Supplementary Information for

Local hybrids as a perturbation to global hybrid functionals

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Charge, spin multiplicity, and geometries of calculated systems (bond lengths and Cartesian coordinates are in Angstrom and angles in degree)

AE6 and BH6 test sets:

Hydrogen

0 2
H

Carbon

0 3
C

Oxygen

0 3
O

Silicon

0 3
Si

```
Sulfur

0 3
S


Hydrogen molecule

0 1
H
H 1 r1

r1=0.74187646


Hydroxyl radical

0 2
O
H 1 r1

r1=0.96889819


SH radical

0 2
S
H 1 r1
```

```
r1=1.34020229



CH3

0 2
C
H,1,CH
H,1,CH,2,120.
H,1,CH,2,120.,3,180.,0

CH=1.07731727



CH4

0 1
C
H,1,RCH
H,1,RCH,2,109.471221
H,1,RCH,2,109.471221,3,109.471221,1
H,1,RCH,2,109.471221,3,109.471221,-1

RCH=1.08744517



H2O
```

```
0 1
O
H,1,OH
H,1,OH,2,HOH

 OH=0.95691441
 HOH=104.51706026



H2S

0 1
S         0.000000     0.000000     0.102519
H         0.000000     0.966249    -0.820154
H         0.000000    -0.966249    -0.820154


Silane

0 1
Si
H,1,R
H,1,R,2,109.471221
H,1,R,2,109.471221,3,120.,0
H,1,R,2,109.471221,3,-120.,0

R=1.47670511


SiO
```

```
0 1
Si
O,1,sio

sio=1.51266699


S2

0 3
S
S,1,R

R=1.89259426


Propyne

0 1
C        0.000000    0.000000    0.219507
C        0.000000    0.000000    1.423958
C        0.000000    0.000000   -1.243764
H        0.000000    0.000000    2.486256
H        0.000000    1.019009   -1.628154
H        0.882487   -0.509504   -1.628154
H       -0.882487   -0.509504   -1.628154


Glyoxal

0 1
C
```

```
C,1,rcc
O,1,rco,2,a1
H,1,rch,2,a2,3,180.,0
O,2,rco,1,a1,3,180.,0
H,2,rch,1,a2,3,0.,0

rcc=1.52071235
rco=1.20370135
rch=1.10078486
a1=121.36275989
a2=115.12063284
```

```
Cyclobutane

0 1
C         0.000000    1.076294    0.142865
C         0.000000   -1.076294    0.142865
C        -1.076294    0.000000   -0.142865
C         1.076294    0.000000   -0.142865
H         0.000000    1.979204   -0.465165
H         0.000000    1.359222    1.195822
H         0.000000   -1.979204   -0.465165
H         0.000000   -1.359222    1.195822
H        -1.979204    0.000000    0.465165
H        -1.359222    0.000000   -1.195822
H         1.979204    0.000000    0.465165
H         1.359222    0.000000   -1.195822
```

```
CH4OH sad pt
```

```
0 2
C       -1.211487     .007968     .000407
O        1.293965    -.108694     .000133
H         .009476    -.118020     .002799
H       -1.525529    -.233250    1.010070
H       -1.430665    1.033233    -.278082
H       -1.552710    -.710114    -.737702
H        1.416636     .849894    -.000591


OH2 sad pt

0 3
H         .000000     .000000    -.860287
O         .000000     .000000     .329024
H         .000000     .000000   -1.771905


SH2 sad pt

0 2
H        1.262097    -.220097     .000000
S         .000000     .223153     .000000
H        -.500576   -1.115445     .000000
H        -.761521   -2.234913     .000000


spin orbit corrected barriers in kcal/mol:

OH + CH4 -> CH4 H2O: 6.54
CH4 H2O -> OH + CH4: 19.61
```

```
H + OH -> O + H2: 10.45
O + H2 -> H + OH: 12.9
H + H2S -> H2 + SH: 3.55
H2 + SH -> H + H2S: 17.27

spin orbit corrected atomization energies in kcal/mol:

SiH4: 322.83
SiO: 192.74
S2: 102.79
propyne: 705.06
glyoxal: 633.99
cyclobutane: 1149.37

HTBH38/04 and NHTBH38/04 test sets:

H

0 2
         H


HCl

0,1
Cl
H,1,R

R=1.27444789


H2
```

```
0,1
H
H,1,r

r=0.74187646


Cl

0 2
          Cl




OH

0,2
O
H,1,ROH

ROH=0.96889819



H2O

0,1
O
H,1,OH
H,1,OH,2,HOH
```

```
 OH=0.95691441
 HOH=104.51706026



CH3

0,2
C
H,1,CH
H,1,CH,2,120.
H,1,CH,2,120.,3,180.,0

CH=1.07731727



CH4

0,1
C
H,1,RCH
H,1,RCH,2,109.471221
H,1,RCH,2,109.471221,3,109.471221,1
H,1,RCH,2,109.471221,3,109.471221,-1

RCH=1.08744517



NH3
```

```
0,1
N         0.000000    0.000000    0.112890
H         0.000000    0.938024   -0.263409
H         0.812353   -0.469012   -0.263409
H        -0.812353   -0.469012   -0.263409


NH2

0,2
N
H,1,RBH
H,1,RBH,2,HBH

 RBH=1.02404748
 HBH=103.15937043


C2H6

0,1
 C
 C,1,r1
 H,2,r2,1,a1
 H,1,r3,2,a2,3,d1,0
 H,2,r4,1,a3,4,d2,0
 H,2,r5,1,a4,4,d3,0
 H,1,r6,2,a5,3,d4,0
 H,1,r7,2,a6,3,d5,0
      Variables:
 r1=1.5261835
 r2=1.09022525
```

```
 r3=1.09022621
 r4=1.09022696
 r5=1.09022598
 r6=1.09022516
 r7=1.09022636
 a1=111.25460068
 a2=111.2544043
 a3=111.25444241
 a4=111.25438925
 a5=111.25444374
 a6=111.25438374
 d1=59.89832127
 d2=-60.10130556
 d3=179.89872252
 d4=179.89831085
 d5=-60.10183867



C2H5

0,2
 C
 C,1,r1
 H,2,r2,1,a1
 H,1,r3,2,a2,3,d1,0
 H,2,r4,1,a3,4,d2,0
 H,2,r5,1,a4,4,d3,0
 H,1,r6,2,a5,3,d4,0
      Variables:
 r1=1.49013941
 r2=1.09019546
```

```
 r3=1.0796627
 r4=1.09710761
 r5=1.09036205
 r6=1.07961412
 a1=111.58154811
 a2=120.80192292
 a3=111.7033882
 a4=111.57275888
 a5=120.84716124
 d1=-156.20674238
 d2=84.35050762
 d3=-35.02413072
 d4=33.58250018



F

0 2
     F



HF

0,1
F
H,1,R

R=0.91538107
```

PH3

0,1

P	0.000000	0.000000	0.126411
H	1.191339	0.000000	-0.632056
H	-0.595669	-1.031730	-0.632056
H	-0.595669	1.031730	-0.632056

