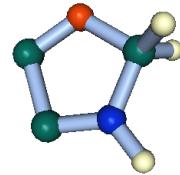
E= -245.996895994 au

ZPE= 0.055825 au

LUMO_eps= -0.10895 au

HOMO_eps= -0.22720 au

Dipole= 6.222 debye



8

O	-0.353454	-1.104461	0.000000
N	0.000000	1.089677	0.000000
C	-1.093179	0.134053	0.000000
C	0.952187	-0.943381	0.000000
C	1.214335	0.602031	0.000000
H	-0.198428	2.081953	0.000000
H	-1.707000	0.184886	0.898569
H	-1.707000	0.184886	-0.898569

Molecule# 1364

2,3-dihydro-1,3,4-thiadiazole-2-thiol

PointGroup: C1

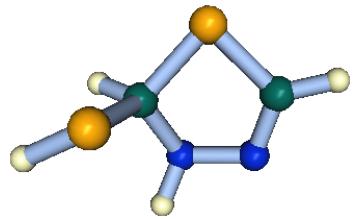
E= -984.595558470 au

ZPE= 0.065173 au

LUMO_eps= -0.02967 au

HOMO_eps= -0.22961 au

Dipole= 1.253 debye



10

S	0.807257	-1.220346	0.197198
S	-1.948226	-0.076615	-0.421874
N	0.326375	1.278014	0.589110
N	1.350166	1.260862	-0.340449
C	-0.427430	0.038051	0.678459
C	1.721627	0.074068	-0.599627
H	-2.794969	0.485790	0.462355
H	-0.239031	2.107672	0.478029
H	-0.761306	-0.139902	1.694067
H	2.549843	-0.147039	-1.253252

Molecule# 1365

2,3-dihydro-5-methylfuran

PointGroup: C1

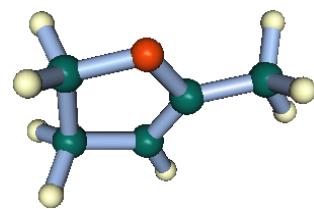
E= -270.652413007 au

ZPE= 0.120243 au

LUMO_eps= -0.01008 au

HOMO_eps= -0.21235 au

Dipole= 0.838 debye



14

C	-1.368345	-0.812936	0.080163
H	-1.906003	-1.388570	-0.670058
H	-1.661689	-1.161174	1.072427
O	0.046311	-1.092004	-0.079668
C	-1.532303	0.714437	-0.061297
H	-2.174500	1.121723	0.721203
H	-1.979486	0.993680	-1.020378
C	-0.096949	1.168984	0.041568
H	0.227483	2.195282	0.084198
C	2.190006	0.000476	0.008583
H	2.539202	-0.503258	-0.895119
H	2.646994	0.986271	0.059826
H	2.528636	-0.591735	0.860936
C	0.709071	0.109674	0.001700

Molecule# 1366

2,3-dihydrofuran

PointGroup: C1

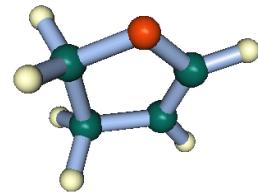
E= -231.314245299 au

ZPE= 0.092555 au

LUMO_eps= -0.01039 au

HOMO_eps= -0.21920 au

Dipole= 1.260 debye



11

H	1.090374	2.042312	0.076465
C	0.596544	1.086224	0.038981
H	2.249849	-0.338572	0.019187
C	1.198765	-0.096252	0.008788
O	0.365290	-1.176016	-0.062866
H	-1.297406	1.237768	-1.005784
H	-1.452898	1.372804	0.739281
C	-0.896855	0.873537	-0.055484
H	-1.592748	-1.131233	-0.710934
H	-1.364629	-0.974542	1.041627
C	-0.990931	-0.663577	0.064896

Molecule# 1367

2,3-dihydrothiophene-1-oxide

PointGroup: C1

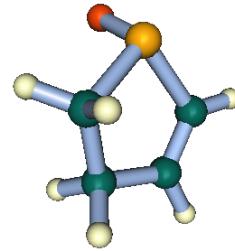
E= -629.516865012 au

ZPE= 0.092913 au

LUMO_eps= -0.04086 au

HOMO_eps= -0.23622 au

Dipole= 4.588 debye



12

C	-1.465797	0.872297	0.156005
C	-1.620855	-0.609455	0.335459
C	-0.276897	1.302884	-0.242595
C	-0.393911	-1.261059	-0.306555
O	1.765599	-0.030829	0.858773
S	0.967718	0.002094	-0.419379
H	-2.288404	1.542755	0.376595
H	-1.699412	-0.844109	1.400319
H	-2.540491	-0.970774	-0.129233
H	0.033910	2.327308	-0.379703
H	0.024673	-2.096585	0.248885
H	-0.593786	-1.573461	-1.330850

Molecule# 1368

2,3-dihydrothiophene-1,1-dioxide

PointGroup: C1

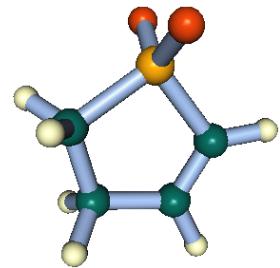
E= -704.766801608 au

ZPE= 0.098393 au

LUMO_eps= -0.04374 au

HOMO_eps= -0.29012 au

Dipole= 5.640 debye



13

O	1.368073	-0.041927	1.328654
S	0.744052	0.002026	0.009543
O	1.597344	0.012383	-1.173724
C	-0.537812	-1.301973	-0.132311
C	-1.894471	-0.605338	0.038088
C	-1.683857	0.887280	-0.028918
C	-0.438708	1.331798	-0.052416
H	-0.319494	-2.041155	0.632439
H	-0.409741	-1.736972	-1.119449
H	-2.352765	-0.862446	0.995568
H	-2.595132	-0.923617	-0.735185
H	-2.540636	1.548631	-0.035815
H	-0.081319	2.348887	-0.076348

Molecule# 1369

2,3-dihydrothiophene-2-ol

PointGroup: C1

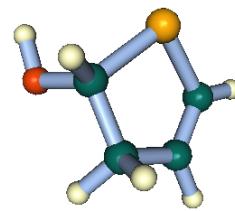
E= -629.551752735 au

ZPE= 0.093663 au

LUMO_eps= -0.01783 au

HOMO_eps= -0.22085 au

Dipole= 0.750 debye



12

S	-0.392972	-1.265072	0.210669
C	0.940796	0.017803	0.413655
C	0.214759	1.365119	0.480256
C	-1.100528	1.217508	-0.232047
C	-1.506870	-0.035217	-0.406130
O	1.821436	0.051740	-0.690597
H	1.477232	-0.222620	1.331943
H	0.856678	2.126104	0.033990
H	-1.678395	2.075102	-0.546595
H	-2.430535	-0.355577	-0.862849
H	0.048224	1.648671	1.524486
H	2.153911	-0.835724	-0.861306

Molecule# 1370

2,3-dihydrothiophene

PointGroup: C1

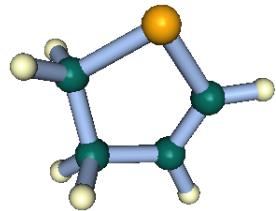
E= -554.300241298 au

ZPE= 0.089395 au

LUMO_eps= -0.01264 au

HOMO_eps= -0.20959 au

Dipole= 1.643 debye



11

C	-0.078596	-1.271647	0.190282
H	-0.054339	-1.558641	1.240593
H	0.112578	-2.148979	-0.421154
C	-1.395081	-0.560009	-0.160033
H	-2.213837	-0.949245	0.447464
H	-1.665515	-0.738605	-1.207404
C	0.114747	1.280233	0.074877
H	0.490719	2.289118	0.151229
C	-1.163345	0.913938	0.056193
H	-1.979816	1.619897	0.117529
S	1.277741	-0.043040	-0.081011

Molecule# 1371

2,3-dimethyl-1-butene

PointGroup: C1

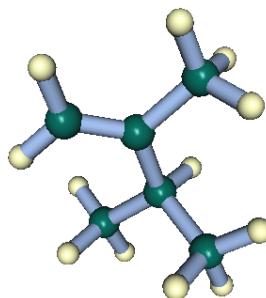
E= -235.944160614 au

ZPE= 0.164231 au

LUMO_eps= -0.01239 au

HOMO_eps= -0.25126 au

Dipole= 0.590 debye



18

C -1.071798 1.395295 -0.516943

H -2.097308 1.655846 -0.745207

H -0.324065 2.139068 -0.752121

C -1.846494 -0.781611 0.354048

H -1.822725 -1.041562 1.416022

H -2.835490 -0.389471 0.122101

H -1.717430 -1.714418 -0.199086

C -0.767616 0.217558 0.024788

C 1.126951 -1.341248 -0.574524

H 2.119063 -1.686706 -0.279687

H 0.459313 -2.201864 -0.554699

H 1.185647 -0.984025 -1.604310

C 0.651228 -0.212141 0.359200

H 0.614475 -0.630270 1.372557

C 1.673172 0.925370 0.370849

H 1.815739 1.345990 -0.626310

H 1.368190 1.732615 1.036949

H 2.641935 0.555459 0.709287

Molecule# 1372

2,3-dimethyl-2-butene

PointGroup: D2h

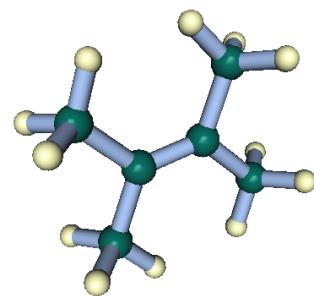
E= -235.947601108 au

ZPE= 0.162967 au

LUMO_eps= -0.01240 au

HOMO_eps= -0.22746 au

Dipole= 0.000 debye



18

C	0.671348	0.000000	0.000000
C	-0.671348	0.000000	0.000000
C	1.522644	1.246022	0.000000
C	1.522644	-1.246022	0.000000
C	-1.522644	-1.246022	0.000000
C	-1.522644	1.246022	0.000000
H	2.179680	1.256485	0.874962
H	2.179680	1.256485	-0.874962
H	0.958985	2.173276	0.000000
H	2.179680	-1.256485	0.874962
H	0.958985	-2.173276	0.000000
H	2.179680	-1.256485	-0.874962
H	-2.179680	-1.256485	-0.874962
H	-2.179680	-1.256485	0.874962
H	-0.958985	-2.173276	0.000000
H	-2.179680	1.256485	-0.874962
H	-2.179680	1.256485	0.874962
H	-0.958985	2.173276	0.000000

Molecule# 1373

2,3-dimethylbutadiene

PointGroup: C2

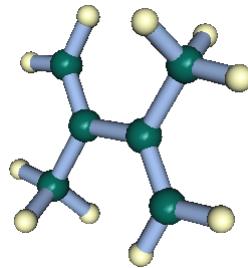
E= -234.719001305 au

ZPE= 0.141473 au

LUMO_eps= -0.03921 au

HOMO_eps= -0.23784 au

Dipole= 0.000 debye



16

C	0.046940	0.737664	0.000000
C	-0.046940	-0.737664	0.000000
C	1.229298	-1.540526	0.000000
C	-1.229298	-1.365802	-0.000001
C	-1.229298	1.540526	0.000000
C	1.229298	1.365802	-0.000001
H	1.011005	-2.606697	0.000002
H	1.839074	-1.319891	-0.878346
H	1.839074	-1.319889	0.878347
H	-1.285187	-2.445953	-0.000001
H	-2.170393	-0.836461	-0.000001
H	-1.839074	1.319889	0.878347
H	-1.011005	2.606697	0.000002
H	-1.839074	1.319891	-0.878346
H	2.170393	0.836461	-0.000001
H	1.285187	2.445953	-0.000001

Molecule# 1374

2,3-dimethylbutane

PointGroup: C2h

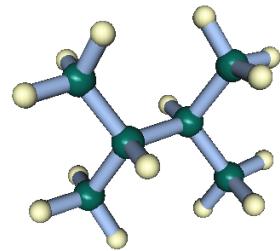
E= -237.173995345 au

ZPE= 0.187213 au

LUMO_eps= -0.00989 au

HOMO_eps= -0.30934 au

Dipole= 0.000 debye



20

C	-0.230967	0.739015	0.000000
C	0.230967	1.496803	1.250954
C	0.230967	1.496803	-1.250954
H	-0.181582	1.079091	2.167949
H	1.320994	1.480162	1.335695
H	1.320994	1.480162	-1.335695
H	-0.181582	1.079091	-2.167949
H	-0.077437	2.542265	1.200790
H	-0.077437	2.542265	-1.200790
H	-1.328230	0.732224	0.000000
C	0.230967	-0.739015	0.000000
C	-0.230967	-1.496803	1.250954
C	-0.230967	-1.496803	-1.250954
H	0.181582	-1.079091	2.167949
H	-1.320994	-1.480162	1.335695
H	-1.320994	-1.480162	-1.335695
H	0.077437	-2.542265	-1.200790
H	0.181582	-1.079091	-2.167949
H	0.077437	-2.542265	1.200790
H	1.328230	-0.732224	0.000000

Molecule# 1375

2,3-dimethylnaphthalene

PointGroup: C2v

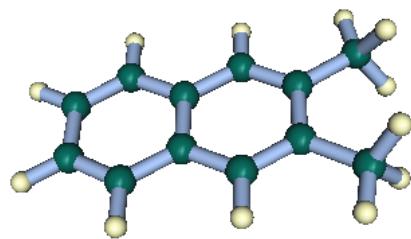
E= -464.691555047 au

ZPE= 0.202296 au

LUMO_eps= -0.04370 au

HOMO_eps= -0.21813 au

Dipole= 0.958 debye



24

C	0.000000	0.705545	3.172599
C	0.000000	-0.705545	3.172599
C	0.000000	1.396736	1.988558
C	0.000000	-1.396736	1.988558
C	0.000000	1.384878	-0.494217
C	0.000000	-1.384878	-0.494217
C	0.000000	0.711893	0.749997
C	0.000000	-0.711893	0.749997
C	0.000000	0.714904	-1.692605
C	0.000000	-0.714904	-1.692605
C	0.000000	1.476613	-2.990942
C	0.000000	-1.476613	-2.990942
H	0.000000	1.240249	4.113143
H	0.000000	-1.240249	4.113143
H	0.000000	2.479711	1.986908
H	0.000000	-2.479711	1.986908
H	0.000000	2.468780	-0.491189
H	0.000000	-2.468780	-0.491189
H	-0.876451	1.238572	-3.598523
H	0.000000	2.550606	-2.812154
H	0.876451	1.238572	-3.598523
H	-0.876451	-1.238572	-3.598523
H	0.876451	-1.238572	-3.598523
H	0.000000	-2.550606	-2.812154

Molecule# 1376

2,3-dimethylphenol

PointGroup: C1

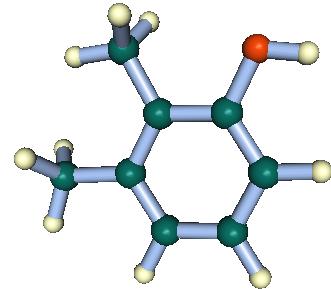
E= -386.250948013 au

ZPE= 0.159534 au

LUMO_eps= -0.01537 au

HOMO_eps= -0.22546 au

Dipole= 0.614 debye



19

C	-0.213058	2.110789	-0.000013
C	1.042586	1.522127	0.000007
C	-1.349117	1.314820	-0.000027
C	1.187094	0.132469	-0.000047
C	0.046570	-0.684289	-0.000161
C	-1.210519	-0.067972	-0.000041
C	2.574664	-0.460211	0.000086
C	0.106756	-2.189188	-0.000088
O	-2.303561	-0.899154	0.000146
H	-0.310027	3.188042	0.000026
H	1.926806	2.145506	0.000092
H	-2.337118	1.760334	0.000039
H	2.748533	-1.085830	0.877800
H	2.749167	-1.084718	-0.878307
H	3.326642	0.326983	0.000827
H	-0.398378	-2.599980	0.876317
H	-0.408082	-2.600325	-0.870566
H	1.128274	-2.557539	-0.005554
H	-3.107182	-0.370501	-0.000145

Molecule# 1377

2,3-dimethylpyridine

PointGroup: Cs

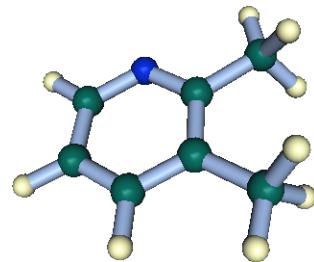
E= -327.042023871 au

ZPE= 0.143369 au

LUMO_eps= -0.03049 au

HOMO_eps= -0.25253 au

Dipole= 2.200 debye



17

C	1.299716	-1.582465	0.000000
C	-0.088674	-1.564388	0.000000
C	1.965699	-0.367634	0.000000
C	-0.770283	-0.353502	0.000000
C	0.000000	0.825444	0.000000
C	-2.273731	-0.308186	0.000000
C	-0.652970	2.180273	0.000000
N	1.335751	0.807581	0.000000
H	1.849802	-2.513184	0.000000
H	-0.646412	-2.492987	0.000000
H	3.049088	-0.329331	0.000000
H	-2.693885	-1.312990	0.000000
H	-2.659868	0.216687	0.876553
H	-2.659868	0.216687	-0.876553
H	-1.290044	2.316709	0.877173
H	0.112433	2.951380	0.000000
H	-1.290044	2.316709	-0.877173

Molecule# 1378

2,3-furo-1,3,2-dioxathiole

PointGroup: C1

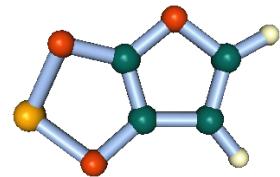
E= -777.535114091 au

ZPE= 0.057389 au

LUMO_eps= -0.08448 au

HOMO_eps= -0.21097 au

Dipole= 1.396 debye



10

S	1.989323	-0.009549	-0.145290
O	0.854042	-1.274861	0.212013
O	0.929171	1.296398	0.203214
O	-1.541919	-1.139480	-0.026054
C	-0.315704	-0.615131	-0.021948
C	-0.319252	0.726214	-0.022953
C	-1.682955	1.131606	-0.022667
C	-2.386914	-0.036529	-0.038427
H	-2.098136	2.123419	-0.033853
H	-3.432428	-0.264049	-0.118917

Molecule# 1379

2,3-pentadiene

PointGroup: C2

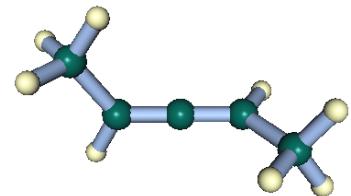
E= -195.371470235 au

ZPE= 0.112010 au

LUMO_eps= -0.01307 au

HOMO_eps= -0.25322 au

Dipole= 0.225 debye



13

C	0.000000	0.000000	0.410032
C	0.000000	1.303082	0.410018
C	0.000000	-1.303082	0.410018
C	-0.871882	2.172515	-0.457285
C	0.871882	-2.172515	-0.457285
H	0.676863	1.817656	1.088068
H	-0.676863	-1.817656	1.088068
H	-1.504967	2.819715	0.154671
H	-0.264433	2.825078	-1.089145
H	-1.514184	1.573281	-1.100088
H	1.504967	-2.819715	0.154671
H	0.264433	-2.825078	-1.089145
H	1.514184	-1.573281	-1.100088

Molecule# 1380

2,3-thieno-1,3,2-dioxathiole

PointGroup: C1

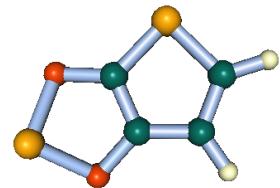
E= -1100.533202450 au

ZPE= 0.054288 au

LUMO_eps= -0.08176 au

HOMO_eps= -0.21246 au

Dipole= 1.471 debye



10

S	1.786816	-0.999206	-0.026846
S	-2.245223	-0.148491	-0.179660
O	-1.005016	-1.270226	0.235149
O	-1.330231	1.236629	0.220211
C	0.134146	-0.525701	0.028191
C	-0.017500	0.819744	0.026189
C	1.196636	1.540976	-0.022378
C	2.258331	0.681032	-0.056911
H	1.283391	2.615343	-0.042028
H	3.303414	0.920280	-0.147308

Molecule# 1381

2,3,2',3'-dipyrrolopyrrole

PointGroup: C1

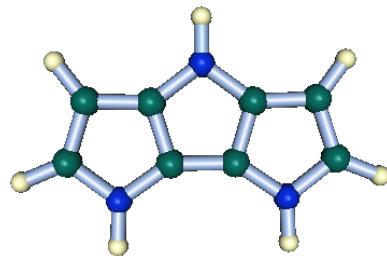
E= -473.444232049 au

ZPE= 0.139707 au

LUMO_eps= -0.01917 au

HOMO_eps= -0.16952 au

Dipole= 1.725 debye



18

C	2.531827	0.838284	0.000719
C	-2.531828	0.838284	0.000727
C	2.945670	-0.478119	0.001541
C	-2.945670	-0.478119	0.001498
C	1.115603	0.798316	-0.000163
C	-1.115604	0.798316	-0.000047
C	0.708404	-0.539305	0.000275
C	-0.708404	-0.539305	0.000396
N	1.844970	-1.314880	0.000405
N	-1.844969	-1.314880	0.000310
N	0.000000	1.623424	-0.012899
H	3.182514	1.695453	0.001317
H	-3.182515	1.695453	0.001272
H	3.941593	-0.883817	0.003112
H	-3.941593	-0.883818	0.003098
H	1.888002	-2.315552	-0.003863
H	-1.887996	-2.315553	-0.003452
H	0.000005	2.622059	0.054138

Molecule# 1382

2,3,3-trifluoropropene

PointGroup: Cs

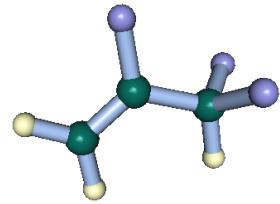
E= -415.788926576 au

ZPE= 0.057429 au

LUMO_eps= -0.03856 au

HOMO_eps= -0.30206 au

Dipole= 3.088 debye



9

C	-1.639261	1.150479	0.000000
H	-2.490302	0.487611	0.000000
H	-1.809141	2.216402	0.000000
C	-0.417478	0.652524	0.000000
F	0.670083	1.440552	0.000000
C	-0.079576	-0.806625	0.000000
H	-0.974900	-1.428241	0.000000
F	0.670083	-1.123278	1.097373
F	0.670083	-1.123278	-1.097373

Molecule# 1383

2,3,4-trimethylpentane

PointGroup: C1

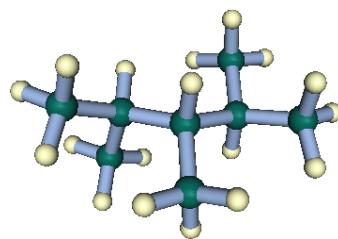
E= -315.824838531 au

ZPE= 0.243952 au

LUMO_eps= -0.01192 au

HOMO_eps= -0.30050 au

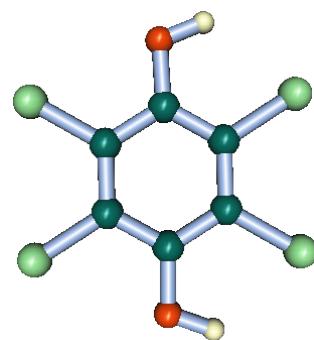
Dipole= 0.106 debye



26

C	-1.643780	-0.744140	1.267860
C	-2.416221	0.092866	-0.979081
C	1.568432	-1.626417	-0.343229
C	2.566669	0.643816	-0.042519
C	-0.183821	1.829717	0.314524
C	-1.228311	-0.457857	-0.180043
C	1.328673	-0.222989	0.228474
C	0.031928	0.441798	-0.307623
H	-2.484667	-1.439569	1.291217
H	-0.835389	-1.189503	1.848803
H	-1.961332	0.164639	1.782113
H	-2.136078	0.303073	-2.013245
H	-2.813834	1.012725	-0.547434
H	-3.231892	-0.632223	-0.997675
H	2.532205	-2.012895	-0.007877
H	0.808890	-2.343326	-0.035097
H	1.585518	-1.607030	-1.436276
H	2.520811	1.609052	0.458909
H	2.684972	0.828086	-1.113860
H	3.469540	0.139486	0.305210
H	-1.127132	2.269864	-0.006227
H	0.602929	2.524328	0.025850
H	-0.194597	1.779952	1.405178
H	-0.977247	-1.415409	-0.640316
H	1.230226	-0.318172	1.315434
H	0.185662	0.586165	-1.384882

Molecule# 1384
 2,3,5,6-tetrachlorobenzene-1,4-diol
 PointGroup: C2v
 E= -2221.352454810 au
 ZPE= 0.070634 au
 LUMO_eps= -0.05696 au
 HOMO_eps= -0.24195 au
 Dipole= 2.616 debye



14

C1	0.000000	1.591361	2.692912
C	0.000000	0.696756	1.212282
C	0.000000	-0.696756	1.212282
C1	0.000000	-1.591361	2.692912
C	0.000000	-1.409756	0.008295
O	0.000000	-2.759999	0.052901
C	0.000000	-0.695960	-1.189657
C1	0.000000	-1.601358	-2.678734
C	0.000000	0.695960	-1.189657
C	0.000000	1.409756	0.008295
O	0.000000	2.759999	0.052901
C1	0.000000	1.601358	-2.678734
H	0.000000	-3.106114	-0.849754
H	0.000000	3.106114	-0.849754

Molecule# 1385

2,3,6,7-tetraazanaphthalene

PointGroup: D2h

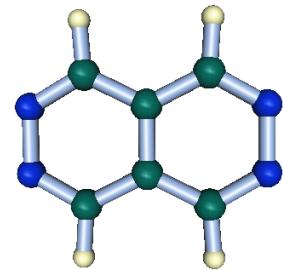
E= -450.122871530 au

ZPE= 0.098367 au

LUMO_eps= -0.10674 au

HOMO_eps= -0.25959 au

Dipole= 0.000 debye



14

C	0.000000	0.000000	0.697725
C	0.000000	1.263786	1.332760
C	0.000000	0.000000	-0.697725
N	0.000000	2.398784	0.679888
C	0.000000	1.263786	-1.332760
N	0.000000	2.398784	-0.679888
C	0.000000	-1.263786	-1.332760
N	0.000000	-2.398784	-0.679888
C	0.000000	-1.263786	1.332760
N	0.000000	-2.398784	0.679888
H	0.000000	-1.340928	-2.414429
H	0.000000	1.340928	2.414429
H	0.000000	-1.340928	2.414429
H	0.000000	1.340928	-2.414429

Molecule# 1386

2,3H-pyridinone

PointGroup: C1

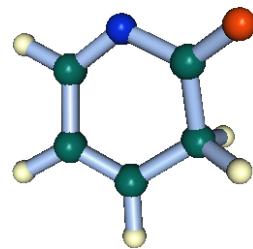
E= -323.603746898 au

ZPE= 0.091208 au

LUMO_eps= -0.09966 au

HOMO_eps= -0.26031 au

Dipole= 5.340 debye



12

N	0.359121	-1.270880	0.172755
C	1.043903	-0.042270	0.020425
C	0.260787	1.248686	0.217829
C	-1.197071	1.126889	-0.072399
C	-1.753015	-0.083323	-0.174172
C	-0.920479	-1.259790	0.050067
O	2.221256	-0.028129	-0.243650
H	0.736325	2.029916	-0.376191
H	-1.785070	2.030930	-0.170963
H	-2.808335	-0.220042	-0.363668
H	-1.424810	-2.220985	0.136930
H	0.393242	1.560219	1.263311

Molecule# 1387

2,4-cyclohexadienone

PointGroup: C1

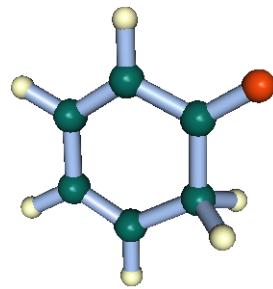
E= -307.559016780 au

ZPE= 0.102937 au

LUMO_eps= -0.08673 au

HOMO_eps= -0.25151 au

Dipole= 3.790 debye



13

C	-1.079574	0.025415	-0.000044
C	-0.317064	1.276053	0.000024
C	1.029994	1.272817	0.000051
C	1.811253	0.048223	-0.000048
C	1.208607	-1.145981	-0.000088
C	-0.278700	-1.273628	0.000176
O	-2.298529	0.003675	-0.000115
H	-0.888882	2.193888	0.000022
H	1.565350	2.214743	0.000240
H	2.890068	0.123598	-0.000248
H	1.792087	-2.058324	-0.000305
H	-0.608643	-1.860082	0.864683
H	-0.608845	-1.860624	-0.863902

Molecule# 1388

2,4-dichloropyrimidine

PointGroup: C1

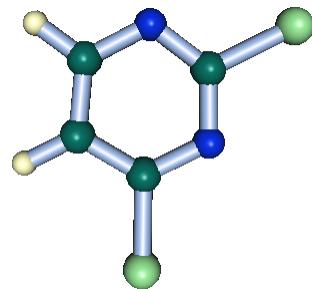
E= -1183.686507790 au

ZPE= 0.057345 au

LUMO_eps= -0.07938 au

HOMO_eps= -0.29447 au

Dipole= 3.145 debye



10

C1	-2.599175	-0.886996	-0.000001
C1	2.613285	-0.893714	0.000000
N	0.001967	-0.687993	0.000000
N	-1.233601	1.339871	0.000000
C	-1.116676	0.025543	0.000000
C	1.121365	0.005739	0.000000
C	1.154461	1.395274	0.000000
C	-0.082104	2.017431	0.000000
H	2.080180	1.947300	0.000000
H	-0.160883	3.097694	0.000002

Molecule# 1389

2,4-dicyanothiophene

PointGroup: C1

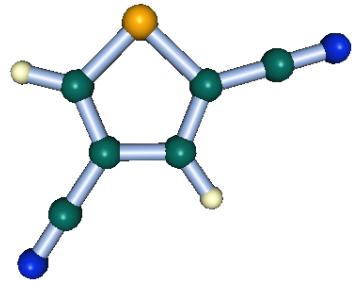
E= -737.643602132 au

ZPE= 0.063992 au

LUMO_eps= -0.10135 au

HOMO_eps= -0.29080 au

Dipole= 2.905 debye



11

S	-0.785680	1.458954	-0.000008
N	-3.431367	-1.222926	0.000007
N	3.697033	-0.916364	0.000004
C	-1.052269	-0.263674	0.000002
C	1.258799	-0.088174	0.000000
C	0.130306	-0.953110	0.000005
C	0.907286	1.241520	-0.000007
C	-2.359652	-0.797434	0.000005
C	2.606930	-0.544009	0.000002
H	0.193528	-2.029602	0.000011
H	1.569280	2.090663	-0.000012

Molecule# 1390

2,4-difluorofuran

PointGroup: C1

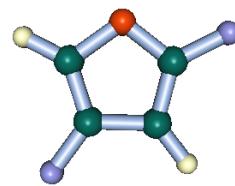
E= -428.650763826 au

ZPE= 0.053981 au

LUMO_eps= -0.01109 au

HOMO_eps= -0.24801 au

Dipole= 0.196 debye



9

F	-2.349093	-0.439318	0.000000
F	2.398437	-0.465192	0.000000
O	-0.734830	1.107764	0.000000
C	-1.057992	-0.187509	0.000000
C	1.115249	-0.099449	0.000000
C	0.013570	-1.010677	0.000000
C	0.647558	1.167846	0.000000
H	0.028831	-2.084299	0.000001
H	1.095398	2.141517	0.000000

Molecule# 1391

2,4-difluoropyrimidine

PointGroup: C1

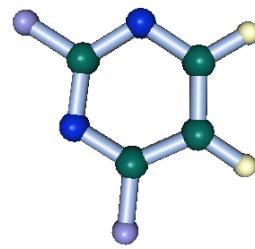
E= -462.992316004 au

ZPE= 0.061058 au

LUMO_eps= -0.07364 au

HOMO_eps= -0.30506 au

Dipole= 3.420 debye



10

F	2.232197	-0.973360	0.000000
F	-2.243497	-1.002072	0.000000
N	-0.001263	-1.004142	0.000000
N	1.229175	1.028037	0.000001
C	1.103378	-0.278453	0.000000
C	-1.109868	-0.306047	0.000000
C	-1.160118	1.080797	0.000001
C	0.074651	1.704920	0.000001
H	-2.093703	1.619545	0.000001
H	0.151768	2.784779	0.000002

Molecule# 1392

2,4-dihydro-1,2,4-triazol-3-one

PointGroup: Cs

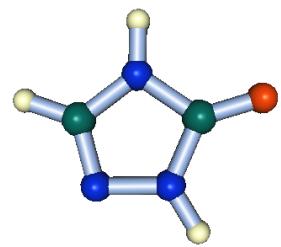
E= -317.617197686 au

ZPE= 0.064065 au

LUMO_eps= -0.02200 au

HOMO_eps= -0.24618 au

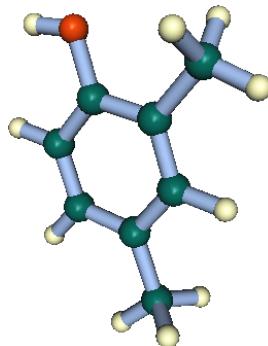
Dipole= 3.002 debye



9

C	0.585236	-1.371153	0.000000
C	0.000000	0.803622	0.000000
N	-0.706083	-1.394643	0.000000
N	1.075996	-0.090990	0.000000
N	-1.065835	-0.067566	0.000000
O	0.019362	2.016386	0.000000
H	1.203231	-2.252103	0.000000
H	2.035972	0.202774	0.000000
H	-2.034065	0.195812	0.000000

Molecule# 1393
 2,4-dimethylphenol
 PointGroup: C1
 E= -386.252603172 au
 ZPE= 0.159218 au
 LUMO_eps= -0.01529 au
 HOMO_eps= -0.22034 au
 Dipole= 0.908 debye



19

C	-1.194148	-1.273079	-0.003365
C	0.157194	-1.604887	-0.000788
C	-0.609182	1.039610	-0.002377
C	-1.601991	0.056026	-0.003248
C	0.749394	0.743892	-0.000095
C	1.120492	-0.606384	0.001279
C	-3.061050	0.433615	0.003949
C	1.799096	1.819578	-0.000742
O	2.465444	-0.884994	0.002866
H	-1.932914	-2.064353	-0.006041
H	0.460474	-2.645819	-0.001658
H	-0.904309	2.082983	-0.004426
H	-3.301613	1.113926	-0.815300
H	-3.696847	-0.445427	-0.096389
H	-3.338323	0.937663	0.932716
H	2.446613	1.742179	0.874661
H	2.448306	1.739421	-0.874651
H	1.340514	2.807196	-0.002729
H	2.595723	-1.838040	0.003211

Molecule# 1394

2,4-dimethylpyridine

PointGroup: C1

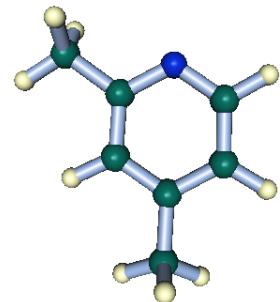
E= -327.044134674 au

ZPE= 0.143000 au

LUMO_eps= -0.03229 au

HOMO_eps= -0.25707 au

Dipole= 2.381 debye



17

C	1.153465	1.135016	-0.007007
C	0.013587	-0.948032	-0.008764
C	-0.091847	1.747296	0.002284
C	1.221900	-0.256301	-0.010428
C	-1.196914	-0.255109	0.000772
C	2.541088	-0.977755	0.007212
C	-2.516394	-0.975301	0.001562
N	-1.245756	1.082383	0.006775
H	2.053167	1.736401	-0.014432
H	0.010024	-2.030698	-0.017846
H	-0.165664	2.829419	0.003732
H	2.444441	-1.995475	-0.368921
H	3.285505	-0.457038	-0.595106
H	2.932172	-1.038201	1.025756
H	-2.388031	-2.056557	-0.001058
H	-3.098551	-0.693608	0.880030
H	-3.102079	-0.689810	-0.873359

Molecule# 1395

2,4-hexadiyne

PointGroup: D3h

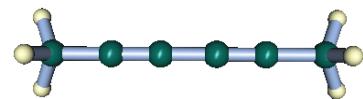
E= -232.228793075 au

ZPE= 0.093962 au

LUMO_eps= -0.01239 au

HOMO_eps= -0.23916 au

Dipole= 0.000 debye



12

C	0.000000	0.000000	0.681952
C	0.000000	0.000000	-0.681952
C	0.000000	0.000000	1.889462
C	0.000000	0.000000	-1.889462
C	0.000000	0.000000	3.341026
C	0.000000	0.000000	-3.341026
H	0.000000	1.019522	3.732419
H	-0.882932	-0.509761	3.732419
H	0.882932	-0.509761	3.732419
H	0.000000	1.019522	-3.732419
H	0.882932	-0.509761	-3.732419
H	-0.882932	-0.509761	-3.732419

Molecule# 1396

2,4-hexadiynedial

PointGroup: C1

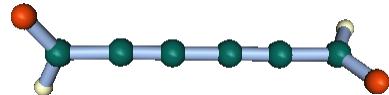
E= -380.272366648 au

ZPE= 0.056904 au

LUMO_eps= -0.12224 au

HOMO_eps= -0.30400 au

Dipole= 2.681 debye



10

O	4.066762	0.495957	0.360134
O	-4.066767	0.495911	-0.360185
C	0.673589	-0.167678	-0.057506
C	-0.673588	-0.167673	0.057516
C	1.882141	-0.160213	-0.149051
C	-1.882140	-0.160196	0.149061
C	3.314251	-0.185757	-0.295724
C	-3.314249	-0.185720	0.295752
H	3.682946	-0.885828	-1.064540
H	-3.682935	-0.885690	1.064664

