TABS: A database of molecular structures

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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
(disulfanylmethylene)malononitrile
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
Cl   -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
Cl   -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
Cl   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'']tripyrrole
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
Cl   -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
Cl   0.454804   -1.139246   1.304813
Cl   -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
Cl   -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
Cl   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
Cl   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
Cl   -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
Cl   0.000000   1.489376   -0.216532
Cl   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
Cl   -3.711306   -0.250025   -0.222443
Cl   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
Cl   2.462394   -0.834112   0.000000
Cl   -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
Cl   -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
Cl   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
ethynylsulfanylmethylsulfanylethyne
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-yloxymethanethioic 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-mercaptoacrylate
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
methylenecyclobutane
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
Cl   -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
Cl   -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
Cl	-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
Cl   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
Cl   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
Cl	-1.403966	1.580358	-0.186597
Cl	-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
Cl   0.728531   1.497292   0.772640
Cl   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-ynenitrile
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
Cl   -0.963836   1.196188   -1.568576
Cl   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
Cl   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
sulfanylmethylthiocyanate
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[4.2.0.02,5]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
tetranitromethane
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
thiirane
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
Cl   0.000000   1.435076   -0.846417
C   0.000000   0.000000   0.142885
Cl   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
trioxidanylmethane
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
Cl   -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
Cl   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
Cl   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-bromooctane
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-diazonioethenolate
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
Cl   -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
Cl   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
Cl   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
Cl   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
Cl   -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
Cl   -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
Cl   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
Cl   -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
Cl   -2.228128   -1.021501   -0.416681
Cl   -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-methylsulfanylethanimine
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-ylnitrite
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-pentanethiol
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-propoxypropane
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-ylethanone
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
Cl   0.249784   -0.974350   1.469255
Cl   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
Cl   -2.158879   -0.834991   0.460362
Cl   -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
Cl   -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
Cl   0.551587   1.629115   0.087511
Cl   -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
Cl   0.166446   2.029748   -0.534405
Cl   -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
Cl   -0.802776   1.542890   -0.140419
Cl   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-thiatriazolidine
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
Cl   1.969671   -1.392624   -0.227155
Cl   -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-thioperoxol
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'-disulfanediyldiacetonitrile
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
Cl   -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-nitrosofuran
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
Cl   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
Cl   -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
Cl   1.196824   -1.594182   -0.748571
Cl   -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
Cl   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
Cl   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
Cl   -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
Cl   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
Cl   -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
Cl   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
Cl   -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
O   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-piperidinecarbaldehyde
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
Cl   -0.526261   1.700246   -0.274259
Cl   -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
Cl   1.404145   1.587201   0.000000
Cl   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
Cl   0.000000   1.591361   2.692912
C   0.000000   0.696756   1.212282
C   0.000000   -0.696756   1.212282
Cl   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
Cl   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
Cl   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
Cl   -2.599175   -0.886996   -0.000001
Cl   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
Cl   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
Cl   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
Cl   -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
Cl   -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
O   -2.290204   -0.882999   -0.151424
O   1.444926   1.959948   0.003154
O   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
Cl   0.811282   1.486375   -0.113059
Cl   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
Cl   2.402272   -0.042853   0.000005
Cl   -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
Cl   -1.455409   -1.648364   0.000000
Cl   -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
Cl   -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
Cl   -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
Cl   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
Cl   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
Cl   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
Cl   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
Cl   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
Cl   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
Cl   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
Cl   -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
Cl   -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-mercaptopyrimidine-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
Cl   -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
Cl   -1.769018   -1.402538   0.178117
Cl   -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
Cl   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
Cl	-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
Cl   -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
Cl   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
Cl	-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