PH2

0,2

P	0.000000	0.000000	-0.115657
H	1.020130	0.000000	0.867427
H	-1.020130	0.000000	0.867427

O

0 3

o

N2H2

0 1

H	-0.984975	-0.915252	0.000000
N	0.000000	-0.621592	0.000000
N	0.000000	0.621592	0.000000

```
H         0.984975     0.915251     0.000000
```

```
N2H

0 2
H          0.874485    -0.985654     0.000000
N         -0.062463    -0.518712     0.000000
N         -0.062463     0.659520     0.000000
```

```
H2S

0,1
S         0.000000     0.000000     0.102519
H         0.000000     0.966249    -0.820154
H         0.000000    -0.966249    -0.820154
```

```
HS

0,2
S
H,1,R

R=1.34020229
```

```
NH

0,3
N
H,1,RNH

RNH=1.03673136



C5H8

0 1
C       -2.055638   -0.612272    0.000007
C       -1.231096    0.640448    0.000049
C        0.105634    0.734273    0.000026
C        1.057555   -0.374407   -0.000044
C        2.383583   -0.198936   -0.000036
H       -2.705085   -0.641597    0.877132
H       -2.705129   -0.641508   -0.877089
H       -1.451332   -1.516079   -0.000055
H       -1.793665    1.567586    0.000103
H        0.545756    1.725643    0.000064
H        0.665262   -1.383242   -0.000105
H        3.064689   -1.037719   -0.000088
H        2.819275    0.792285    0.000023



H-HCl_H2-Cl_ts

0 2
```

```
H         0.000480   -1.340627    0.000000
Cl        0.000000    0.203252    0.000000
H        -0.000480   -2.114659    0.000000
```

```
OH-H2_H-H2O_ts

0 2
O         -.301064    -.108049    -.000008
H         -.427945     .851569     .000016
H         1.015486    -.100367     .000119
H         1.820968     .113187    -.000073
```

```
CH3-H2_H-CH4_ts

0 2
C          .000000     .264813     .000000
H         1.053429     .516668     .000000
H         -.526627     .517025     .912250
H         -.526627     .517025    -.912250
H         -.000260   -1.117771     .000000
H          .000084   -2.021825     .000000
```

```
OH-CH4_CH3-H2O_ts

0 2
C        -1.211487     .007968     .000407
```

```
O         1.293965    -.108694     .000133
H          .009476    -.118020     .002799
H        -1.525529    -.233250    1.010070
H        -1.430665    1.033233    -.278082
H        -1.552710    -.710114    -.737702
H         1.416636     .849894    -.000591
```

H-H2_H2-H_ts

```
0 2
H         0.000000    0.000000    0.000000
H         0.000000    0.000000    0.929474
H         0.000000    0.000000   -0.929474
```

OH-NH3_H2O-NH2_ts

```
0 2
N        -1.150816    -.043932    -.102559
O         1.179186    -.092696    -.010290
H        -1.303185    -.547638     .766571
H        -1.338913     .935808     .091854
H         -.030687    -.153834    -.353184
H         1.295009     .814753     .294991
```

HCl-CH3_Cl-CH4_ts

```
0 2
C          .244117      .599916    1.702423
H         -.675597      .278482    2.172939
H          .351910    1.663786    1.537672
H         1.140686      .065787    1.987822
H          .057163      .139973     .397112
Cl        -.137580     -.338090    -.959416
```

OH-C2H6_H2O-C2H5_ts

```
0 2
C         1.458334     -.446365     .025478
C          .469423      .697422    -.027493
O        -1.853037     -.314659    -.053055
H         1.301764    -1.061079     .910737
H         1.366585    -1.086189    -.851118
H         2.482245     -.066879     .057150
H          .471069     1.325443     .861037
H          .533524     1.303495    -.928560
H         -.630232      .207816    -.078465
H        -2.267207      .388321     .465751
```

F-H2_HF-H_ts

```
0 2
H          .146568    -1.128390     .000000
F          .000000      .330422     .000000
H         -.146568    -1.845410     .000000
```

O-CH4_OH-CH3_ts

0 3

C	0.000290	-1.142289	0.000000
H	-1.055957	-1.384735	0.000000
H	0.520167	-1.407389	0.912447
H	0.520167	-1.407389	-0.912447
H	0.011560	0.160099	0.000000
O	0.000290	1.361643	0.000000

H-PH3_PH2-H2_ts

0 2

P	.217429	.000088	-.111249
H	.246609	1.034668	.852164
H	.262661	-1.025058	.861623
H	-1.266418	-.010952	-.150626
H	-2.504290	.000028	.105575

H-OH_H2-O_ts

0 3

H	.000000	.000000	-.860287
O	.000000	.000000	.329024
H	.000000	.000000	-1.771905

H-H2S_H2-HS_ts

0 2

H	1.262097	-.220097	.000000
S	.000000	.223153	.000000
H	-.500576	-1.115445	.000000
H	-.761521	-2.234913	.000000

O-HCl_OH-Cl_ts

0 3

Cl	.018820	-.817301	.000000
H	-.470488	.569480	.000000
O	.018820	1.665579	.000000

NH2-CH3_CH4-NH_ts

0 3

C	-1.199577	-.011126	-.000030
N	1.400715	.129862	.000015
H	-1.426660	-.512932	.933057
H	-1.419907	-.591382	-.888143
H	-1.520237	1.022806	-.045783
H	.188926	.126896	.001001
H	1.570338	-.887667	-.000053

NH2-C2H5_C2H6-NH_ts

0 3

C	-1.394984	-0.449661	0.000703
C	-0.435746	0.714063	0.002027
N	1.927570	-0.378352	0.003036
H	-1.200087	-1.120951	-0.835687
H	-1.322095	-1.027884	0.921773
H	-2.428713	-0.105352	-0.089334
H	-0.417688	1.308482	-0.907201
H	-0.441127	1.329095	0.897467
H	0.828501	0.180593	-0.028561
H	2.472592	0.498073	0.003910