Molecule# 1397

2,4-hexadiynedioic acid

PointGroup: C1

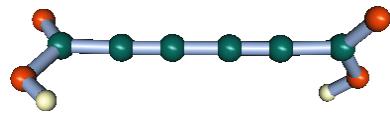
E= -530.831477000 au

ZPE= 0.068197 au

LUMO_eps= -0.11709 au

HOMO_eps= -0.30675 au

Dipole= 3.229 debye



12

O	3.930220	0.922903	-0.701602
O	-3.930220	-0.922899	-0.701611
O	3.973285	-0.836514	0.665513
O	-3.973285	0.836512	0.665510
C	3.332555	0.099218	-0.070156
C	-3.332555	-0.099217	-0.070161
C	1.886554	0.027690	-0.032419
C	-1.886554	-0.027691	-0.032422
C	0.677478	0.008906	-0.032785
C	-0.677478	-0.008907	-0.032786
H	3.342337	-1.424609	1.100947
H	-3.342337	1.424605	1.100948

Molecule# 1398

2,4-pentanedione

PointGroup: C2

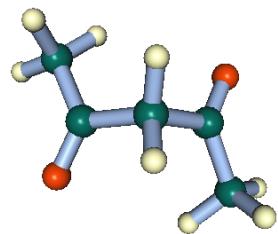
E= -345.933830260 au

ZPE= 0.121398 au

LUMO_eps= -0.05899 au

HOMO_eps= -0.26472 au

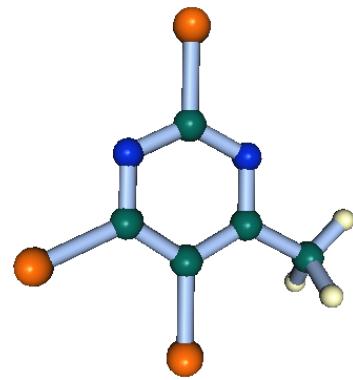
Dipole= 1.573 debye



15

C	0.000000	1.243074	0.098143
C	0.000000	-1.243074	0.098143
C	1.350214	1.778331	-0.300826
C	-1.350214	-1.778331	-0.300826
C	0.000000	0.000000	0.994477
O	-1.040368	1.730141	-0.279145
O	1.040368	-1.730141	-0.279145
H	1.852898	2.184930	0.580181
H	1.978873	0.968481	-0.675930
H	1.241245	2.557857	-1.049844
H	-1.241245	-2.557857	-1.049844
H	-1.852898	-2.184930	0.580181
H	-1.978873	-0.968481	-0.675930
H	-0.895614	0.031398	1.611420
H	0.895614	-0.031398	1.611420

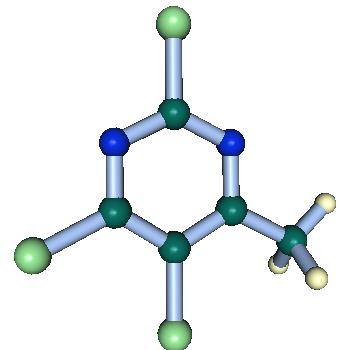
Molecule# 1399
 2,4,5-tribromo-6-methylpyrimidine
 PointGroup: Cs
 E= -8024.626624160 au
 ZPE= 0.072976 au
 LUMO_eps= -0.07901 au
 HOMO_eps= -0.27498 au
 Dipole= 2.765 debye



13

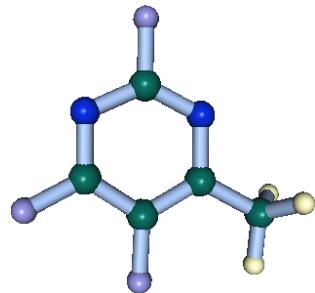
C	1.049437	-0.211037	0.000000
C	0.705144	-1.570612	0.000000
C	0.000000	0.707995	0.000000
C	-1.482500	-0.974742	0.000000
C	1.721025	-2.668583	0.000000
N	-0.583207	-1.936825	0.000000
N	-1.262789	0.327100	0.000000
Br	2.868516	0.315811	0.000000
Br	0.298749	2.584662	0.000000
Br	-3.309658	-1.517798	0.000000
H	2.367812	-2.598209	0.875665
H	1.211458	-3.627237	0.000000
H	2.367812	-2.598209	-0.875665

Molecule# 1400
 2,4,5-trichloro-6-methylpyrimidine
 PointGroup: Cs
 E= -1682.648280940 au
 ZPE= 0.075019 au
 LUMO_eps= -0.07851 au
 HOMO_eps= -0.28198 au
 Dipole= 2.772 debye



13
 C 1.021460 0.038369 0.000000
 C 0.640074 -1.308976 0.000000
 C 0.000000 0.987794 0.000000
 C -1.528760 -0.650022 0.000000
 C 1.636021 -2.424461 0.000000
 N -0.656618 -1.639019 0.000000
 N -1.273552 0.646231 0.000000
 Cl 2.695285 0.484019 0.000000
 Cl 0.352375 2.685355 0.000000
 Cl -3.211246 -1.098954 0.000000
 H 2.284076 -2.364524 0.875642
 H 1.111227 -3.374788 0.000000
 H 2.284076 -2.364524 -0.875642

Molecule# 1401
2,4,5-trifluoro-6-methylpyrimidine
PointGroup: C1
E= -601.594924807 au
ZPE= 0.080108 au
LUMO_eps= -0.07580 au
HOMO_eps= -0.29536 au
Dipole= 2.941 debye



13

C	-1.022816	0.186174	-0.000039
C	-0.513038	-1.102920	-0.000143
C	-0.116583	1.240174	0.000005
C	1.559349	-0.205422	0.000000
C	-1.388160	-2.314502	0.000022
N	0.818742	-1.284102	-0.000133
N	1.178216	1.060469	0.000038
F	-2.341445	0.427343	0.000001
F	-0.566309	2.486423	0.000014
F	2.872628	-0.397773	0.000055
H	-1.162280	-2.925605	-0.874234
H	-1.170278	-2.919635	0.880532
H	-2.442518	-2.054287	-0.005320

Molecule# 1402

2,4,6-trichloro-1,3,5-triazine

PointGroup: D3h

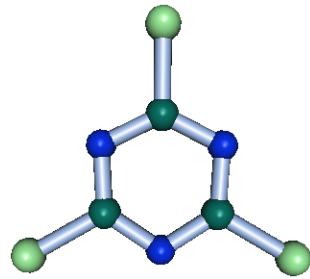
E= -1659.363504380 au

ZPE= 0.035685 au

LUMO_eps= -0.09595 au

HOMO_eps= -0.32521 au

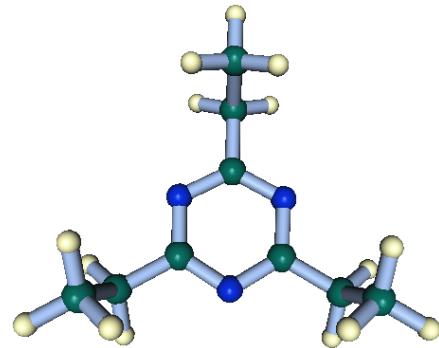
Dipole= 0.000 debye



9

C	0.000000	1.278542	0.000000
C	1.107250	-0.639271	0.000000
C	-1.107250	-0.639271	0.000000
N	0.000000	-1.366438	0.000000
N	-1.183370	0.683219	0.000000
N	1.183370	0.683219	0.000000
Cl	0.000000	3.006062	0.000000
Cl	2.603326	-1.503031	0.000000
Cl	-2.603326	-1.503031	0.000000

Molecule# 1403
 2,4,6-triethyl-1,3,5-triazine
 PointGroup: C1
 E= -516.465728582 au
 ZPE= 0.232949 au
 LUMO_eps= -0.04662 au
 HOMO_eps= -0.26643 au
 Dipole= 0.382 debye



27

C	1.213746	-0.485195	-0.451299
C	-0.186751	1.291886	-0.452061
C	-1.025519	-0.809540	-0.451492
C	3.106193	-1.226077	1.022311
C	-0.489286	3.302497	1.020270
C	-2.620272	-2.070057	1.021573
C	2.607524	-1.040956	-0.418867
C	-0.402257	2.776850	-0.420576
C	-2.203885	-1.738495	-0.419487
N	1.071093	0.842916	-0.451579
N	0.196001	-1.350037	-0.450873
N	-1.265574	0.504278	-0.451645
H	3.118887	-0.274436	1.553900
H	4.118823	-1.629272	1.024095
H	2.464865	-1.917378	1.569345
H	-1.319148	2.838266	1.553364
H	-0.646245	4.381085	1.021356
H	0.430754	3.093039	1.566254
H	-1.805223	-2.554587	1.559462
H	-3.476138	-2.744948	1.022972
H	-2.900234	-1.165995	1.562599
H	2.608917	-2.000696	-0.934359
H	3.265833	-0.353860	-0.949473
H	0.427560	3.257459	-0.937555
H	-1.327118	3.003015	-0.950185
H	-3.033410	-1.262410	-0.941151
H	-1.935724	-2.654865	-0.944181

Molecule# 1404

2,5-cyclohexadienone

PointGroup: C2v

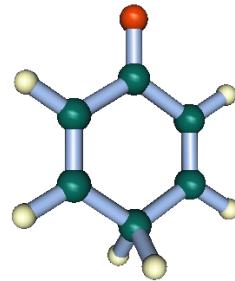
E= -307.561020375 au

ZPE= 0.103373 au

LUMO_eps= -0.07090 au

HOMO_eps= -0.25339 au

Dipole= 4.843 debye



13

C	0.000000	0.000000	1.108167
C	0.000000	1.252736	0.329165
C	0.000000	1.253135	-1.006331
C	0.000000	0.000000	-1.814407
C	0.000000	-1.253135	-1.006331
C	0.000000	-1.252736	0.329165
O	0.000000	0.000000	2.331070
H	0.000000	2.170549	0.902157
H	0.000000	2.189815	-1.551879
H	-0.863698	0.000000	-2.492840
H	0.863698	0.000000	-2.492840
H	0.000000	-2.189815	-1.551879
H	0.000000	-2.170549	0.902157

Molecule# 1405

2,5-dihydro-1,2-oxazole

PointGroup: C1

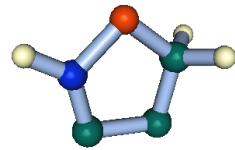
E= -245.926151959 au

ZPE= 0.052011 au

LUMO_eps= -0.13981 au

HOMO_eps= -0.23371 au

Dipole= 3.694 debye



8

O	0.216355	-1.131231	-0.000019
N	-1.034393	-0.361708	0.000007
C	1.141200	-0.042903	0.000000
C	-1.003508	0.912444	0.000005
C	0.486277	1.267077	-0.000055
H	-1.812094	-1.012004	0.000017
H	1.788873	-0.112783	0.883419
H	1.789317	-0.113121	-0.883034

Molecule# 1406

2,5-dihydro-1,2-thiazole-1-oxide

PointGroup: C1

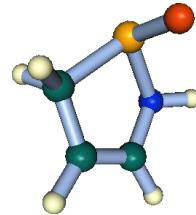
E= -645.568209336 au

ZPE= 0.081095 au

LUMO_eps= -0.02172 au

HOMO_eps= -0.23834 au

Dipole= 2.997 debye



11

C	-1.589968	0.591998	0.318003
C	-1.482626	-0.731595	0.240541
C	-0.409779	1.297050	-0.271302
N	-0.319737	-1.200523	-0.391951
O	1.667032	-0.003415	0.897793
S	0.936297	0.011580	-0.400006
H	-2.429540	1.112221	0.749196
H	-2.206329	-1.457624	0.580961
H	-0.583145	1.663910	-1.286760
H	0.010173	2.099326	0.334185
H	0.024228	-2.116844	-0.139614

Molecule# 1407

2,5-dihydro-2-methylthiophene-1,1-dioxide

PointGroup: C1

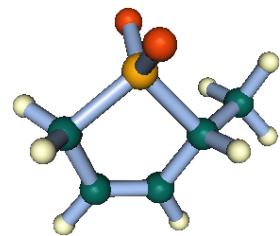
E= -744.099659925 au

ZPE= 0.126087 au

LUMO_eps= -0.03054 au

HOMO_eps= -0.28894 au

Dipole= 4.812 debye



16

C	1.685700	-1.598566	0.155043
C	1.000120	-0.422584	-0.529065
C	1.568891	0.929035	-0.216112
C	0.733478	1.900514	0.142277
C	-0.724568	1.573344	0.203570
S	-0.774100	-0.249045	-0.007386
O	-0.956176	-0.865654	1.303800
O	-1.661019	-0.613275	-1.108479
H	1.194401	-2.537785	-0.094112
H	2.721514	-1.657362	-0.182632
H	1.674864	-1.482978	1.236789
H	0.941234	-0.587664	-1.606882
H	2.639629	1.076501	-0.276618
H	1.070634	2.897063	0.393682
H	-1.307196	2.010364	-0.607179
H	-1.193646	1.807560	1.158274

Molecule# 1408

2,5-dihydrofuran

PointGroup: Cs

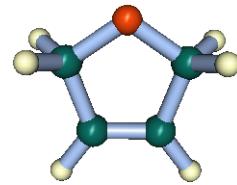
E= -231.309057164 au

ZPE= 0.092099 au

LUMO_eps= -0.01045 au

HOMO_eps= -0.24300 au

Dipole= 1.625 debye



11

O	-0.000005	1.187716	0.000000
C	0.000009	0.367981	1.174300
C	0.000009	-1.040764	0.662346
C	0.000009	-1.040764	-0.662346
C	0.000009	0.367981	-1.174300
H	-0.884524	0.596428	1.780702
H	0.884421	0.596465	1.780810
H	0.884421	0.596465	-1.780810
H	-0.884524	0.596428	-1.780702
H	0.000016	-1.907063	1.307178
H	0.000016	-1.907063	-1.307178

Molecule# 1409

2,5-dihydrothiophene-1-oxide

PointGroup: C1

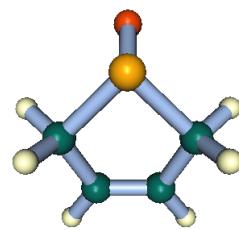
E= -629.519525467 au

ZPE= 0.092341 au

LUMO_eps= -0.01762 au

HOMO_eps= -0.23893 au

Dipole= 4.105 debye



12

C	1.587197	-0.663411	0.266045
C	1.587197	0.663411	0.266045
C	0.353161	-1.327115	-0.256480
C	0.353161	1.327115	-0.256480
O	-1.726065	0.000000	0.869953
S	-0.946541	0.000000	-0.417329
H	2.420926	-1.255926	0.620455
H	2.420926	1.255926	0.620455
H	0.494961	-1.789128	-1.236410
H	-0.081439	-2.065993	0.417387
H	-0.081439	2.065993	0.417387
H	0.494961	1.789128	-1.236410

Molecule# 1410

2,5-dihydrothiophene-1,1-dioxide

PointGroup: Cs

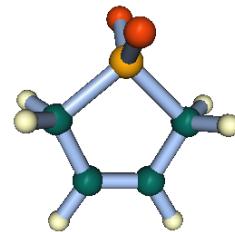
E= -704.769239706 au

ZPE= 0.098056 au

LUMO_eps= -0.02871 au

HOMO_eps= -0.29315 au

Dipole= 4.925 debye



13

O	1.270824	-1.445451	0.000000
S	0.002229	-0.724554	0.000000
O	-1.257213	-1.461278	0.000000
C	-0.004596	0.507527	1.362305
C	-0.004596	1.830288	0.665220
C	-0.004596	1.830288	-0.665220
C	-0.004596	0.507527	-1.362305
H	0.883848	0.328649	1.967200
H	-0.896445	0.325784	1.961332
H	-0.004535	2.742025	1.247250
H	-0.004535	2.742025	-1.247250
H	0.883848	0.328649	-1.967200
H	-0.896445	0.325784	-1.961332

Molecule# 1411

2,5-dihydrothiophene-3-ol

PointGroup: Cs

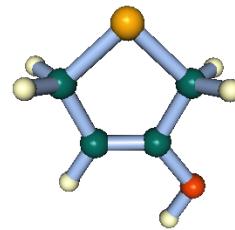
E= -629.555014351 au

ZPE= 0.093809 au

LUMO_eps= -0.02301 au

HOMO_eps= -0.22289 au

Dipole= 2.439 debye



12

S	0.486424	-1.562232	0.000000
C	1.185552	0.135916	0.000000
C	0.000000	1.049246	0.000000
C	-1.213614	0.503766	0.000000
C	-1.274556	-0.989952	0.000000
O	0.322895	2.373917	0.000000
H	1.804678	0.296812	0.883239
H	-2.125549	1.088447	0.000000
H	-1.777269	-1.389274	-0.882273
H	1.804678	0.296812	-0.883239
H	-1.777269	-1.389274	0.882273
H	-0.479502	2.906985	0.000000

Molecule# 1412

2,5-dihydrothiophene

PointGroup: C2v

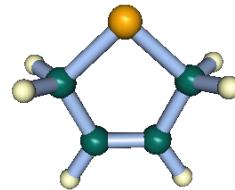
E= -554.300004788 au

ZPE= 0.089164 au

LUMO_eps= -0.01293 au

HOMO_eps= -0.22182 au

Dipole= 1.794 debye



11

S	0.000000	0.000000	1.252467
C	0.000000	1.350899	-0.004471
C	0.000000	-1.350899	-0.004471
C	0.000000	0.662535	-1.335066
C	0.000000	-0.662535	-1.335066
H	-0.881617	1.980110	0.130213
H	0.881617	1.980110	0.130213
H	0.881617	-1.980110	0.130213
H	-0.881617	-1.980110	0.130213
H	0.000000	1.252912	-2.242943
H	0.000000	-1.252912	-2.242943

Molecule# 1413

2,5-dimethylphenol

PointGroup: C1

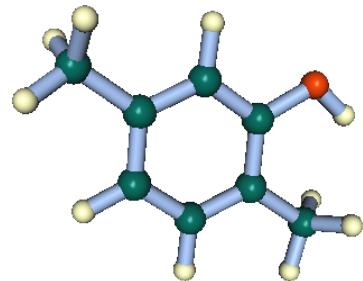
E= -386.252790738 au

ZPE= 0.159156 au

LUMO_eps= -0.01646 au

HOMO_eps= -0.22484 au

Dipole= 1.333 debye



19

C	1.129531	-1.313585	-0.008560
C	-0.238510	-1.556011	-0.001692
C	0.696232	1.038980	-0.007975
C	1.615630	-0.006887	-0.009477
C	-1.168888	-0.520347	0.002959
C	-0.670298	0.788304	-0.000863
C	3.095047	0.276324	0.010869
C	-2.651007	-0.783942	0.006802
O	-1.498806	1.880695	-0.001109
H	1.821316	-2.145686	-0.015281
H	-0.597329	-2.578032	-0.002925
H	1.028405	2.069063	-0.014268
H	3.349610	1.113290	-0.640203
H	3.430665	0.535881	1.018029
H	3.668352	-0.591678	-0.312831
H	-3.141766	-0.362979	0.890092
H	-3.146115	-0.365455	-0.875291
H	-2.851563	-1.853728	0.008728
H	-2.417548	1.596761	0.000440

Molecule# 1414

2,5-dimethylpyridine

PointGroup: Cs

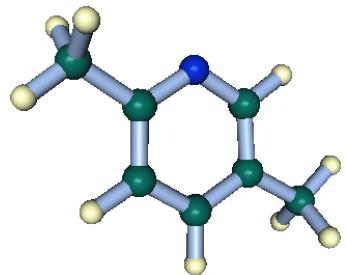
E= -327.042947753 au

ZPE= 0.143053 au

LUMO_eps= -0.03635 au

HOMO_eps= -0.25127 au

Dipole= 2.093 debye



17

C	-1.178683	-0.742088	0.000000
C	0.047290	-1.388143	0.000000
C	0.000000	1.309459	0.000000
C	-1.228041	0.649909	0.000000
C	1.221409	-0.633508	0.000000
C	-2.528268	1.405525	0.000000
C	2.580459	-1.275923	0.000000
N	1.185094	0.702648	0.000000
H	-2.095720	-1.319232	0.000000
H	0.097475	-2.468673	0.000000
H	0.024650	2.395020	0.000000
H	-3.128947	1.163181	0.878919
H	-2.357997	2.481564	0.000000
H	-3.128947	1.163181	-0.878919
H	3.147907	-0.961093	-0.876888
H	3.147907	-0.961093	0.876888
H	2.513018	-2.362770	0.000000

Molecule# 1415

2,5-dimethyltetrahydrofuran

PointGroup: C2

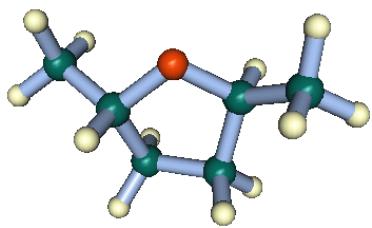
E= -311.209263035 au

ZPE= 0.171690 au

LUMO_eps= -0.01097 au

HOMO_eps= -0.24860 au

Dipole= 1.596 debye



19

C	0.000000	0.764255	-1.297167
C	0.000000	-0.764255	-1.297167
C	-0.468541	1.090526	0.123716
C	0.468541	-1.090526	0.123716
C	0.032579	2.405081	0.690505
C	-0.032579	-2.405081	0.690505
O	0.000000	0.000000	0.938605
H	1.011237	1.147828	-1.454012
H	-0.646734	1.200592	-2.057687
H	-1.011237	-1.147828	-1.454012
H	0.646734	-1.200592	-2.057687
H	-1.565793	1.083362	0.154246
H	1.565793	-1.083362	0.154246
H	-0.297960	2.529471	1.721560
H	1.122913	2.439253	0.673182
H	-0.351842	3.243340	0.105964
H	-1.122913	-2.439253	0.673182
H	0.351842	-3.243340	0.105964
H	0.297960	-2.529471	1.721560

Molecule# 1416

2,5H-pyridinone

PointGroup: Cs

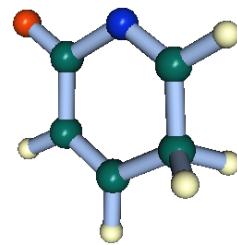
E= -323.604884903 au

ZPE= 0.091305 au

LUMO_eps= -0.08066 au

HOMO_eps= -0.26086 au

Dipole= 6.087 debye



12

N	-1.254654	0.394118	0.000000
C	0.000000	1.081090	0.000000
C	1.244764	0.286621	0.000000
C	1.223615	-1.045676	0.000000
C	-0.067291	-1.783582	0.000000
C	-1.258745	-0.878361	0.000000
O	0.015804	2.291171	0.000000
H	2.166216	0.852058	0.000000
H	2.142475	-1.619589	0.000000
H	-0.136811	-2.456207	0.864752
H	-2.232984	-1.368807	0.000000
H	-0.136811	-2.456207	-0.864752

Molecule# 1417

2,6-diazabicyclo-3,3,0-octa-3,7,9-triene

PointGroup: C2h

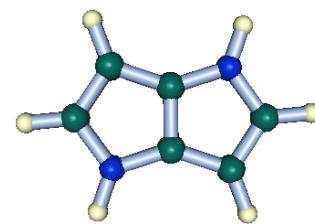
E= -341.848341422 au

ZPE= 0.111420 au

LUMO_eps= -0.01054 au

HOMO_eps= -0.18788 au

Dipole= 0.000 debye



14

C	1.327665	1.176379	0.000000
C	-1.327665	-1.176379	0.000000
C	2.119092	0.047739	0.000000
C	-2.119092	-0.047739	0.000000
C	-0.008256	0.695795	0.000000
C	0.008256	-0.695795	0.000000
N	1.327665	-1.085752	0.000000
N	-1.327665	1.085752	0.000000
H	1.685808	2.190986	0.000000
H	-1.685808	-2.190986	0.000000
H	3.191771	-0.033733	0.000000
H	-3.191771	0.033733	0.000000
H	1.673163	-2.026299	0.000000
H	-1.673163	2.026299	0.000000

Molecule# 1418

2,6-difluoropyridine

PointGroup: C2v

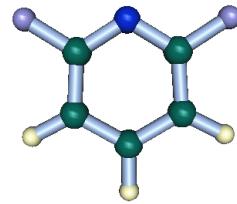
E= -446.945543536 au

ZPE= 0.072608 au

LUMO_eps= -0.05609 au

HOMO_eps= -0.27798 au

Dipole= 3.836 debye



11

N	0.000000	0.000000	1.004348
C	0.000000	0.000000	-1.763705
C	0.000000	1.116033	0.313567
C	0.000000	-1.116033	0.313567
C	0.000000	1.202637	-1.069047
C	0.000000	-1.202637	-1.069047
H	0.000000	0.000000	-2.844744
F	0.000000	2.245286	1.032550
F	0.000000	-2.245286	1.032550
H	0.000000	2.162100	-1.561803
H	0.000000	-2.162100	-1.561803

Molecule# 1419

2,6-dimethyl-4H-pyran-4-one

PointGroup: C2v

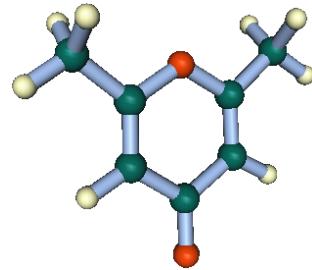
E= -422.162513495 au

ZPE= 0.135289 au

LUMO_eps= -0.04503 au

HOMO_eps= -0.24343 au

Dipole= 5.176 debye



17

C	0.000000	2.348442	-1.472492
C	0.000000	1.181572	-0.546325
C	0.000000	1.220509	0.796168
C	0.000000	0.000000	1.597720
O	0.000000	0.000000	2.824812
O	0.000000	0.000000	-1.229567
C	0.000000	-1.220509	0.796168
C	0.000000	-1.181572	-0.546325
C	0.000000	-2.348442	-1.472492
H	0.879762	2.324369	-2.118001
H	0.000000	3.279116	-0.911282
H	-0.879762	2.324369	-2.118001
H	0.000000	2.170852	1.309034
H	0.000000	-2.170852	1.309034
H	0.000000	-3.279116	-0.911282
H	0.879762	-2.324369	-2.118001
H	-0.879762	-2.324369	-2.118001

Molecule# 1420

2,6-dimethyl-4H-pyran-4-thione

PointGroup: C2v

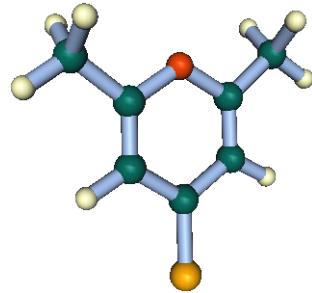
E= -745.127826195 au

ZPE= 0.133314 au

LUMO_eps= -0.07574 au

HOMO_eps= -0.20494 au

Dipole= 5.859 debye

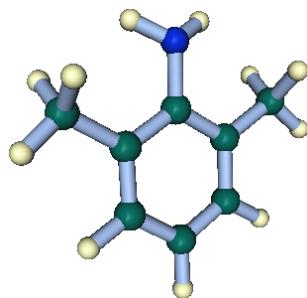


17

S	0.000000	0.000000	2.851009
C	0.000000	0.000000	1.185615
C	0.000000	1.206883	0.400792
C	0.000000	2.352278	-1.861101
C	0.000000	1.178354	-0.946461
O	0.000000	0.000000	-1.631977
C	0.000000	-1.206883	0.400792
C	0.000000	-1.178354	-0.946461
C	0.000000	-2.352278	-1.861101
H	0.000000	2.159035	0.909125
H	-0.879753	2.334551	-2.507116
H	0.879753	2.334551	-2.507116
H	0.000000	3.277663	-1.291277
H	0.000000	-2.159035	0.909125
H	-0.879753	-2.334551	-2.507116
H	0.000000	-3.277663	-1.291277
H	0.879753	-2.334551	-2.507116

Molecule# 1421
2,6-dimethylaniline
PointGroup: Cs

E= -366.379389348 au
ZPE= 0.172267 au
LUMO_eps= -0.01760 au
HOMO_eps= -0.20581 au
Dipole= 1.697 debye



20

C	0.031636	2.129960	0.000000
C	0.022160	1.426629	1.197036
C	0.022160	1.426629	-1.197036
C	0.000741	0.035768	1.220838
C	0.000741	0.035768	-1.220838
C	-0.014016	-0.663674	0.000000
C	0.000741	-0.713836	2.525634
C	0.000741	-0.713836	-2.525634
N	0.019170	-2.060830	0.000000
H	0.048473	3.210934	0.000000
H	0.033219	1.964237	2.137086
H	0.033219	1.964237	-2.137086
H	-0.899053	-1.326444	2.647724
H	0.860065	-1.385263	2.606507
H	0.037075	-0.025129	3.367762
H	0.860065	-1.385263	-2.606507
H	-0.899053	-1.326444	-2.647724
H	0.037075	-0.025129	-3.367762
H	-0.317355	-2.510195	-0.834773
H	-0.317355	-2.510195	0.834773

Molecule# 1422

2,6-dimethylphenol

PointGroup: Cs

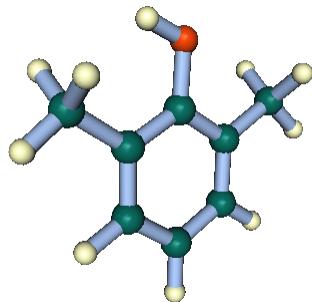
E= -386.253020505 au

ZPE= 0.159607 au

LUMO_eps= -0.01753 au

HOMO_eps= -0.22432 au

Dipole= 1.420 debye



19

C	0.029432	-2.115963	0.000000
C	-1.177779	-1.432184	0.000000
C	1.221499	-1.401498	0.000000
C	-1.215878	-0.038978	0.000000
C	1.232186	-0.009912	0.000000
C	0.000000	0.652782	0.000000
C	-2.522797	0.709811	0.000000
C	2.513155	0.776894	0.000000
O	0.045187	2.025498	0.000000
H	0.042486	-3.197090	0.000000
H	-2.110575	-1.981915	0.000000
H	2.166310	-1.930240	0.000000
H	-2.631669	1.347832	0.882868
H	-2.631669	1.347832	-0.882868
H	-3.362725	0.017813	0.000000
H	2.580324	1.426517	-0.874653
H	2.580324	1.426517	0.874653
H	3.374227	0.110457	0.000000
H	-0.847434	2.382583	0.000000

Molecule# 1423

2,6-dimethylpyridine

PointGroup: C2v

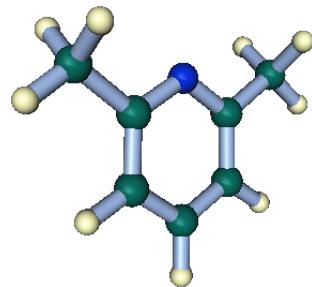
E= -327.045990062 au

ZPE= 0.142863 au

LUMO_eps= -0.03468 au

HOMO_eps= -0.25281 au

Dipole= 1.474 debye



17

C	0.000000	0.000000	-1.831849
C	0.000000	1.195324	-1.129066
C	0.000000	-1.195324	-1.129066
C	0.000000	1.155404	0.265392
C	0.000000	-1.155404	0.265392
C	0.000000	2.411589	1.091716
C	0.000000	-2.411589	1.091716
N	0.000000	0.000000	0.937784
H	0.000000	0.000000	-2.914051
H	0.000000	2.144159	-1.647425
H	0.000000	-2.144159	-1.647425
H	-0.876787	2.436350	1.740225
H	0.876787	2.436350	1.740225
H	0.000000	3.304826	0.469053
H	0.000000	-3.304826	0.469053
H	0.876787	-2.436350	1.740225
H	-0.876787	-2.436350	1.740225

Molecule# 1424

2,6-dioxabicyclo-3,3,0-octa-3,7,9-triene

PointGroup: C2h

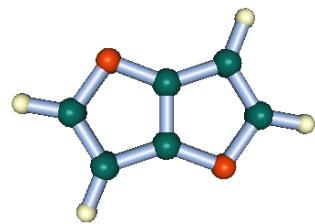
E= -381.564704484 au

ZPE= 0.086721 au

LUMO_eps= -0.02326 au

HOMO_eps= -0.21803 au

Dipole= 0.000 debye



12

C	1.309093	1.172916	0.000000
C	-1.309093	-1.172916	0.000000
C	2.068867	0.039777	0.000000
C	-2.068867	-0.039777	0.000000
C	-0.023065	0.680222	0.000000
C	0.023065	-0.680222	0.000000
O	1.309093	-1.111529	0.000000
O	-1.309093	1.111529	0.000000
H	1.675271	2.183812	0.000000
H	-1.675271	-2.183812	0.000000
H	3.132307	-0.112935	0.000000
H	-3.132307	0.112935	0.000000

Molecule# 1425

2,6-dithiabicyclo-3,3,0-octa-3,7,9-triene

PointGroup: C2h

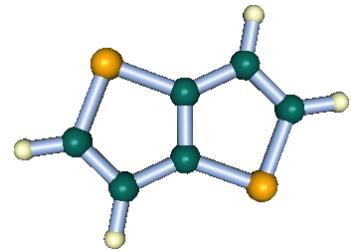
E= -1027.559792710 au

ZPE= 0.080576 au

LUMO_eps= -0.03969 au

HOMO_eps= -0.22631 au

Dipole= 0.000 debye



12

C	1.447868	1.099623	0.000000
C	-1.447868	-1.099623	0.000000
C	2.286737	0.027705	0.000000
C	-2.286737	-0.027705	0.000000
C	0.088213	0.687881	0.000000
C	-0.088213	-0.687881	0.000000
S	1.447868	-1.498577	0.000000
S	-1.447868	1.498577	0.000000
H	1.786562	2.124058	0.000000
H	-1.786562	-2.124058	0.000000
H	3.363551	0.035733	0.000000
H	-3.363551	-0.035733	0.000000

Molecule# 1426

2H-imidazole

PointGroup: C2v

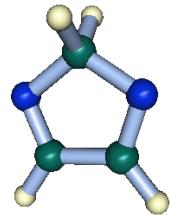
E= -226.276090624 au

ZPE= 0.069785 au

LUMO_eps= -0.07346 au

HOMO_eps= -0.28861 au

Dipole= 1.267 debye

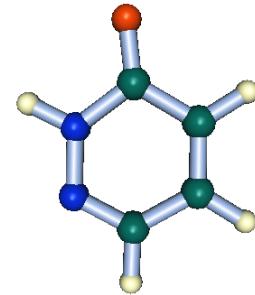


9

C	0.000000	0.000000	1.130632
N	0.000000	1.186666	0.292106
N	0.000000	-1.186666	0.292106
C	0.000000	0.737561	-0.907000
C	0.000000	-0.737561	-0.907000
H	-0.879628	0.000000	1.780422
H	0.879628	0.000000	1.780422
H	0.000000	1.384794	-1.775054
H	0.000000	-1.384794	-1.775054

Molecule# 1427
2H-pyridazin-3-one
PointGroup: Cs

E= -339.664589540 au
ZPE= 0.081527 au
LUMO_eps= -0.08362 au
HOMO_eps= -0.25763 au
Dipole= 3.484 debye



11

C	1.231266	-1.050200	0.000000
C	1.247252	0.302719	0.000000
C	-0.014010	-1.744866	0.000000
C	0.000000	1.044703	0.000000
N	-1.158816	-1.129309	0.000000
N	-1.120005	0.204852	0.000000
O	-0.133213	2.257718	0.000000
H	2.151945	-1.618873	0.000000
H	2.161023	0.878599	0.000000
H	-0.060616	-2.824365	0.000000
H	-2.021955	0.659959	0.000000

Molecule# 1428

2H-thiete-1,1-dioxide

PointGroup: C1

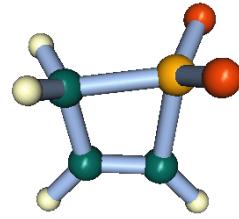
E= -665.407921195 au

ZPE= 0.068804 au

LUMO_eps= -0.05636 au

HOMO_eps= -0.30338 au

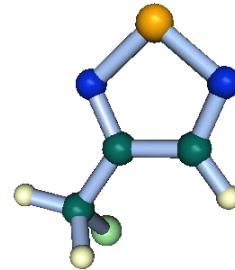
Dipole= 5.098 debye



10

O	1.238707	-1.255661	0.004628
S	0.503569	-0.000001	0.014979
O	1.238698	1.255665	0.004692
C	-0.961544	0.000030	-1.129930
C	-1.794509	-0.000009	0.132105
C	-0.911283	-0.000031	1.127195
H	-1.013806	-0.899488	-1.740062
H	-1.013804	0.899596	-1.739990
H	-2.873692	-0.000011	0.186098
H	-0.971028	-0.000045	2.203515

Molecule# 1429
3-(chloromethyl)-1,2,5-thiadiazole
PointGroup: C1
E= -1084.154104960 au
ZPE= 0.062515 au
LUMO_eps= -0.07980 au
HOMO_eps= -0.28592 au
Dipole= 1.683 debye



10

C1	2.634618	0.089972	-0.472541
S	-2.226941	-0.407927	-0.293740
N	-0.782002	-1.097257	0.085205
N	-1.805293	1.168792	-0.048337
C	0.046472	-0.123793	0.406185
C	-0.547869	1.172036	0.326492
C	1.448200	-0.422078	0.812171
H	-0.047158	2.105902	0.539835
H	1.735384	0.120694	1.707773
H	1.584567	-1.487017	0.958257