C2H6-NH2_NH3-C2H5_ts

0 2

C	-1.485700	-0.448156	-0.000019
C	-0.505042	0.701740	0.000029
N	1.865161	-0.340167	-0.000057
H	-1.354193	-1.076505	-0.880503
H	-1.354159	-1.076611	0.880385
H	-2.517025	-0.086173	0.000025
H	-0.522224	1.316118	-0.897218
H	-0.522205	1.316029	0.897338
H	0.665047	0.147961	-0.000034
H	2.246644	0.159717	-0.804806

```
H        2.246439    0.159133    0.805151
```

```
NH2-CH4_CH3-NH3_ts

0 2
C       -1.260750   -0.000006    0.012291
N        1.313255   -0.000005   -0.136782
H       -1.583987    0.908538   -0.484744
H       -1.463672   -0.004573    1.077302
H       -1.584748   -0.903880   -0.492700
H        0.043108   -0.000064   -0.151692
H        1.480459    0.805577    0.467751
H        1.480557   -0.805524    0.467808
```

```
C5H8_C5H8_ts

0 1
C       -1.299623   -0.904853   -0.020155
C       -1.205947    0.505817   -0.013414
C        0.000000    1.183361    0.153301
C        1.205948    0.505814   -0.013422
C        1.299626   -0.904851   -0.020147
H        2.168797   -1.327549   -0.515697
H        1.032041   -1.454385    0.873166
H        2.037130    1.085583   -0.398504
H        0.000001    2.262913    0.085905
H       -2.037133    1.085587   -0.398481
H       -2.168796   -1.327540   -0.515716
```

```
H       -0.000011   -1.181942   -0.520808
H       -1.032059   -1.454394    0.873158


H

O 2
H


N2O

0,1
 N
 N,1,r1
 O,2,r2,1,180.
      Variables:
 r1=1.12056262
 r2=1.1870483


OH

0,2
O
H,1,ROH

ROH=0.96889819


N2
```

```
0,1
N
N,1,NN

NN=1.09710935


H-N2O_OH-N2_ts

0,2
      1             0        -.303286   -1.930712     .000000
      8             0        -.861006    -.621526     .000000
      7             0         .000000     .257027     .000000
      7             0        1.027333     .729104     .000000


F

0 2
 F


HF

0,1
F
H,1,R

R=0.91538107


H-HF_HF-H_ts
```

```
0  2
      1             0        0.000000    0.000000    1.137217
      9             0        0.000000    0.000000    0.000000
      1             0        0.000000    0.000000   -1.137217


HCl

0,1
Cl
H,1,R

R=1.27444789


H-HCl_HCl-H_ts

0 2
H        0.000000    0.000000    1.485800
Cl       0.000000    0.000000    0.000000
H        0.000000    0.000000   -1.485800


CH3F

0 1
      6             0       -0.632074    0.000001   -0.000000
      9             0        0.749117    0.000002   -0.000002
      1             0       -0.983182   -0.338489    0.972625
      1             0       -0.983222    1.011553   -0.193172
      1             0       -0.983203   -0.673084   -0.779437
```

```
CH3

0,2
C
H,1,CH
H,1,CH,2,120.
H,1,CH,2,120.,3,180.,0

CH=1.07731727


H-CH3F_HF-CH3_ts

0  2
      1             0        -.039764     .000000     .044106
      9             0        -.049321     .000000    1.282554
      6             0        -.061544     .000000    2.951157
      1             0         .990497     .000000    3.194275
      1             0        -.590070     .912355    3.183481
      1             0        -.590070    -.912355    3.183481


F2

0,1
F
F,1,FF

 FF=1.3952041
```

H-F2_HF-F_ts

0 2

1	0	0.000000	0.000000	-2.231273
9	0	0.000000	0.000000	-0.616218
9	0	0.000000	0.000000	0.864138

ClF

0,1

F

Cl,1,R1

R1=1.63033021

Cl

0 2

Cl

CH3-ClF_CH3F-Cl_ts

0 2

17	0	1.454749	-0.001237	-0.000040
9	0	-0.323587	0.004631	0.000124
6	0	-2.387418	-0.002147	-0.000073
1	0	-2.495086	-0.855361	-0.649404
1	0	-2.497313	-0.138673	1.063139

```
      1             0       -2.501537    0.986269   -0.413734


Fmin

-1 1
F


Fmin-CH3F_CH3F-Fmin_ts

-1 1
      9             0         .003098    -.018892    -.015456
      6             0        -.000149    -.000140    1.807857
      1             0        1.069449     .001708    1.809761
      1             0        -.536607     .925133    1.796935
      1             0        -.532601    -.927783    1.817058
      9             0        -.003191     .019974    3.631845


Fmin...CH3F

-1 1
      9             0         .000000     .000000   -1.847626
      6             0         .000000     .000000    -.421873
      1             0         .000000    1.023581    -.073843
      1             0        -.886447    -.511791    -.073843
      1             0         .886447    -.511791    -.073843
      9             0         .000000     .000000    2.153489


Fmin...CH3F_Fmin...CH3F_ts
```

```
-1 1
      9             0          .003098    -.018892    -.015456
      6             0         -.000149    -.000140    1.807857
      1             0         1.069449     .001708    1.809761
      1             0         -.536607     .925133    1.796935
      1             0         -.532601    -.927783    1.817058
      9             0         -.003191     .019974    3.631845


Clmin

-1 1
Cl


CH3Cl

0,1
C        0.000000    0.000000   -1.125886
Cl       0.000000    0.000000    0.656830
H        0.000000    1.027993   -1.470264
H        0.890268   -0.513997   -1.470264
H       -0.890268   -0.513997   -1.470264


Clmin-CH3Cl_CH3Cl-Clmin_ts

-1 1
     17             0         2.322581    -.000132     .000140
      6             0         -.000085     .000491    -.000509
      1             0          .000077    -.744290    -.767605
```

```
      1             0        -.000320    -.291443    1.028021
      1             0         .000081    1.037218    -.261959
     17             0       -2.322542    -.000129     .000130


Clmin...CH3Cl

-1 1
     17             0         .000000     .000000   -2.384735
      6             0         .000000     .000000    -.566331
      1             0         .000000    1.025066    -.224379
      1             0        -.887734    -.512533    -.224379
      1             0         .887734    -.512533    -.224379
     17             0         .000000     .000000    2.624213


Clmin...CH3Cl_Clmin...CH3Cl_ts

-1 1
     17             0        2.322581    -.000132     .000140
      6             0        -.000085     .000491    -.000509
      1             0         .000077    -.744290    -.767605
      1             0        -.000320    -.291443    1.028021
      1             0         .000081    1.037218    -.261959
     17             0       -2.322542    -.000129     .000130


Fmin-CH3Cl_CH3F-Clmin_ts

-1 1
      9             0         .000000     .000000   -2.537929
      6             0         .000000     .000000    -.488372
```

```
      1             0          .000000    1.062087    -.614972
      1             0         -.919795    -.531044    -.614972
      1             0          .919795    -.531044    -.614972
     17             0          .000000     .000000    1.624501


Fmin...CH3Cl

-1 1
     17             0          .000000     .000000    1.623138
      6             0          .000000     .000000    -.227358
      1             0          .000000    1.026321    -.555141
      1             0          .888820    -.513160    -.555141
      1             0         -.888820    -.513160    -.555141
      9             0          .000000     .000000   -2.729308


CH3F...Clmin

-1 1
      9             0          .000000     .000000   -2.648539
      6             0          .000000     .000000   -1.240170
      1             0          .000000    1.024719    -.886406
      1             0         -.887432    -.512359    -.886406
      1             0          .887432    -.512359    -.886406
     17             0          .000000     .000000    1.996299


Fmin...CH3Cl_CH3F...Clmin_ts

-1 1
      9             0          .000000     .000000   -2.537929
```

```
      6             0          .000000      .000000     -.488372
      1             0          .000000     1.062087     -.614972
      1             0         -.919795     -.531044     -.614972
      1             0          .919795     -.531044     -.614972
     17             0          .000000      .000000     1.624501


OHmin

-1,1
O
H,1,r

r=0.96204317


CH3OH

0,1
C       -0.046423    0.663069    0.000000
O       -0.046423   -0.755063    0.000000
H       -1.086956    0.975938    0.000000
H        0.860592   -1.057039    0.000000
H        0.438145    1.071594    0.889539
H        0.438145    1.071594   -0.889539


OHmin-CH3F_CH3OH-Fmin_ts

-1,1
      9             0          .022536     -.007453      .005529
      6             0         -.018420      .005037     1.764925
```

1	0	1.048050	.005240	1.854146
1	0	-.547819	.934707	1.792224
1	0	-.548955	-.923433	1.805762
8	0	.001265	.019200	3.750599
1	0	-.926763	.031615	3.997581

OHmin...CH3F

-1,1

9	0	.000371	-2.468340	.021390
6	0	-.276642	-1.074418	-.002690
1	0	.649290	-.516500	-.009016
1	0	-.841989	-.847119	-.897075
1	0	-.851028	-.826589	.881417
8	0	-.301713	1.582524	-.206544
1	0	-.605112	2.492434	-.164305

CH3OH...Fmin

-1,1

6	0	-1.297997	-.389518	-.000034
8	0	-.477223	.728021	.000054
1	0	-2.351922	-.080232	-.008639
1	0	-1.140853	-1.035821	-.878101
1	0	-1.153178	-1.027513	.886359
1	0	.510580	.371160	.000243
9	0	1.749016	-.190517	-.000010

OHmin...CH3F_CH3OH...Fmin_ts

```
-1,1
      9              0          .022536    -.007453     .005529
      6              0        -.018420     .005037    1.764925
      1              0        1.048050     .005240    1.854146
      1              0        -.547819     .934707    1.792224
      1              0        -.548955    -.923433    1.805762
      8              0         .001265     .019200    3.750599
      1              0        -.926763     .031615    3.997581


HN2

0 2
 n
 n   1 nn2
 h   2 hn3        1 hnn3

nn2         1.1782
hn3         1.0465
hnn3        116.4892


H-N2_HN2_ts

0 2
 n
 n   1 nn2
 h   2 hn3        1 hnn3

nn2         1.122811
hn3         1.430583
```

```
hnn3        117.543


CO

0,1
O
C,1,RCO

RCO=1.12960815


HCO

0  2
      1             0        -.009057     .000000    -.007086
      6             0        -.007035     .000000    1.109678
      8             0         .956040     .000000    1.785656


H-CO_HCO_ts

0  2
      1             0       -1.520864    1.388829     .000000
      6             0         .108633     .549329     .000000
      8             0         .108633    -.585601     .000000


C2H4

0   1
      6         -0.000000    0.000000    0.665593
```

```
      6           0.000000   -0.000000   -0.665593
      1           0.000000    0.921495    1.231668
      1          -0.000000   -0.921495    1.231668
      1           0.000000    0.921495   -1.231668
      1          -0.000000   -0.921495   -1.231668


C2H5

0  2
C 0   -0.258719   -0.816829    0.000000
C 0   -0.250987    0.674191    0.000000
H 0    0.758830   -1.225939    0.000000
H 0   -0.758830   -1.213866    0.883419
H 0   -0.758830   -1.213866   -0.883419
H 0   -0.170021    1.225939   -0.924320
H 0   -0.170021    1.225939    0.924320


H-C2H4_C2H5_ts

0   2
      6           0       -0.567877    0.000051   -0.218958
      6           0        0.751139   -0.000036    0.041932
      1           0       -1.493884   -0.000488    1.531765
      1           0       -1.101691    0.920651   -0.408626
      1           0       -1.102022   -0.920234   -0.409110
      1           0        1.299128   -0.922344    0.173763
      1           0        1.298899    0.922325    0.174363


C3H7
```

0 2

6	1.208440	-0.287189	0.000057
6	-0.065359	0.576132	-0.000057
6	-1.314787	-0.239518	-0.000011
1	1.241369	-0.928395	0.881234
1	1.241394	-0.928586	-0.880980
1	2.101871	0.338727	0.000000
1	-0.048218	1.226851	-0.877089
1	-0.048272	1.227037	0.876834
1	-1.729146	-0.615771	0.924435
1	-1.728763	-0.616415	-0.924369

CH3-C2H4_C3H7_ts

0 2

6	-0.472132	0.645933	-0.000043
6	-1.382617	-0.363885	-0.000002
1	-0.232044	1.164575	-0.917264
1	-0.232342	1.164759	0.917169
1	-1.727128	-0.809810	0.922519
1	-1.726936	-0.810131	-0.922435
6	1.612015	-0.242189	0.000035
1	2.195182	0.668671	-0.001269
1	1.589423	-0.809619	-0.918632
1	1.590245	-0.807598	0.919969

HCN

0 1

```
C         0.000000    0.000000   -0.500365
N         0.000000    0.000000    0.652640
H         0.000000    0.000000   -1.566291


HNC

0  1
      6             0          .000000     .000000    -.737248
      7             0          .000000     .000000     .432089
      1             0          .000000     .000000    1.426960


HCN_HNC_ts

0  1
      6             0          .080319     .620258     .000000
      7             0          .080319    -.568095     .000000
      1             0        -1.044148     .255121     .000000


Reference values for HTBH38/04 barriers (without spin-orbit corrections) in kcal/mol:

forward:
 H-HCl_H2-Cl_ts: 5.7
 OH-H2_H-H2O_ts: 5.1
 CH3-H2_H-CH4_ts: 12.1
 OH-CH4_CH3-H2O_ts: 6.7
 H-H2_H2-H_ts: 9.6
 OH-NH3_H2O-NH2_ts: 3.2
 HCl-CH3_Cl-CH4_ts: 1.7
 OH-C2H6_H2O-C2H5_ts: 3.4
```

```
 F-H2_HF-H_ts: 1.8
 O-CH4_OH-CH3_ts: 13.7
 H-PH3_PH2-H2_ts: 3.1
 H-OH_H2-O_ts: 10.7
 H-H2S_H2-HS_ts: 3.5
 O-HCl_OH-Cl_ts: 9.8
 NH2-CH3_CH4-NH_ts: 8.0
 NH2-C2H5_C2H6-NH_ts: 7.5
 C2H6-NH2_NH3-C2H5_ts: 10.4
 NH2-CH4_CH3-NH3_ts: 14.5
 C5H8_C5H8_ts: 38.4'

reverse:
 H-HCl_H2-Cl_ts: 8.7
 OH-H2_H-H2O_ts: 21.2
 CH3-H2_H-CH4_ts: 15.3
 OH-CH4_CH3-H2O_ts: 19.6
 H-H2_H2-H_ts: 9.6
 OH-NH3_H2O-NH2_ts: 12.7
 HCl-CH3_Cl-CH4_ts: 7.9
 OH-C2H6_H2O-C2H5_ts: 19.9
 F-H2_HF-H_ts: 33.4
 O-CH4_OH-CH3_ts: 8.1
 H-PH3_PH2-H2_ts: 23.2
 H-OH_H2-O_ts: 13.1
 H-H2S_H2-HS_ts: 17.3
 O-HCl_OH-Cl_ts: 10.4
 NH2-CH3_CH4-NH_ts: 22.4
 NH2-C2H5_C2H6-NH_ts: 18.3
 C2H6-NH2_NH3-C2H5_ts: 17.4
 NH2-CH4_CH3-NH3_ts: 17.8
 C5H8_C5H8_ts: 38.4'
```

```
Reference values for NHTBH38/04 barriers (without spin-orbit corrections) in kcal/mol

forward:
H-N2O_OH-N2_ts: 18.14
H-HF_HF-H_ts: 42.18
H-HCl_HCl-H_ts: 18.00
H-CH3F_HF-CH3_ts: 30.38
H-F2_HF-F_ts: 2.27
CH3-ClF_CH3F-Cl_ts: 7.43
Fmin-CH3F_CH3F-Fmin_ts: -0.34
Fmin...CH3F_Fmin...CH3F_ts: 13.38
Clmin-CH3Cl_CH3Cl-Clmin_ts: 3.10
Clmin...CH3Cl_Clmin...CH3Cl_ts: 13.61
Fmin-CH3Cl_CH3F-Clmin_ts: -12.54
Fmin...CH3Cl_CH3F...Clmin_ts: 2.89
OHmin-CH3F_CH3OH-Fmin_ts: -2.78
OHmin...CH3F_CH3OH...Fmin_ts: 10.96
H-N2_HN2_ts: 14.69
H-CO_HCO_ts: 3.17
H-C2H4_C2H5_ts: 1.72
CH3-C2H4_C3H7_ts: 6.85
HCN_HNC_ts: 48.16

reverse:
H-N2O_OH-N2_ts: 83.22
H-HF_HF-H_ts: 42.18
H-HCl_HCl-H_ts: 18.00
H-CH3F_HF-CH3_ts: 57.02
H-F2_HF-F_ts: 106.18
CH3-ClF_CH3F-Cl_ts: 60.17
```

```
Fmin-CH3F_CH3F-Fmin_ts: -0.34
Fmin...CH3F_Fmin...CH3F_ts: 13.38
Clmin-CH3Cl_CH3Cl-Clmin_ts: 3.10
Clmin...CH3Cl_Clmin...CH3Cl_ts: 13.61
Fmin-CH3Cl_CH3F-Clmin_ts: 20.11
Fmin...CH3Cl_CH3F...Clmin_ts: 29.62
OHmin-CH3F_CH3OH-Fmin_ts: 17.33
OHmin...CH3F_CH3OH...Fmin_ts: 47.20
H-N2_HN2_ts: 10.72
H-CO_HCO_ts: 22.68
H-C2H4_C2H5_ts: 41.75
CH3-C2H4_C3H7_ts: 32.97
HCN_HNC_ts: 33.11


G2/97, G3-3 test sets:

0,2
H



0,2
Li



0,1
Be
```