Molecule# 1430

3-(difluoroamino)propanenitrile

PointGroup: C1

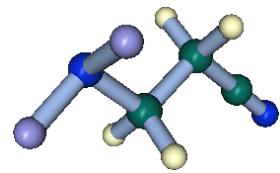
E= -425.934690186 au

ZPE= 0.074269 au

LUMO_eps= -0.02395 au

HOMO_eps= -0.32646 au

Dipole= 1.413 debye



11

F	2.284114	-0.947156	-0.058625
F	1.675956	1.135447	-0.349163
N	1.368083	-0.002087	0.430483
N	-3.383243	-0.343586	-0.277416
C	0.067845	-0.461845	-0.080232
C	-1.014437	0.516543	0.390152
C	-2.342864	0.043335	0.020269
H	-0.078651	-1.445718	0.361181
H	0.101207	-0.548538	-1.166096
H	-0.967408	0.631463	1.474281
H	-0.852917	1.499687	-0.051863

Molecule# 1431

3-(difluoromethyl)-1H-pyrazole

PointGroup: C1

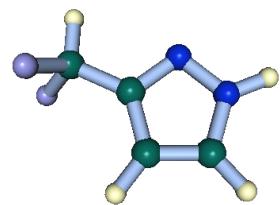
E= -464.179389677 au

ZPE= 0.084174 au

LUMO_eps= -0.02131 au

HOMO_eps= -0.27714 au

Dipole= 4.086 debye



12

F	1.978702	0.162047	1.097252
F	1.978699	0.162110	-1.097247
N	-0.935444	-1.145511	-0.000034
N	-2.145699	-0.572385	-0.000016
C	-0.086571	-0.124026	-0.000003
C	1.374341	-0.401214	-0.000013
C	-0.758309	1.116762	0.000036
C	-2.090320	0.782498	0.000026
H	-2.962960	-1.156749	-0.000033
H	1.588333	-1.468840	-0.000044
H	-0.328803	2.101756	0.000066
H	-2.980019	1.387567	0.000046

Molecule# 1432

3-(ethylsulphonyl)-1-propene

PointGroup: C1

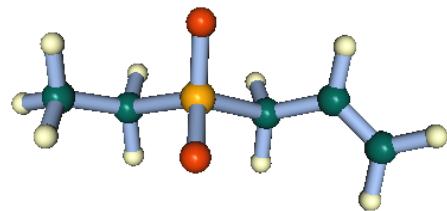
E= -745.308522971 au

ZPE= 0.146632 au

LUMO_eps= -0.03034 au

HOMO_eps= -0.27644 au

Dipole= 4.358 debye



18

C	-3.048752	-0.233601	0.036674
C	-1.747093	-0.694147	-0.606769
S	-0.333206	0.184684	0.124046
O	-0.241241	-0.192676	1.531689
O	-0.432759	1.596855	-0.241566
C	1.104634	-0.526657	-0.766862
C	2.358790	0.197724	-0.407998
C	3.357139	-0.350923	0.271282
H	-3.045989	-0.433495	1.106557
H	-3.203625	0.832669	-0.117926
H	-3.884192	-0.770832	-0.411908
H	-1.719025	-0.479926	-1.674605
H	-1.562290	-1.755515	-0.442909
H	1.142724	-1.579964	-0.494282
H	0.862845	-0.421743	-1.825556
H	2.417087	1.230864	-0.727347
H	3.318293	-1.376763	0.615663
H	4.249152	0.211954	0.508629

Molecule# 1433

3-(methylsulphonyl)-1-propene

PointGroup: C1

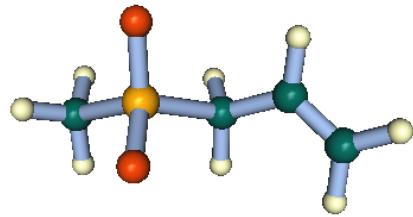
E= -705.979215774 au

ZPE= 0.118024 au

LUMO_eps= -0.03170 au

HOMO_eps= -0.27956 au

Dipole= 4.475 debye



15

C	-2.115162	-0.859134	-0.446944
S	-0.736952	0.145568	0.134592
O	-0.603003	-0.070176	1.570701
O	-0.913666	1.497805	-0.387410
C	0.712310	-0.599546	-0.708204
C	1.940525	0.209848	-0.457486
C	2.972177	-0.220038	0.256620
H	-1.957196	-1.891564	-0.146285
H	-2.996316	-0.452994	0.044646
H	-2.202825	-0.759745	-1.525431
H	0.446453	-0.619309	-1.766218
H	0.799645	-1.614868	-0.324996
H	1.949759	1.202936	-0.889296
H	2.982692	-1.202462	0.711754
H	3.843275	0.401100	0.412111

Molecule# 1434

3-amino-2-propynoic acid

PointGroup: C1

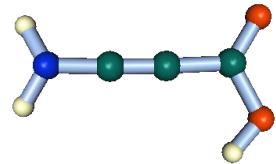
E= -321.395671175 au

ZPE= 0.059971 au

LUMO_eps= -0.03914 au

HOMO_eps= -0.26322 au

Dipole= 6.831 debye



9

O	1.772604	-1.164175	0.005094
O	1.810770	1.063763	0.003743
N	-2.805856	0.007250	-0.044985
C	1.155229	-0.132919	0.000440
C	-0.273472	-0.038262	-0.008028
C	-1.481370	-0.002709	-0.003032
H	1.173225	1.788219	-0.008235
H	-3.302718	-0.848895	0.140583
H	-3.298834	0.856562	0.175579

Molecule# 1435

3-amino-2,2-difluoropropanoic acid

PointGroup: C1

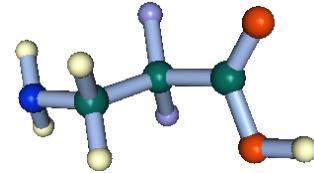
E= -522.436054952 au

ZPE= 0.091940 au

LUMO_eps= -0.04452 au

HOMO_eps= -0.27075 au

Dipole= 1.928 debye



13

F	0.465018	1.425630	0.535618
F	0.389467	-0.599318	1.371080
O	-1.954835	0.979221	-0.552404
O	-1.763085	-1.212817	-0.059693
N	2.517481	-0.276918	-0.574374
C	0.176013	0.131313	0.230920
C	-1.311942	0.050048	-0.156467
C	1.107414	-0.362137	-0.884322
H	-2.687110	-1.216711	-0.352628
H	2.799763	0.676454	-0.387399
H	2.755145	-0.838551	0.232905
H	0.841761	-1.396806	-1.101889
H	0.892172	0.230650	-1.774659

Molecule# 1436

3-amino-3-cyano-2-iminopropanoic acid

PointGroup: C1

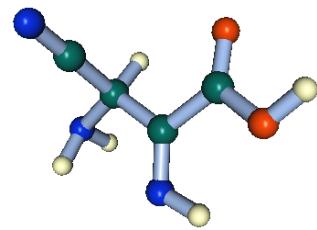
E= -470.291616422 au

ZPE= 0.100060 au

LUMO_eps= -0.10361 au

HOMO_eps= -0.28468 au

Dipole= 5.227 debye



14

O	-1.415386	1.150290	1.034869
O	-2.526884	-0.061738	-0.504591
N	-0.329637	-1.734260	-0.686231
N	2.142867	-1.152163	0.543205
N	1.836613	1.901711	-0.939641
C	-0.259663	-0.639128	-0.066281
C	-1.442454	0.263798	0.223360
C	1.089974	-0.157905	0.501868
C	1.523271	1.007131	-0.290019
H	-3.243142	0.541726	-0.256306
H	-1.276668	-1.925711	-1.010760
H	2.219932	-1.620473	-0.352294
H	1.916260	-1.862476	1.227909
H	0.906095	0.208124	1.514324

Molecule# 1437

3-aminobutyronitrile

PointGroup: C1

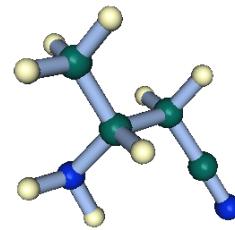
E= -266.838574063 au

ZPE= 0.119633 au

LUMO_eps= -0.02285 au

HOMO_eps= -0.26470 au

Dipole= 4.064 debye



14

N	2.719618	0.153377	-0.188334
C	1.682004	-0.289004	0.037142
C	0.346430	-0.814715	0.299669
C	-0.763293	0.051501	-0.329333
C	-2.127718	-0.576818	-0.072382
N	-0.717065	1.384780	0.269645
H	0.293437	-1.831487	-0.093339
H	0.196590	-0.861421	1.380188
H	-0.587244	0.069181	-1.413475
H	-2.916735	0.027258	-0.522652
H	-2.188243	-1.576132	-0.504413
H	-2.323569	-0.642517	0.998642
H	0.153061	1.858327	0.055880
H	-1.469698	1.963912	-0.080591

Molecule# 1438

3-aminopropionitrile

PointGroup: Cs

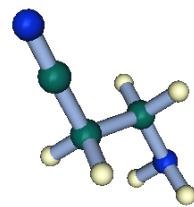
E= -227.506101517 au

ZPE= 0.091689 au

LUMO_eps= -0.02823 au

HOMO_eps= -0.26925 au

Dipole= 4.088 debye



11

H	2.562959	-0.097562	0.819589
H	2.562959	-0.097562	-0.819589
N	2.216312	-0.578879	0.000000
H	0.469894	-1.278430	0.874317
H	0.469894	-1.278430	-0.874317
C	0.770226	-0.700586	0.000000
H	0.275992	1.231576	0.878759
H	0.275992	1.231576	-0.878759
C	0.000000	0.644465	0.000000
N	-2.581961	0.274773	0.000000
C	-1.446584	0.459050	0.000000

Molecule# 1439

3-azido-2-fluoro-1-propene

PointGroup: C1

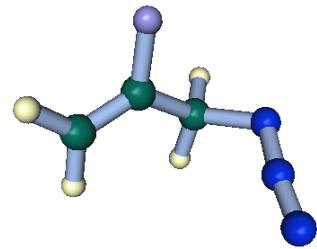
E= -380.875944346 au

ZPE= 0.076093 au

LUMO_eps= -0.04817 au

HOMO_eps= -0.27514 au

Dipole= 2.606 debye



11

F	-1.641036	-0.642024	-0.961587
N	1.087050	-0.943365	0.151427
N	1.749753	0.051367	-0.134059
N	2.441943	0.885774	-0.448358
C	-0.170884	-0.683104	0.894190
C	-1.185976	0.068769	0.096722
C	-1.642697	1.288657	0.320483
H	-0.554963	-1.669771	1.144246
H	0.032320	-0.144959	1.821789
H	-2.385849	1.733728	-0.323978
H	-1.276059	1.856850	1.160784

Molecule# 1440

3-azido-2-hydroxypropanal

PointGroup: C1

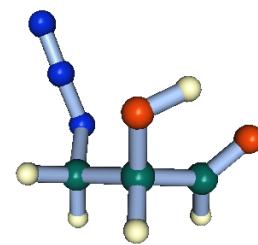
E= -432.114384522 au

ZPE= 0.093046 au

LUMO_eps= -0.06655 au

HOMO_eps= -0.27148 au

Dipole= 3.651 debye



13

O	-0.600225	-0.593424	1.360417
O	-2.161412	-0.986180	-0.769034
N	1.130210	0.592913	-0.768875
N	1.938772	-0.211377	-0.307642
N	2.733579	-0.958359	-0.022308
C	-0.951945	0.534649	0.607097
C	0.297309	1.321982	0.196777
C	-1.791724	0.146454	-0.592557
H	-1.576131	1.219785	1.205469
H	0.000108	2.247521	-0.295100
H	0.858777	1.579106	1.096908
H	-2.066282	0.961562	-1.285775
H	-1.063155	-1.351900	0.971304

Molecule# 1441

3-azidoprop-1-yne

PointGroup: C1

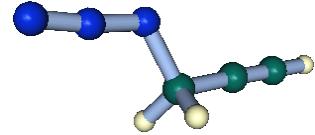
E= -280.337637079 au

ZPE= 0.059575 au

LUMO_eps= -0.05017 au

HOMO_eps= -0.27265 au

Dipole= 2.004 debye



9

N	-0.530767	-0.509584	-0.000040
N	-1.711032	-0.172686	0.000014
N	-2.824957	0.016559	0.000057
C	0.434644	0.619527	0.000002
C	1.797538	0.114494	-0.000012
C	2.931476	-0.269581	-0.000026
H	0.275495	1.245353	0.883766
H	0.275500	1.245412	-0.883722
H	3.934346	-0.617438	-0.000035

Molecule# 1442

3-azidotetrahydropyran-4-one

PointGroup: C1

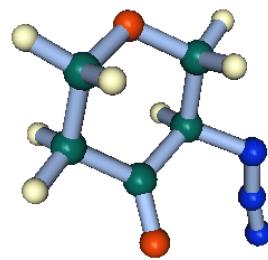
E= -509.556159283 au

ZPE= 0.129760 au

LUMO_eps= -0.05367 au

HOMO_eps= -0.26141 au

Dipole= 3.574 debye



17

O	-2.132717	-1.095340	0.252518
O	0.610471	1.752049	-0.467087
N	1.491407	-0.901688	-0.337217
N	2.510476	-0.318967	0.031214
N	3.520422	0.108687	0.290218
C	0.232239	-0.500781	0.281776
C	-1.595681	1.278882	0.363472
C	-0.861691	-1.447344	-0.252856
C	-0.161431	0.954486	0.005105
C	-2.543735	0.195754	-0.169896
H	0.271704	-0.619788	1.372356
H	-1.844528	2.263920	-0.029043
H	-1.679931	1.309068	1.453493
H	-0.657202	-2.466746	0.065853
H	-0.850944	-1.418392	-1.349027
H	-3.551721	0.340673	0.213185
H	-2.583755	0.235389	-1.265368

Molecule# 1443

3-bromo-1H-pyrazol-1-ol

PointGroup: C1

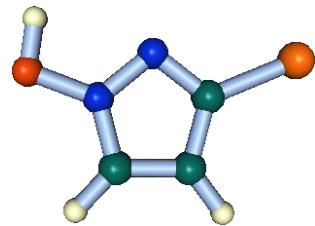
E= -2875.104108110 au

ZPE= 0.063717 au

LUMO_eps= -0.01807 au

HOMO_eps= -0.24688 au

Dipole= 2.036 debye



10

Br	1.886361	-0.162682	0.000002
O	-3.179826	-0.885749	-0.000052
N	-2.009809	-0.162878	-0.000002
N	-0.844863	-0.793270	-0.000030
C	0.041031	0.205520	-0.000015
C	-1.934087	1.175591	0.000021
C	-0.575323	1.460936	0.000003
H	-2.869407	-1.804465	0.000448
H	-2.811416	1.796172	0.000051
H	-0.110220	2.428917	0.000015

Molecule# 1444

3-bromomethyl-1,2,4-oxadiazole

PointGroup: C1

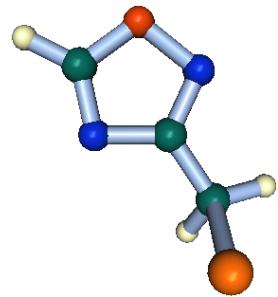
E= -2875.146060470 au

ZPE= 0.065034 au

LUMO_eps= -0.06620 au

HOMO_eps= -0.29346 au

Dipole= 1.855 debye



10

Br	-1.866540	-0.137088	-0.203360
O	2.819813	0.357476	-0.563875
N	1.671972	1.110528	-0.281156
N	1.463046	-0.977641	0.546283
C	0.911573	0.273259	0.367763
C	2.603840	-0.851410	-0.039704
C	-0.419727	0.668697	0.875839
H	3.385034	-1.585402	-0.151350
H	-0.577417	0.309096	1.886116
H	-0.556443	1.741076	0.814547

Molecule# 1445

3-bromoprop-1-yn-1-ol

PointGroup: C1

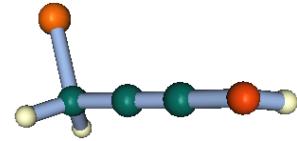
E= -2765.569672250 au

ZPE= 0.051667 au

LUMO_eps= -0.04266 au

HOMO_eps= -0.26160 au

Dipole= 2.927 debye



8

Br	-1.519719	-0.252861	-0.000984
O	3.544485	-0.493180	-0.104174
C	1.263353	0.534506	-0.000844
C	-0.045903	1.116960	0.014116
C	2.353998	0.034853	-0.003672
H	3.887031	-0.740541	0.764645
H	-0.239300	1.696424	0.910815
H	-0.242149	1.721763	-0.865232

Molecule# 1446

3-bromopropyne

PointGroup: C1

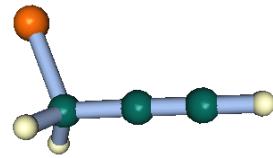
E= -2690.326320180 au

ZPE= 0.046740 au

LUMO_eps= -0.05412 au

HOMO_eps= -0.28673 au

Dipole= 1.723 debye



7

Br 1.036449 -0.159394 0.000000

C -0.618003 0.948377 0.000005

C -1.811728 0.145758 0.000000

C -2.818217 -0.505788 -0.000005

H -0.540319 1.567071 0.888490

H -0.540319 1.567081 -0.888473

H -3.707400 -1.085428 -0.000008

Molecule# 1447

3-bromopyruvicacid

PointGroup: C1

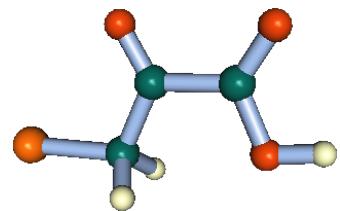
E= -2916.157074720 au

ZPE= 0.061312 au

LUMO_eps= -0.10750 au

HOMO_eps= -0.29398 au

Dipole= 4.269 debye



10

Br	-2.032775	-0.044594	0.000004
O	0.595136	1.597293	-0.000025
O	3.246009	0.723435	0.000020
O	2.430682	-1.379138	-0.000014
C	0.830055	0.425933	-0.000008
C	2.321702	-0.031722	0.000000
C	-0.197302	-0.684821	0.000008
H	3.374686	-1.601695	-0.000008
H	-0.064463	-1.313305	-0.877640
H	-0.064460	-1.313284	0.877670

Molecule# 1448

3-butenal

PointGroup: C1

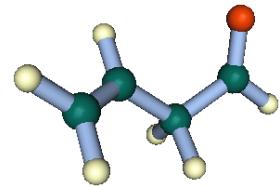
E= -231.315715581 au

ZPE= 0.088853 au

LUMO_eps= -0.04105 au

HOMO_eps= -0.26569 au

Dipole= 2.707 debye



11

C	-2.171508	-0.232104	-0.260028
H	-2.449028	0.531540	-0.977091
H	-2.897472	-1.011714	-0.074136
C	-0.999134	-0.216949	0.359116
H	-0.751263	-1.006444	1.058838
C	0.047693	0.833307	0.160729
H	-0.219239	1.524237	-0.645289
H	0.146644	1.464630	1.055798
C	1.439026	0.311691	-0.117058
H	2.190418	1.104526	-0.313882
O	1.760435	-0.847806	-0.120099

Molecule# 1449

3-chloro-1-propene

PointGroup: C1

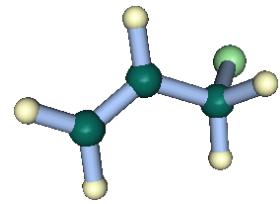
E= -577.588835203 au

ZPE= 0.071332 au

LUMO_eps= -0.03461 au

HOMO_eps= -0.28490 au

Dipole= 2.114 debye



9

C	2.222154	-0.206522	-0.305896
C	1.135350	-0.117984	0.450291
C	-0.025341	0.749869	0.122211
Cl	-1.546037	-0.242264	-0.108197
H	3.058152	-0.830798	-0.022178
H	2.314549	0.344401	-1.233886
H	1.060566	-0.687381	1.369728
H	-0.264925	1.439219	0.927711
H	0.121308	1.300880	-0.801666

Molecule# 1450

3-chloro-1,3-oxazinane

PointGroup: C1

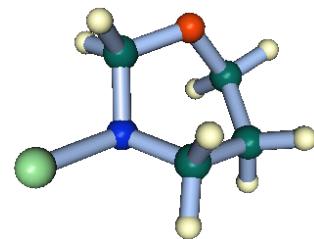
E= -747.499578735 au

ZPE= 0.124211 au

LUMO_eps= -0.04085 au

HOMO_eps= -0.24636 au

Dipole= 1.771 debye



15

C1	2.255385	0.055886	-0.086072
O	-1.387172	-1.150321	0.406249
N	0.508488	0.064813	-0.326125
C	-1.587319	1.218175	-0.062742
C	-0.127098	1.153328	0.423310
C	-2.077147	-0.196737	-0.403529
C	-0.016309	-1.252187	0.102890
H	-1.663879	1.854374	-0.945176
H	-2.199448	1.662233	0.722962
H	0.401358	2.076079	0.198723
H	-0.078803	0.986178	1.505841
H	-1.918611	-0.422066	-1.462420
H	-3.133523	-0.327195	-0.179940
H	0.473099	-1.609500	1.013006
H	0.163451	-1.956766	-0.716465

Molecule# 1451

3-chloro-2-isothiocyanatopropanal

PointGroup: C1

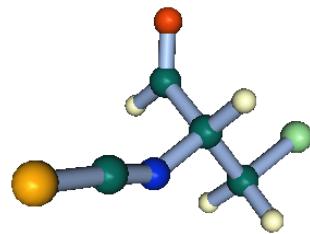
E= -1143.348302000 au

ZPE= 0.076607 au

LUMO_eps= -0.07606 au

HOMO_eps= -0.26928 au

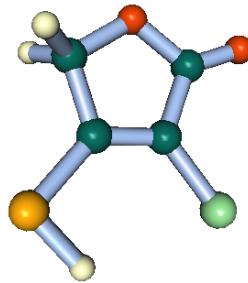
Dipole= 2.456 debye



12

C1	-3.091891	-0.553378	-0.200574
S	3.632310	-0.266570	-0.128147
O	-0.699111	2.368642	-0.205516
N	0.897212	-0.474689	0.245548
C	-0.405066	-0.025285	-0.173044
C	-1.436255	-1.039052	0.315660
C	-0.633145	1.364267	0.442426
C	2.069088	-0.345652	0.048062
H	-0.443611	0.071906	-1.258723
H	-1.234330	-2.019402	-0.103642
H	-1.437139	-1.102639	1.400744
H	-0.695064	1.370700	1.548388

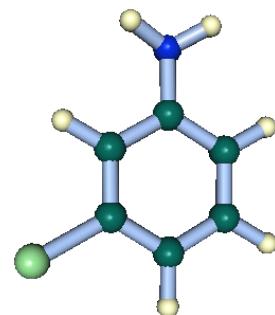
Molecule# 1452
3-chloro-4-sulfanyl-2(5H)-furanone
PointGroup: C1
E= -1163.243205730 au
ZPE= 0.064637 au
LUMO_eps= -0.06922 au
HOMO_eps= -0.26483 au
Dipole= 4.828 debye



11

C1	-0.294090	2.071082	-0.000003
S	2.440221	-0.174159	0.000001
O	-1.231702	-1.742984	0.000002
O	-2.709242	-0.031225	0.000000
C	-0.315568	0.356447	0.000000
C	0.729367	-0.479618	0.000001
C	-1.577506	-0.412007	0.000000
C	0.190782	-1.883495	0.000003
H	2.338062	1.169452	0.000000
H	0.491515	-2.442798	0.888008
H	0.491515	-2.442801	-0.888000

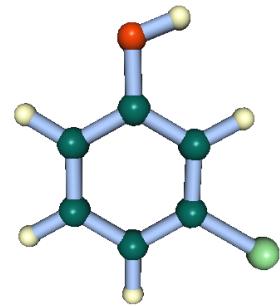
Molecule# 1453
3-chloroaniline
PointGroup: C1
E= -747.350258158 au
ZPE= 0.107304 au
LUMO_eps= -0.02553 au
HOMO_eps= -0.22317 au
Dipole= 2.973 debye



14

C	-0.725688	1.839957	0.003904
C	-1.772672	0.931790	-0.002269
C	0.599144	1.416167	0.004591
C	-0.184148	-0.880797	-0.007062
C	-1.513782	-0.444159	-0.007235
C	0.841141	0.050127	-0.000913
N	-2.554624	-1.364322	-0.068662
Cl	2.499376	-0.526961	0.002399
H	-0.942366	2.899755	0.008952
H	-2.796213	1.283658	-0.007912
H	1.416937	2.119885	0.009926
H	0.045646	-1.937052	-0.016153
H	-3.451270	-1.039482	0.252768
H	-2.343722	-2.296693	0.246175

Molecule# 1454
 3-chlorophenol
 PointGroup: Cs
 E= -767.222310810 au
 ZPE= 0.094934 au
 LUMO_eps= -0.03307 au
 HOMO_eps= -0.24400 au
 Dipole= 0.955 debye



13
 C 1.869828 -0.647799 0.000000
 C 1.019117 -1.742447 0.000000
 C 1.374486 0.652998 0.000000
 C -0.877502 -0.243979 0.000000
 C -0.358346 -1.536330 0.000000
 C 0.000000 0.831402 0.000000
 O -1.160637 -2.640733 0.000000
 Cl -0.660272 2.455830 0.000000
 H 2.939624 -0.806173 0.000000
 H 1.400483 -2.753177 0.000000
 H 2.036335 1.505248 0.000000
 H -1.945745 -0.074236 0.000000
 H -2.086473 -2.377981 0.000000

Molecule# 1455

3-chloropyridine

PointGroup: Cs

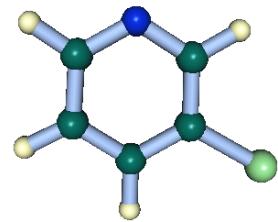
E= -708.007117762 au

ZPE= 0.079048 au

LUMO_eps= -0.05415 au

HOMO_eps= -0.27064 au

Dipole= 2.072 debye



11

C	1.207137	-1.555590	0.000000
C	1.220086	-0.167956	0.000000
C	-0.016035	-2.214360	0.000000
C	-1.179306	-0.248424	0.000000
C	0.000000	0.488855	0.000000
N	-1.187738	-1.578485	0.000000
Cl	-0.068149	2.235327	0.000000
H	2.132085	-2.115420	0.000000
H	2.145085	0.390219	0.000000
H	-0.058137	-3.297055	0.000000
H	-2.137626	0.255941	0.000000

Molecule# 1456

3-cyanoisoxazole

PointGroup: C1

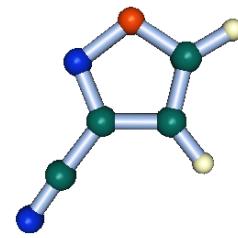
E= -338.395831694 au

ZPE= 0.056393 au

LUMO_eps= -0.08074 au

HOMO_eps= -0.31238 au

Dipole= 4.919 debye



9

O	-1.681498	-0.743311	0.000016
N	-0.355469	-1.123275	0.000007
N	2.897391	0.029139	-0.000024
C	0.323220	0.004011	-0.000002
C	-0.528654	1.144183	0.000000
C	-1.764853	0.597636	0.000012
C	1.747751	-0.010163	-0.000014
H	-0.247836	2.180702	-0.000006
H	-2.758422	1.010746	0.000018

Molecule# 1457

3-diazopropanenitrile

PointGroup: C1

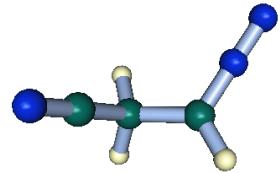
E= -280.397941572 au

ZPE= 0.060038 au

LUMO_eps= -0.07828 au

HOMO_eps= -0.24764 au

Dipole= 3.523 debye



9

N	-1.616715	-0.101498	0.115335
N	-2.512940	-0.696208	-0.240366
N	2.592445	-0.787850	0.164792
C	-0.601166	0.598614	0.503988
C	0.580873	0.787284	-0.409301
C	1.711258	-0.097097	-0.096653
H	-0.609112	0.927289	1.529719
H	0.289318	0.620071	-1.447202
H	0.934469	1.818720	-0.349050

Molecule# 1458

3-ethylphenol

PointGroup: C1

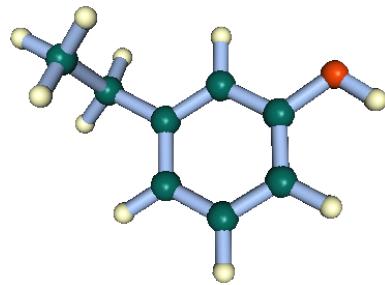
E= -386.249403637 au

ZPE= 0.160473 au

LUMO_eps= -0.01867 au

HOMO_eps= -0.23019 au

Dipole= 0.934 debye



19

C	-0.901148	1.795527	0.122367
C	0.418569	1.454846	-0.142196
C	-1.883647	0.815844	0.200910
C	-0.208669	-0.860797	-0.256980
C	0.778487	0.118510	-0.333408
C	-1.530238	-0.516572	0.009051
C	2.984093	-0.577570	0.712281
C	2.217039	-0.266854	-0.580918
O	-2.444462	-1.534667	0.066317
H	-1.173015	2.832920	0.265293
H	1.172655	2.228454	-0.206139
H	-2.913718	1.083750	0.403866
H	0.034043	-1.904816	-0.407043
H	2.994645	0.286561	1.377704
H	4.017795	-0.850368	0.494569
H	2.521714	-1.405294	1.251253
H	2.251433	-1.139150	-1.236927
H	2.720909	0.543479	-1.111640
H	-3.317676	-1.175798	0.251885

Molecule# 1459

3-ethylpyridine

PointGroup: C1

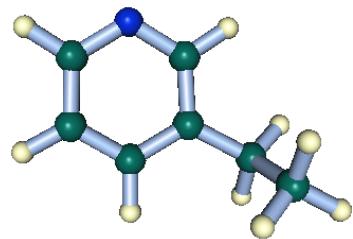
E= -327.035863779 au

ZPE= 0.144581 au

LUMO_eps= -0.03733 au

HOMO_eps= -0.25957 au

Dipole= 2.534 debye



17

C	1.635229	1.169984	0.080429
C	0.276934	1.186693	-0.201516
C	2.267258	-0.057658	0.237114
C	0.324908	-1.186647	-0.148460
C	-0.416052	-0.015986	-0.320449
C	-2.745423	0.061771	0.682967
C	-1.897892	-0.062347	-0.591011
N	1.628799	-1.222087	0.123692
H	2.197669	2.088931	0.173539
H	-0.242156	2.128401	-0.334054
H	3.327219	-0.108700	0.457919
H	-0.166546	-2.150313	-0.242291
H	-2.523086	-0.747211	1.379701
H	-3.809451	0.022818	0.446195
H	-2.548064	1.004033	1.195978
H	-2.164854	0.740982	-1.281320
H	-2.142103	-0.999187	-1.095962

Molecule# 1460

3-ethylthio-1-propene

PointGroup: Cs

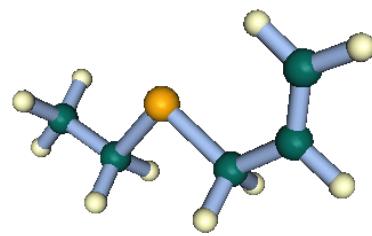
E= -594.831806932 au

ZPE= 0.137214 au

LUMO_eps= -0.01330 au

HOMO_eps= -0.22457 au

Dipole= 1.815 debye



16

H	-3.802515	-1.239154	0.000000
H	-2.689478	0.229953	0.000000
C	-2.794898	-0.846771	0.000000
H	-1.915495	-2.733395	0.000000
C	-1.747715	-1.660126	0.000000
H	0.189038	-1.709801	0.877836
H	0.189038	-1.709801	-0.877836
C	-0.299553	-1.277902	0.000000
S	0.000000	0.525942	0.000000
H	2.174574	-0.032527	0.883368
H	2.174574	-0.032527	-0.883368
C	1.831485	0.507447	0.000000
H	3.459524	1.922130	0.000000
H	2.036376	2.479514	-0.882479
H	2.036376	2.479514	0.882479
C	2.368679	1.932523	0.000000

Molecule# 1461

3-ethynoxy-1-hydroxy-1-methyl-urea

PointGroup: C1

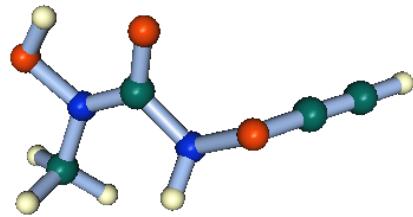
E= -491.202636472 au

ZPE= 0.106904 au

LUMO_eps= -0.02946 au

HOMO_eps= -0.25166 au

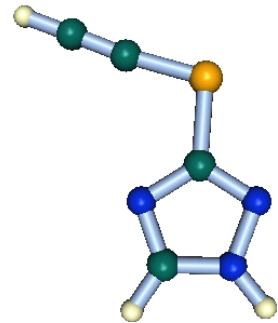
Dipole= 3.936 debye



15

O	1.731880	0.108377	-0.831919
O	-0.233133	-1.544013	-0.196714
O	-2.691735	-0.847458	0.265518
N	-1.675720	0.124252	0.257316
N	0.522172	0.666970	-0.284536
C	-0.460475	-0.351147	-0.115603
C	-2.198971	1.462610	0.154511
C	2.699348	0.095191	0.044841
C	3.640521	0.058237	0.782977
H	-2.181394	-1.673843	0.154736
H	0.256709	1.383325	-0.950263
H	-2.597488	1.677053	-0.841848
H	-2.998686	1.573387	0.884085
H	-1.411630	2.169530	0.406162
H	4.468689	0.007404	1.442234

Molecule# 1462
3-ethynylsulfanyl-1H-1,2,4-triazole
PointGroup: C1
E= -716.725639768 au
ZPE= 0.069414 au
LUMO_eps= -0.02600 au
HOMO_eps= -0.23303 au
Dipole= 3.600 debye



11

S	-1.131399	-1.070775	-0.000017
N	1.538046	-1.000510	-0.000058
N	0.653008	1.084197	0.000038
N	2.510851	-0.057395	-0.000035
C	0.445498	-0.256528	-0.000012
C	1.967699	1.170963	0.000021
C	-2.199076	0.233648	0.000030
C	-3.054062	1.079168	0.000059
H	3.478056	-0.332882	-0.000061
H	2.546140	2.079525	0.000047
H	-3.795499	1.838204	0.000079

Molecule# 1463

3-fluoro-2-nitropyridine

PointGroup: C1

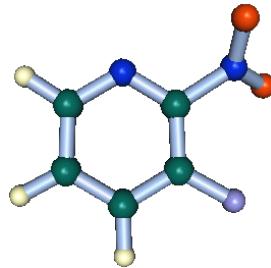
E= -552.220342209 au

ZPE= 0.082507 au

LUMO_eps= -0.10455 au

HOMO_eps= -0.29694 au

Dipole= 5.998 debye



13

F	0.201937	2.092857	-0.235362
O	2.218016	-1.126868	-0.702067
O	2.244199	0.459327	0.785864
N	-0.418686	-1.425726	0.129866
N	1.685363	-0.319981	0.031773
C	0.196563	-0.271665	0.023108
C	-0.463634	0.946200	-0.091353
C	-1.846644	0.947840	-0.089972
C	-2.503225	-0.267010	0.041067
C	-1.749398	-1.430562	0.150722
H	-2.376584	1.884122	-0.192026
H	-3.582748	-0.311349	0.052145
H	-2.224534	-2.397029	0.254856

Molecule# 1464

3-fluoro-propyne

PointGroup: C1

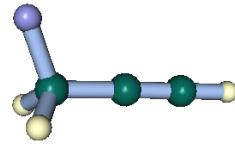
E= -215.970421531 au

ZPE= 0.048832 au

LUMO_eps= -0.02000 au

HOMO_eps= -0.29525 au

Dipole= 1.841 debye



7

F -1.495654 -0.534690 0.000025

C 0.759246 0.134886 -0.000021

C -0.629994 0.562044 0.000074

C 1.910455 -0.197047 -0.000106

H 2.928597 -0.497755 -0.000166

H -0.852940 1.155263 0.888657

H -0.853016 1.155403 -0.888397

Molecule# 1465

3-hexanol

PointGroup: C1

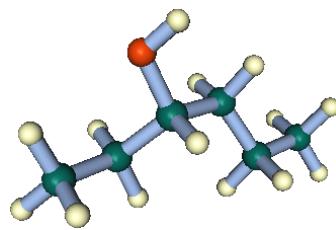
E= -312.425172785 au

ZPE= 0.192585 au

LUMO_eps= -0.01362 au

HOMO_eps= -0.27510 au

Dipole= 1.643 debye



21

C	-3.258638	-0.287523	0.090842
C	2.749710	-0.958717	-0.125572
C	-1.803228	-0.542577	-0.299578
C	1.324767	-0.757447	0.387390
C	-0.859239	0.560574	0.183682
C	0.597669	0.413820	-0.263537
O	1.346525	1.592486	0.069305
H	-3.369799	-0.222411	1.174974
H	-3.623837	0.649674	-0.334114
H	-3.910731	-1.087613	-0.261728
H	3.360328	-0.076592	0.059161
H	3.223088	-1.809507	0.366235
H	2.756534	-1.152346	-1.200530
H	-1.487941	-1.506260	0.106282
H	-1.729119	-0.630970	-1.387734
H	1.337132	-0.587285	1.467729
H	0.744175	-1.665979	0.216421
H	-1.230746	1.521745	-0.190767
H	-0.885745	0.627798	1.275431
H	0.618632	0.275514	-1.354253
H	0.919582	2.355577	-0.330907