0,2
B

0,3
C

0,4
N

0,3
O

0,2
F

0,2
Na

0,1
Mg

```
0,2
Al



0,3
Si



0,4
P



0,3
S



0,2
Cl


LiH, B3LYP/6-31G(2df,p) geometry

0,1
Li
H,1,R
```

```
R=1.61452972


BeH, B3LYP/6-31G(2df,p) geometry

0,2
Be
H,1,RBEH

RBEH=1.34380733


CH radical, B3LYP/6-31G(2df,p) geometry

0,2
C
H,1,RCH

RCH=1.13062603


CH2 (3B1), B3LYP/6-31G(2df,p) geometry

0,3
C
H,1,RCH
H,1,RCH,2,HCH

RCH=1.08097342
HCH=133.83742404
```

```
CH2 (1A1), B3LYP/6-31G(2df,p) geometry

0,1
C
H,1,CH
H,1,CH,2,HCH

CH=1.11792921
HCH=99.85526193


CH3 radical, D3h, B3LYP/6-31G(2df,p) geometry

0,2
C
H,1,CH
H,1,CH,2,120.
H,1,CH,2,120.,3,180.,0

CH=1.08130823


CH4, B3LYP/6-31G(2df,p) geometry

0,1
C
H,1,RCH
H,1,RCH,2,109.47122063
H,1,RCH,2,109.47122063,3,109.47122063,1
H,1,RCH,2,109.47122063,3,109.47122063,-1
```

```
RCH=1.09185419


NH radical, B3LYP/6-31G(2df,p) geometry

0,3
N
H,1,RNH

RNH=1.0447328


NH2 (2B1), B3LYP/6-31G(2df,p) geometry

0,2
N
H,1,RBH
H,1,RBH,2,HBH

RBH=1.03128471
HBH=101.91770685


Ammonia, B3LYP/6-31G(2df,p) geometry

0,1
N
X,1,1.
H,1,RNH,2,XNH
H,1,RNH,2,XNH,3,120.,0
H,1,RNH,2,XNH,3,240.,0
```

```
RNH=1.01719433
XNH=113.26166981


OH radical, B3LYP/6-31G(2df,p) geometry

0,2
O
H,1,ROH

ROH=0.97613331


H2O, B3LYP/6-31G(2df,p) geometry

0,1
O
H,1,OH
H,1,OH,2,HOH

OH=0.96210248
HOH=103.71685008


HF, B3LYP/6-31G(2df,p) geometry

0,1
F
H,1,R

R=0.91945793
```

```
SiH2 (1A1), B3LYP/6-31G(2df,p) geometry

0,1
Si
X,1,1.
H,1,R,2,A
H,1,R,2,A,3,180.,0

R=1.52561661
A=45.67372696


SiH2 (3B1), B3LYP/6-31G(2df,p) geometry

0,3
Si
X,1,1.
H,1,R,2,A
H,1,R,2,A,3,180.,0

R=1.48656291
A=59.20730743


SiH3, c3v, B3LYP/6-31G(2df,p) geometry

0,2
Si
X,1,1.
H,1,R,2,BETA
H,1,R,2,BETA,3,120.,0
```

```
H,1,R,2,BETA,3,-120.,0

R=1.48480778
BETA=107.89090342


SiH4, B3LYP/6-31G(2df,p) geometry

0,1
Si
H,1,R
H,1,R,2,109.47122063
H,1,R,2,109.47122063,3,120.,0
H,1,R,2,109.47122063,3,-120.,0

R=1.48241986


PH2 doublet, B3LYP/6-31G(2df,p) geometry

0,2
P
X,1,1.
H,1,R,2,A
H,1,R,2,A,3,180.,0

R=1.42692167
A=45.79311753


PH3, c3v, B3LYP/6-31G(2df,p) geometry
```

```
0,1
P
X,1,1.
H,1,R,2,BETA
H,1,R,2,BETA,3,120.,0
H,1,R,2,BETA,3,-120.,0

R=1.42205572
BETA=122.9486097


H2S, B3LYP/6-31G(2df,p) geometry

0,1
S
X,1,1.
H,1,R,2,A
H,1,R,2,A,3,180.,0

R=1.34531822
A=46.20925632


HCl, B3LYP/6-31G(2df,p) geometry

0,1
Cl
H,1,R

R=1.28367324
```

```
Li2, B3LYP/6-31G(2df,p) geometry

0,1
Li
Li,1,R

R=2.72127987


LiF, B3LYP/6-31G(2df,p) geometry

0,1
Li
F,1,LiF

LiF=1.56359565


Acetylene, B3LYP/6-31G(2df,p) geometry

0,1
C
C,1,CC
X,2,1.,1,90.
H,2,CH,3,90.,1,180.,0
X,1,1.,2,90.,3,180.,0
H,1,CH,5,90.,2,180.,0

CC=1.1989086
CH=1.06216907
```

```
Ethylene, B3LYP/6-31G(2df,p) geometry

0,1
C
C,1,RCC
H,1,RCH,2,HCC
H,1,RCH,2,HCC,3,180.,0
H,2,RCH,1,HCC,3,0.,0
H,2,RCH,1,HCC,3,180.,0

RCC=1.32718886
RCH=1.08577456
HCC=121.95017938


Ethane, B3LYP/6-31G(2df,p) geometry

0,1
C
C,1,AA
H,1,AH,2,HAA
H,1,AH,2,HAA,3,120.,0
H,1,AH,2,HAA,3,-120.,0
H,2,AH,1,HAA,3,180.,0
H,2,AH,1,HAA,6,120.,0
H,2,AH,1,HAA,6,-120.,0

AA=1.53003633
AH=1.09484731
HAA=111.3741399
```

```
CN radical, 2-SIGMA-PLUS, B3LYP/6-31G(2df,p) geometry

0,2
C
N,1,R

R=1.16945125


HCN, B3LYP/6-31G(2df,p) geometry

0,1
C
N,1,AB
X,1,1.,2,90.
H,1,AH,3,90.,2,180.,0

AB=1.15174191
AH=1.06658792


CO, B3LYP/6-31G(2df,p) geometry

0,1
O
C,1,RCO

RCO=1.1309114


HCO, BENT CS, B3LYP/6-31G(2df,p) geometry
```

```
0,2
C
O,1,CO
H,1,CH,2,HCO

CO=1.17621067
CH=1.12859543
HCO=124.03532275


H2CO, B3LYP/6-31G(2df,p) geometry

0,1
O
C,1,RCO
H,2,RH,1,THETA
H,2,RH,1,THETA,3,180.,0

RCO=1.19995954
THETA=122.47953272
RH=1.1108676


Methanol, B3LYP/6-31G(2df,p) geometry

0,1
C
O,1,AB
H,1,AH3,2,H3AB
H,2,BH9,1,H9BA,3,180.,0
X,1,1.,2,BAH12,3,180.,0
H,1,AH1,5,H1AH2,2,90.,0
```

```
H,1,AH1,5,H1AH2,2,-90.,0

AB=1.41526798
AH1=1.10037418
AH3=1.09348232
BH9=0.96129158
H1AH2=54.13726394
BAH12=131.31510075
H3AB=106.94071399
H9BA=107.8511363


Nitrogen N2, B3LYP/6-31G(2df,p) geometry opt=z-matrix

0,1
N
N,1,NN

NN=1.0987918


H2NNH2, B3LYP/6-31G(2df,p) geometry opt=z-matrix

0,1
N
N,1,AA
H,1,AH4,2,H4AA
H,1,AH5,2,H5AA,3,H4AH5,1
H,2,AH4,1,H4AA,3,H4AAH7,0
H,2,AH5,1,H5AA,5,H4AH5,1

AA=1.43687706
```

```
AH4=1.01893091
AH5=1.01495037
H4AA=111.61361711
H5AA=106.79854321
H4AH5=106.64730213
H4AAH7=27.6651151


NO radical, 2pi, B3LYP/6-31G(2df,p) geometry opt=z-matrix

0,2
N
O,1,r

r=1.15122729


Oxygen O2, B3LYP/6-31G(2df,p) geometry opt=z-matrix

0,3
O
O,1,r

r=1.20639068


H2O2, B3LYP/6-31G(2df,p) geometry opt=z-matrix

0,1
O
O,1,AA
H,1,AH4,2,H4AA
```

```
H,2,AH4,1,H4AA,3,H4AAH8,0

AA=1.44582784
AH4=0.9672488
H4AA=100.44937014
H4AAH8=112.33679746


Fluorine F2, B3LYP/6-31G(2df,p) geometry opt=z-matrix

0,1
F
F,1,FF

FF=1.38792514


CO2, B3LYP/6-31G(2df,p) geometry

0,1
C
O,1,R
X,1,1.,2,90.
O,1,R,3,90.,2,180.,0

R=1.16287946


Na2, B3LYP/6-31G(2df,p) geometry

0,1
Na
```

```
Na,1,R

R=3.0149584


Si2 3-SGG, B3LYP/6-31G(2df,p) geometry

0,3
Si
Si,1,R

R=2.27042797


P2, B3LYP/6-31G(2df,p) geometry

0,1
P
P,1,PP

PP=1.8953162


S2, B3LYP/6-31G(2df,p) geometry

0,3
S
S,1,R

R=1.91215538
```

```
Cl2, B3LYP/6-31G(2df,p) geometry

0,1
Cl
Cl,1,R

R=2.01648224


NaCl, B3LYP/6-31G(2df,p) geometry

0,1
Na
Cl,1,NaCl

NaCl=2.3607642


SiO, B3LYP/6-31G(2df,p) geometry

0,1
Si
O,1,sio

sio=1.51282579


CS, B3LYP/6-31G(2df,p) geometry

0,1
C
S,1,CS
```

```
CS=1.54093216


SO, B3LYP/6-31G(2df,p) geometry opt=z-matrix

0,3
O
S,1,OS

OS=1.49681906


ClO 2-PI, B3LYP/6-31G(2df,p) geometry

0,2
Cl
O,1,R

R=1.59262773


ClF 1-SG, B3LYP/6-31G(2df,p) geometry

0,1
F
Cl,1,R1

R1=1.64275079


Si2H6, B3LYP/6-31G(2df,p) geometry
```

```
0,1
Si
Si,1,R
H,1,SIH,2,SICC
H,1,SIH,2,SICC,3,120.,0
H,1,SIH,2,SICC,3,-120.,0
H,2,SIH,1,SICC,3,180.,0
H,2,SIH,1,SICC,6,120.,0
H,2,SIH,1,SICC,6,-120.,0

SICC=110.49912192
SIH=1.48548901
R=2.35421744


CH3Cl, B3LYP/6-31G(2df,p) geometry

0,1
C
Cl,1,CCl
H,1,CH,2,HCCl
H,1,CH,2,HCCl,3,120.,0
H,1,CH,2,HCCl,3,240.,0

CCl=1.79885648
CH=1.08881113
HCCl=108.3077969


CH3SH, METHANETHIOL STAGGERED, B3LYP/6-31G(2df,p) geometry
```

```
0,1
C
S,1,CS
H,2,SH,1,CSH
H,1,CHA,2,HACS,3,180.,0
X,1,1.,2,XCS,3,0.,0
H,1,CHB,5,HALF,2,90.,0
H,1,CHB,5,HALF,2,-90.,0

CS=1.82939003
SH=1.34584251
CHA=1.09139903
CHB=1.09069821
CSH=97.1035912
HACS=106.02325623
XCS=129.48465195
HALF=55.21415843


HOCl, B3LYP/6-31G(2df,p) geometry

0,1
O
H,1,OH
Cl,1,OCl,2,HOCl

OH=0.96804646
OCl=1.7074574
HOCl=102.46612245


SO2, B3LYP/6-31G(2df,p) geometry
```

```
0,1
S
O,1,SO
O,1,SO,2,OSO

SO=1.44255426
OSO=119.22404594


BF3 (planar), B3LYP/6-31G(2df,p) geometry

0,1
B
F,1,BF
F,1,BF,2,120.
F,1,BF,2,120.,3,180.,0