Molecule# 1466

3-hexene

PointGroup: C1

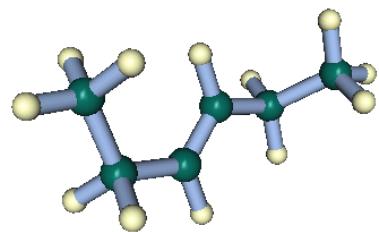
E= -235.945449487 au

ZPE= 0.164704 au

LUMO_eps= -0.00962 au

HOMO_eps= -0.24607 au

Dipole= 0.136 debye



18

C	0.392949	0.006753	-0.314271
C	1.845922	-0.344618	-0.447971
C	2.755670	0.526135	0.427735
C	-2.464073	0.895132	-0.087612
C	-2.023839	-0.525165	0.253168
C	-0.559417	-0.825207	0.095654
H	0.134394	1.030172	-0.571721
H	2.150834	-0.225520	-1.493272
H	1.992029	-1.398584	-0.200685
H	2.631761	1.584844	0.191968
H	2.523122	0.393155	1.485148
H	3.806004	0.272696	0.276534
H	-1.961620	1.631077	0.541868
H	-2.247135	1.142851	-1.127808
H	-3.538045	1.008319	0.062785
H	-2.588225	-1.237015	-0.359875
H	-2.312564	-0.756467	1.284752
H	-0.273824	-1.843703	0.350091

Molecule# 1467

3-hexyne

PointGroup: C2

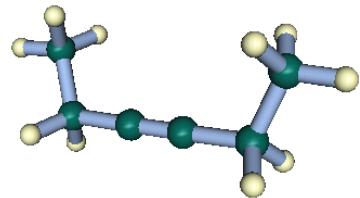
E= -234.698569426 au

ZPE= 0.141502 au

LUMO_eps= -0.01119 au

HOMO_eps= -0.25215 au

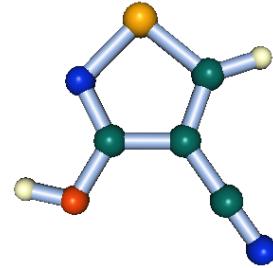
Dipole= 0.096 debye



16

C	-0.218611	-2.656740	0.856457
C	0.218611	2.656740	0.856457
C	0.001222	2.061425	-0.542357
C	-0.001222	-2.061425	-0.542357
C	0.001222	-0.601199	-0.556308
C	-0.001222	0.601199	-0.556308
H	-0.212880	-3.746339	0.811070
H	0.212880	3.746339	0.811070
H	1.174145	2.335610	1.270132
H	-0.567645	2.337886	1.540172
H	0.567645	-2.337886	1.540172
H	-1.174145	-2.335610	1.270132
H	0.780734	2.424674	-1.217851
H	-0.945635	2.426023	-0.950275
H	0.945635	-2.426023	-0.950275
H	-0.780734	-2.424674	-1.217851

Molecule# 1468
3-hydroxy-1,2-thiazole-4-carbonitrile
PointGroup: C1
E= -736.679192448 au
ZPE= 0.058411 au
LUMO_eps= -0.07999 au
HOMO_eps= -0.27432 au
Dipole= 3.695 debye



10

S	-1.919398	-0.623306	-0.000004
O	0.684500	2.053364	0.000006
N	-1.349126	0.945938	0.000001
N	3.124988	-0.766794	0.000002
C	0.587079	-0.360579	0.000000
C	-0.044852	0.929530	0.000002
C	-0.373055	-1.340201	-0.000004
C	1.987770	-0.580577	0.000001
H	0.082922	2.809754	0.000007
H	-0.221242	-2.406813	-0.000007

Molecule# 1469

3-hydroxy-1,3-oxazinan-4-one

PointGroup: C1

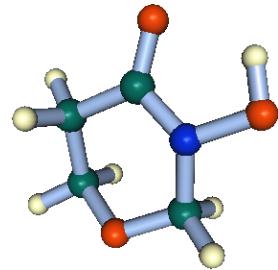
E= -437.178811390 au

ZPE= 0.119528 au

LUMO_eps= -0.02404 au

HOMO_eps= -0.25022 au

Dipole= 2.883 debye



15

C	-0.625254	0.796229	-0.069321
C	0.748082	1.424367	-0.171862
C	1.831447	0.472172	0.325884
C	0.493068	-1.432208	0.084495
N	-0.642039	-0.552571	-0.197890
O	-1.673211	1.417918	0.082626
O	1.681886	-0.808195	-0.288855
O	-1.868778	-1.171591	0.063455
H	0.927139	1.687106	-1.216193
H	0.732774	2.348662	0.404513
H	2.826636	0.822192	0.062253
H	1.780973	0.363978	1.416043
H	0.486076	-1.691814	1.152629
H	0.385931	-2.336757	-0.510335
H	-2.448486	-0.393788	0.203331

Molecule# 1470

3-hydroxy-1,3-thiazole-2(3H)-thione

PointGroup: C1

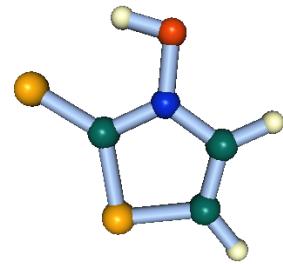
E= -1042.581363560 au

ZPE= 0.061195 au

LUMO_eps= -0.05624 au

HOMO_eps= -0.22396 au

Dipole= 4.158 debye



10

S	1.022965	-1.331872	0.000004
S	-2.014356	-0.693644	-0.000004
O	-0.819041	2.032145	-0.000005
N	0.058506	0.978276	0.000000
C	1.414989	1.194251	0.000002
C	-0.395063	-0.296584	0.000000
C	2.103807	0.039075	0.000005
H	1.783115	2.205430	0.000001
H	3.171199	-0.084468	0.000008
H	-1.691668	1.561773	-0.000006

Molecule# 1471

3-hydroxy-2-propynoic acid

PointGroup: C1

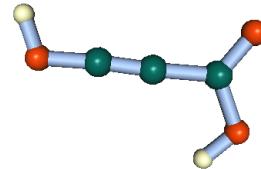
E= -341.255144615 au

ZPE= 0.047981 au

LUMO_eps= -0.04543 au

HOMO_eps= -0.29192 au

Dipole= 4.970 debye



8

O	-1.742727	-1.171659	-0.000001
O	-1.798817	1.053904	0.000000
O	2.791456	0.110796	0.000000
C	-1.139153	-0.134860	0.000000
C	0.298037	-0.026971	0.000000
C	1.499219	0.000183	0.000000
H	-1.166265	1.783255	0.000000
H	3.218346	-0.757686	0.000000

Molecule# 1472

3-hydroxy-4a,7a-dihydrofuro[2,3-d][1,2,3]triazin-4(3H)-one

PointGroup: C1

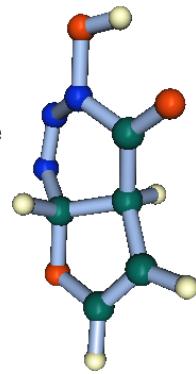
E= -583.521079722 au

ZPE= 0.110925 au

LUMO_eps= -0.08770 au

HOMO_eps= -0.26543 au

Dipole= 3.151 debye



16

0	-2.290204	-0.882999	-0.151424
0	1.444926	1.959948	0.003154
0	2.919242	-0.207425	-0.239915
N	-0.081213	-1.807611	0.272914
N	1.538222	-0.300125	-0.183639
N	1.139137	-1.556445	0.277999
C	-0.561361	0.592228	0.420127
C	-0.879772	-0.732796	-0.252028
C	-1.815431	1.347987	0.067672
C	0.851036	0.905794	0.038355
C	-2.746502	0.420002	-0.163318
H	-0.516052	0.455732	1.514116
H	-0.629924	-0.648724	-1.323073
H	-1.972359	2.408820	0.151036
H	-3.804155	0.525826	-0.340190
H	3.069933	0.752129	-0.132165

Molecule# 1473

3-hydroxybenzaldehyde

PointGroup: Cs

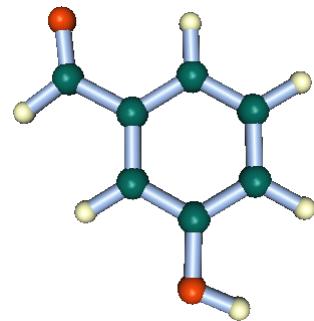
E= -420.957131511 au

ZPE= 0.113618 au

LUMO_eps= -0.07874 au

HOMO_eps= -0.25141 au

Dipole= 4.252 debye



15

C	1.664907	-0.863089	0.000000
C	1.344951	0.483532	0.000000
C	0.661934	-1.830509	0.000000
C	-1.007329	-0.096986	0.000000
C	0.000000	0.864343	0.000000
C	-0.676595	-1.448300	0.000000
C	-0.383063	2.293828	0.000000
O	0.394376	3.219298	0.000000
O	-1.703952	-2.348067	0.000000
H	2.700183	-1.175867	0.000000
H	2.108986	1.247054	0.000000
H	0.922411	-2.882429	0.000000
H	-2.049997	0.193551	0.000000
H	-1.476268	2.476862	0.000000
H	-1.357529	-3.245935	0.000000

Molecule# 1474

3-hydroxybenzonitrile

PointGroup: Cs

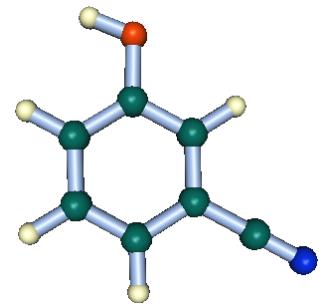
E= -399.864268300 au

ZPE= 0.103122 au

LUMO_eps= -0.06738 au

HOMO_eps= -0.26010 au

Dipole= 5.854 debye



14

C	2.334677	0.206360	0.000000
C	-0.822717	-1.740768	0.000000
C	0.532576	-1.450511	0.000000
C	-1.767452	-0.721730	0.000000
C	0.000000	0.919953	0.000000
C	0.939278	-0.111681	0.000000
C	-1.355148	0.609356	0.000000
N	3.459374	0.456490	0.000000
O	-2.231417	1.653229	0.000000
H	-1.151422	-2.770634	0.000000
H	1.270287	-2.238560	0.000000
H	-2.824291	-0.959587	0.000000
H	0.311031	1.954012	0.000000
H	-3.137157	1.327635	0.000000

Molecule# 1475

3-imino-1-allenone

PointGroup: C1

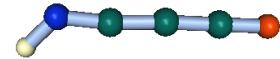
E= -244.922587600 au

ZPE= 0.031051 au

LUMO_eps= -0.07838 au

HOMO_eps= -0.26764 au

Dipole= 2.726 debye



6

O	2.465982	0.020631	-0.000235
N	-2.444823	-0.094872	-0.000289
C	0.032526	-0.028629	0.000643
C	1.301270	-0.000338	-0.000035
C	-1.244363	0.008532	0.000055
H	-3.150699	0.621669	-0.000074

Molecule# 1476

3-imino-2-propenoicacid

PointGroup: C1

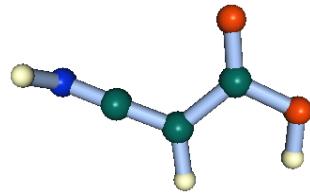
E= -321.418484669 au

ZPE= 0.059506 au

LUMO_eps= -0.05076 au

HOMO_eps= -0.27464 au

Dipole= 4.767 debye



9

O	0.832747	1.359187	0.006513
O	2.144989	-0.432647	-0.013277
N	-2.578092	0.122693	-0.135032
C	0.917327	0.160721	0.006423
C	-0.225737	-0.768608	0.030257
C	-1.459445	-0.297235	0.010407
H	2.070121	-1.393038	-0.029288
H	-3.142970	0.393415	0.664093
H	-0.095256	-1.840812	0.082007

Molecule# 1477

3-iminoacrylonitrile

PointGroup: C1

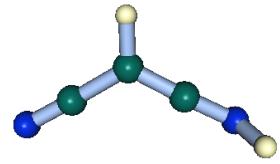
E= -225.044274159 au

ZPE= 0.043540 au

LUMO_eps= -0.05847 au

HOMO_eps= -0.27311 au

Dipole= 4.683 debye



7

N 2.167803 -0.419703 -0.124405

N -2.312485 -0.509274 -0.000062

C -0.068587 0.741058 0.011284

C 1.098133 0.121401 0.008582

C -1.296379 0.036975 0.003444

H -0.082728 1.822552 0.039789

H 2.696506 -0.716315 0.691622

Molecule# 1478

3-isothiocyanato-1-propyne

PointGroup: C1

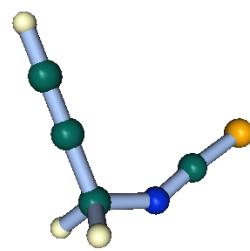
E= -607.197725807 au

ZPE= 0.057677 au

LUMO_eps= -0.04574 au

HOMO_eps= -0.25710 au

Dipole= 2.743 debye



9

S	2.304780	0.469076	0.000055
N	-0.000276	-1.064889	-0.000264
C	-1.440161	-1.078448	0.000154
C	-2.045252	0.250085	0.000038
C	0.961067	-0.361593	-0.000087
C	-2.535008	1.342919	-0.000048
H	-1.775353	-1.640578	-0.874688
H	-1.774829	-1.640184	0.875452
H	-2.968251	2.311985	-0.000143

Molecule# 1479

3-isothiocyanatopropanenitrile

PointGroup: C1

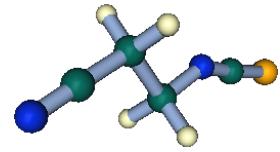
E= -662.634618919 au

ZPE= 0.075646 au

LUMO_eps= -0.05463 au

HOMO_eps= -0.26886 au

Dipole= 1.306 debye



11

S	3.337777	-0.078999	-0.008241
N	0.585203	0.215569	0.016899
N	-4.172513	-0.426062	-0.009011
C	-0.703901	-0.405684	0.011919
C	-1.805058	0.666399	-0.001765
C	-3.134377	0.067327	-0.005912
C	1.762573	0.040262	0.005120
H	-0.797866	-1.046210	-0.866960
H	-0.809327	-1.034429	0.897962
H	-1.695465	1.298430	-0.884021
H	-1.706021	1.309821	0.873498

Molecule# 1480

3-methoxyaniline

PointGroup: C1

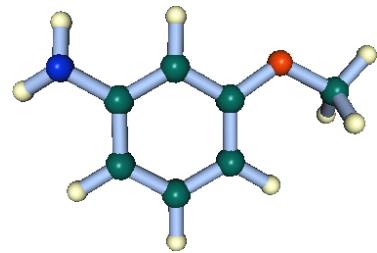
E= -402.285750006 au

ZPE= 0.149180 au

LUMO_eps= -0.01395 au

HOMO_eps= -0.20942 au

Dipole= 0.902 debye



18

C	-0.533337	1.799111	0.003615
C	-1.705095	1.064563	-0.002894
C	0.717403	1.184420	0.004395
C	-0.402266	-0.962277	-0.006106
C	-1.646552	-0.337109	-0.007512
C	0.770726	-0.209050	-0.000830
C	3.162146	-0.235899	0.003261
N	-2.816974	-1.091799	-0.070750
O	1.927453	-0.933333	0.000800
H	-0.586702	2.879891	0.008420
H	-2.664991	1.564249	-0.010323
H	1.613061	1.784526	0.009583
H	-0.323439	-2.041438	-0.015180
H	3.268427	0.385502	0.896029
H	3.269501	0.389402	-0.886596
H	3.936497	-0.998414	0.002060
H	-3.647664	-0.634953	0.267787
H	-2.743642	-2.042069	0.253499

Molecule# 1481

3-methoxyphenol

PointGroup: Cs

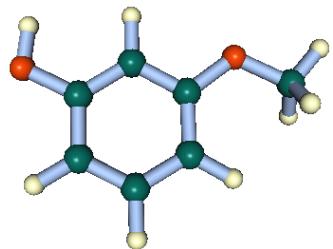
E= -422.158639224 au

ZPE= 0.136848 au

LUMO_eps= -0.01425 au

HOMO_eps= -0.22516 au

Dipole= 1.787 debye



17

C	-1.579132	-1.018404	0.000000
C	-0.556518	-1.950256	0.000000
C	-1.323399	0.352438	0.000000
C	1.044493	-0.139672	0.000000
C	0.763417	-1.497487	0.000000
C	0.000000	0.787801	0.000000
C	-0.623241	3.096404	0.000000
O	1.751266	-2.443316	0.000000
O	0.383127	2.095674	0.000000
H	-2.605756	-1.359527	0.000000
H	-0.754444	-3.011972	0.000000
H	-2.144558	1.051118	0.000000
H	2.064483	0.223401	0.000000
H	-1.251546	3.030018	0.891559
H	-1.251546	3.030018	-0.891559
H	-0.098191	4.047676	0.000000
H	2.612695	-2.014536	0.000000

Molecule# 1482

3-methyl-1-butanethiol

PointGroup: Cs

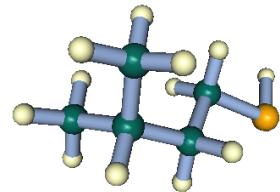
E= -596.067798984 au

ZPE= 0.159316 au

LUMO_eps= -0.01798 au

HOMO_eps= -0.23939 au

Dipole= 1.767 debye



18

C	1.606387	-0.480067	0.000000
H	2.540581	0.090664	0.000000
S	-2.130950	1.425864	0.000000
H	-3.258675	0.692401	0.000000
C	-0.938661	0.019058	0.000000
C	0.482787	0.577197	0.000000
C	1.606387	-1.344668	1.264784
C	1.606387	-1.344668	-1.264784
H	-1.123532	-0.585866	0.884604
H	-1.123532	-0.585866	-0.884604
H	0.607472	1.219754	-0.875670
H	0.607472	1.219754	0.875670
H	2.487666	-1.987485	-1.291990
H	2.487666	-1.987485	1.291990
H	0.730680	-1.994906	1.310682
H	0.730680	-1.994906	-1.310682
H	1.614497	-0.730494	2.167099
H	1.614497	-0.730494	-2.167099

Molecule# 1483

3-methyl-1-butanol

PointGroup: C1

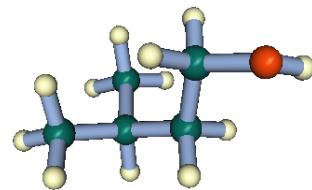
E= -273.091182433 au

ZPE= 0.164668 au

LUMO_eps= -0.01553 au

HOMO_eps= -0.27555 au

Dipole= 1.856 debye



18

C	1.596556	-1.266774	-0.239032
C	1.596587	1.262126	-0.295667
C	-0.382487	0.015965	0.749058
C	-1.297520	-0.031192	-0.471402
C	1.132440	0.013943	0.463905
O	-2.679318	-0.078760	-0.109803
H	2.685123	-1.295615	-0.309213
H	1.204663	-1.335770	-1.255520
H	1.274126	-2.157267	0.303519
H	1.204440	1.286519	-1.313980
H	2.685176	1.287631	-0.367323
H	1.275953	2.176485	0.207423
H	-0.625987	0.914555	1.327581
H	-0.629303	-0.837820	1.385322
H	-1.111212	0.820023	-1.133951
H	-1.127626	-0.938783	-1.049056
H	1.619002	0.036154	1.444159
H	-2.893279	0.709561	0.398292

Molecule# 1484

3-methyl-1-butene

PointGroup: Cs

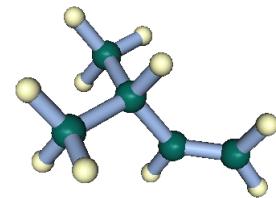
E= -196.614298997 au

ZPE= 0.135922 au

LUMO_eps= -0.00865 au

HOMO_eps= -0.26346 au

Dipole= 0.385 debye



15

C	0.038790	-2.151291	0.000000
C	-0.466392	-0.924162	0.000000
C	0.038790	1.174358	1.264341
C	0.038790	1.174358	-1.264341
C	0.328419	0.351813	0.000000
H	-0.595889	-3.027411	0.000000
H	1.108765	-2.324083	0.000000
H	-1.547581	-0.800215	0.000000
H	0.621162	2.097450	1.268423
H	0.283840	0.612320	2.165774
H	-1.017756	1.447586	1.316867
H	-1.017756	1.447586	-1.316867
H	0.621162	2.097450	-1.268423
H	0.283840	0.612320	-2.165774
H	1.389834	0.086538	0.000000

Molecule# 1485

3-methyl-1,2-butadiene

PointGroup: C2v

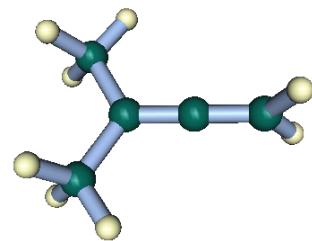
E= -195.371781607 au

ZPE= 0.111684 au

LUMO_eps= -0.01198 au

HOMO_eps= -0.24624 au

Dipole= 0.642 debye



13

C	0.000000	0.000000	2.232657
C	0.000000	0.000000	0.930096
H	-0.923706	0.000000	2.800709
H	0.923706	0.000000	2.800709
C	0.000000	0.000000	-0.374142
C	0.000000	1.284198	-1.168462
C	0.000000	-1.284198	-1.168462
H	0.000000	2.158725	-0.521798
H	0.000000	-2.158725	-0.521798
H	0.878905	1.332755	-1.816985
H	-0.878905	1.332755	-1.816985
H	-0.878905	-1.332755	-1.816985
H	0.878905	-1.332755	-1.816985

Molecule# 1486

3-methyl-1,2-oxazole

PointGroup: Cs

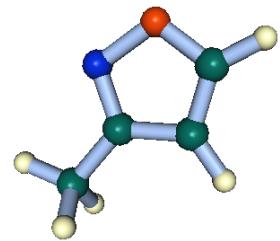
E= -285.466223416 au

ZPE= 0.085392 au

LUMO_eps= -0.02521 au

HOMO_eps= -0.27509 au

Dipole= 3.050 debye



11

C	0.053087	2.127284	0.000000
H	-0.448036	2.532049	0.880290
H	1.086611	2.465817	0.000000
H	-0.448036	2.532049	-0.880290
C	-0.629178	-1.458575	0.000000
O	0.709685	-1.409033	0.000000
N	1.104596	-0.064916	0.000000
C	0.000000	0.635944	0.000000
C	-1.148537	-0.210735	0.000000
H	-2.184862	0.075240	0.000000
H	-1.067559	-2.441986	0.000000

Molecule# 1487

3-methyl-1H-indole

PointGroup: Cs

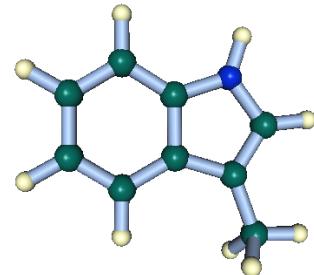
E= -403.283545674 au

ZPE= 0.156992 au

LUMO_eps= -0.02156 au

HOMO_eps= -0.20684 au

Dipole= 2.003 debye



19

C	2.400164	0.371989	0.000000
C	2.378036	-1.032831	0.000000
C	1.225975	1.104452	0.000000
C	1.182367	-1.731751	0.000000
C	-2.128810	-0.282841	0.000000
C	0.000000	0.426694	0.000000
C	-1.373591	0.855619	0.000000
C	0.002265	-0.990913	0.000000
C	-1.867833	2.265725	0.000000
N	-1.311240	-1.397591	0.000000
H	3.352447	0.884837	0.000000
H	3.311976	-1.578318	0.000000
H	1.256605	2.186234	0.000000
H	1.169380	-2.813921	0.000000
H	-3.200520	-0.392058	0.000000
H	-1.518424	2.813683	0.878543
H	-1.518424	2.813683	-0.878543
H	-2.957161	2.300824	0.000000
H	-1.628625	-2.348693	0.000000

Molecule# 1488

3-methyl-2-butanethiol

PointGroup: C1

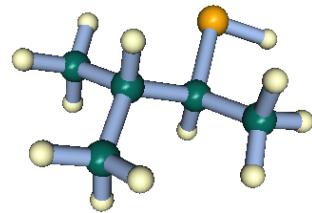
E= -596.068416119 au

ZPE= 0.158902 au

LUMO_eps= -0.01483 au

HOMO_eps= -0.23851 au

Dipole= 1.710 debye



18

C	-1.178493	-1.652194	0.116805
H	-2.072764	-2.053240	-0.361889
H	-0.342512	-2.298223	-0.146619
H	-1.321481	-1.719640	1.198086
C	0.547343	1.874508	-0.035601
H	-0.265216	2.515201	0.308948
H	1.466983	2.246656	0.415537
H	0.637818	1.980802	-1.117431
S	1.773454	-0.622977	-0.100054
H	2.704710	0.202406	0.408749
C	0.298134	0.419562	0.349892
H	0.183677	0.344478	1.433269
C	-0.951456	-0.197739	-0.311553
H	-0.786007	-0.181121	-1.393993
C	-2.209169	0.629016	-0.010608
H	-2.374526	0.713213	1.066488
H	-2.158055	1.634905	-0.423808
H	-3.086048	0.143279	-0.440087

Molecule# 1489

3-methyl-2-butanol

PointGroup: C1

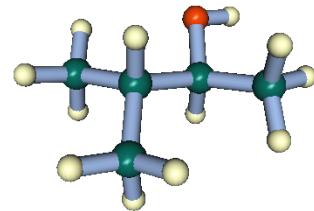
E= -273.097346522 au

ZPE= 0.163910 au

LUMO_eps= -0.01379 au

HOMO_eps= -0.27816 au

Dipole= 1.507 debye



18

C	-1.572019	-1.152435	0.064704
H	-2.544151	-1.085014	-0.426242
H	-1.109397	-2.095497	-0.217069
H	-1.747322	-1.170696	1.143837
C	1.649859	1.062268	-0.055942
H	1.313035	2.014631	0.352183
H	2.646218	0.870729	0.349265
H	1.737758	1.156202	-1.139611
O	1.248482	-1.330506	-0.129077
H	2.137286	-1.421916	0.225802
C	0.703049	-0.076396	0.308494
H	0.580650	-0.102704	1.400853
C	-0.691524	0.040475	-0.320727
H	-0.545223	0.020911	-1.406038
C	-1.380726	1.356806	0.052990
H	-1.468276	1.460678	1.137735
H	-0.850062	2.229463	-0.326308
H	-2.390195	1.382956	-0.358897

Molecule# 1490

3-methyl-2-butanone

PointGroup: C1

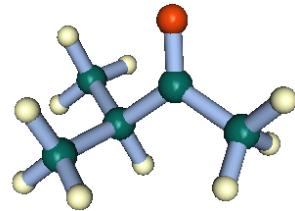
E= -271.891312894 au

ZPE= 0.140162 au

LUMO_eps= -0.02610 au

HOMO_eps= -0.25297 au

Dipole= 2.923 debye



16

C	0.753389	-0.242774	-0.066189
C	1.950166	0.504928	0.480694
C	-1.111331	1.335203	-0.553983
C	-1.623252	-0.926800	0.469523
C	-0.624754	0.227078	0.399162
O	0.883709	-1.161368	-0.844108
H	1.795440	1.584352	0.445517
H	2.847365	0.235724	-0.070490
H	2.082848	0.238822	1.532800
H	-1.240580	0.938427	-1.561561
H	-2.071930	1.724975	-0.215890
H	-0.412270	2.170887	-0.605134
H	-1.294846	-1.694619	1.170584
H	-1.735386	-1.397170	-0.506315
H	-2.599221	-0.564364	0.794752
H	-0.506399	0.668094	1.393352

Molecule# 1491

3-methyl-2-peroxycyclopentanol

PointGroup: C1

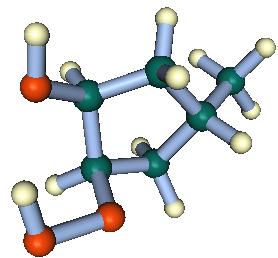
E= -461.619620652 au

ZPE= 0.180618 au

LUMO_eps= -0.02214 au

HOMO_eps= -0.26400 au

Dipole= 4.067 debye



21

O	1.270396	-1.072639	-0.506582
O	1.517293	1.629822	0.199626
O	2.683542	-0.799493	-0.331343
C	0.563240	-0.576995	0.629280
C	0.307919	0.934523	0.521011
C	-1.624769	-0.258153	-0.451572
C	-0.849525	-1.149198	0.553638
C	-0.801644	1.058787	-0.534497
C	-3.086772	-0.053090	-0.062299
H	1.309055	2.536080	-0.044132
H	2.700175	0.168020	-0.431915
H	1.109271	-0.857959	1.530822
H	-0.053565	1.281853	1.495981
H	-1.598532	-0.739344	-1.429450
H	-1.302471	-1.082953	1.545764
H	-0.834433	-2.200567	0.271677
H	-0.336755	1.157769	-1.515782
H	-1.419865	1.942579	-0.368709
H	-3.610629	-1.007454	0.018344
H	-3.169359	0.453398	0.902715
H	-3.613427	0.551813	-0.802280

Molecule# 1492

3-methyl-2,5-dihydrothiophene-1,1-dioxide

PointGroup: C1

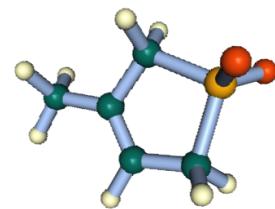
E= -744.104380498 au

ZPE= 0.125779 au

LUMO_eps= -0.02262 au

HOMO_eps= -0.27955 au

Dipole= 5.341 debye



16

O	-1.801585	-0.353946	-1.263177
S	-1.102837	-0.138972	0.000074
O	-1.800137	-0.353814	1.264151
C	0.470647	-1.077138	-0.000655
C	1.551977	-0.034521	-0.000177
C	2.979502	-0.481812	0.000109
C	-0.322179	1.520248	-0.000351
C	1.145332	1.235846	-0.000038
H	0.476225	-1.706442	-0.890781
H	0.476388	-1.707450	0.888755
H	3.659750	0.368607	0.000410
H	3.197004	-1.095951	-0.877283
H	3.196558	-1.096217	0.877425
H	-0.672041	2.042715	-0.890512
H	-0.672325	2.043260	0.889375
H	1.845935	2.061374	0.000310

Molecule# 1493

3-methylbutanoic acid

PointGroup: C1

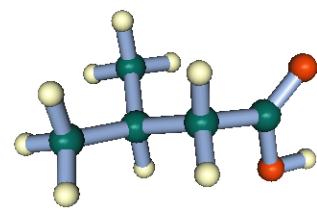
E= -347.169449086 au

ZPE= 0.146622 au

LUMO_eps= -0.01832 au

HOMO_eps= -0.28535 au

Dipole= 1.994 debye



17

C	-1.385093	-0.119037	-0.191443
C	1.198586	1.436061	0.377759
C	2.456843	-0.677449	-0.193579
C	-0.014446	-0.553958	-0.640655
C	1.127999	-0.090146	0.287288
O	-2.127693	0.617199	-0.789592
O	-1.722647	-0.661713	1.007831
H	0.267397	1.867338	0.747324
H	1.400121	1.875664	-0.601872
H	1.997897	1.744882	1.052719
H	2.699166	-0.326079	-1.199339
H	3.273423	-0.380691	0.466040
H	2.426108	-1.767952	-0.218522
H	-0.012100	-1.645227	-0.691635
H	0.133247	-0.165542	-1.647605
H	0.921724	-0.484958	1.284881
H	-2.607598	-0.334141	1.225892

Molecule# 1494

3-methylcyclopentene

PointGroup: C1

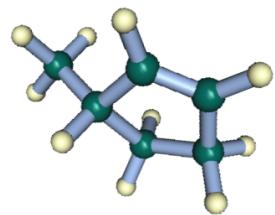
E= -234.730451402 au

ZPE= 0.144225 au

LUMO_eps= -0.01001 au

HOMO_eps= -0.24490 au

Dipole= 0.271 debye



16

H	-0.288253	2.211377	0.113712
C	0.103075	1.202002	0.097091
H	2.155830	1.583915	-0.380964
C	1.366429	0.878250	-0.158285
H	2.158926	-0.837607	0.868606
H	2.190120	-1.009750	-0.873105
C	1.601620	-0.607266	-0.046137
H	0.072016	-2.042382	0.656132
H	-0.122787	-1.505070	-1.005335
C	0.165989	-1.180038	-0.003279
H	-0.908864	-0.034062	1.507559
C	-0.750290	-0.003256	0.421562
H	-2.727516	0.841153	0.071891
H	-2.677022	-0.918993	-0.000210
H	-2.025849	0.037111	-1.334613
C	-2.124590	-0.010641	-0.248232

Molecule# 1495

3-methylenecyclopentene

PointGroup: C1

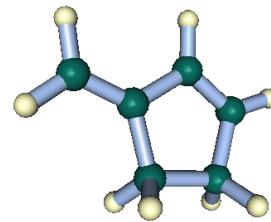
E= -233.506648679 au

ZPE= 0.120890 au

LUMO_eps= -0.02933 au

HOMO_eps= -0.22289 au

Dipole= 0.885 debye



14

C	-0.101375	-1.193285	0.000050
H	0.073644	-1.818598	0.875674
H	0.073697	-1.818666	-0.875519
C	-1.534643	-0.600290	-0.000041
H	-2.112333	-0.914628	0.873359
H	-2.112265	-0.914644	-0.873479
C	2.169627	-0.018400	-0.000040
H	2.749486	0.894993	-0.000074
H	2.721180	-0.949106	-0.000022
C	0.834976	0.009041	0.000011
C	-1.306567	0.887577	-0.000018
H	-2.117586	1.602915	-0.000019
C	-0.007168	1.200885	0.000034
H	0.395073	2.204577	0.000103

Molecule# 1496

3-methylenepentane

PointGroup: C2

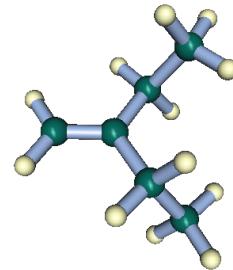
E= -235.944073445 au

ZPE= 0.164952 au

LUMO_eps= -0.01151 au

HOMO_eps= -0.25101 au

Dipole= 0.564 debye



18

C	0.000000	1.958176	-0.987741
H	0.566649	1.430602	-1.755450
H	-0.650438	2.672727	-1.493685
H	0.707866	2.520346	-0.377078
C	-0.827026	0.996208	-0.123763
H	-1.529824	0.461466	-0.769662
H	-1.433305	1.572550	0.576719
C	0.000000	-1.958176	-0.987741
H	-0.566649	-1.430602	-1.755450
H	0.650438	-2.672727	-1.493685
H	-0.707866	-2.520346	-0.377078
C	0.827026	-0.996208	-0.123763
H	1.529824	-0.461466	-0.769662
H	1.433305	-1.572550	0.576719
C	0.000000	0.000000	0.656119
C	0.000000	0.000000	1.987937
H	-0.592649	0.706057	2.556012
H	0.592649	-0.706057	2.556012

Molecule# 1497

3-methylfuran

PointGroup: Cs

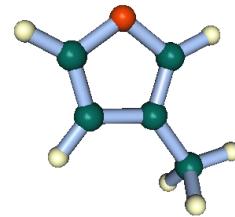
E= -269.444255720 au

ZPE= 0.097494 au

LUMO_eps= -0.00894 au

HOMO_eps= -0.23218 au

Dipole= 1.017 debye



12

O	-0.697958	-1.455911	0.000000
C	-1.079484	-0.145052	0.000000
C	0.661528	-1.463672	0.000000
C	0.000000	0.676627	0.000000
C	1.141177	-0.197619	0.000000
C	0.006984	2.171398	0.000000
H	-2.139263	0.036670	0.000000
H	1.128523	-2.431792	0.000000
H	2.178895	0.090679	0.000000
H	-1.007010	2.569914	0.000000
H	0.520643	2.565867	0.878993
H	0.520643	2.565867	-0.878993

Molecule# 1498

3-methylheptane

PointGroup: C1

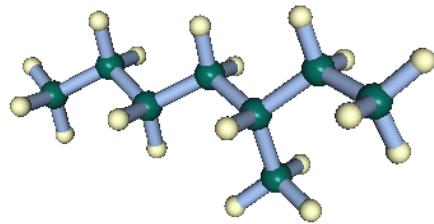
E= -315.830697076 au

ZPE= 0.244403 au

LUMO_eps= -0.01048 au

HOMO_eps= -0.30316 au

Dipole= 0.092 debye



26

C	4.015672	0.099100	0.289449
C	-3.659890	-0.381305	0.397793
C	-1.312953	1.589945	-0.274353
C	2.736727	-0.537959	-0.251184
C	-2.319478	-0.745039	-0.241002
C	1.463534	0.175911	0.206921
C	0.184875	-0.466156	-0.335149
C	-1.132203	0.137622	0.180181
H	4.109221	1.136544	-0.038345
H	4.025788	0.097510	1.381427
H	4.903264	-0.436410	-0.050520
H	-3.592023	-0.395135	1.487967
H	-4.434015	-1.093105	0.107456
H	-4.003439	0.609778	0.100382
H	-0.491110	2.223149	0.059161
H	-1.356401	1.648509	-1.365506
H	-2.232244	2.024627	0.117681
H	2.769370	-0.548538	-1.344870
H	2.692400	-1.586189	0.059526
H	-2.414267	-0.714025	-1.331790
H	-2.082615	-1.782577	0.011079
H	1.429172	0.178672	1.301980
H	1.519308	1.224408	-0.097653
H	0.198956	-1.530706	-0.080311
H	0.192317	-0.418766	-1.430343
H	-1.091387	0.129538	1.276747