BF=1.30881545


BCl3 (D3h), B3LYP/6-31G(2df,p) geometry

0,1
B
X,1,1.
X,1,1.,2,90.
Cl,1,R2,2,ALPHA,3,0.,0
Cl,1,R2,2,ALPHA,3,120.,0
Cl,1,R2,2,ALPHA,3,-120.,0

R2=1.75062062
```

```
ALPHA=90.


AlF3, B3LYP/6-31G(2df,p) geometry

0,1
Al
X,1,1.
X,1,1.,2,90.
F,1,R2,2,ALPHA,3,0.,0
F,1,R2,2,ALPHA,3,120.,0
F,1,R2,2,ALPHA,3,-120.,0

R2=1.63152469
ALPHA=90.


AlCl3, B3LYP/6-31G(2df,p) geometry

0,1
Al
X,1,1.
X,1,1.,2,90.
Cl,1,R2,2,ALPHA,3,0.,0
Cl,1,R2,2,ALPHA,3,120.,0
Cl,1,R2,2,ALPHA,3,-120.,0

R2=2.08019057
ALPHA=90.


CF4, B3LYP/6-31G(2df,p) geometry
```

```
0,1
C
F,1,R
F,1,R,2,A
F,1,R,2,A,3,120.,0
F,1,R,2,A,3,-120.,0

R=1.32143587
A=109.47122063


CCl4, B3LYP/6-31G(2df,p) geometry

0,1
C
Cl,1,R
Cl,1,R,2,A
Cl,1,R,2,A,3,120.,0
Cl,1,R,2,A,3,-120.,0

R=1.78422687
A=109.47122063


O=C=S, Singlet Sigma(+) B3LYP/6-31G(2df,p) geometry

0,1
O
C,1,C-O
X,2,1.,1,90.
S,2,C-S,3,90.,1,180.,0
```

```
C-O=1.15765333
C-S=1.56701428


CS2, B3LYP/6-31G(2df,p) geometry

0,1
S
C,1,r1
X,2,1.,1,90.
S,2,r1,3,90.,1,180.,0

r1=1.55605459


COF2, B3LYP/6-31G(2df,p) geometry

0,1
O
C,1,CO
F,2,CF,1,FCO
F,2,CF,1,FCO,3,180.,0

CO=1.17477079
CF=1.31218225
FCO=126.07585309


SiF4, B3LYP/6-31G(2df,p) geometry

0,1
```

```
Si
F,1,sif
F,1,sif,2,109.47122063
F,1,sif,2,109.47122063,3,120.,0
F,1,sif,2,109.47122063,3,-120.,0

sif=1.56479184


SiCl4, Td 1a1, B3LYP/6-31G(2df,p) geometry

0,1
Si
Cl,1,r
Cl,1,r,2,109.47122063
Cl,1,r,2,109.47122063,3,109.47122063,1
Cl,1,r,2,109.47122063,3,109.47122063,-1

r=2.04091393


N2O, B3LYP/6-31G(2df,p) geometry

0,1
N
N,1,r1
X,2,1.,1,90.
O,2,r2,3,90.,1,180.,0

r1=1.12774303
r2=1.18577044
```

```
ClNO, B3LYP/6-31G(2df,p) geometry

0,1
Cl
N,1,r1
O,2,r2,1,a

r1=1.98909401
r2=1.13450032
a=113.88561238


NF3, c3v B3LYP/6-31G(2df,p) geometry

0,1
N
X,1,1.
F,1,R,2,BETA
F,1,R,2,BETA,3,120.,0
F,1,R,2,BETA,3,-120.,0

R=1.37292515
BETA=116.21894033


PF3, c3v B3LYP/6-31G(2df,p) geometry

0,1
P
X,1,1.
F,1,R,2,BETA
```

```
F,1,R,2,BETA,3,120.,0
F,1,R,2,BETA,3,-120.,0

R=1.57615131
BETA=119.55957178


Ozone O3, 1-a1 B3LYP/6-31G(2df,p) geometry

O,1
O
O,1,r
O,2,r,1,a

r=1.25530878
a=117.9490422


F2O, B3LYP/6-31G(2df,p) geometry

O,1
F
O,1,r1
X,2,1.,1,90.
F,2,r1,3,a,1,180.,0

r1=1.39565115
a=166.16423883


ClF3, C2V B3LYP/6-31G(2df,p) geometry
```

```
0,1
Cl
F,1,R1
F,1,R2,2,A1
F,1,R2,2,A1,3,180.,0

R1=1.62598019
R2=1.71440648
A1=87.36101111


CF2=CF2, D2H SINGLET B3LYP/6-31G(2df,p) geometry

0,1
C
C,1,C2-C1
F,1,C-F,2,F-C-C
F,1,C-F,2,F-C-C,3,180.,0
F,2,C-F,1,F-C-C,3,0.,0
F,2,C-F,1,F-C-C,3,180.,0

C2-C1=1.32349394
C-F=1.31429908
F-C-C=123.30251259


Cl2C=CCl2, B3LYP/6-31G(2df,p) geometry

0,1
C
C,1,cc
Cl,1,ccl,2,cccl
```

```
Cl,1,ccl,2,cccl,3,180.,0
Cl,2,ccl,1,cccl,3,180.,0
Cl,2,ccl,1,cccl,3,0.,0

cc=1.34358034
ccl=1.72387501
cccl=122.46213503


CF3CN, B3LYP/6-31G(2df,p) geometry

0,1
C
C,1,r1
F,1,R,2,A
F,1,R,2,A,3,120.,0
F,1,R,2,A,3,-120.,0
X,2,1.,1,90.,3,0.,0
N,2,r2,6,90.,1,180.,0

r1=1.48569112
r2=1.15235052
R=1.32924825
A=110.06152181


Propyne, C3V B3LYP/6-31G(2df,p) geometry

0,1
C
C,1,R1
X,1,1.,2,90.
```

```
C,1,R2,3,90.,2,180.,0
X,2,1.,1,90.,3,0.,0
H,2,R3,5,90.,1,180.,0
H,4,R4,1,THETA1,3,0.,0
H,4,R4,1,THETA1,7,120.,0
H,4,R4,1,THETA1,7,-120.,0

R1=1.20145885
R2=1.45496349
R3=1.06146513
R4=1.09526757
THETA1=111.19520898
```