Molecule# 1499

3-methylhexane

PointGroup: C1

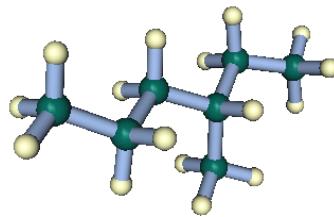
E= -276.502643554 au

ZPE= 0.216104 au

LUMO_eps= -0.01020 au

HOMO_eps= -0.30607 au

Dipole= 0.081 debye



23

C	-3.327207	-0.419023	0.041928
C	3.090721	-0.451140	-0.274255
C	-0.788431	-0.412239	0.253951
C	0.571113	0.141230	-0.203853
C	1.708576	-0.763650	0.299514
C	-2.017419	0.251736	-0.371051
H	3.827406	-1.178545	0.069812
H	-4.188029	0.070172	-0.416159
H	-3.463898	-0.383764	1.124825
H	-3.344052	-1.469173	-0.256997
H	3.079369	-0.485016	-1.366025
H	3.447082	0.535638	0.022419
H	-1.923476	0.224375	-1.461206
H	-2.055863	1.307823	-0.095365
H	1.456099	-1.799914	0.057534
H	1.746302	-0.710073	1.392821
H	-0.853981	-0.337240	1.345824
H	-0.821582	-1.482078	0.023681
H	0.587534	0.107539	-1.300667
C	0.769883	1.598721	0.226172
H	-0.014695	2.245965	-0.165115
H	1.720804	1.997706	-0.126289
H	0.757558	1.682770	1.316470

Molecule# 1500

3-methylpentane

PointGroup: Cs

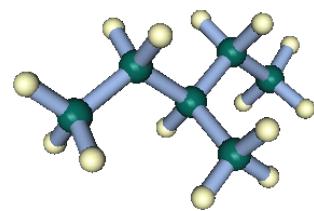
E= -237.174743700 au

ZPE= 0.187690 au

LUMO_eps= -0.01028 au

HOMO_eps= -0.31141 au

Dipole= 0.099 debye



20

C	0.332422	-0.120738	2.576193
C	0.332422	-0.120738	-2.576193
C	-1.326599	-0.799534	0.000000
C	0.332422	0.658899	1.260993
C	0.332422	0.658899	-1.260993
C	0.076207	-0.183223	0.000000
H	1.064695	-0.930894	2.552760
H	0.589136	0.530437	3.413029
H	-0.640971	-0.560347	2.794714
H	0.589136	0.530437	-3.413029
H	-0.640971	-0.560347	-2.794714
H	1.064695	-0.930894	-2.552760
H	-2.090417	-0.016871	0.000000
H	-1.492605	-1.425260	0.876651
H	-1.492605	-1.425260	-0.876651
H	1.299473	1.157680	1.150999
H	-0.414951	1.458132	1.311128
H	-0.414951	1.458132	-1.311128
H	1.299473	1.157680	-1.150999
H	0.805074	-1.004008	0.000000

Molecule# 1501

3-methylpyridine

PointGroup: Cs

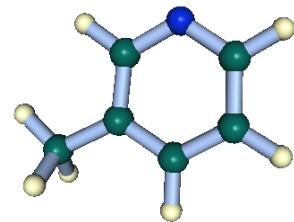
E= -287.708301969 au

ZPE= 0.115861 au

LUMO_eps= -0.03933 au

HOMO_eps= -0.26052 au

Dipole= 2.535 debye



14

C	-1.174839	-1.203589	0.000000
C	-1.199799	0.182128	0.000000
C	0.057339	-1.847450	0.000000
C	1.173702	0.138239	0.000000
C	0.000000	0.891573	0.000000
C	0.034480	2.395305	0.000000
N	1.217307	-1.194023	0.000000
H	-2.090952	-1.778442	0.000000
H	-2.144751	0.712153	0.000000
H	0.113787	-2.930206	0.000000
H	2.134084	0.644651	0.000000
H	-0.468705	2.803456	0.878765
H	1.058791	2.765852	0.000000
H	-0.468705	2.803456	-0.878765

Molecule# 1502

3-methylsulfanylprop-2-ynenitrile

PointGroup: C1

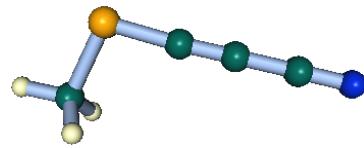
E= -607.201966111 au

ZPE= 0.056785 au

LUMO_eps= -0.07774 au

HOMO_eps= -0.26076 au

Dipole= 5.672 debye



9

S	1.646373	-0.642200	-0.000046
N	-3.679210	0.273566	0.000060
C	2.361907	1.048758	0.000007
C	0.007828	-0.301890	-0.000011
C	-1.191000	-0.121742	0.000012
C	-2.535848	0.090366	0.000037
H	2.057644	1.581413	0.895536
H	3.439906	0.904390	-0.000013
H	2.057620	1.581480	-0.895474

Molecule# 1503

3-methylthiophene

PointGroup: Cs

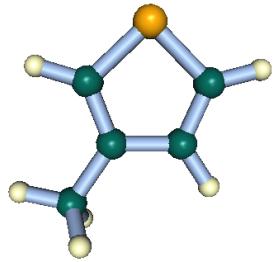
E= -592.432396252 au

ZPE= 0.094105 au

LUMO_eps= -0.01971 au

HOMO_eps= -0.23861 au

Dipole= 0.953 debye



12

H	-2.208077	0.786344	0.000000
C	-1.250002	0.285807	0.000000
C	0.000000	0.979789	0.000000
C	1.052965	0.110970	0.000000
H	-1.892989	-1.815714	0.000000
C	-1.117544	-1.068772	0.000000
S	0.542369	-1.539521	0.000000
H	1.168494	2.786598	0.000000
H	-0.354771	2.912496	0.878798
H	-0.354771	2.912496	-0.878798
C	0.124666	2.475760	0.000000
H	2.103691	0.348795	0.000000

Molecule# 1504

3-nitroaniline

PointGroup: C1

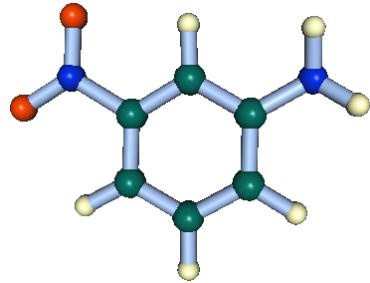
E= -492.300851981 au

ZPE= 0.119340 au

LUMO_eps= -0.09821 au

HOMO_eps= -0.23863 au

Dipole= 5.748 debye



16

C	-1.019949	1.869903	0.005061
C	-2.035560	0.925894	-0.000762
C	0.315136	1.486331	0.004036
C	-0.402977	-0.840723	-0.007286
C	-1.742943	-0.445332	-0.006521
C	0.587891	0.126743	-0.001813
N	-2.757551	-1.389060	-0.067066
N	1.997431	-0.318897	0.000986
O	2.865495	0.541162	-0.001230
O	2.215470	-1.522514	0.006001
H	-1.272850	2.921047	0.010796
H	-3.069081	1.248201	-0.005007
H	1.119865	2.202562	0.008669
H	-0.125177	-1.883684	-0.015106
H	-3.666794	-1.094774	0.247033
H	-2.522433	-2.323737	0.221720

Molecule# 1505

3-nitroso-3H-dithiole

PointGroup: C1

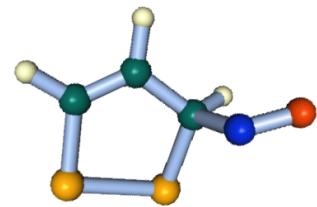
E= -1042.529751530 au

ZPE= 0.058792 au

LUMO_eps= -0.11069 au

HOMO_eps= -0.22079 au

Dipole= 2.646 debye



10

S	0.262272	-1.270575	0.351509
S	1.911534	-0.165680	-0.415891
O	-2.958453	-0.023467	-0.342226
N	-1.819104	0.125111	-0.669138
C	-0.854816	0.161427	0.535168
C	-0.048735	1.415196	0.494290
C	1.197951	1.369932	0.028995
H	-1.455073	0.027442	1.436830
H	-0.518659	2.347856	0.774850
H	1.827781	2.237414	-0.110510

Molecule# 1506

3-oxoprop-2-enoicacid

PointGroup: C1

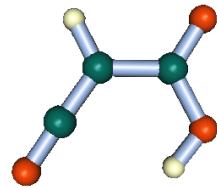
E= -341.309678416 au

ZPE= 0.047793 au

LUMO_eps= -0.09295 au

HOMO_eps= -0.29218 au

Dipole= 3.540 debye



8

O	-2.088631	-0.584833	-0.000019
O	-0.935596	1.306407	0.000008
O	2.497307	0.192352	-0.000016
C	-1.014648	-0.052431	0.000002
C	0.243940	-0.824199	0.000019
C	1.450682	-0.297452	0.000000
H	-0.029116	1.634178	0.000053
H	0.164626	-1.901098	0.000033

Molecule# 1507

3-oxopropanoic acid

PointGroup: C1

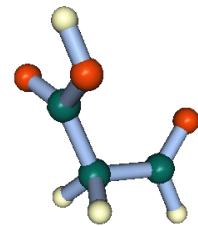
E= -342.539137730 au

ZPE= 0.071043 au

LUMO_eps= -0.05452 au

HOMO_eps= -0.28542 au

Dipole= 3.104 debye



10

C	1.643090	-0.157443	0.153934
C	-0.880250	-0.166831	0.029956
C	0.347276	-0.704458	0.723932
O	1.723698	0.647413	-0.732257
O	-1.466392	-0.723024	-0.859094
O	-1.245723	1.033301	0.528366
H	2.550479	-0.574965	0.632776
H	0.367812	-1.791023	0.624453
H	0.330267	-0.468364	1.790806
H	-2.001918	1.345224	0.008912

Molecule# 1508

3-pentanol

PointGroup: Cs

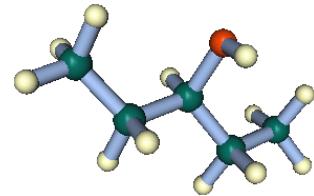
E= -273.097769875 au

ZPE= 0.164132 au

LUMO_eps= -0.01435 au

HOMO_eps= -0.27677 au

Dipole= 1.620 debye



18

C	0.256059	-0.145790	2.557816
C	0.256059	-0.145790	-2.557816
C	0.256059	0.678253	1.272070
C	0.256059	0.678253	-1.272070
C	0.123504	-0.161251	0.000000
O	-1.093205	-0.921538	0.000000
H	0.329959	0.496804	3.435919
H	-0.654055	-0.737969	2.645405
H	1.102179	-0.835589	2.578827
H	0.329959	0.496804	-3.435919
H	1.102179	-0.835589	-2.578827
H	-0.654055	-0.737969	-2.645405
H	-0.562591	1.406988	1.294805
H	1.178723	1.261415	1.206832
H	-0.562591	1.406988	-1.294805
H	1.178723	1.261415	-1.206832
H	0.906368	-0.925655	0.000000
H	-1.835609	-0.307374	0.000000

Molecule# 1509

3-pentanone

PointGroup: C2v

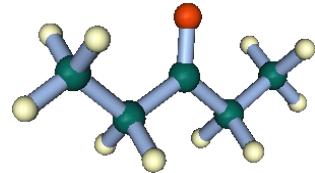
E= -271.892831520 au

ZPE= 0.140358 au

LUMO_eps= -0.02367 au

HOMO_eps= -0.25456 au

Dipole= 2.796 debye



16

C	0.000000	0.000000	0.077636
C	0.000000	2.555166	0.122397
C	0.000000	-2.555166	0.122397
C	0.000000	1.291000	-0.726245
C	0.000000	-1.291000	-0.726245
O	0.000000	0.000000	1.288225
H	0.000000	3.442073	-0.511364
H	-0.876892	2.593353	0.767222
H	0.876892	2.593353	0.767222
H	-0.876892	-2.593353	0.767222
H	0.876892	-2.593353	0.767222
H	0.000000	-3.442073	-0.511364
H	-0.868213	1.265230	-1.392902
H	0.868213	1.265230	-1.392902
H	0.868213	-1.265230	-1.392902
H	-0.868213	-1.265230	-1.392902

Molecule# 1510

3-phenyl-1-propanol

PointGroup: C1

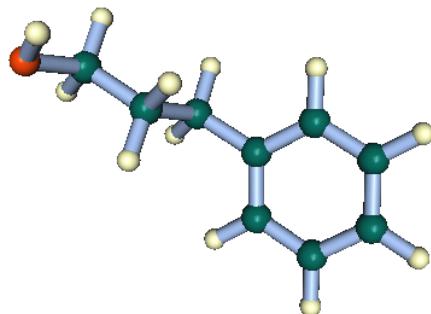
E= -425.567341504 au

ZPE= 0.189684 au

LUMO_eps= -0.01904 au

HOMO_eps= -0.25058 au

Dipole= 1.481 debye



22

C	-3.309215	-0.035048	-0.489887
C	-2.671442	1.180652	-0.272279
C	-2.629106	-1.220002	-0.231542
C	-1.363124	1.208399	0.197144
C	-1.321483	-1.186224	0.237822
C	-0.666846	0.027201	0.456848
C	0.765821	0.059305	0.929966
C	1.782430	-0.026705	-0.220241
C	3.223262	0.025404	0.272641
O	4.180079	-0.117662	-0.774765
H	-4.328143	-0.059056	-0.851886
H	-3.193934	2.108670	-0.463436
H	-3.118515	-2.171659	-0.391314
H	-0.877699	2.161375	0.369864
H	-0.803093	-2.115354	0.441580
H	0.940283	-0.770099	1.620194
H	0.940705	0.977696	1.495854
H	1.606106	0.797260	-0.919162
H	1.631807	-0.951245	-0.781323
H	3.399381	0.953589	0.829929
H	3.418890	-0.803311	0.954619
H	4.081795	0.615535	-1.389632

Molecule# 1511

3-phenylpyridazine

PointGroup: C1

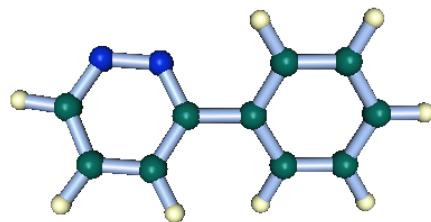
E= -495.522189106 au

ZPE= 0.156872 au

LUMO_eps= -0.06486 au

HOMO_eps= -0.24042 au

Dipole= 3.758 debye



20

C	0.771928	0.031892	0.002176
N	1.373089	-1.135533	-0.268058
C	1.517491	1.185214	0.283493
C	2.888656	1.088544	0.253045
C	3.435576	-0.156370	-0.042961
N	2.692576	-1.231573	-0.286051
C	-0.709720	0.022857	-0.000158
C	-1.402884	-1.169419	0.234804
C	-2.789799	-1.189168	0.240834
C	-3.510661	-0.022683	0.006144
C	-2.832600	1.165699	-0.237604
C	-1.444071	1.188439	-0.239574
H	4.505517	-0.314225	-0.081356
H	3.523963	1.938063	0.462583
H	1.028770	2.114805	0.536243
H	-3.383886	2.075335	-0.434047
H	-4.592120	-0.040627	0.009324
H	-3.310530	-2.118188	0.430151
H	-0.839342	-2.073585	0.409647
H	-0.935526	2.118137	-0.454969

Molecule# 1512

3-pyridinol

PointGroup: Cs

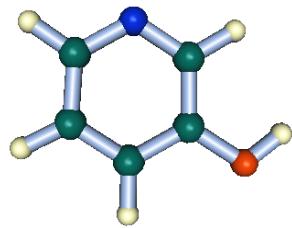
E= -323.630199456 au

ZPE= 0.092719 au

LUMO_eps= -0.04196 au

HOMO_eps= -0.24961 au

Dipole= 1.297 debye



12

N	-1.199731	-1.156343	0.000000
C	-1.178706	0.173175	0.000000
C	0.000000	0.918177	0.000000
C	1.213975	0.242243	0.000000
C	1.190617	-1.143321	0.000000
C	-0.034471	-1.802433	0.000000
O	0.013506	2.282556	0.000000
H	-2.141010	0.679327	0.000000
H	2.140074	0.800041	0.000000
H	2.112543	-1.708300	0.000000
H	-0.081634	-2.884350	0.000000
H	-0.888395	2.620187	0.000000

Molecule# 1513

3-sulfanyl-1H-imidazole-2-thione

PointGroup: C1

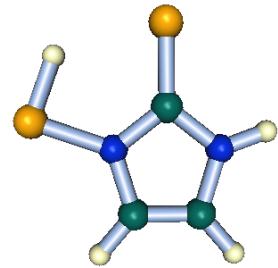
E= -1022.744577780 au

ZPE= 0.072127 au

LUMO_eps= -0.04347 au

HOMO_eps= -0.20870 au

Dipole= 4.568 debye



11

S	1.423113	-1.504035	-0.000003
S	1.033270	1.806919	0.000000
N	-0.098633	-0.682408	0.000000
N	-1.561189	0.904248	0.000002
C	-0.213029	0.685854	0.000000
C	-1.351292	-1.279776	0.000001
C	-2.265069	-0.285493	0.000003
H	2.055117	-0.283372	-0.000002
H	-1.946319	1.831522	0.000004
H	-1.478172	-2.345480	0.000001
H	-3.337664	-0.325200	0.000003

Molecule# 1514

3-sulfanyl-2H-thiadiazole

PointGroup: C1

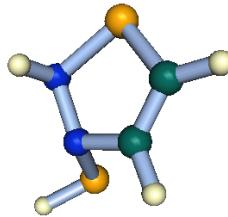
E= -984.547322289 au

ZPE= 0.064479 au

LUMO_eps= -0.04112 au

HOMO_eps= -0.21375 au

Dipole= 1.841 debye



10

S	-1.704462	-0.551936	-0.348464
S	2.023603	-0.133580	-0.423222
N	0.632814	0.094551	0.642941
N	-0.297676	-0.998966	0.631752
C	-0.067494	1.302057	0.352543
C	-1.293811	1.155566	-0.146389
H	2.855091	-0.564541	0.544789
H	-0.635754	-1.053433	1.588426
H	0.457833	2.229855	0.510423
H	-1.961569	1.941553	-0.456436

Molecule# 1515

3-sulfanylideneprop-2-enoicacid

PointGroup: C1

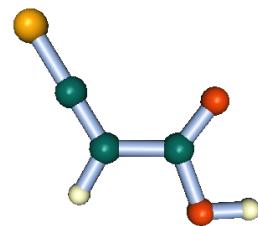
E= -664.275503456 au

ZPE= 0.046002 au

LUMO_eps= -0.11047 au

HOMO_eps= -0.26002 au

Dipole= 1.814 debye



8

S	-2.444945	0.114711	-0.000002
O	1.338014	1.334195	0.000002
O	2.574349	-0.551462	0.000001
C	1.397186	0.128744	0.000001
C	0.265164	-0.804020	0.000000
C	-0.982040	-0.381913	0.000000
H	3.277153	0.114294	0.000002
H	0.461205	-1.868401	0.000000

Molecule# 1516

3-thioxo-1,2-oxazolidin-5-one

PointGroup: C1

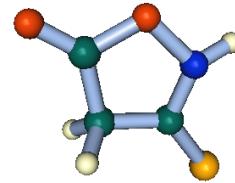
E= -719.620674843 au

ZPE= 0.063769 au

LUMO_eps= -0.08153 au

HOMO_eps= -0.24691 au

Dipole= 0.669 debye



10

S	2.388840	-0.228485	-0.065926
O	-1.264798	1.114379	-0.020009
O	-2.745689	-0.568829	-0.105351
N	0.144946	1.180968	0.131545
C	0.766882	-0.013837	0.054715
C	-1.610527	-0.229493	-0.016169
C	-0.337581	-1.036321	0.118536
H	0.526739	2.051909	-0.206611
H	-0.336392	-1.568271	1.071151
H	-0.255164	-1.781153	-0.670150

Molecule# 1517

3(2H)-pyridinone

PointGroup: C1

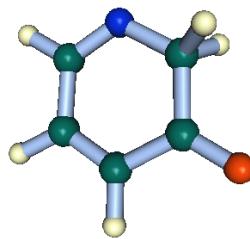
E= -323.597874565 au

ZPE= 0.091295 au

LUMO_eps= -0.10546 au

HOMO_eps= -0.25125 au

Dipole= 3.128 debye



12

N	1.200532	-1.192190	0.000009
C	-0.248247	-1.251538	0.000100
C	-1.059500	0.036614	0.000061
C	-0.288709	1.286859	0.000113
C	1.051418	1.235550	-0.000006
C	1.757680	-0.047837	-0.000095
O	-2.276005	0.018306	-0.000145
H	-0.559635	-1.846968	0.864275
H	-0.843315	2.215844	0.000201
H	1.646021	2.141077	-0.000054
H	2.845073	-0.022117	-0.000226
H	-0.559677	-1.846841	-0.864144

Molecule# 1518

3(4H)-pyridinone

PointGroup: C1

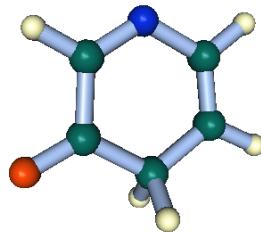
E= -323.592645805 au

ZPE= 0.090833 au

LUMO_eps= -0.10829 au

HOMO_eps= -0.25657 au

Dipole= 3.005 debye



12

N	1.003702	-1.321515	-0.000044
C	-0.274008	-1.255389	0.000230
C	-1.057493	0.010593	0.000105
C	-0.250299	1.293437	0.000138
C	1.227716	1.089202	0.000005
C	1.758426	-0.135993	-0.000177
O	-2.271435	-0.003688	-0.000258
H	-0.853456	-2.175087	0.000425
H	-0.562854	1.887548	-0.865857
H	1.870338	1.960254	0.000050
H	2.828067	-0.291154	-0.000357
H	-0.562581	1.887450	0.866314

Molecule# 1519

3(6H)-pyridinone

PointGroup: Cs

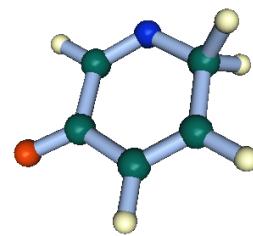
E= -323.597953405 au

ZPE= 0.091528 au

LUMO_eps= -0.09071 au

HOMO_eps= -0.25207 au

Dipole= 3.890 debye



12

N	-1.271596	-1.030212	0.000000
C	-1.236096	0.239527	0.000000
C	0.000000	1.085157	0.000000
C	1.263984	0.348634	0.000000
C	1.244327	-0.987977	0.000000
C	-0.025532	-1.764497	0.000000
O	-0.082178	2.301599	0.000000
H	-2.173830	0.792159	0.000000
H	2.180630	0.923062	0.000000
H	2.167680	-1.557260	0.000000
H	-0.047988	-2.442167	0.862672
H	-0.047988	-2.442167	-0.862672

Molecule# 1520

3,3'-iminobis(2-propynoic acid)

PointGroup: C1

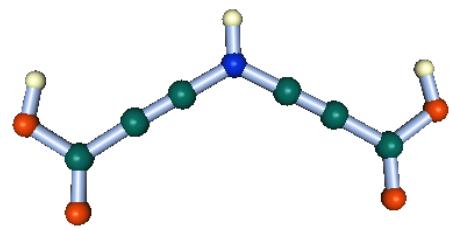
E= -586.187804226 au

ZPE= 0.084794 au

LUMO_eps= -0.07547 au

HOMO_eps= -0.27888 au

Dipole= 9.160 debye



14

O	3.552425	-1.677314	-0.000076
O	-3.552425	-1.677314	-0.000133
O	4.601741	0.288643	0.000051
O	-4.601741	0.288643	-0.000016
N	0.000000	1.455001	0.000098
C	3.482204	-0.481149	-0.000003
C	-3.482204	-0.481149	-0.000058
C	2.240625	0.251308	0.000033
C	-2.240624	0.251308	-0.000006
C	1.181312	0.822939	0.000062
C	-1.181312	0.822939	0.000041
H	4.369566	1.225617	0.000108
H	-4.369566	1.225617	0.000046
H	0.000000	2.465308	0.000146

Molecule# 1521

3,3-dichloropropyne

PointGroup: C1

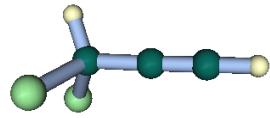
E= -1035.951748340 au

ZPE= 0.037992 au

LUMO_eps= -0.04948 au

HOMO_eps= -0.30478 au

Dipole= 1.870 debye



7

C1 0.811282 1.486375 -0.113059

C1 0.811397 -1.486324 -0.112983

C -0.023639 0.000009 0.490782

C -1.414266 -0.000051 0.121661

C -2.577535 -0.000087 -0.162983

H 0.115063 0.000040 1.565162

H -3.607963 -0.000119 -0.419211

Molecule# 1522

3,3-dimethyl-2-butanone

PointGroup: C1

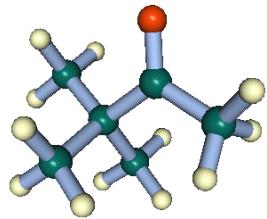
E= -311.217166878 au

ZPE= 0.167847 au

LUMO_eps= -0.02467 au

HOMO_eps= -0.25078 au

Dipole= 2.885 debye



19

C	0.906853	0.321148	-0.017128
C	1.943934	-0.786999	-0.005884
C	-0.933612	-0.544883	1.418768
C	-0.861053	-1.193432	-1.015538
C	-1.437212	1.161991	-0.352359
C	-0.585568	-0.063766	-0.006852
O	1.259489	1.479477	-0.029986
H	2.897115	-0.377609	0.318312
H	1.660429	-1.625395	0.628697
H	2.062196	-1.175511	-1.020006
H	-0.366445	-1.430877	1.704810
H	-0.740904	0.236991	2.154158
H	-1.993325	-0.800366	1.469308
H	-0.315821	-2.105697	-0.774352
H	-0.592539	-0.894537	-2.030268
H	-1.924863	-1.435703	-1.013178
H	-1.207435	1.532654	-1.351356
H	-1.258629	1.976552	0.346678
H	-2.495732	0.899320	-0.318958

Molecule# 1523

3,3-dimethylbutyne

PointGroup: C3v

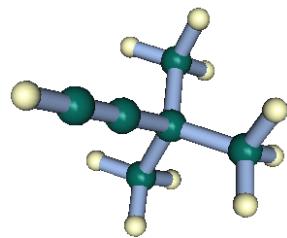
E= -234.688976530 au

ZPE= 0.139998 au

LUMO_eps= -0.01197 au

HOMO_eps= -0.27326 au

Dipole= 0.750 debye



16

C	0.000000	0.000000	1.171492
C	0.000000	0.000000	-0.297053
C	0.000000	1.456381	-0.805220
C	1.261263	-0.728190	-0.805220
C	-1.261263	-0.728190	-0.805220
C	0.000000	0.000000	2.371824
H	0.000000	0.000000	3.433077
H	0.000000	1.469839	-1.896499
H	1.272918	-0.734919	-1.896499
H	-1.272918	-0.734919	-1.896499
H	-0.882465	1.990948	-0.454532
H	0.882465	1.990948	-0.454532
H	2.165444	-0.231237	-0.454532
H	1.282979	-1.759711	-0.454532
H	-1.282979	-1.759711	-0.454532
H	-2.165444	-0.231237	-0.454532

Molecule# 1524

3,3-dimethyloxetane

PointGroup: Cs

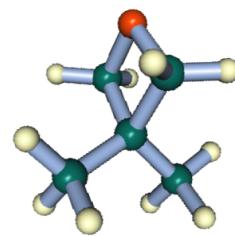
E= -271.844350346 au

ZPE= 0.141982 au

LUMO_eps= -0.01454 au

HOMO_eps= -0.25588 au

Dipole= 2.078 debye



16

C	-1.264788	1.284808	0.000000
H	-1.283550	1.930106	0.881130
H	-1.283550	1.930106	-0.881130
H	-2.179327	0.690156	0.000000
C	1.255285	1.225783	0.000000
H	2.138334	0.585269	0.000000
H	1.305127	1.868005	-0.882100
H	1.305127	1.868005	0.882100
C	-0.026045	0.399811	0.000000
C	-0.026045	-0.751630	1.036255
C	-0.026045	-0.751630	-1.036255
H	0.817961	-0.777877	1.729654
H	0.817961	-0.777877	-1.729654
H	-0.958286	-0.870369	1.595908
H	-0.958286	-0.870369	-1.595908
O	0.100540	-1.752252	0.000000

Molecule# 1525

3,3-dimethylpentane

PointGroup: C2

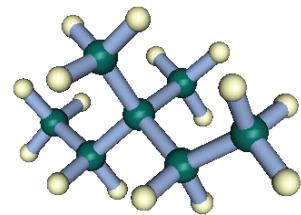
E= -276.499461719 au

ZPE= 0.215718 au

LUMO_eps= -0.01286 au

HOMO_eps= -0.30663 au

Dipole= 0.088 debye



23

C	0.000000	0.000000	0.065284
C	-0.000119	1.241984	-0.861684
C	0.000119	-1.241984	-0.861684
C	0.000000	2.618031	-0.193199
C	0.000000	-2.618031	-0.193199
C	1.255287	0.000120	0.952178
C	-1.255287	-0.000120	0.952178
H	0.872906	1.172573	-1.518050
H	-0.873342	1.172588	-1.517788
H	-0.872906	-1.172573	-1.518050
H	0.873342	-1.172588	-1.517788
H	-0.000193	3.402590	-0.951355
H	0.000193	-3.402590	-0.951355
H	-0.880980	2.772125	0.430603
H	0.881256	2.772164	0.430201
H	0.880980	-2.772125	0.430603
H	-0.881256	-2.772164	0.430201
H	-1.284762	-0.876517	1.599898
H	-2.165042	-0.000409	0.347245
H	-1.285140	0.876465	1.599626
H	1.284762	0.876517	1.599898
H	2.165042	0.000409	0.347245
H	1.285140	-0.876465	1.599626

Molecule# 1526

3,3-disulfanylacrylonitrile

PointGroup: C1

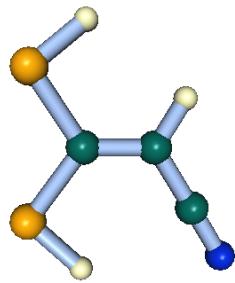
E= -967.351168273 au

ZPE= 0.049493 au

LUMO_eps= -0.07161 au

HOMO_eps= -0.25579 au

Dipole= 3.589 debye



9

S	-2.060348	-0.589692	-0.009626
S	-0.161916	1.601569	0.011242
N	3.126547	-0.356597	0.009543
C	-0.350403	-0.148815	-0.003521
C	0.655072	-1.051986	-0.012853
C	2.016548	-0.678636	0.001914
H	0.437308	-2.110497	-0.041709
H	-1.873141	-1.910659	0.164177
H	1.178921	1.603923	-0.128368

Molecule# 1527

3,3,3-trifluoropropene

PointGroup: Cs

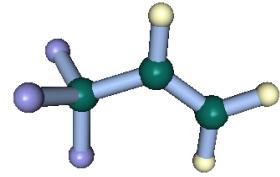
E= -415.807201479 au

ZPE= 0.056984 au

LUMO_eps= -0.04474 au

HOMO_eps= -0.31640 au

Dipole= 2.518 debye



9

C	0.296563	-2.092194	0.000000
H	1.369761	-1.964827	0.000000
H	-0.086440	-3.102651	0.000000
C	-0.524953	-1.056203	0.000000
H	-1.601322	-1.166159	0.000000
C	-0.061543	0.365426	0.000000
F	1.278529	0.488309	0.000000
F	-0.524953	1.029816	1.084366
F	-0.524953	1.029816	-1.084366

Molecule# 1528

3,3,3-trimethoxypropanenitrile

PointGroup: C1

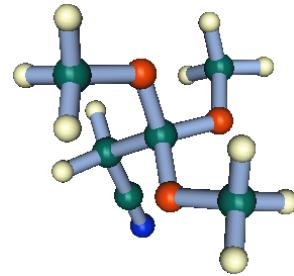
E= -515.838609665 au

ZPE= 0.171385 au

LUMO_eps= -0.01954 au

HOMO_eps= -0.29563 au

Dipole= 4.960 debye



21

C	2.151772	-0.572496	-0.560545
C	-2.062713	-0.100817	-1.587752
C	0.451205	2.241234	0.698532
C	-1.313679	-1.261876	1.680440
C	0.859422	-0.182791	-1.105501
C	-0.223077	0.034236	-0.014933
N	3.188160	-0.864297	-0.158479
O	-1.377593	0.628217	-0.574436
O	0.199911	0.871969	1.008392
O	-0.475157	-1.218770	0.519329
H	-2.222341	-1.139012	-1.294351
H	-1.527238	-0.071217	-2.540553
H	-3.024533	0.389798	-1.715392
H	1.291753	2.348187	0.008318
H	0.717315	2.710667	1.641691
H	-0.432534	2.723319	0.283632
H	-2.243086	-0.715593	1.516465
H	-0.797455	-0.851306	2.545921
H	-1.529699	-2.314243	1.843635
H	0.519543	-0.961831	-1.786348
H	0.976294	0.735039	-1.681386

Molecule# 1529

3,4-dichloro-2(5H)-furanone

PointGroup: C1

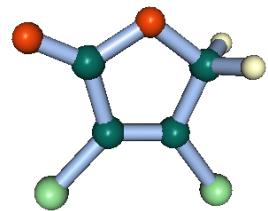
E= -1224.643643630 au

ZPE= 0.055941 au

LUMO_eps= -0.07797 au

HOMO_eps= -0.28804 au

Dipole= 4.119 debye



10

C1	2.402272	-0.042853	0.000005
C1	-0.367556	2.071610	-0.000009
O	-1.150299	-1.778024	0.000004
O	-2.691642	-0.125824	-0.000006
C	0.277438	-1.865987	0.000008
C	0.741846	-0.443903	0.000003
C	-0.314842	0.367425	-0.000002
C	-1.548384	-0.464123	-0.000002
H	0.604505	-2.409285	-0.888461
H	0.604501	-2.409278	0.888482

Molecule# 1530

3,4-dichloropyridazine

PointGroup: Cs

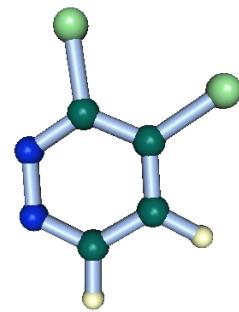
E= -1183.642579640 au

ZPE= 0.056717 au

LUMO_eps= -0.08710 au

HOMO_eps= -0.26939 au

Dipole= 3.665 debye



10

C1	-1.455409	-1.648364	0.000000
C1	-1.486903	1.583880	0.000000
N	1.107307	1.406825	0.000000
N	2.295689	0.818349	0.000000
C	-0.000224	-0.713003	0.000000
C	1.231764	-1.327063	0.000000
C	0.000000	0.689684	0.000000
C	2.356394	-0.507545	0.000000
H	1.317692	-2.403602	0.000000
H	3.353030	-0.928842	0.000000

Molecule# 1531

3,4-difluoro-2,3-dihydro-1,3-thiazole

PointGroup: C1

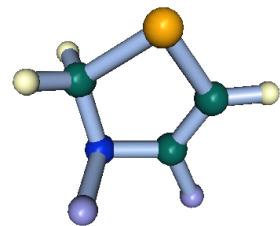
E= -768.822937829 au

ZPE= 0.060595 au

LUMO_eps= -0.07213 au

HOMO_eps= -0.24205 au

Dipole= 2.878 debye



10

S	-1.754466	-0.335189	-0.197249
F	1.013789	1.522561	-0.771068
F	2.045030	-1.036519	0.178958
N	0.632941	0.772412	0.482854
C	0.799133	-0.571033	0.149039
C	-0.780143	1.004087	0.668274
C	-0.280485	-1.267924	-0.221740
H	-0.988442	0.907291	1.731910
H	-1.050908	1.989954	0.309837
H	-0.280179	-2.306271	-0.510189

Molecule# 1532

3,4-difluorofuran

PointGroup: C1

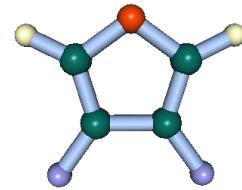
E= -428.641496724 au

ZPE= 0.054142 au

LUMO_eps= -0.02381 au

HOMO_eps= -0.25561 au

Dipole= 1.592 debye



9

F	1.398463	1.484940	-0.000003
F	1.398463	-1.484940	-0.000003
O	-1.779157	0.000000	0.000004
C	0.314030	0.712057	0.000000
C	0.314030	-0.712057	0.000000
C	-0.981873	1.104503	0.000002
C	-0.981873	-1.104503	0.000002
H	-1.462488	2.064029	0.000004
H	-1.462488	-2.064029	0.000003

Molecule# 1533

3,4-dihydro-2H-pyran

PointGroup: C1

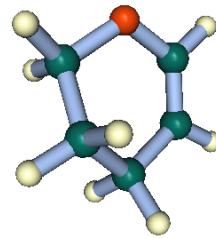
E= -270.649934051 au

ZPE= 0.122160 au

LUMO_eps= -0.01284 au

HOMO_eps= -0.22386 au

Dipole= 1.417 debye



14

H	1.698238	1.800485	-0.192826
C	0.918237	1.060294	-0.079962
H	-0.642305	2.415460	0.088334
C	-0.370105	1.369715	0.059818
H	-2.282342	0.596748	-0.513812
H	-1.850400	0.242473	1.140159
C	-1.442186	0.317252	0.126593
H	-0.784776	-1.061303	-1.405706
H	-1.516006	-1.859353	-0.019166
C	-0.868229	-1.033211	-0.317152
H	0.970892	-2.166720	-0.038422
H	0.456412	-1.234431	1.379263
C	0.514350	-1.233647	0.285501
O	1.429736	-0.201972	-0.110826

Molecule# 1534

3,4-dihydro-2H-pyrrol-2-ol

PointGroup: C1

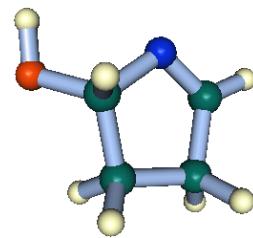
E= -286.706590784 au

ZPE= 0.109343 au

LUMO_eps= -0.02125 au

HOMO_eps= -0.27385 au

Dipole= 2.054 debye

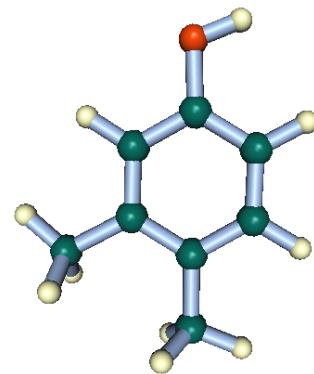


13

O	1.940466	0.100077	-0.356377
H	2.421588	-0.726471	-0.237956
N	0.023471	-1.215094	0.138296
C	-1.181592	-0.930797	-0.131038
H	-1.898279	-1.715924	-0.357940
C	0.758775	0.029689	0.415101
H	1.011317	0.022646	1.482130
C	-1.554766	0.529531	-0.103113
H	-2.214713	0.732484	0.745109
H	-2.099834	0.828700	-0.999730
C	-0.174244	1.197650	0.045596
H	-0.160808	1.988315	0.792056
H	0.163676	1.618849	-0.900003

Molecule# 1535
3,4-dimethylphenol
PointGroup: Cs

E= -386.251759875 au
ZPE= 0.159425 au
LUMO_eps= -0.01403 au
HOMO_eps= -0.22143 au
Dipole= 1.091 debye



19

C	1.129792	-1.107674	0.000000
C	-0.086067	-1.782624	0.000000
C	-1.216225	0.338498	0.000000
C	1.202373	0.281815	0.000000
C	0.000000	1.013650	0.000000
C	-1.265989	-1.051728	0.000000
C	2.538691	0.976753	0.000000
C	0.014913	2.519608	0.000000
O	-2.504718	-1.638916	0.000000
H	2.046577	-1.683971	0.000000
H	-0.110692	-2.865937	0.000000
H	-2.147731	0.888906	0.000000
H	2.663768	1.616923	0.876838
H	3.353135	0.253692	0.000000
H	2.663768	1.616923	-0.876838
H	-0.996299	2.922450	0.000000
H	0.534083	2.914310	0.876468
H	0.534083	2.914310	-0.876468
H	-2.407882	-2.596061	0.000000

Molecule# 1536

3,4-dimethylpyridine

PointGroup: Cs

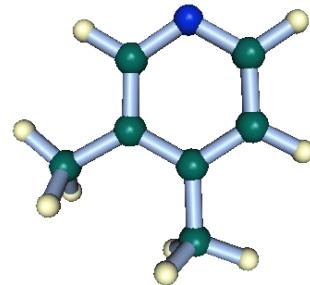
E= -327.040742256 au

ZPE= 0.143567 au

LUMO_eps= -0.03119 au

HOMO_eps= -0.25735 au

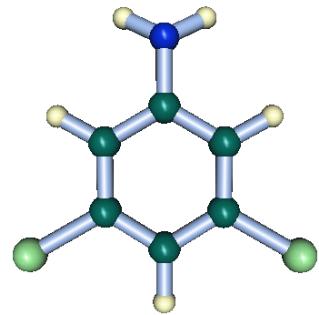
Dipole= 3.003 debye



17

C	0.121338	-1.552985	0.000000
C	-1.266480	-1.587989	0.000000
C	-1.384777	0.677563	0.000000
C	0.784658	-0.329802	0.000000
C	0.000000	0.833406	0.000000
C	2.286145	-0.262994	0.000000
C	0.610891	2.207110	0.000000
N	-2.022279	-0.492366	0.000000
H	0.683596	-2.478145	0.000000
H	-1.790838	-2.537250	0.000000
H	-2.015999	1.561189	0.000000
H	2.660028	0.271394	0.876276
H	2.724758	-1.259274	0.000000
H	2.660028	0.271394	-0.876276
H	1.242218	2.367833	-0.877127
H	-0.160709	2.975727	0.000000
H	1.242218	2.367833	0.877127

Molecule# 1537
 3,5-dichloroaniline
 PointGroup: Cs
 E= -1206.981645910 au
 ZPE= 0.097677 au
 LUMO_eps= -0.03611 au
 HOMO_eps= -0.23356 au
 Dipole= 3.351 debye



14			
C	-0.002611	-1.733711	0.000000
C	-0.002408	-1.024146	1.207301
C	-0.002408	0.359331	1.183235
C	-0.002586	1.085107	0.000000
C	-0.002408	0.359331	-1.183235
C	-0.002408	-1.024146	-1.207301
N	-0.060193	-3.118911	0.000000
H	-0.007345	-1.548683	2.151914
Cl	0.000346	1.229076	2.704581
H	-0.002009	2.162516	0.000000
Cl	0.000346	1.229076	-2.704581
H	-0.007345	-1.548683	-2.151914
H	0.257626	-3.575977	-0.838380
H	0.257626	-3.575977	0.838380

Molecule# 1538

3,5-difluoro-2-pyridinecarbonitrile

PointGroup: C1

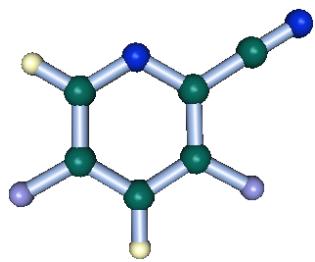
E= -539.191104344 au

ZPE= 0.070553 au

LUMO_eps= -0.09473 au

HOMO_eps= -0.29615 au

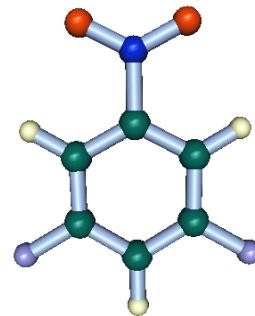
Dipole= 4.760 debye



12

F	-1.107399	1.972598	-0.000008
F	3.142849	-0.010796	0.000001
N	-0.115794	-1.478474	0.000005
N	-3.450688	-0.659364	0.000001
C	-0.881069	-0.381590	0.000001
C	-0.318666	0.896498	-0.000003
C	1.807176	-0.095422	0.000001
C	1.053220	1.060726	-0.000003
C	1.201271	-1.347746	0.000005
C	-2.305482	-0.546687	0.000001
H	1.504868	2.041454	-0.000006
H	1.802744	-2.247483	0.000009

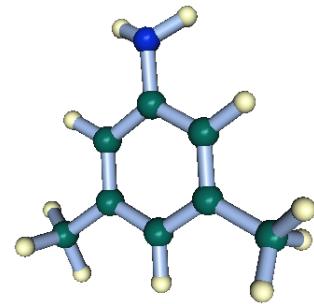
Molecule# 1539
3,5-difluoronitrobenzene
PointGroup: C2
E= -635.466539039 au
ZPE= 0.086259 au
LUMO_eps= -0.12002 au
HOMO_eps= -0.29345 au
Dipole= 2.940 debye



14

F	0.000000	2.343179	-1.982060
F	0.000000	-2.343179	-1.982060
O	0.000003	-1.083137	2.779892
O	-0.000003	1.083137	2.779892
N	0.000000	0.000000	2.217668
C	0.000000	0.000000	0.737023
C	0.000000	1.183547	-1.305000
C	0.000000	-1.183547	-1.305000
C	0.000000	-1.219150	0.077114
C	0.000000	1.219150	0.077114
C	0.000000	0.000000	-2.024499
H	0.000000	-2.150455	0.619296
H	0.000000	2.150455	0.619296
H	0.000000	0.000000	-3.103967

Molecule# 1540
 3,5-dimethylaniline
 PointGroup: C1
 E= -366.379970693 au
 ZPE= 0.171143 au
 LUMO_eps= -0.01499 au
 HOMO_eps= -0.20639 au
 Dipole= 1.257 debye



20

C	2.517544	-1.436630	-0.005275
C	1.212170	-0.683611	0.014104
C	-0.002777	-1.367699	0.003328
C	-1.215431	-0.678269	-0.013052
C	-2.523027	-1.427228	0.013340
C	-1.202251	0.712541	-0.023179
C	0.003078	1.420199	-0.008027
C	1.204894	0.707957	0.012682
N	0.006024	2.814868	-0.071872
H	2.865912	-1.586339	-1.030476
H	2.415107	-2.420997	0.451010
H	3.299264	-0.894762	0.527510
H	-0.005117	-2.450862	0.008225
H	-3.318321	-0.859422	-0.469576
H	-2.839478	-1.624369	1.040910
H	-2.438852	-2.390051	-0.490594
H	-2.138287	1.258871	-0.046205
H	2.143579	1.250287	0.019305
H	0.839819	3.263374	0.270906
H	-0.830989	3.266634	0.258566

Molecule# 1541

3,5-dimethylphenol

PointGroup: C1

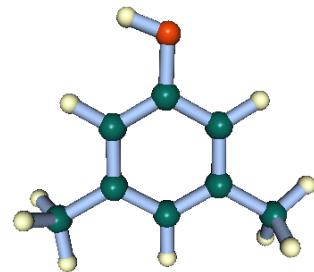
E= -386.253227583 au

ZPE= 0.158880 au

LUMO_eps= -0.01532 au

HOMO_eps= -0.22651 au

Dipole= 1.336 debye



19

C	0.135051	-1.341137	-0.005889
C	-1.264169	0.607942	0.005249
C	1.139570	0.840940	-0.006939
C	-1.138604	-0.783210	0.001330
C	1.282088	-0.540466	-0.008323
C	-0.131706	1.410882	0.000566
C	-2.369752	-1.651925	0.000466
C	2.650233	-1.171347	0.006646
O	-0.202773	2.778770	0.000841
H	0.240904	-2.419111	-0.011504
H	-2.248573	1.063933	0.008732
H	2.003339	1.491882	-0.012720
H	-2.995986	-1.450770	0.871977
H	-2.981562	-1.469036	-0.885355
H	-2.107933	-2.708818	0.013301
H	3.426357	-0.446250	-0.234263
H	2.878024	-1.585952	0.991583
H	2.715992	-1.990403	-0.710787
H	-1.124645	3.054300	0.003665

Molecule# 1542

3,5-dimethylpyridine

PointGroup: C2

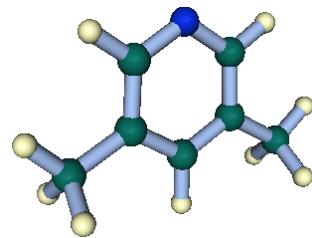
E= -327.040236831 au

ZPE= 0.143091 au

LUMO_eps= -0.03808 au

HOMO_eps= -0.25424 au

Dipole= 2.710 debye



17

C	0.000000	0.000000	-0.952610
C	0.000001	1.139799	1.130184
C	-0.000001	-1.139799	1.130184
C	0.000000	1.209041	-0.263066
C	0.000000	-1.209041	-0.263066
C	-0.000008	2.530903	-0.981213
C	0.000008	-2.530903	-0.981213
N	0.000000	0.000000	1.817942
H	0.000000	0.000000	-2.037504
H	0.000003	2.053289	1.716116
H	-0.000003	-2.053289	1.716116
H	0.000077	3.361966	-0.277021
H	0.878860	2.634607	-1.620442
H	-0.878973	2.634672	-1.620300
H	0.878973	-2.634672	-1.620300
H	-0.000077	-3.361966	-0.277021
H	-0.878860	-2.634607	-1.620442

Molecule# 1543

3,7(lambda^4)-dithia-6,8-diazabicyclo[3.3.0]octa-1,4,6,7-tetraene

PointGroup: C2v

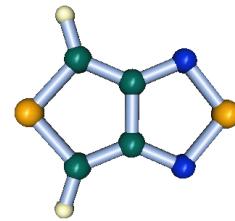
E= -1059.621571040 au

ZPE= 0.056441 au

LUMO_eps= -0.11052 au

HOMO_eps= -0.23274 au

Dipole= 1.602 debye



10

S	0.000000	0.000000	2.365328
S	0.000000	0.000000	-2.307684
N	0.000000	1.264006	-1.291328
N	0.000000	-1.264006	-1.291328
C	0.000000	0.729665	-0.053183
C	0.000000	-0.729665	-0.053183
C	0.000000	1.267958	1.226307
C	0.000000	-1.267958	1.226307
H	0.000000	2.296156	1.539395
H	0.000000	-2.296156	1.539395

Molecule# 1544

3H-1,2-dithiole-3-carboxylic acid

PointGroup: C1

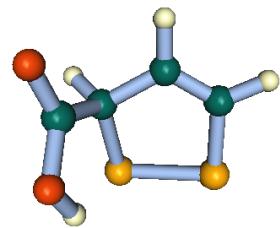
E= -1101.839263670 au

ZPE= 0.077328 au

LUMO_eps= -0.08132 au

HOMO_eps= -0.23225 au

Dipole= 3.200 debye



12

S	-0.671855	-1.153928	0.660705
S	-2.102626	-0.073495	-0.487708
O	2.806302	0.706910	0.014558
O	1.840814	-1.023297	-0.999049
C	0.592505	0.197419	0.742618
C	1.861261	-0.020299	-0.114890
C	-0.080754	1.484200	0.342170
C	-1.272181	1.455845	-0.241430
H	0.997209	-1.505143	-0.912903
H	0.933145	0.237738	1.777666
H	0.468066	2.404340	0.484590
H	-1.788640	2.329941	-0.612187

Molecule# 1545

3H-1,2-dithiole-4,5-dicarbonitrile

PointGroup: C1

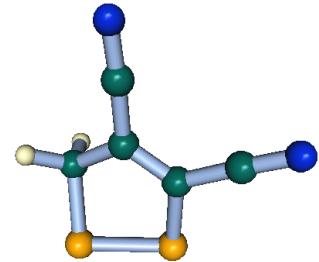
E= -1097.734168050 au

ZPE= 0.059902 au

LUMO_eps= -0.12355 au

HOMO_eps= -0.25614 au

Dipole= 5.143 debye



11

S	-1.222640	1.296701	0.169140
S	-2.161882	-0.546051	-0.275063
N	2.326633	2.291015	-0.116594
N	2.731829	-2.027823	-0.080487
C	0.395120	0.601936	0.030052
C	0.511175	-0.743969	0.062000
C	-0.745707	-1.549818	0.310030
C	1.476896	1.515274	-0.054572
C	1.752199	-1.421097	-0.020140
H	-0.759980	-2.475318	-0.261951
H	-0.835001	-1.791373	1.372058

Molecule# 1546

3H-1,2-dithiolene

PointGroup: C1

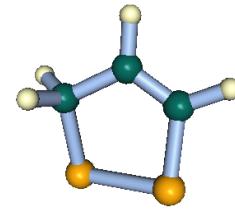
E= -913.197043473 au

ZPE= 0.062469 au

LUMO_eps= -0.05606 au

HOMO_eps= -0.20697 au

Dipole= 2.282 debye



9

S	1.327006	-0.375637	0.105858
S	-0.627900	-1.176631	-0.128471
C	0.766846	1.280061	-0.119461
C	-1.496295	0.415715	0.204467
C	-0.535996	1.534602	-0.083959
H	1.537200	2.027810	-0.243628
H	-1.848317	0.454829	1.239330
H	-2.365633	0.428755	-0.452364
H	-0.916283	2.542633	-0.187804

Molecule# 1547

3H-1,2,3-oxathiazole

PointGroup: C1

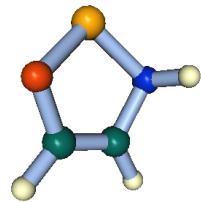
E= -606.219773707 au

ZPE= 0.053377 au

LUMO_eps= -0.05464 au

HOMO_eps= -0.21468 au

Dipole= 1.921 debye



8

S	-1.154148	-0.066919	-0.130433
O	0.068806	-1.262764	0.214972
N	-0.111862	1.263970	0.119104
C	1.205240	0.713893	-0.140345
C	1.248577	-0.612642	-0.043800
H	2.033948	1.375479	-0.327363
H	-0.169651	1.597164	1.080067
H	2.111755	-1.255125	-0.114406

Molecule# 1548

3H-1,2,4-dithiazole

PointGroup: C1

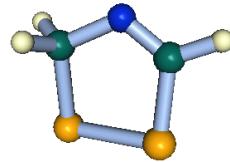
E= -929.251181905 au

ZPE= 0.051166 au

LUMO_eps= -0.06485 au

HOMO_eps= -0.22199 au

Dipole= 0.686 debye



8

S	1.295602	-0.412017	0.082747
S	-0.664803	-1.162627	-0.093069
N	-0.479291	1.584298	-0.083568
C	0.738128	1.267662	-0.100668
C	-1.435059	0.543003	0.155054
H	1.524832	2.007293	-0.203172
H	-2.263985	0.603202	-0.546612
H	-1.817015	0.629721	1.173604

Molecule# 1549

3H-diazirine

PointGroup: C2v

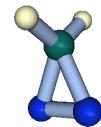
E= -148.775979394 au

ZPE= 0.033258 au

LUMO_eps= -0.07744 au

HOMO_eps= -0.28595 au

Dipole= 1.714 debye



5

C 0.000000 0.000000 0.808471

N 0.000000 0.607849 -0.539787

N 0.000000 -0.607849 -0.539787

H 0.931674 0.000000 1.353097

H -0.931674 0.000000 1.353097

Molecule# 1550

3H-dithiazole

PointGroup: C1

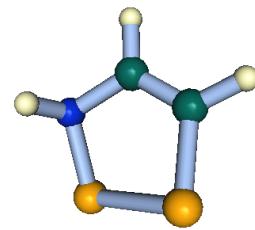
E= -929.225411389 au

ZPE= 0.050943 au

LUMO_eps= -0.06507 au

HOMO_eps= -0.20860 au

Dipole= 1.998 debye



8

S	-0.665329	-1.105340	-0.182687
S	1.328505	-0.380755	0.146421
N	-1.448431	0.367384	0.222713
C	0.727116	1.257202	-0.172811
C	-0.585503	1.466416	-0.095672
H	-1.727963	0.395573	1.201544
H	1.454698	2.032027	-0.360302
H	-1.048226	2.436538	-0.209095

Molecule# 1551

3H,1,2,4-dioxazole

PointGroup: C1

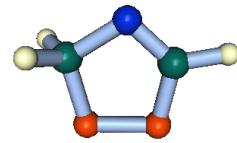
E= -283.210364590 au

ZPE= 0.055764 au

LUMO_eps= -0.03401 au

HOMO_eps= -0.26169 au

Dipole= 0.689 debye



8

O	0.891155	-0.824592	0.000333
O	-0.557923	-1.054738	-0.000461
N	-0.044878	1.222226	-0.000283
C	1.000131	0.519722	-0.000070
C	-1.143632	0.283846	0.000324
H	2.022843	0.872053	-0.000125
H	-1.756107	0.392727	0.898645
H	-1.757438	0.392866	-0.897042

Molecule# 1552

3H,1,2,4-dithiazol-3-amine

PointGroup: C1

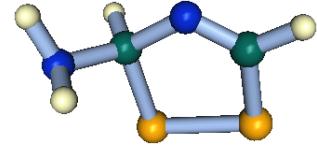
E= -984.630972058 au

ZPE= 0.068079 au

LUMO_eps= -0.05553 au

HOMO_eps= -0.22220 au

Dipole= 1.670 debye



10

S	-0.028479	-1.298792	0.113208
S	-1.706091	-0.067083	-0.155054
N	0.494117	1.411130	0.230341
N	2.316910	-0.066084	-0.430930
C	1.182581	0.157135	0.412230
C	-0.739922	1.410171	-0.021635
H	2.101161	0.113195	-1.403505
H	3.105494	0.503334	-0.149239
H	1.509307	0.087909	1.449130
H	-1.295978	2.330405	-0.166289

Molecule# 1553

4-(2-methyl-2-propanyl)phenol

PointGroup: Cs

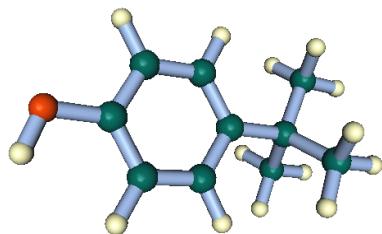
E= -464.899950093 au

ZPE= 0.216298 au

LUMO_eps= -0.01721 au

HOMO_eps= -0.22517 au

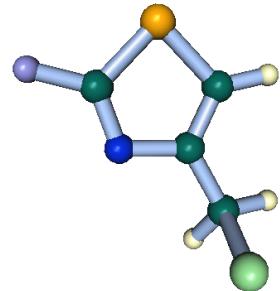
Dipole= 1.341 debye



25

C	-1.115443	-0.498903	0.000000
C	1.250967	-0.260855	0.000000
C	-0.986607	-1.880476	0.000000
C	1.399896	-1.643053	0.000000
C	-0.004568	0.350470	0.000000
C	0.278520	-2.460677	0.000000
C	-0.986607	2.295203	1.257771
C	-0.986607	2.295203	-1.257771
C	1.138805	2.629595	0.000000
C	-0.198372	1.873754	0.000000
O	0.472057	-3.816729	0.000000
H	-2.113690	-0.082584	0.000000
H	2.147758	0.340453	0.000000
H	-1.871422	-2.506840	0.000000
H	2.382431	-2.094241	0.000000
H	-1.134610	3.376937	1.269176
H	-1.969239	1.825058	1.295308
H	-0.449010	2.016368	2.165116
H	-1.969239	1.825058	-1.295308
H	-1.134610	3.376937	-1.269176
H	-0.449010	2.016368	-2.165116
H	0.952247	3.704407	0.000000
H	1.735409	2.400064	0.883926
H	1.735409	2.400064	-0.883926
H	-0.378786	-4.265777	0.000000

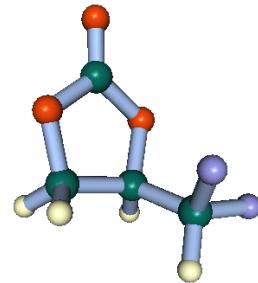
Molecule# 1554
 4-(chloromethyl)-2-fluoro-1,3-thiazole
 PointGroup: C1
 E= -1167.385546180 au
 ZPE= 0.066378 au
 LUMO_eps= -0.05496 au
 HOMO_eps= -0.26877 au
 Dipole= 3.352 debye



11

C1	-2.893971	-0.323448	-0.516915
S	1.947247	0.982404	-0.300395
F	2.454522	-1.612150	-0.075441
N	0.331438	-0.906310	0.410222
C	-0.387056	0.275290	0.443852
C	1.530280	-0.673246	0.042767
C	0.310052	1.391096	0.099770
C	-1.816007	0.247130	0.843769
H	-0.036503	2.408900	0.047814
H	-2.175019	1.233905	1.114544
H	-1.981283	-0.450741	1.657975

Molecule# 1555
 4-(difluoromethyl)-1,3-dioxolan-2-one
 PointGroup: C1
 E= -580.422747684 au
 ZPE= 0.087627 au
 LUMO_eps= -0.03042 au
 HOMO_eps= -0.32045 au
 Dipole= 6.191 debye



13

F	-1.348626	-0.049956	1.364939
F	-2.375705	-0.844928	-0.412965
O	0.433224	-0.723724	-0.682853
O	1.618313	0.882499	0.312093
O	2.419188	-1.228012	0.268661
C	-0.406254	0.422707	-0.759710
C	1.578879	-0.436900	0.000770
C	-1.668924	0.213355	0.065480
C	0.485739	1.562976	-0.229668
H	-0.703392	0.567543	-1.797832
H	-2.315882	1.094850	0.045598
H	0.016202	2.142547	0.562716
H	0.819614	2.230086	-1.022680

Molecule# 1556

4-(difluoromethyl)-2-ethynyl-5H-isoxazole

PointGroup: C1

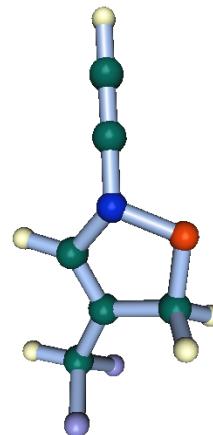
E= -561.350131560 au

ZPE= 0.101320 au

LUMO_eps= -0.03472 au

HOMO_eps= -0.22388 au

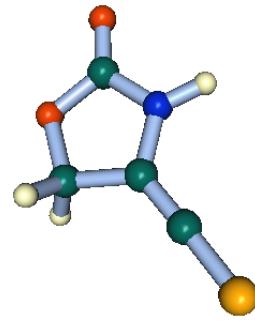
Dipole= 2.127 debye



15

F	-2.610592	-0.327834	1.201239
F	-2.811525	-0.037318	-0.964662
O	1.182464	1.333129	0.117243
N	1.584817	0.016648	-0.354989
C	-0.642997	-0.097857	-0.059740
C	0.463626	-0.798090	-0.297934
C	-2.016538	-0.627408	-0.004321
C	-0.262774	1.356137	0.055783
C	2.824717	-0.333007	-0.014553
C	3.962621	-0.634351	0.227184
H	0.589733	-1.853786	-0.474588
H	-2.071144	-1.706782	-0.144639
H	-0.624227	1.838730	0.964570
H	-0.584651	1.938157	-0.814947
H	4.963978	-0.904064	0.448868

Molecule# 1557
4-(thioxomethylene)-1,3-oxazolidin-2-one
PointGroup: C1
E= -757.752806566 au
ZPE= 0.070135 au
LUMO_eps= -0.11719 au
HOMO_eps= -0.22056 au
Dipole= 3.225 debye



11

S	-3.117372	-0.219151	-0.000042
O	1.880210	1.021564	-0.000017
O	3.047958	-0.924185	0.000000
N	0.735994	-0.877231	0.000067
C	-0.262689	0.101627	0.000020
C	2.003640	-0.340666	0.000015
C	0.502611	1.419673	0.000015
C	-1.560452	-0.063026	-0.000009
H	0.587091	-1.870027	0.000039
H	0.307433	2.016200	-0.890818
H	0.307471	2.016180	0.890870

Molecule# 1558

4-amino-1,2-thiazole-5-carbonitrile

PointGroup: C1

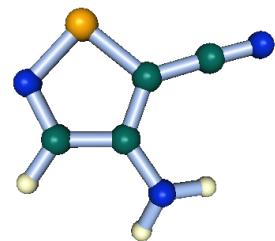
E= -716.798425218 au

ZPE= 0.070447 au

LUMO_eps= -0.08138 au

HOMO_eps= -0.24718 au

Dipole= 4.091 debye



11

S	0.849093	-1.404452	-0.001478
N	2.043738	-0.263167	0.010200
N	-0.588772	2.219969	-0.067972
N	-2.942184	-0.775655	0.010632
C	-0.440552	-0.233849	-0.006414
C	0.105987	1.037713	-0.005426
C	1.531170	0.941099	0.004087
C	-1.808893	-0.550499	-0.000160
H	-0.122155	3.047725	0.260526
H	-1.574094	2.192039	0.137048
H	2.195028	1.796650	0.003525

Molecule# 1559

4-amino-1,3-thiazole-5-carbonitrile

PointGroup: C1

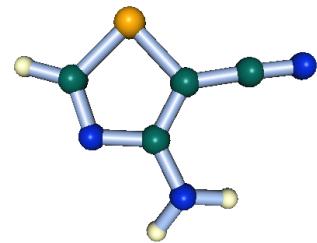
E= -716.811253277 au

ZPE= 0.070619 au

LUMO_eps= -0.07219 au

HOMO_eps= -0.23986 au

Dipole= 3.657 debye



11

S	-0.844455	-1.432131	-0.001735
N	-1.485615	1.063138	0.005370
N	0.565464	2.204052	-0.054581
N	2.937529	-0.771304	0.008341
C	-0.117671	1.028945	-0.005236
C	0.435762	-0.243451	-0.005215
C	-1.980824	-0.136886	0.007729
C	1.800797	-0.558509	-0.000399
H	-3.040901	-0.340536	0.015885
H	0.051496	3.036922	0.173244
H	1.550661	2.205914	0.143440

Molecule# 1560

4-amino-3-chloro-5-hydroxy-2(5H)-furanone

PointGroup: C1

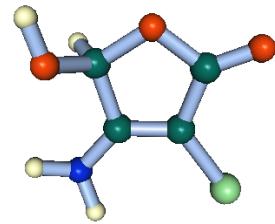
E= -895.663755234 au

ZPE= 0.086704 au

LUMO_eps= -0.05396 au

HOMO_eps= -0.25018 au

Dipole= 6.283 debye



13

C1	-2.280642	-0.628707	-0.145550
O	1.092025	1.391278	0.220496
O	-0.955684	2.323645	-0.050493
O	2.553373	-0.218210	-0.655230
N	0.574476	-2.183960	0.238082
C	-0.663800	-0.075616	0.058842
C	0.431472	-0.842507	0.189010
C	-0.290734	1.338463	0.058027
C	1.619020	0.075759	0.341980
H	3.324738	0.348497	-0.543164
H	-0.217906	-2.752537	-0.012740
H	1.479328	-2.567370	0.021871
H	2.069968	-0.003146	1.336481

Molecule# 1561

4-bromo-1-methyl-1H-1,2,3-triazole

PointGroup: C1

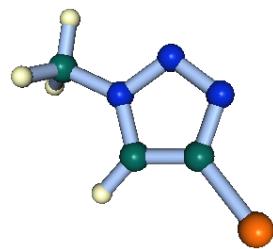
E= -2855.265054000 au

ZPE= 0.076450 au

LUMO_eps= -0.03334 au

HOMO_eps= -0.26043 au

Dipole= 5.099 debye



11

Br	-1.940021	-0.130890	0.000013
N	2.047656	-0.135415	-0.000005
N	1.787271	1.183026	-0.000054
N	0.493084	1.336424	-0.000054
C	0.900174	-0.848615	0.000028
C	3.420046	-0.607084	0.000012
C	-0.078964	0.114124	-0.000004
H	0.863908	-1.921772	0.000069
H	3.616542	-1.202920	-0.889841
H	4.060128	0.269835	-0.000059
H	3.616565	-1.202793	0.889946

Molecule# 1562

4-bromo-1,2-thiazole

PointGroup: Cs

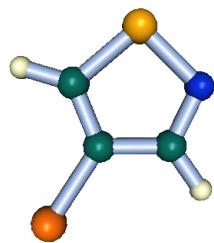
E= -3142.767754390 au

ZPE= 0.045043 au

LUMO_eps= -0.06050 au

HOMO_eps= -0.26436 au

Dipole= 1.446 debye



8

Br	-1.244668	-1.381034	0.000000
S	2.057420	1.464213	0.000000
N	0.605990	2.281940	0.000000
C	0.000000	0.045842	0.000000
C	1.355837	-0.098699	0.000000
C	-0.377613	1.415359	0.000000
H	1.933457	-1.006977	0.000000
H	-1.400074	1.767181	0.000000

Molecule# 1563

4-bromo-1,3-dioxolan-2-one

PointGroup: C1

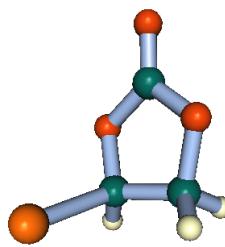
E= -2916.164183630 au

ZPE= 0.064630 au

LUMO_eps= -0.05187 au

HOMO_eps= -0.30870 au

Dipole= 4.579 debye



10

Br	-1.679281	-0.222549	-0.171503
O	0.904198	-0.596180	0.859473
O	1.724404	0.868550	-0.607082
O	2.767002	-1.118360	-0.322274
C	-0.059419	0.412716	0.795866
C	1.898097	-0.357530	-0.066646
C	0.648879	1.543670	0.054380
H	-0.412430	0.651047	1.790346
H	1.064262	2.270895	0.754952
H	0.032846	2.042043	-0.685213

Molecule# 1564

4-bromo-1,3-thiazole

PointGroup: C1

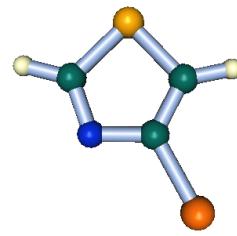
E= -3142.772036880 au

ZPE= 0.044963 au

LUMO_eps= -0.05552 au

HOMO_eps= -0.25749 au

Dipole= 2.503 debye



8

Br	1.848237	-0.043396	-0.000002
S	-2.496229	-0.509277	0.000004
N	-0.646434	1.272501	-0.000002
C	-0.042288	0.052832	0.000000
C	-0.854899	-1.038080	0.000003
C	-1.936788	1.132192	0.000000
H	-0.587694	-2.079025	0.000005
H	-2.632061	1.957134	-0.000001

Molecule# 1565

4-bromo-1,4-dihydro-1,2,3-triazine

PointGroup: C1

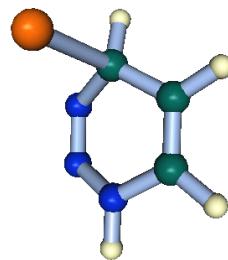
E= -2855.237123200 au

ZPE= 0.077226 au

LUMO_eps= -0.07319 au

HOMO_eps= -0.25384 au

Dipole= 4.999 debye



11

Br	1.581452	-0.005498	-0.231010
N	-0.815865	-1.152029	0.820491
N	-1.695128	-1.287808	-0.054949
N	-2.067917	-0.198682	-0.791747
C	-0.130345	0.114237	0.970519
C	-0.928850	1.276706	0.603133
C	-1.865214	1.081753	-0.335199
H	-2.826799	-0.411009	-1.416720
H	0.341662	0.149095	1.940961
H	-0.758833	2.240031	1.056350
H	-2.508024	1.847756	-0.742521

Molecule# 1566

4-bromo-1H-imidazol-5-amine

PointGroup: C1

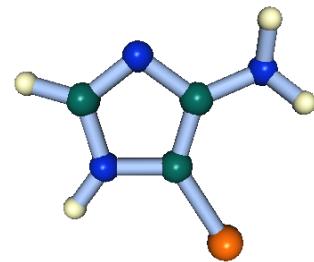
E= -2855.309401400 au

ZPE= 0.077854 au

LUMO_eps= -0.01941 au

HOMO_eps= -0.20595 au

Dipole= 2.132 debye



11

Br	1.654489	-0.043411	-0.000256
N	-0.844475	-1.454312	0.006560
N	-2.428718	0.083865	-0.001573
N	-1.121691	2.096676	-0.082186
C	-0.212074	-0.222400	-0.003153
C	-1.212764	0.716064	-0.008737
C	-2.175221	-1.206191	0.006024
H	-0.387701	-2.348953	0.012452
H	-1.957262	2.559042	0.241182
H	-0.284725	2.491263	0.317113
H	-2.912900	-1.990420	0.013814

Molecule# 1567

4-bromophenol

PointGroup: Cs

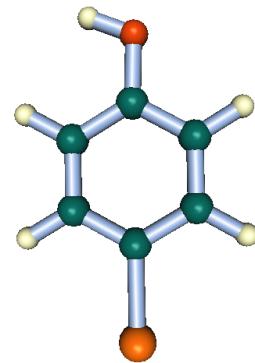
E= -2881.215385130 au

ZPE= 0.094370 au

LUMO_eps= -0.03521 au

HOMO_eps= -0.23522 au

Dipole= 2.299 debye



13

C	1.224864	-1.755744	0.000000
C	-1.184580	-1.776314	0.000000
C	1.212391	-0.368570	0.000000
C	-1.199101	-0.386210	0.000000
C	0.025862	-2.463626	0.000000
C	0.000000	0.309383	0.000000
O	0.100361	-3.827816	0.000000
Br	-0.015329	2.222061	0.000000
H	2.158827	-2.299537	0.000000
H	-2.120681	-2.321643	0.000000
H	2.142842	0.179709	0.000000
H	-2.139593	0.144523	0.000000
H	-0.784392	-4.206178	0.000000

Molecule# 1568

4-chloro-1-butene

PointGroup: C1

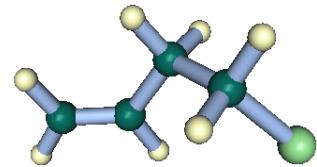
E= -616.917432420 au

ZPE= 0.099769 au

LUMO_eps= -0.01674 au

HOMO_eps= -0.27434 au

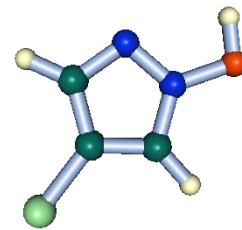
Dipole= 2.023 debye



12

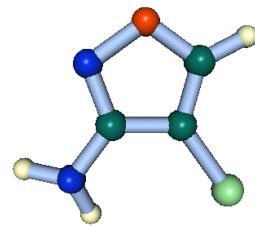
H	3.260702	-1.294214	-0.401232
C	1.438044	-0.423931	0.191330
H	3.206899	0.548451	-0.421234
C	2.695041	-0.387967	-0.232098
H	0.306468	0.824211	1.506818
C	0.591287	0.786117	0.451638
H	-1.211253	1.787841	-0.217654
H	-0.463260	0.753418	-1.450887
C	-0.675702	0.859133	-0.390868
H	0.963360	-1.382561	0.370238
H	1.169489	1.691325	0.243452
Cl	-1.854378	-0.466387	0.014735

Molecule# 1569
4-chloro-1-hydroxy-pyrazole
PointGroup: C1
E= -761.108333688 au
ZPE= 0.064500 au
LUMO_eps= -0.01765 au
HOMO_eps= -0.24970 au
Dipole= 1.350 debye



10
C1 2.401410 -0.258167 -0.000042
O -2.704169 -0.697729 0.000040
N -1.435056 -0.167750 0.000025
N -1.265034 1.139232 0.000023
C 0.703455 0.056232 -0.000012
C -0.307179 -0.895635 0.000004
C 0.067053 1.299981 0.000002
H -3.268039 0.091657 0.000098
H -0.301932 -1.969154 0.000002
H 0.500000 2.284319 -0.000003

Molecule# 1570
4-chloro-1,2-oxazol-3-amine
PointGroup: C1
E= -761.140901736 au
ZPE= 0.065393 au
LUMO_eps= -0.03188 au
HOMO_eps= -0.25545 au
Dipole= 2.181 debye



10
C1 2.032090 -0.194629 -0.000258
O -1.737574 -1.136233 0.004416
N -1.857611 0.269811 0.007343
N -0.338436 2.066229 -0.073485
C 0.315301 -0.344216 -0.003266
C -0.628792 0.728757 -0.004720
C -0.442310 -1.462994 0.002464
H 0.555469 2.341498 0.298227
H -1.096227 2.686160 0.162543
H -0.197051 -2.510661 0.004428

Molecule# 1571

4-chloro-1,2-thiazole-5-carbaldehyde

PointGroup: Cs

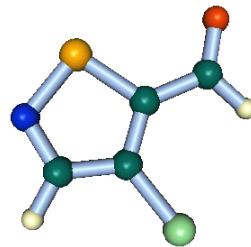
E= -1142.135885030 au

ZPE= 0.054862 au

LUMO_eps= -0.11354 au

HOMO_eps= -0.28473 au

Dipole= 2.403 debye



10

C1	1.997780	-1.371459	0.000000
S	-1.725995	0.605097	0.000000
O	0.396341	2.866951	0.000000
N	-1.923957	-1.041509	0.000000
C	0.000000	0.542410	0.000000
C	0.370267	-0.782870	0.000000
C	-0.756625	-1.641068	0.000000
C	0.840877	1.741435	0.000000
H	-0.703404	-2.720895	0.000000
H	1.926917	1.549668	0.000000

Molecule# 1572

4-chloro-1,2,3-oxathiazolidine

PointGroup: C1

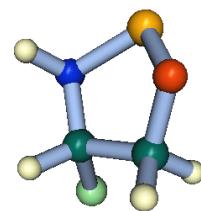
E= -1067.087797870 au

ZPE= 0.068414 au

LUMO_eps= -0.04599 au

HOMO_eps= -0.24026 au

Dipole= 2.138 debye



10

C1	2.146887	-0.158355	-0.305057
S	-1.585845	-0.628523	-0.400452
O	-1.548273	1.014367	0.043950
N	-0.277672	-1.009832	0.627787
C	0.609969	0.131067	0.637735
C	-0.158865	1.344018	0.027468
H	-0.595129	-1.227421	1.564642
H	0.945527	0.317665	1.652134
H	0.182044	1.521159	-0.992647
H	-0.032741	2.240381	0.631744

Molecule# 1573

4-chloro-2-butyn-1-ylthiocyanate

PointGroup: C1

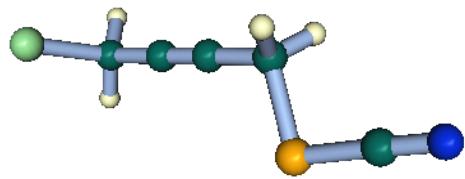
E= -1106.150122170 au

ZPE= 0.076072 au

LUMO_eps= -0.06307 au

HOMO_eps= -0.28153 au

Dipole= 3.896 debye



12

C1	3.790159	-0.565860	-0.387381
S	-2.085317	-0.503553	0.546804
N	-4.695349	-0.036278	-0.498130
C	-1.119696	0.706179	-0.506380
C	2.801833	0.572983	0.637702
C	0.267289	0.664830	-0.108118
C	1.418175	0.614979	0.230597
C	-3.630791	-0.216125	-0.084152
H	-1.553731	1.692329	-0.354795
H	-1.245536	0.411120	-1.546247
H	3.273951	1.547665	0.545309
H	2.904272	0.222241	1.661369

Molecule# 1574

4-chloro-2-butynoic acid

PointGroup: C1

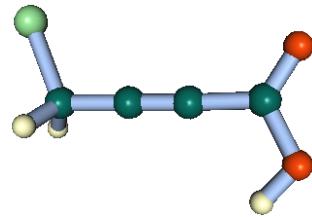
E= -764.972167220 au

ZPE= 0.062748 au

LUMO_eps= -0.06993 au

HOMO_eps= -0.30434 au

Dipole= 5.241 debye



10

C1	2.873531	0.486714	0.000430
O	-2.513569	1.387263	-0.000565
O	-3.095526	-0.762540	-0.000395
C	-2.179793	0.237520	-0.000377
C	-0.799428	-0.203129	-0.000117
C	0.356403	-0.534339	0.000095
C	1.742195	-0.935325	0.000352
H	-2.655104	-1.621927	-0.000224
H	1.980933	-1.519238	-0.885367
H	1.980645	-1.519107	0.886235

Molecule# 1575

4-chloro-3H-1,2-dioxole

PointGroup: C1

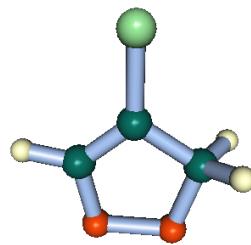
E= -726.772710413 au

ZPE= 0.057604 au

LUMO_eps= -0.03911 au

HOMO_eps= -0.23459 au

Dipole= 1.212 debye



9

C1	2.035348	-0.011575	-0.003987
O	-1.801008	-0.820277	0.011276
O	-1.875262	0.660254	-0.028353
C	0.315681	-0.055902	-0.001214
C	-0.477853	-1.114474	0.001648
C	-0.531551	1.179920	0.019645
H	-0.253678	-2.168788	0.002003
H	-0.374491	1.821150	-0.853262
H	-0.400253	1.767328	0.935181

Molecule# 1576

4-chloro-pyrazole

PointGroup: C1

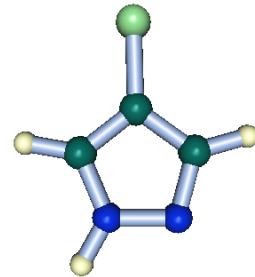
E= -685.915170210 au

ZPE= 0.061846 au

LUMO_eps= -0.01977 au

HOMO_eps= -0.25465 au

Dipole= 2.438 debye



9

C1	-2.003064	-0.016547	-0.000005
N	1.843891	0.756301	0.000005
N	1.813601	-0.586654	0.000004
C	-0.275304	-0.001147	0.000000
C	0.569529	1.124682	0.000002
C	0.559203	-1.094849	0.000001
H	2.680219	-1.094481	0.000006
H	0.296397	2.165829	0.000002
H	0.352459	-2.149705	0.000000

Molecule# 1577

4-chlorodithiolan-3-one

PointGroup: C1

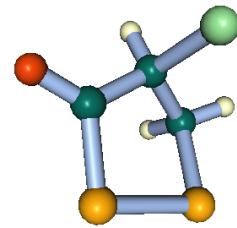
E= -1448.105218900 au

ZPE= 0.058362 au

LUMO_eps= -0.07574 au

HOMO_eps= -0.24442 au

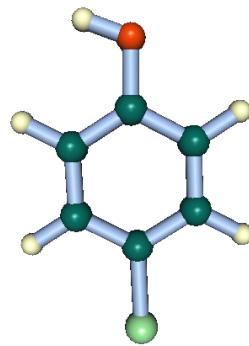
Dipole= 3.244 debye



10

C1	-2.010456	-0.590268	-0.599839
S	1.409201	-1.226558	-0.189113
S	1.477785	0.867297	-0.404520
O	-0.613216	2.315389	0.315501
C	-0.892502	-0.061929	0.726505
C	0.101019	-1.136073	1.098478
C	-0.172173	1.206202	0.240534
H	-1.528841	0.214376	1.562461
H	0.561916	-0.885355	2.054656
H	-0.359432	-2.118613	1.161173

Molecule# 1578
4-chlorophenol
PointGroup: Cs
E= -767.221547391 au
ZPE= 0.094896 au
LUMO_eps= -0.03463 au
HOMO_eps= -0.23600 au
Dipole= 2.268 debye



13

C	1.214937	-1.114720	0.000000
C	-1.194532	-1.123734	0.000000
C	1.208906	0.272121	0.000000
C	-1.202251	0.266088	0.000000
C	0.012562	-1.816947	0.000000
C	0.000000	0.956110	0.000000
O	0.080600	-3.181991	0.000000
Cl	-0.005372	2.710582	0.000000
H	2.146145	-1.663099	0.000000
H	-2.133071	-1.664730	0.000000
H	2.139489	0.820428	0.000000
H	-2.137764	0.805811	0.000000
H	-0.805998	-3.555873	0.000000

Molecule# 1579

4-cyclopentene-1,3-dione

PointGroup: C2v

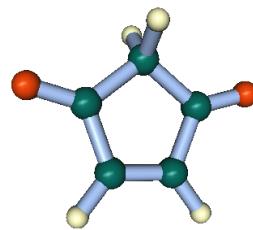
E= -343.493434143 au

ZPE= 0.078515 au

LUMO_eps= -0.11272 au

HOMO_eps= -0.26916 au

Dipole= 1.796 debye



11

C	0.000000	0.000000	1.088734
C	0.000000	1.198351	0.149259
C	0.000000	-1.198351	0.149259
C	0.000000	0.669044	-1.243983
C	0.000000	-0.669044	-1.243983
O	0.000000	2.365037	0.458652
O	0.000000	-2.365037	0.458652
H	0.878958	0.000000	1.734426
H	-0.878958	0.000000	1.734426
H	0.000000	1.326391	-2.101506
H	0.000000	-1.326391	-2.101506

Molecule# 1580

4-ethylphenol

PointGroup: C1

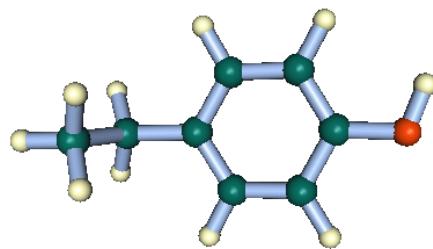
E= -386.248532353 au

ZPE= 0.160413 au

LUMO_eps= -0.01864 au

HOMO_eps= -0.22543 au

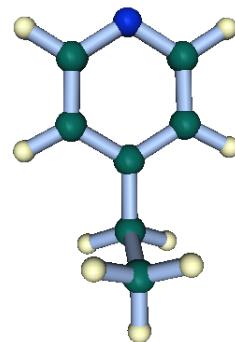
Dipole= 1.318 debye



19

C	0.182296	-1.194600	-0.232278
C	0.200946	1.190822	-0.237286
C	-1.192318	-1.189355	-0.023350
C	-1.170510	1.215647	-0.029025
C	0.907341	-0.009408	-0.342365
C	-1.872642	0.019468	0.080035
C	3.186098	0.002643	0.787434
C	2.404665	-0.021419	-0.533621
O	-3.225765	0.093049	0.281877
H	0.695495	-2.144808	-0.315944
H	0.733105	2.130212	-0.325596
H	-1.733693	-2.125233	0.053648
H	-1.708215	2.150587	0.045495
H	2.948053	0.896107	1.366309
H	4.262069	-0.005627	0.605398
H	2.940274	-0.864143	1.402489
H	2.689551	-0.909460	-1.102288
H	2.698617	0.839070	-1.138965
H	-3.594392	-0.793890	0.337165

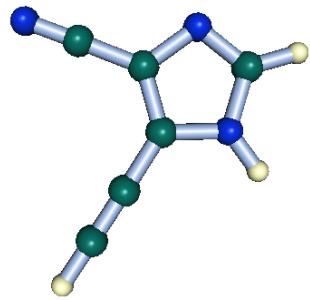
Molecule# 1581
 4-ethylpyridine
 PointGroup: Cs
 E= -327.036817944 au
 ZPE= 0.144593 au
 LUMO_eps= -0.03600 au
 HOMO_eps= -0.26082 au
 Dipole= 2.850 debye



17

C	0.233751	-0.248858	1.186174
C	0.233751	-0.248858	-1.186174
C	0.233751	-1.636587	1.135286
C	0.233751	-1.636587	-1.135286
C	0.232164	0.482399	0.000000
C	-1.236306	2.546240	0.000000
C	0.194870	1.988942	0.000000
N	0.233121	-2.335890	0.000000
H	0.240621	0.255199	2.144492
H	0.240621	0.255199	-2.144492
H	0.238122	-2.214612	2.053040
H	0.238122	-2.214612	-2.053040
H	-1.786360	2.212834	-0.880654
H	-1.225706	3.636797	0.000000
H	-1.786360	2.212834	0.880654
H	0.727349	2.363720	0.876427
H	0.727349	2.363720	-0.876427

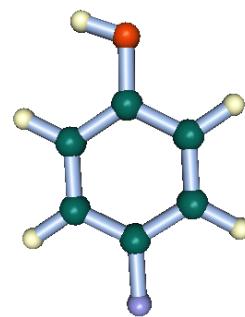
Molecule# 1582
4-ethynyl-1H-imidazole-5-carbonitrile
PointGroup: C1
E= -394.753575151 au
ZPE= 0.078858 au
LUMO_eps= -0.06924 au
HOMO_eps= -0.25848 au
Dipole= 7.189 debye



12

N	-0.276322	-1.723967	0.000021
N	-1.849466	-0.170596	-0.000023
N	-0.289475	2.979967	-0.000049
C	0.394581	-0.521917	0.000012
C	-0.614933	0.430613	-0.000017
C	-1.610732	-1.456201	0.000000
C	1.794759	-0.410634	0.000031
C	-0.446188	1.838684	-0.000036
C	2.991406	-0.303459	0.000049
H	0.162004	-2.629700	0.000046
H	-2.356541	-2.233190	0.000003
H	4.048019	-0.197456	0.000073

Molecule# 1583
4-fluorophenol
PointGroup: Cs
E= -406.865584544 au
ZPE= 0.096185 au
LUMO_eps= -0.03300 au
HOMO_eps= -0.23507 au
Dipole= 2.007 debye



13

C	1.209009	0.686001	0.000000
C	-1.202025	0.675134	0.000000
C	1.216005	-0.701909	0.000000
C	-1.199895	-0.715998	0.000000
C	0.000000	1.377007	0.000000
C	0.010446	-1.381379	0.000000
O	0.057288	2.745374	0.000000
F	0.018013	-2.736527	0.000000
H	2.134342	1.243985	0.000000
H	-2.143868	1.210090	0.000000
H	2.143774	-1.255723	0.000000
H	-2.123419	-1.276673	0.000000
H	-0.832492	3.110943	0.000000

Molecule# 1584

4-heptanone

PointGroup: C2

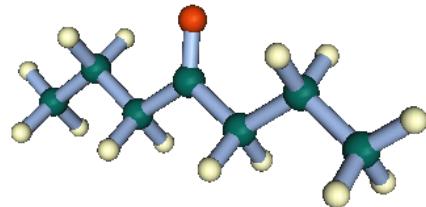
E= -350.548366842 au

ZPE= 0.197113 au

LUMO_eps= -0.02292 au

HOMO_eps= -0.25269 au

Dipole= 2.575 debye



22

C	0.000000	0.000000	0.295876
C	0.000056	3.828834	-0.530290
C	-0.000056	-3.828834	-0.530290
C	0.000000	1.290026	-0.509256
C	0.000000	-1.290026	-0.509256
C	0.000059	2.564624	0.327131
C	-0.000059	-2.564624	0.327131
O	0.000000	0.000000	1.506774
H	-0.880828	3.873562	-1.174448
H	0.000099	4.725217	0.090803
H	0.880894	3.873522	-1.174514
H	0.880828	-3.873562	-1.174448
H	-0.000099	-4.725217	0.090803
H	-0.880894	-3.873522	-1.174514
H	0.868429	1.265284	-1.177370
H	-0.868485	1.265321	-1.177299
H	0.868485	-1.265321	-1.177299
H	-0.868429	-1.265284	-1.177370
H	-0.869532	2.558992	0.986328
H	0.869698	2.558953	0.986265
H	0.869532	-2.558992	0.986328
H	-0.869698	-2.558953	0.986265

Molecule# 1585

4-hydroxy-2-mercaptopurine-5-carbonitrile

PointGroup: C1

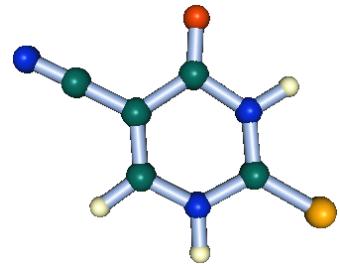
E= -830.207630713 au

ZPE= 0.083298 au

LUMO_eps= -0.10720 au

HOMO_eps= -0.26294 au

Dipole= 4.879 debye



13

S	3.132710	-0.028210	0.000007
O	-1.337989	2.079383	-0.000019
N	0.658787	0.991064	-0.000007
N	0.797722	-1.297239	0.000012
N	-3.917479	-0.575246	-0.000004
C	-1.360122	-0.311158	0.000000
C	-0.749660	1.025767	-0.000010
C	-0.554818	-1.403788	0.000010
C	1.482361	-0.097815	0.000004
C	-2.773022	-0.442707	-0.000002
H	1.112595	1.894358	-0.000013
H	-0.951396	-2.408389	0.000017
H	1.377708	-2.121519	0.000020

Molecule# 1586

4-hydroxy-2,3-dihydrothiophene

PointGroup: C1

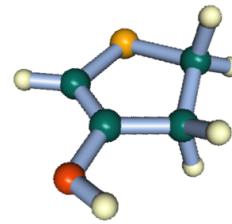
E= -629.550478011 au

ZPE= 0.093696 au

LUMO_eps= -0.02418 au

HOMO_eps= -0.19507 au

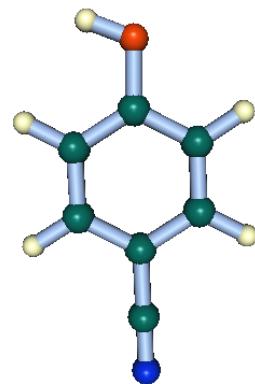
Dipole= 3.022 debye



12

S	-1.557947	-0.547420	-0.078355
C	0.113521	-1.121692	0.074303
C	1.026808	-0.155065	0.016891
C	0.488759	1.236776	-0.190699
C	-0.987946	1.187007	0.215046
O	2.374694	-0.392412	0.019811
H	0.314952	-2.177612	0.152421
H	1.028571	1.980024	0.403180
H	-1.614058	1.868088	-0.353978
H	0.605870	1.517008	-1.244505
H	-1.102813	1.398424	1.277082
H	2.850231	0.429936	0.167745

Molecule# 1587
 4-hydroxybenzonitrile
 PointGroup: Cs
 E= -399.866343121 au
 ZPE= 0.103261 au
 LUMO_eps= -0.05544 au
 HOMO_eps= -0.25681 au
 Dipole= 5.239 debye



14

C	-0.005988	2.507272	0.000000
C	-1.204001	0.369123	0.000000
C	1.211150	0.375851	0.000000
C	-1.197969	-1.015172	0.000000
C	1.219241	-1.005857	0.000000
C	0.000000	1.080084	0.000000
C	0.013220	-1.706493	0.000000
N	-0.011295	3.660282	0.000000
O	0.081551	-3.064394	0.000000
H	-2.141968	0.905432	0.000000
H	2.144005	0.921085	0.000000
H	-2.133901	-1.560076	0.000000
H	2.147877	-1.558073	0.000000
H	-0.803265	-3.444050	0.000000

Molecule# 1588

4-imino-1,3-thiazolidine-2-thione

PointGroup: C1

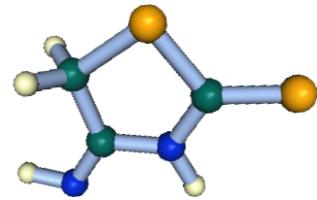
E= -1022.768761300 au

ZPE= 0.074652 au

LUMO_eps= -0.07308 au

HOMO_eps= -0.23940 au

Dipole= 4.068 debye



11

S	0.212246	1.503595	0.000013
S	2.374967	-0.597531	-0.000005
N	-0.270384	-1.016336	-0.000009
N	-2.558616	-1.309203	-0.000011
C	0.793728	-0.164480	-0.000001
C	-1.566028	-0.523204	-0.000005
C	-1.550107	0.995182	0.000009
H	-0.112586	-2.013711	-0.000018
H	-3.442358	-0.809316	-0.000007
H	-2.051518	1.379900	-0.885946
H	-2.051518	1.379884	0.885970

Molecule# 1589

4-methoxy-N,N-dimethylbenzamide

PointGroup: C1

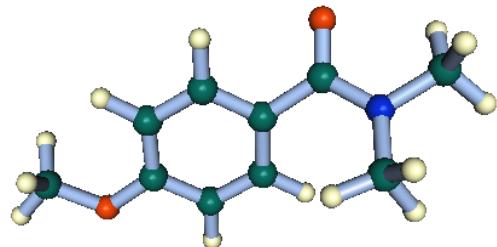
E= -594.312390858 au

ZPE= 0.215310 au

LUMO_eps= -0.02986 au

HOMO_eps= -0.23142 au

Dipole= 3.308 debye



26

C	-0.490195	1.181024	0.380923
C	-0.087273	-0.940362	-0.656437
C	-1.855971	0.926677	0.397595
C	-1.445482	-1.198966	-0.668128
C	0.414573	0.251972	-0.124372
C	-2.340707	-0.270667	-0.129777
C	1.862691	0.635548	-0.187993
C	4.207575	0.027914	-0.102161
C	2.582085	-1.485876	0.935530
C	-4.617266	0.290682	0.342564
N	2.808906	-0.316370	0.101874
O	2.178901	1.768129	-0.533865
O	-3.654834	-0.618058	-0.172296
H	-0.115377	2.122535	0.757231
H	0.588383	-1.664528	-1.090945
H	-2.526213	1.665397	0.809027
H	-1.837104	-2.111604	-1.095000
H	4.753810	-0.863416	-0.414276
H	4.664605	0.410445	0.816274
H	4.282830	0.793784	-0.866477
H	3.181135	-1.412773	1.848519
H	2.873534	-2.401982	0.415066
H	1.539541	-1.562042	1.221072
H	-4.602392	1.237341	-0.202758
H	-4.455250	0.481757	1.406130
H	-5.582559	-0.188564	0.205851

Molecule# 1590

4-methyl-1,3-thiazole

PointGroup: Cs

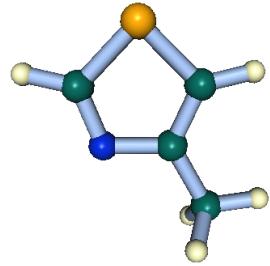
E= -608.484124374 au

ZPE= 0.082549 au

LUMO_eps= -0.03608 au

HOMO_eps= -0.25083 au

Dipole= 1.303 debye



11

H	1.956440	-1.637058	0.000000
C	0.000000	0.950174	0.000000
C	1.120691	-0.954132	0.000000
H	0.432261	2.850247	0.878324
H	-1.103247	2.790379	0.000000
H	0.432261	2.850247	-0.878324
C	-0.071430	2.443743	0.000000
S	-0.511579	-1.544954	0.000000
N	1.234040	0.335533	0.000000
H	-2.109532	0.327724	0.000000
C	-1.059462	0.091715	0.000000

Molecule# 1591

4-methyl-1H-imidazole

PointGroup: Cs

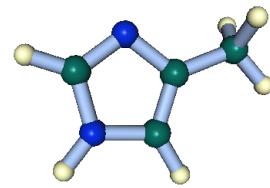
E= -265.640035948 au

ZPE= 0.098493 au

LUMO_eps= -0.01886 au

HOMO_eps= -0.23012 au

Dipole= 3.365 debye



12

C	1.108723	-0.145442	0.000000
C	-0.725124	-1.365652	0.000000
C	0.000000	0.658242	0.000000
C	-0.075878	2.147531	0.000000
N	-1.137354	-0.122450	0.000000
N	0.632730	-1.439852	0.000000
H	2.160529	0.077190	0.000000
H	-1.353102	-2.241108	0.000000
H	-0.613019	2.509034	0.878479
H	0.918810	2.592122	0.000000
H	-0.613019	2.509034	-0.878479
H	1.185847	-2.278231	0.000000

Molecule# 1592

4-methyl-2-pentanone

PointGroup: C1

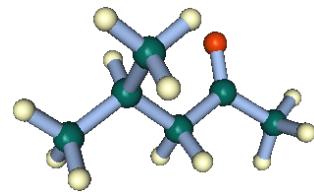
E= -311.220395068 au

ZPE= 0.168211 au

LUMO_eps= -0.02612 au

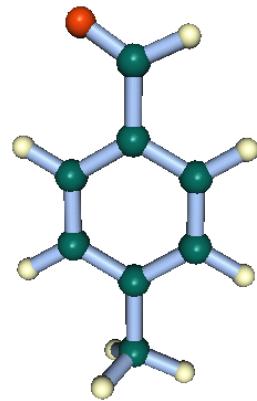
HOMO_eps= -0.25561 au

Dipole= 2.697 debye



19

C	1.363855	0.030075	-0.170042
C	2.606929	-0.557824	0.463532
C	-1.455280	1.225604	0.713644
C	-2.421092	-0.889332	-0.272124
C	0.061163	-0.705726	0.102479
C	-1.218410	0.057722	-0.248330
O	1.416645	1.020203	-0.864763
H	2.642224	-1.640680	0.332842
H	3.496393	-0.099039	0.039705
H	2.584875	-0.368191	1.539724
H	-2.352545	1.781025	0.436354
H	-1.594220	0.865028	1.736746
H	-0.618385	1.922898	0.706321
H	-3.332967	-0.354649	-0.542235
H	-2.584846	-1.345226	0.707862
H	-2.281272	-1.695729	-0.994592
H	0.119090	-1.634373	-0.479035
H	0.049131	-1.027199	1.149683
H	-1.083622	0.471398	-1.250224



Molecule# 1593

4-methylbenzaldehyde

PointGroup: C1

E= -385.035481371 au
 ZPE= 0.136752 au
 LUMO_eps= -0.07375 au
 HOMO_eps= -0.26436 au
 Dipole= 4.084 debye

17

C	-0.225569	1.332966	-0.000002
C	-0.455485	-1.064735	-0.000006
C	1.156764	1.200181	-0.000032
C	0.920244	-1.190395	-0.000036
C	-1.043674	0.204925	0.000012
C	1.751261	-0.060989	-0.000040
C	-2.509207	0.366017	0.000015
C	3.247030	-0.218201	0.000041
O	-3.310674	-0.540952	0.000015
H	-0.675329	2.318557	-0.000006
H	-1.096676	-1.935469	-0.000014
H	1.781369	2.084082	-0.000052
H	1.367447	-2.176702	-0.000067
H	-2.854814	1.419797	0.000014
H	3.582124	-0.775241	-0.877101
H	3.750856	0.746927	-0.001219
H	3.582235	-0.772949	0.878607

Molecule# 1594

4-methylcyclopentene

PointGroup: Cs

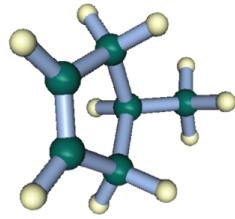
E= -234.730190535 au

ZPE= 0.144213 au

LUMO_eps= -0.01028 au

HOMO_eps= -0.24420 au

Dipole= 0.260 debye



16

H	0.028003	-2.438976	1.284839
C	-0.009038	-1.553163	0.664724
H	0.028003	-2.438976	-1.284839
C	-0.009038	-1.553163	-0.664724
H	0.979678	0.096300	1.630209
H	-0.717848	-0.020955	2.047210
C	-0.009038	-0.154824	1.227012
H	-0.717848	-0.020955	-2.047210
H	0.979678	0.096300	-1.630209
C	-0.009038	-0.154824	-1.227012
H	-1.442190	0.863921	0.000000
C	-0.357295	0.727796	0.000000
H	0.014739	2.680869	0.880857
H	0.014739	2.680869	-0.880857
H	1.389603	2.014165	0.000000
C	0.300687	2.102752	0.000000

Molecule# 1595

4-methylene-2-oxetanone

PointGroup: Cs

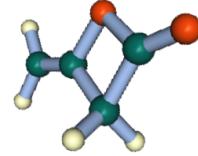
E= -305.359788964 au

ZPE= 0.072318 au

LUMO_eps= -0.02381 au

HOMO_eps= -0.27333 au

Dipole= 3.614 debye



10

C	0.232599	2.252569	0.000000
H	1.240702	2.639284	0.000000
H	-0.591492	2.949028	0.000000
O	0.964439	-0.073898	0.000000
C	-0.031516	-1.052379	0.000000
O	0.109849	-2.226036	0.000000
C	-1.150253	-0.013443	0.000000
H	-1.774247	-0.027961	0.891486
H	-1.774247	-0.027961	-0.891486
C	0.000000	0.957768	0.000000

Molecule# 1596

4-methylmorpholine

PointGroup: Cs

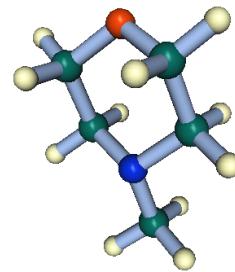
E= -327.232302250 au

ZPE= 0.161819 au

LUMO_eps= -0.01056 au

HOMO_eps= -0.22639 au

Dipole= 1.331 debye



18

C	0.106519	0.321839	1.198642
C	0.106519	0.321839	-1.198642
C	0.106519	-1.199020	1.172521
C	0.106519	-1.199020	-1.172521
C	-0.609708	2.294708	0.000000
N	-0.539239	0.845250	0.000000
O	0.737364	-1.697303	0.000000
H	-0.440093	0.670990	2.077415
H	1.146930	0.681983	1.286343
H	1.146930	0.681983	-1.286343
H	-0.440093	0.670990	-2.077415
H	0.665003	-1.599068	2.017754
H	-0.925754	-1.568194	1.224034
H	-0.925754	-1.568194	-1.224034
H	0.665003	-1.599068	-2.017754
H	0.384828	2.772550	0.000000
H	-1.149724	2.637811	0.883102
H	-1.149724	2.637811	-0.883102

Molecule# 1597

4-methylpyridine

PointGroup: C1

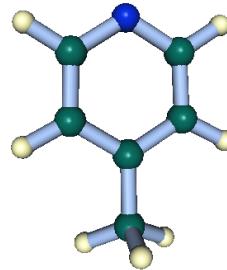
E= -287.709303398 au

ZPE= 0.115779 au

LUMO_eps= -0.03545 au

HOMO_eps= -0.26127 au

Dipole= 2.788 debye



14

C	0.170112	1.186351	-0.008143
C	0.170422	-1.186190	-0.008142
C	-1.217953	1.135555	0.002250
C	-1.217513	-1.135808	0.002253
C	0.901466	0.000262	-0.011063
C	2.404775	0.000161	0.007281
N	-1.916745	-0.000180	0.008110
H	0.673396	2.144679	-0.017182
H	0.673970	-2.144393	-0.017199
H	-1.795666	2.053142	0.003167
H	-1.794994	-2.053533	0.003164
H	2.808502	-0.876247	-0.498790
H	2.808455	0.891635	-0.471579
H	2.775701	-0.016004	1.035029

Molecule# 1598

4-nitro-1H-pyrrole-2-carbonitrile

PointGroup: C1

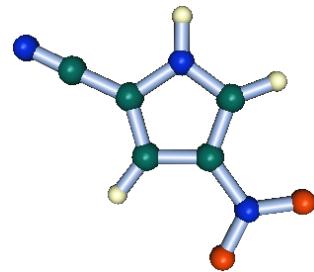
E= -507.108366912 au

ZPE= 0.084080 au

LUMO_eps= -0.10630 au

HOMO_eps= -0.28250 au

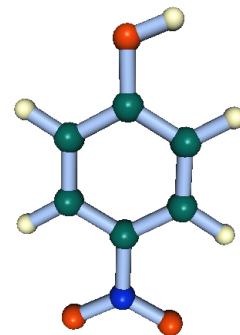
Dipole= 3.945 debye



13

O	2.409384	-1.476771	-0.000003
O	2.963804	0.626484	0.000002
N	-1.062861	1.308586	0.000003
N	2.141777	-0.283046	0.000000
N	-3.957177	-0.642796	-0.000002
C	0.751730	0.081376	0.000000
C	-0.341936	-0.807462	-0.000002
C	0.284912	1.380757	0.000003
C	-1.469753	-0.017320	0.000000
C	-2.836470	-0.370988	-0.000001
H	-0.303559	-1.881146	-0.000005
H	0.823963	2.309913	0.000006
H	-1.688970	2.096140	0.000005

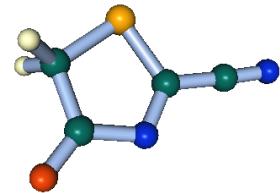
Molecule# 1599
 4-nitrophenol
 PointGroup: Cs
 E= -512.174815684 au
 ZPE= 0.107134 au
 LUMO_eps= -0.09740 au
 HOMO_eps= -0.26830 au
 Dipole= 5.376 debye



15

C	-1.206951	0.001465	0.000000
C	1.216264	0.012824	0.000000
C	-1.196872	-1.382293	0.000000
C	1.225228	-1.368685	0.000000
C	0.000000	0.687846	0.000000
C	0.018081	-2.070366	0.000000
N	-0.009275	2.152677	0.000000
O	-1.096069	2.717197	0.000000
O	1.070131	2.730377	0.000000
O	0.088467	-3.425739	0.000000
H	-2.133281	0.554066	0.000000
H	2.135640	0.576959	0.000000
H	-2.130792	-1.930246	0.000000
H	2.153866	-1.920498	0.000000
H	-0.795242	-3.808449	0.000000

Molecule# 1600
4-oxo-4,5-dihydro-1,3-thiazole-2-carbonitrile
PointGroup: C1
E= -736.668623527 au
ZPE= 0.057242 au
LUMO_eps= -0.13147 au
HOMO_eps= -0.29883 au
Dipole= 4.324 debye



10

S	0.234585	1.466163	0.000019
O	-2.496898	-1.266018	-0.000007
N	-0.187033	-1.159171	-0.000015
N	3.238743	-0.724713	-0.000024
C	-1.499104	0.930285	0.000020
C	-1.494441	-0.611498	-0.000002
C	0.703863	-0.238954	-0.000007
C	2.103888	-0.535976	-0.000017
H	-2.012693	1.296805	-0.885980
H	-2.012684	1.296780	0.886036

Molecule# 1601

4-propylphenol

PointGroup: C1

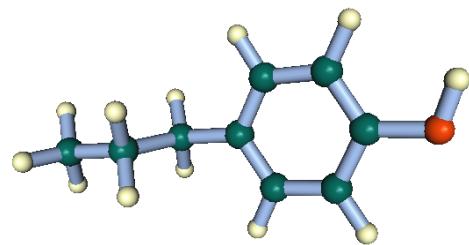
E= -425.576893093 au

ZPE= 0.188737 au

LUMO_eps= -0.01832 au

HOMO_eps= -0.22491 au

Dipole= 1.320 debye



22

C	-0.358008	-1.192497	-0.280254
C	-0.343198	1.192831	-0.282150
C	-1.721958	-1.189747	-0.010477
C	-1.704067	1.215219	-0.013027
C	0.359997	-0.006025	-0.420220
C	-2.398815	0.017812	0.125458
C	4.192562	-0.004905	0.338317
C	1.847021	-0.015398	-0.674427
C	2.689971	0.002765	0.610921
O	-3.741651	0.088900	0.388088
H	0.152278	-2.141809	-0.388206
H	0.183030	2.133209	-0.392492
H	-2.257935	-2.126629	0.088883
H	-2.239210	2.149244	0.086996
H	4.489024	-0.895456	-0.219839
H	4.492677	0.865907	-0.248259
H	4.763947	0.008939	1.267358
H	2.112002	-0.900851	-1.258622
H	2.117837	0.849206	-1.286581
H	2.424357	0.886004	1.197601
H	2.420111	-0.860563	1.224708
H	-4.105938	-0.798727	0.458901

Molecule# 1602

4-pyridinol

PointGroup: Cs

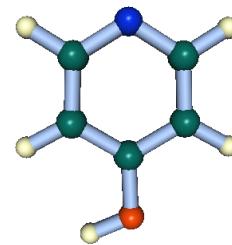
E= -323.633957046 au

ZPE= 0.092948 au

LUMO_eps= -0.02976 au

HOMO_eps= -0.26589 au

Dipole= 2.677 debye



12

N	0.022052	-1.868589	0.000000
C	-1.118779	-1.180044	0.000000
C	-1.190003	0.206824	0.000000
C	0.000000	0.928441	0.000000
C	1.202363	0.228588	0.000000
C	1.152339	-1.156758	0.000000
O	0.047471	2.286339	0.000000
H	-2.032661	-1.763240	0.000000
H	-2.150092	0.708021	0.000000
H	2.143131	0.759763	0.000000
H	2.074927	-1.725725	0.000000
H	-0.844958	2.648295	0.000000

Molecule# 1603

4-sulfanyl-1,3-thiazole-5-carbonitrile

PointGroup: C1

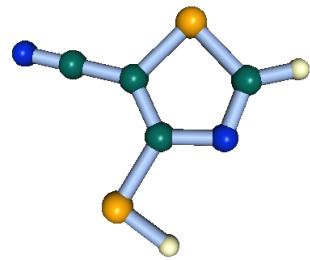
E= -1059.644288380 au

ZPE= 0.052860 au

LUMO_eps= -0.08773 au

HOMO_eps= -0.25452 au

Dipole= 4.354 debye



10

S	-1.958243	0.228807	0.000000
S	2.220685	-0.683816	0.000001
N	-0.289940	-1.729567	0.000001
N	0.650712	2.984496	0.000000
C	-0.252301	0.588485	0.000000
C	0.464268	-0.591163	0.000000
C	-1.558175	-1.448494	0.000000
C	0.241588	1.904998	0.000000
H	2.237266	-2.028192	0.000001
H	-2.334026	-2.199110	0.000000

Molecule# 1604

4-thioxo-1,3-thiazolidin-2-one

PointGroup: C1

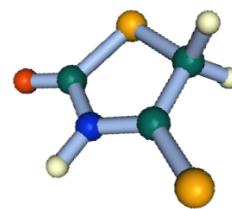
E= -1042.663829390 au

ZPE= 0.062498 au

LUMO_eps= -0.08951 au

HOMO_eps= -0.24951 au

Dipole= 1.614 debye



10

S	1.535241	1.076974	0.000006
S	-2.578025	-0.232305	0.000005
O	2.214634	-1.515497	-0.000019
N	-0.028314	-1.003049	-0.000009
C	-0.279530	1.342985	0.000012
C	-0.953928	-0.011648	0.000002
C	1.338317	-0.698704	-0.000010
H	-0.577310	1.904471	-0.882290
H	-0.577306	1.904457	0.882325
H	-0.308867	-1.974111	-0.000017

Molecule# 1605

4(1H)-pyridinone

PointGroup: C2v

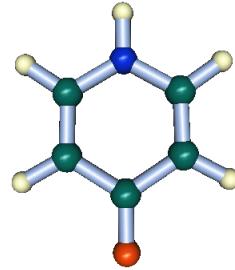
E= -323.631538451 au

ZPE= 0.093421 au

LUMO_eps= -0.03462 au

HOMO_eps= -0.23406 au

Dipole= 6.946 debye



12

C	0.000000	1.224565	0.305825
C	0.000000	-1.224565	0.305825
C	0.000000	1.188942	-1.044134
C	0.000000	-1.188942	-1.044134
C	0.000000	0.000000	1.104808
N	0.000000	0.000000	-1.722199
O	0.000000	0.000000	2.335063
H	0.000000	2.171811	0.824427
H	0.000000	-2.171811	0.824427
H	0.000000	2.077841	-1.658455
H	0.000000	-2.077841	-1.658455
H	0.000000	0.000000	-2.726202

Molecule# 1606

4(3H)-pyridinone

PointGroup: C1

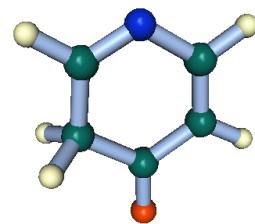
E= -323.600634456 au

ZPE= 0.090917 au

LUMO_eps= -0.09937 au

HOMO_eps= -0.26592 au

Dipole= 2.002 debye



12

N	1.836314	0.047911	-0.000037
C	1.226255	-1.073102	-0.000001
C	-0.257423	-1.256683	0.000068
C	-1.075456	0.025969	-0.000044
C	-0.291026	1.257772	0.000051
C	1.053818	1.213993	-0.000020
O	-2.292236	0.003283	-0.000067
H	1.839628	-1.972339	-0.000073
H	-0.551220	-1.860885	0.865345
H	-0.825378	2.197611	0.000125
H	1.634483	2.127729	0.000039
H	-0.550829	-1.861455	-0.864964

Molecule# 1607

4(3H)-pyrimidinone

PointGroup: Cs

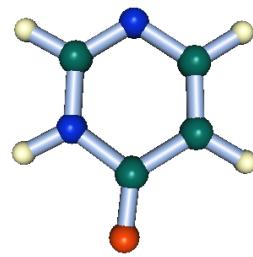
E= -339.694855437 au

ZPE= 0.081883 au

LUMO_eps= -0.06773 au

HOMO_eps= -0.26201 au

Dipole= 2.370 debye



11

C	1.232892	0.302834	0.000000
C	1.206555	-1.054025	0.000000
C	-1.049356	-1.149467	0.000000
C	0.000000	1.055988	0.000000
N	0.061359	-1.812046	0.000000
N	-1.126414	0.202125	0.000000
O	-0.144293	2.264784	0.000000
H	2.159160	0.856946	0.000000
H	2.129679	-1.620129	0.000000
H	-1.994198	-1.680952	0.000000
H	-2.025462	0.663333	0.000000

Molecule# 1608

4,4-difluoro-2-butynoic acid

PointGroup: C1

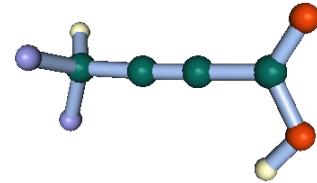
E= -503.891757185 au

ZPE= 0.056719 au

LUMO_eps= -0.09007 au

HOMO_eps= -0.31939 au

Dipole= 2.612 debye



10

F	2.506325	1.085625	-0.291206
F	2.521596	-0.878303	0.707492
O	-2.800863	-1.049313	-0.310556
O	-2.668371	1.055585	0.407816
C	1.976955	-0.173421	-0.324959
C	0.523022	-0.117121	-0.183650
C	-0.674290	-0.101787	-0.111486
C	-2.125829	-0.103987	-0.024120
H	-1.980086	1.705683	0.601006
H	2.283524	-0.643865	-1.260372

Molecule# 1609

4,5-didehydro-1,3-dihydro-2H-imidazol-2-one

PointGroup: C1

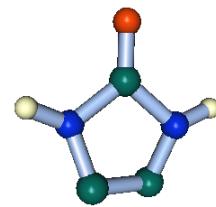
E= -300.200169940 au

ZPE= 0.050006 au

LUMO_eps= -0.13895 au

HOMO_eps= -0.24709 au

Dipole= 1.525 debye



8

O	-1.905063	0.000000	0.000000
N	0.190297	1.107884	0.120754
N	0.190296	-1.107884	-0.120755
C	-0.714324	0.000000	0.000000
C	1.431605	0.685517	-0.183402
C	1.431604	-0.685518	0.183403
H	-0.158479	2.033494	-0.089560
H	-0.158482	-2.033493	0.089561

Molecule# 1610

4,5-dihydro-1,2-thiazole-1-oxide

PointGroup: C1

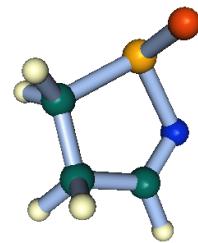
E= -645.570038708 au

ZPE= 0.081029 au

LUMO_eps= -0.05452 au

HOMO_eps= -0.25002 au

Dipole= 5.340 debye



11

C	-1.612174	0.568511	0.325815
C	-1.359474	-0.903273	0.131974
C	-0.398399	1.283143	-0.255369
N	-0.231575	-1.335367	-0.251174
O	1.735392	0.014128	0.833141
S	0.935671	-0.012414	-0.425050
H	-2.539917	0.860498	-0.169257
H	-1.752446	0.764996	1.391742
H	-2.153498	-1.621061	0.337364
H	-0.586582	1.674298	-1.253682
H	0.019870	2.064161	0.373207

Molecule# 1611

4,5-dihydro-1,2,3-thiadiazole-4-thiol

PointGroup: C1

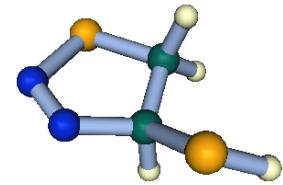
E= -984.585851602 au

ZPE= 0.064049 au

LUMO_eps= -0.07142 au

HOMO_eps= -0.26093 au

Dipole= 3.643 debye



10

S	-1.983658	-0.378275	-0.077921
S	2.278646	-0.016762	-0.202915
N	-0.053374	1.287591	0.110852
N	-1.248787	1.259796	-0.126326
C	0.571612	-0.012113	0.475502
C	-0.332408	-1.149797	-0.006743
H	2.698054	-1.070500	0.520774
H	0.640671	0.011826	1.564772
H	-0.043820	-1.503899	-0.993521
H	-0.334803	-1.977092	0.697118

Molecule# 1612

4,5-dimethyl-1,3-thiazole-2(3H)-thione

PointGroup: C1

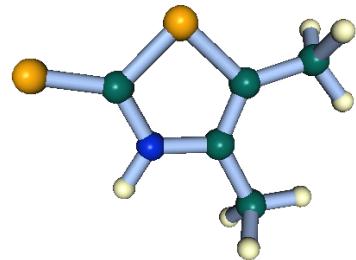
E= -1046.052274610 au

ZPE= 0.113184 au

LUMO_eps= -0.04363 au

HOMO_eps= -0.20746 au

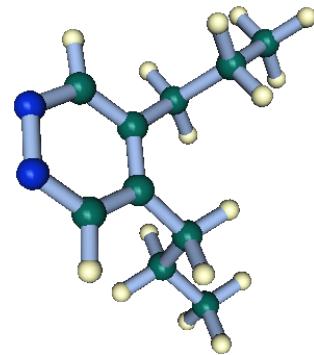
Dipole= 6.279 debye



15

C	2.045287	1.959573	0.000020
C	1.079023	0.821006	0.000009
C	1.317642	-0.506197	0.000000
C	2.614953	-1.243781	0.000000
S	-0.210914	-1.391881	-0.000010
C	-1.168018	0.085615	-0.000003
N	-0.281545	1.116807	0.000007
S	-2.819584	0.202116	-0.000008
H	1.909294	2.589853	-0.881908
H	3.071241	1.602683	0.000021
H	1.909289	2.589840	0.881956
H	2.709293	-1.883500	-0.879789
H	2.709288	-1.883511	0.879781
H	3.456495	-0.553476	0.000007
H	-0.639431	2.059413	0.000012

Molecule# 1613
 4,5-dipropylpyridazine
 PointGroup: C2
 E= -500.361213211 au
 ZPE= 0.245149 au
 LUMO_eps= -0.05085 au
 HOMO_eps= -0.23431 au
 Dipole= 5.397 debye



28

C	-0.550872	1.183343	1.818393
C	0.550872	-1.183343	1.818393
C	-0.290910	0.631581	0.558623
C	0.290910	-0.631581	0.558623
C	0.216434	3.129438	-2.389797
C	-0.216434	-3.129438	-2.389797
C	-0.608822	1.420841	-0.684182
C	0.608822	-1.420841	-0.684182
C	0.550872	2.327591	-1.134342
C	-0.550872	-2.327591	-1.134342
N	-0.282914	0.601718	2.979528
N	0.282914	-0.601718	2.979528
H	-1.012928	2.161604	1.897374
H	1.012928	-2.161604	1.897374
H	-0.012670	2.471736	-3.230631
H	-0.650384	3.773094	-2.228370
H	1.051528	3.765640	-2.684387
H	0.012670	-2.471736	-3.230631
H	0.650384	-3.773094	-2.228370
H	-1.051528	-3.765640	-2.684387
H	-0.878678	0.750885	-1.501953
H	-1.486647	2.042926	-0.493539
H	0.878678	-0.750885	-1.501953
H	1.486647	-2.042926	-0.493539
H	0.807198	3.006117	-0.317347
H	1.439842	1.716802	-1.310001
H	-0.807198	-3.006117	-0.317347
H	-1.439842	-1.716802	-1.310001

Molecule# 1614

4H-imidazole

PointGroup: Cs

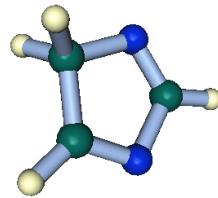
E= -226.276336367 au

ZPE= 0.069493 au

LUMO_eps= -0.06678 au

HOMO_eps= -0.28439 au

Dipole= 2.107 debye



9

N	-1.193024	0.354700	0.000000
C	0.000000	1.136486	0.000000
N	1.111424	0.505412	0.000000
C	0.730867	-0.899567	0.000000
C	-0.764372	-0.854862	0.000000
H	-0.075334	2.215149	0.000000
H	1.139796	-1.410552	0.877155
H	1.139796	-1.410552	-0.877155
H	-1.432029	-1.707173	0.000000

Molecule# 1615

5-(chloromethyl)-1,2,4-thiadiazole

PointGroup: C1

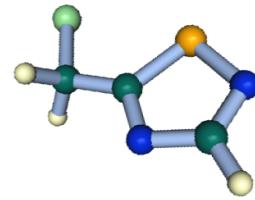
E= -1084.159298900 au

ZPE= 0.062512 au

LUMO_eps= -0.06464 au

HOMO_eps= -0.29221 au

Dipole= 1.492 debye



10

C1	-2.472282	-0.267612	-0.000030
S	0.639929	-1.110653	0.000024
N	1.179481	1.352505	-0.000015
N	2.252013	-0.695943	-0.000013
C	0.152322	0.548818	0.000016
C	2.324073	0.610198	-0.000029
C	-1.251803	1.057260	0.000047
H	3.286720	1.101720	-0.000055
H	-1.432399	1.662317	-0.884472
H	-1.432404	1.662208	0.884642

Molecule# 1616

5-(dichloromethyl)-1,2-oxazole

PointGroup: C1

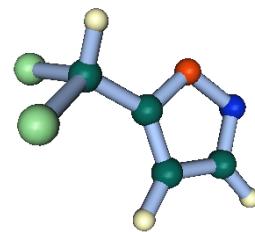
E= -1204.714522770 au

ZPE= 0.067423 au

LUMO_eps= -0.06704 au

HOMO_eps= -0.28882 au

Dipole= 2.015 debye



11

C1	-1.769018	-1.402538	0.178117
C1	-1.547273	1.487912	-0.423243
O	1.460798	0.667411	0.845353
N	2.756231	0.418539	0.391564
C	0.598785	-0.083649	0.134479
C	-0.831962	0.092960	0.483695
C	1.270958	-0.829507	-0.776098
C	2.623928	-0.463831	-0.561859
H	-0.948218	0.336127	1.532441
H	0.868419	-1.532812	-1.480568
H	3.506494	-0.819577	-1.069811

Molecule# 1617

5-amino-1,3-thiazole-2(3H)-thione

PointGroup: C1

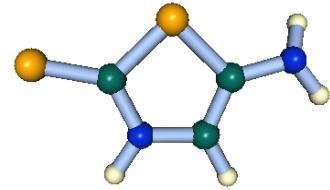
E= -1022.759171430 au

ZPE= 0.074328 au

LUMO_eps= -0.04340 au

HOMO_eps= -0.20277 au

Dipole= 6.418 debye



11

N	2.935965	-0.304877	-0.073828
C	1.606186	0.090118	0.012997
S	0.316726	-1.115816	-0.018860
C	-0.949684	0.127458	-0.004415
S	-2.581806	-0.148817	0.010440
C	1.075661	1.327803	0.016693
N	-0.317561	1.323933	-0.009342
H	3.193890	-1.060264	0.544728
H	3.594248	0.457458	-0.006269
H	1.603851	2.266439	0.028808
H	-0.872523	2.164827	-0.002006

Molecule# 1618

5-bromo-1,2-thiazole

PointGroup: C1

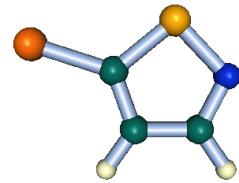
E= -3142.765891730 au

ZPE= 0.045191 au

LUMO_eps= -0.05953 au

HOMO_eps= -0.27214 au

Dipole= 1.720 debye



8

Br	1.729973	0.017382	-0.000001
S	-1.209080	-1.160255	0.000003
N	-2.589158	-0.232176	-0.000005
C	-0.869464	1.346817	0.000008
C	-0.141924	0.190845	-0.000001
C	-2.253218	1.039197	-0.000004
H	-0.449839	2.339613	0.000014
H	-3.042178	1.780191	-0.000008

Molecule# 1619

5-bromo-1H-pyrazole

PointGroup: C1

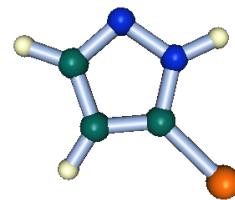
E= -2799.910033770 au

ZPE= 0.061189 au

LUMO_eps= -0.02665 au

HOMO_eps= -0.25626 au

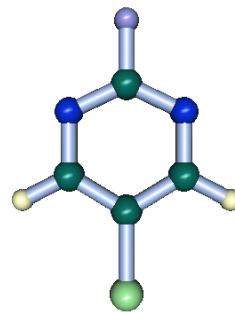
Dipole= 1.044 debye



9

Br	-1.536707	0.008714	-0.000003
N	1.096211	-1.031357	-0.000001
N	2.414134	-0.755321	0.000003
C	0.338351	0.087818	0.000000
C	1.196284	1.162139	0.000006
C	2.475800	0.570639	0.000007
H	0.934042	2.203797	0.000008
H	0.779959	-1.985169	-0.000003
H	3.435711	1.059553	0.000010

Molecule# 1620
5-chloro-2-fluoropyrimidine
PointGroup: C2v
E= -823.334877522 au
ZPE= 0.059320 au
LUMO_eps= -0.08580 au
HOMO_eps= -0.29054 au
Dipole= 2.470 debye



10

C1	0.000000	0.000000	2.639630
F	0.000000	0.000000	-3.046511
N	0.000000	1.187688	-1.149552
N	0.000000	-1.187688	-1.149552
C	0.000000	0.000000	-1.718678
C	0.000000	0.000000	0.901715
C	0.000000	1.186904	0.181469
C	0.000000	-1.186904	0.181469
H	0.000000	2.147124	0.681378
H	0.000000	-2.147124	0.681378

Molecule# 1621

5-chloro-3-ethynyl-1-methyl-1H-1,2,4-triazole

PointGroup: C1

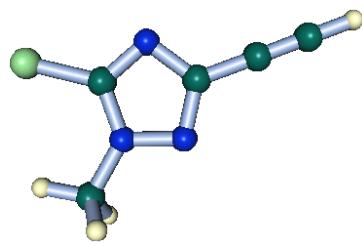
E= -817.467985702 au

ZPE= 0.086491 au

LUMO_eps= -0.04247 au

HOMO_eps= -0.26029 au

Dipole= 2.890 debye



13

C1	-2.273721	-1.145016	0.000007
N	-0.545925	0.931210	-0.000361
N	0.780358	1.189764	-0.000206
N	0.415924	-1.046068	0.000109
C	-1.507346	2.016770	0.000250
C	-0.725032	-0.407416	-0.000057
C	1.323326	-0.022938	0.000027
C	2.726873	-0.228945	0.000057
C	3.911599	-0.413981	0.000075
H	-1.359292	2.633377	-0.883814
H	-2.508410	1.598147	-0.006840
H	-1.368588	2.625200	0.891548
H	4.960520	-0.576746	0.000087

Molecule# 1622

5-chloro-4-methyl-1,2,3-thiadiazole

PointGroup: C1

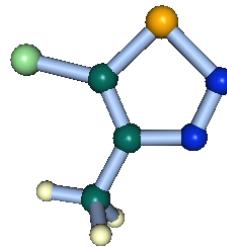
E= -1084.124971420 au

ZPE= 0.060608 au

LUMO_eps= -0.07656 au

HOMO_eps= -0.27432 au

Dipole= 2.528 debye



10

C1	-2.008972	-0.645633	-0.000016
S	0.916995	-1.382670	0.000044
N	1.562136	1.012518	-0.000064
N	2.104548	-0.138903	0.000000
C	-0.342527	-0.225321	-0.000029
C	0.192585	1.037355	-0.000081
C	-0.528302	2.343259	0.000042
H	-0.251761	2.929510	-0.876767
H	-1.605449	2.196556	-0.004895
H	-0.259520	2.925361	0.882074

Molecule# 1623

5-fluoro-3-thiophenecarbonitrile

PointGroup: C1

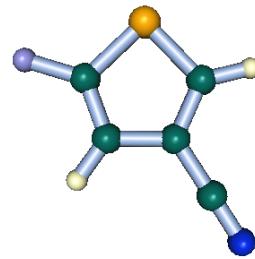
E= -744.638975975 au

ZPE= 0.057325 au

LUMO_eps= -0.07063 au

HOMO_eps= -0.27073 au

Dipole= 3.351 debye



10

S	1.303707	1.137937	-0.000005
F	2.339801	-1.305984	0.000004
N	-3.545099	-0.372952	0.000002
C	-0.996543	-0.005333	0.000000
C	-0.047454	-1.079338	0.000004
C	-0.415563	1.234811	-0.000005
C	1.215353	-0.596779	0.000002
C	-2.404958	-0.204569	0.000001
H	-0.299796	-2.127042	0.000008
H	-0.907038	2.191826	-0.000008

Molecule# 1624

5-fluoro-6-hydroxydihydro-2,4(1H,3H)-pyrimidinedione

PointGroup: C1

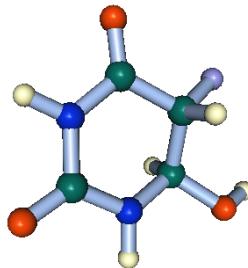
E= -590.716387889 au

ZPE= 0.105992 au

LUMO_eps= -0.05089 au

HOMO_eps= -0.28978 au

Dipole= 2.856 debye



15

F	2.375832	0.341649	-0.121397
O	1.124163	-2.287866	0.174880
O	0.695969	2.490935	-0.051098
O	-2.942224	-0.245940	0.022644
N	-0.875008	-1.207874	0.004582
N	-1.112015	1.111674	-0.020101
C	1.090406	0.142282	0.334810
C	0.527478	-1.113100	-0.322479
C	0.238552	1.381307	0.053108
C	-1.735828	-0.146180	0.002266
H	1.129546	-0.014071	1.416546
H	0.692280	-1.042947	-1.407061
H	2.004927	-2.374716	-0.205212
H	-1.307982	-2.113080	-0.090426
H	-1.739008	1.900491	-0.090282

Molecule# 1625

5-hydroxy-2,3-dihydrothiophene

PointGroup: C1

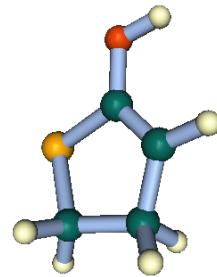
E= -629.551614026 au

ZPE= 0.093898 au

LUMO_eps= -0.01845 au

HOMO_eps= -0.20716 au

Dipole= 2.454 debye



12

S	0.063989	-1.268775	-0.106157
C	-0.855000	0.245265	0.022198
C	-0.124231	1.361916	0.026050
C	1.350842	1.127767	-0.161767
C	1.614187	-0.331940	0.244577
O	-2.200117	0.086742	0.072454
H	-0.557765	2.351675	0.076223
H	1.963154	1.798749	0.443646
H	1.811188	-0.410907	1.312550
H	1.639155	1.290531	-1.207061
H	2.432239	-0.791140	-0.303764
H	-2.625644	0.949515	0.010935

Molecule# 1626

5-hydroxypenta-2,4-diynoic acid

PointGroup: C1

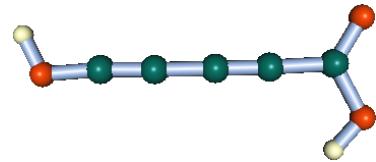
E= -417.436714484 au

ZPE= 0.057793 au

LUMO_eps= -0.07459 au

HOMO_eps= -0.27094 au

Dipole= 6.125 debye



10

O	2.917786	-1.157943	-0.000019
O	2.935541	1.069886	-0.000044
O	-4.203167	0.107734	0.000034
C	2.298217	-0.130187	-0.000019
C	0.859664	-0.051301	0.000006
C	-0.350583	-0.022132	0.000009
C	-1.705579	0.003733	0.000014
C	-2.911532	0.002168	0.000026
H	2.290340	1.788517	-0.000042
H	-4.632743	-0.759617	0.000060

Molecule# 1627

5-isocyanato-1,2-oxazole

PointGroup: C1

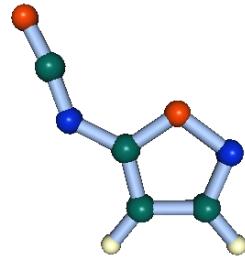
E= -413.677015716 au

ZPE= 0.061385 au

LUMO_eps= -0.05466 au

HOMO_eps= -0.26773 au

Dipole= 2.878 debye



10

O	0.546539	-0.953762	0.000000
O	-3.228086	-0.349170	0.000000
N	-1.101796	0.691502	0.000000
N	1.947764	-1.059792	0.000000
C	0.218242	0.351741	0.000000
C	1.335896	1.124727	0.000000
C	2.382875	0.171585	0.000000
C	-2.155264	0.095523	0.000000
H	1.392435	2.196850	0.000000
H	3.447671	0.343180	0.000001

Molecule# 1628

5-methyl-1,2-oxazole

PointGroup: Cs

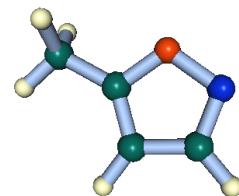
E= -285.467895696 au

ZPE= 0.085332 au

LUMO_eps= -0.02595 au

HOMO_eps= -0.26561 au

Dipole= 3.331 debye



11

C	-0.346200	2.073702	0.000000
H	-0.936846	2.330581	0.880543
H	0.558932	2.676627	0.000000
H	-0.936846	2.330581	-0.880543
C	0.000000	0.630252	0.000000
O	-1.025177	-0.242897	0.000000
N	-0.522613	-1.551143	0.000000
C	0.774494	-1.414513	0.000000
H	1.390658	-2.299799	0.000000
C	1.173944	-0.053727	0.000000
H	2.170386	0.348899	0.000000

Molecule# 1629

5-methyl-1,2,3-oxadithiole

PointGroup: C1

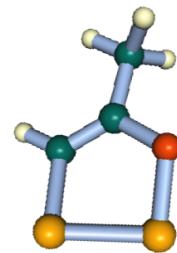
E= -988.424310169 au

ZPE= 0.065938 au

LUMO_eps= -0.06986 au

HOMO_eps= -0.20368 au

Dipole= 2.148 debye



10

S	-1.381222	0.952356	0.131158
S	-1.060922	-1.105763	-0.180184
O	0.561045	-1.063545	0.339172
C	1.148044	0.146398	-0.006454
C	2.633844	0.082759	-0.038161
C	0.357752	1.202401	-0.188373
H	2.975948	-0.613159	-0.805738
H	3.010492	-0.275655	0.922250
H	3.055424	1.065713	-0.234875
H	0.706231	2.196611	-0.412681

Molecule# 1630

5-methyl-2H-tetrazole

PointGroup: Cs

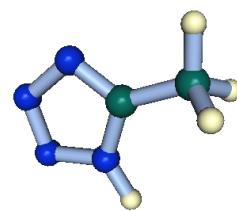
E= -297.689191345 au

ZPE= 0.074386 au

LUMO_eps= -0.03091 au

HOMO_eps= -0.29723 au

Dipole= 5.816 debye



10

N	-1.139760	-0.058016	0.000000
C	0.000000	0.597494	0.000000
C	0.176443	2.072182	0.000000
H	0.723233	2.405707	0.882916
H	0.723233	2.405707	-0.882916
H	-0.803151	2.542233	0.000000
N	0.988808	-0.317104	0.000000
N	0.447343	-1.553756	0.000000
N	-0.823573	-1.381071	0.000000
H	1.988304	-0.202077	0.000000

Molecule# 1631

5-phenylpyrimidine

PointGroup: C2

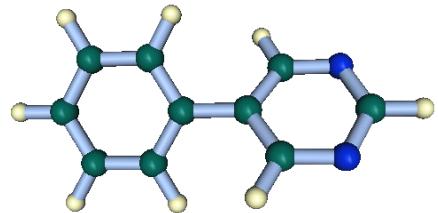
E= -495.555657902 au

ZPE= 0.157776 au

LUMO_eps= -0.06032 au

HOMO_eps= -0.25462 au

Dipole= 2.959 debye



20

C	0.000000	0.000000	-0.758430
C	-0.754120	0.903797	-1.510292
C	0.754120	-0.903797	-1.510292
N	-0.757576	0.915186	-2.840582
C	0.000000	0.000000	-3.441454
N	0.757576	-0.915186	-2.840582
C	0.000000	0.000000	0.718089
C	0.000000	1.201904	1.434398
C	-0.000714	1.201397	2.822810
C	0.000000	0.000000	3.522386
C	0.000714	-1.201397	2.822810
C	0.000000	-1.201904	1.434398
H	0.000000	0.000000	-4.524887
H	-1.389638	1.632242	-1.018874
H	1.389638	-1.632242	-1.018874
H	-0.006602	-2.140956	3.358639
H	0.000000	0.000000	4.603795
H	0.006602	2.140956	3.358639
H	0.024377	2.142989	0.901579
H	-0.024377	-2.142989	0.901579

Molecule# 1632

5,5,5-tribromo-1,3-pentadiyne

PointGroup: Cs

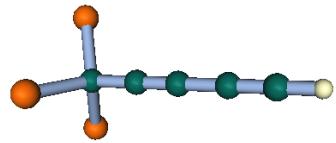
E= -7913.735788180 au

ZPE= 0.035768 au

LUMO_eps= -0.09479 au

HOMO_eps= -0.28123 au

Dipole= 1.956 debye



9

C	2.518920	-0.002174	0.000000
C	1.310377	0.000211	0.000000
C	3.876413	-0.005315	0.000000
C	-0.107815	0.001082	0.000000
C	5.081565	-0.008529	0.000000
H	6.143406	-0.011445	0.000000
Br	-0.783049	-0.929981	1.612817
Br	-0.783049	-0.929981	-1.612817
Br	-0.783049	1.862814	0.000000

Molecule# 1633

5,5,5-trichloro-1,3-pentadiyne

PointGroup: Cs

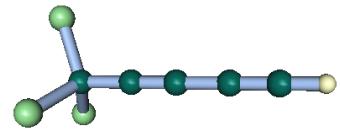
E= -1571.750779410 au

ZPE= 0.037569 au

LUMO_eps= -0.07997 au

HOMO_eps= -0.28800 au

Dipole= 2.204 debye



9

C	1.977238	-0.001331	0.000000
C	0.770993	0.001118	0.000000
C	3.336251	-0.004812	0.000000
C	-0.659885	0.001640	0.000000
C	4.540805	-0.008521	0.000000
H	5.602698	-0.011921	0.000000
Cl	-1.282257	-0.846315	1.468789
Cl	-1.282257	-0.846315	-1.468789
Cl	-1.282257	1.697533	0.000000

Molecule# 1634

5,5,5-trifluoro-1,3-pentadiyne

PointGroup: Cs

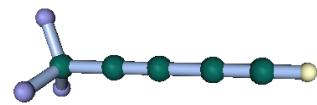
E= -490.720640435 au

ZPE= 0.043007 au

LUMO_eps= -0.07136 au

HOMO_eps= -0.29986 au

Dipole= 3.011 debye



9

C	0.151624	1.390687	0.000000
C	0.020289	0.194427	0.000000
C	0.300477	2.743694	0.000000
C	-0.137549	-1.254142	0.000000
C	0.432336	3.940048	0.000000
H	0.548834	4.995753	0.000000
F	0.432336	-1.811612	1.085585
F	0.432336	-1.811612	-1.085585
F	-1.437103	-1.608337	0.000000

Molecule# 1635

5,6-dihydro-4H-cyclopenta[c]furan

PointGroup: Cs

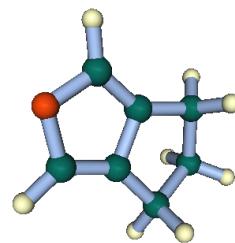
E= -346.877295974 au

ZPE= 0.133997 au

LUMO_eps= -0.01143 au

HOMO_eps= -0.22664 au

Dipole= 1.481 debye



16

C	0.056743	-1.403063	1.105281
C	0.056743	-1.403063	-1.105281
C	0.056743	-0.108428	0.714480
C	0.056743	-0.108428	-0.714480
C	0.061614	1.293990	1.248837
C	0.061614	1.293990	-1.248837
C	-0.362168	2.121493	0.000000
O	0.055843	-2.213536	0.000000
H	0.050540	-1.910773	2.052548
H	0.050540	-1.910773	-2.052548
H	-0.610306	1.450561	2.092349
H	1.064430	1.578481	1.579793
H	1.064430	1.578481	-1.579793
H	-0.610306	1.450561	-2.092349
H	-1.447985	2.228635	0.000000
H	0.063723	3.124156	0.000000

Molecule# 1636

5H-1,2,5-oxathiazole

PointGroup: C1

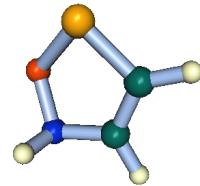
E= -606.182149248 au

ZPE= 0.052494 au

LUMO_eps= -0.06082 au

HOMO_eps= -0.21127 au

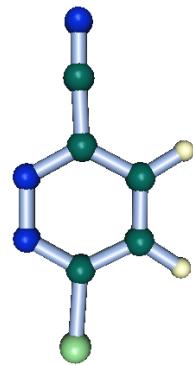
Dipole= 2.676 debye



8

S	-1.220858	0.001998	0.091689
O	-0.018734	-1.194169	-0.271412
N	1.276449	-0.701292	0.081978
C	0.008231	1.252585	-0.070218
C	1.225589	0.721438	-0.045189
H	1.431922	-0.961286	1.061342
H	-0.249835	2.295344	-0.144943
H	2.163454	1.252241	-0.093527

Molecule# 1637
 6-chloro-3-pyridazinecarbonitrile
 PointGroup: C1
 E= -816.281642136 au
 ZPE= 0.064461 au
 LUMO_eps= -0.10647 au
 HOMO_eps= -0.28623 au
 Dipole= 5.215 debye



11			
C1	2.930400	-0.091791	0.000009
N	-0.768407	-1.166317	-0.000008
N	0.553379	-1.155933	-0.000004
N	-4.016345	-0.114795	-0.000012
C	-0.799758	1.241089	0.000003
C	0.573371	1.246721	0.000007
C	-1.433356	-0.007434	-0.000005
C	1.197294	-0.000622	0.000004
C	-2.865884	-0.095394	-0.000009
H	-1.376813	2.154336	0.000005
H	1.149618	2.159260	0.000013

Molecule# 1638

6-chloro-N-hydroxy-3-pyridazinamine

PointGroup: C1

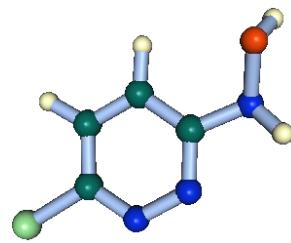
E= -854.598391162 au

ZPE= 0.087343 au

LUMO_eps= -0.07524 au

HOMO_eps= -0.25422 au

Dipole= 4.647 debye



13

C1	-3.081143	0.085415	0.053858
O	3.477026	0.490747	0.348644
N	0.521246	-1.313680	-0.003582
N	-0.801147	-1.191495	0.027950
N	2.647107	-0.500843	-0.241609
C	1.286485	-0.231016	-0.098672
C	-1.337020	0.006725	-0.003734
C	0.766362	1.071813	-0.120508
C	-0.597170	1.192029	-0.066717
H	4.072324	0.747301	-0.364548
H	2.880061	-1.402555	0.159613
H	1.418677	1.929694	-0.168056
H	-1.090219	2.152346	-0.073288

Molecule# 1639

7H-purine

PointGroup: Cs

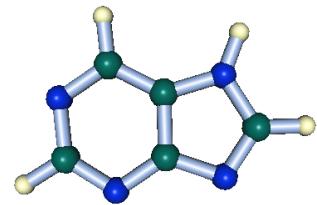
E= -412.089547433 au

ZPE= 0.094761 au

LUMO_eps= -0.06621 au

HOMO_eps= -0.26362 au

Dipole= 5.750 debye



13

C	-1.358848	0.996788	0.000000
C	-1.701599	-1.270252	0.000000
C	2.192531	0.578405	0.000000
C	0.000000	0.735121	0.000000
C	0.431371	-0.608939	0.000000
N	-2.209140	-0.025435	0.000000
N	-0.422841	-1.629439	0.000000
N	1.809446	-0.668802	0.000000
N	1.159397	1.480474	0.000000
H	-1.773845	1.998833	0.000000
H	-2.428333	-2.073138	0.000000
H	3.219520	0.908175	0.000000
H	1.243895	2.481808	0.000000

Molecule# 1640

9H-purine-2,6,8-trione

PointGroup: Cs

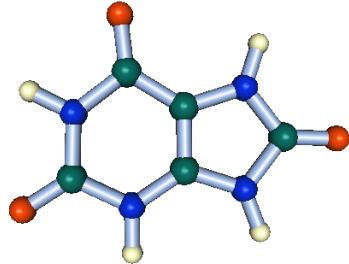
E= -637.929692434 au

ZPE= 0.108738 au

LUMO_eps= -0.05175 au

HOMO_eps= -0.23415 au

Dipole= 3.114 debye



16

C	0.000000	0.690260	0.000000
C	0.612433	-0.524322	0.000000
C	-1.421181	0.815858	0.000000
C	2.250868	1.064696	0.000000
C	-1.472895	-1.715075	0.000000
N	1.008530	1.656063	0.000000
N	1.963364	-0.327181	0.000000
N	-0.075505	-1.702376	0.000000
N	-2.045569	-0.457319	0.000000
O	-2.078366	1.839915	0.000000
O	3.351110	1.564725	0.000000
O	-2.104133	-2.748954	0.000000
H	0.868938	2.650817	0.000000
H	2.693788	-1.017316	0.000000
H	0.372696	-2.603452	0.000000
H	-3.055399	-0.448350	0.000000

Molecule# 1641

9H-purine

PointGroup: Cs

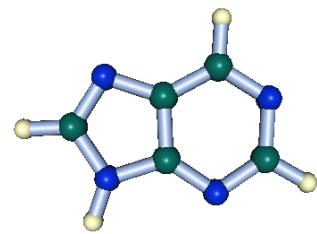
E= -412.095350400 au

ZPE= 0.094940 au

LUMO_eps= -0.06276 au

HOMO_eps= -0.26485 au

Dipole= 3.658 debye



13

C	-2.118438	0.068567	0.000000
N	-1.263191	1.092745	0.000000
C	0.000000	0.698379	0.000000
C	0.447803	-0.635313	0.000000
N	1.831505	-0.681693	0.000000
C	2.197462	0.568529	0.000000
N	1.143662	1.456527	0.000000
N	-1.827298	-1.239681	0.000000
C	-0.545581	-1.604990	0.000000
H	-3.170670	0.323513	0.000000
H	3.218998	0.914021	0.000000
H	1.191504	2.461120	0.000000
H	-0.320055	-2.664970	0.000000