Allene, D2D B3LYP/6-31G(2df,p) geometry

```
0,1
C
C,1,R1
X,1,1.,2,90.
C,1,R1,3,90.,2,180.,0
H,2,R2,1,THETA1,3,0.,0
H,2,R2,1,THETA1,3,180.,0
H,4,R2,1,THETA1,3,90.,0
H,4,R2,1,THETA1,3,-90.,0

R1=1.30139909
R2=1.08618235
THETA1=121.53108121
```

Cyclopropene, C2V B3LYP/6-31G(2df,p) geometry

```
0,1
X
C,1,R1
C,1,R2,2,90.
C,1,R2,2,90.,3,180.,0
H,2,R3,1,THETA1,3,90.,0
H,2,R3,1,THETA1,3,-90.,0
H,3,R4,1,THETA2,2,180.,0
H,4,R4,1,THETA2,2,180.,0

R1=1.3612372
R2=0.64528841
R3=1.09254783
R4=1.07566736
THETA1=123.42119338
THETA2=149.96802304


Propene, CS B3LYP/6-31G(2df,p) geometry

0,1
C
C,1,R1
H,1,R2,2,THETA1
H,1,R3,2,THETA2,3,180.,0
H,2,R4,1,THETA3,4,0.,0
C,2,R5,1,THETA4,5,180.,0
H,6,R6,2,THETA5,5,180.,0
X,6,1.,2,THETA6,5,0.,0
H,6,R7,8,THETA7,2,90.,0
H,6,R7,8,THETA7,2,-90.,0
```

```
R1=1.32925219
R2=1.08677372
R3=1.08483135
R4=1.08961167
R5=1.49980667
R6=1.09387616
R7=1.09717141
THETA1=121.6375825
THETA2=121.91652557
THETA3=118.97790641
THETA4=125.32396106
THETA5=111.5565194
THETA6=127.10533662
THETA7=53.21778134


Cyclopropane, D3H B3LYP/6-31G(2df,p) geometry

0,1
C
X,1,1.
C,1,R1,2,150.
C,1,R1,2,150.,3,180.,0
H,1,R2,2,THETA1,3,90.,0
H,1,R2,2,THETA1,3,-90.,0
X,3,1.,1,150.,2,0.,0
H,3,R2,7,THETA1,1,90.,0
H,3,R2,7,THETA1,1,-90.,0
X,4,1.,1,150.,2,0.,0
H,4,R2,10,THETA1,1,90.,0
H,4,R2,10,THETA1,1,-90.,0
```

```
R1=1.50714694
R2=1.08443318
THETA1=56.99370306


Propane, C2V B3LYP/6-31G(2df,p) geometry

0,1
C
X,1,1.
C,1,R1,2,THETA1
C,1,R1,2,THETA1,3,180.,0
H,1,R2,2,THETA2,3,90.,0
H,1,R2,2,THETA2,3,-90.,0
H,3,R3,1,THETA3,2,180.,0
H,4,R3,1,THETA3,2,180.,0
X,3,1.,1,THETA4,2,0.,0
H,3,R4,9,THETA5,1,90.,0
H,3,R4,9,THETA5,1,-90.,0
X,4,1.,1,THETA4,2,0.,0
H,4,R4,12,THETA5,1,90.,0
H,4,R4,12,THETA5,1,-90.,0

R1=1.53121947
R2=1.09728045
R3=1.09467797
R4=1.09594628
THETA1=56.46081592
THETA2=127.00393303
THETA3=111.58675061
THETA4=127.51157215
```

THETA5=53.70520872

1.3-Butadiene, trans- C2H B3LYP/6-31G(2df,p) geometry

0,1
C
C,1,CDC
C,2,CSC,1,CCC
C,3,CDC,2,CCC,1,180.,0
H,1,CH1,2,CC1,3,180.,0
H,1,CH2,2,CC2,3,0.,0
H,2,CH3,1,CC3,3,180.,0
H,3,CH3,4,CC3,2,180.,0
H,4,CH2,3,CC2,2,0.,0
H,4,CH1,3,CC1,2,180.,0

CDC=1.33634977
CSC=1.45421177
CH1=1.08398245
CH2=1.08621796
CH3=1.08915354
CCC=124.4471241
CC1=121.92595908
CC2=121.45999519
CC3=119.49630428

2-Butyne, D3h (eclipsed). B3LYP/6-31G(2df,p) Geometry

0,1
C

```
C,1,CCS
X,2,1.,1,90.
C,2,CCT,3,90.,1,180.,0
X,4,1.,2,90.,3,0.,0
C,4,CCS,5,90.,2,180.,0
H,1,CH,2,HCC,3,0.,0
H,1,CH,2,HCC,3,120.,0
H,1,CH,2,HCC,3,-120.,0
H,6,CH,4,HCC,7,0.,0
H,6,CH,4,HCC,7,120.,0
H,6,CH,4,HCC,7,-120.,0

CCS=1.45619443
CCT=1.20358637
CH=1.09584236
HCC=111.4025293


Methylene cyclopropane, C2v symm. B3LYP/6-31G(2df,p) Geom.

0,1
C,0.,0.,0.3171760286
C,0.7693069711,0.,-0.9304892921
C,-0.7693069711,0.,-0.9304892921
C,0.,0.,1.6335892725
H,1.2773319304,-0.9111694913,-1.2357350504
H,1.2773319304,0.9111694913,-1.2357350504
H,-1.2773319304,0.9111694913,-1.2357350504
H,-1.2773319304,-0.9111694913,-1.2357350504
H,0.9251490515,0.,2.2021099501
H,-0.9251490515,0.,2.2021099501
```

```
Bicyclo[1.1.0]butane, C2v symm. B3LYP/6-31G(2df,p) Geometry

0,1
C,1.1353522196,0.,0.3145853609
C,-1.1353522196,0.,0.3145853609
C,0.,-0.7432012006,-0.3213258386
C,0.,0.7432012006,-0.3213258386
H,1.2367850377,0.,1.4022375557
H,2.0834670474,0.,-0.2186439415
H,-1.2367850377,0.,1.4022375557
H,-2.0834670474,0.,-0.2186439415
H,0.,-1.4407616032,-1.1431507484
H,0.,1.4407616032,-1.1431507484


Cyclobutene, B3LYP/6-31G(2df,p) geometry

0,1
X
X,1,R
C,1,CDC,2,90.
C,1,CDC,2,90.,3,180.,0
C,2,CSC,1,90.,3,0.,0
C,2,CSC,1,90.,3,180.,0
H,3,CH1,1,HCX,2,180.,0
H,4,CH1,1,HCX,2,180.,0
X,5,1.,2,ZCY,1,180.,0
X,6,1.,2,ZCY,1,180.,0
H,5,CH3,9,HAL,2,90.,0
H,5,CH3,9,HAL,2,-90.,0
H,6,CH3,10,HAL,2,90.,0
```

```
H,6,CH3,10,HAL,2,-90.,0

R=1.51377456
CDC=0.66881993
CSC=0.78605659
CH1=1.08423142
HCX=133.71114872
ZCY=135.93573668
CH3=1.09534589
HAL=54.19084986


Cyclobutane, B3LYP/6-31G(2df,p) geometry

0,1
X
X,1,1.
X,1,1.,2,90.
X,1,1.,3,90.,2,180.,0
C,1,R,2,A,3,0.,0
C,1,R,2,A,3,180.,0
C,1,R,4,A,3,90.,0
C,1,R,4,A,3,-90.,0
H,5,RH1,1,A1,2,180.,0
H,5,RH2,1,A2,2,0.,0
H,6,RH1,1,A1,2,180.,0
H,6,RH2,1,A2,3,0.,0
H,7,RH1,1,A1,4,180.,0
H,7,RH2,1,A2,4,0.,0
H,8,RH1,1,A1,4,180.,0
H,8,RH2,1,A2,4,0.,0
```

R=1.091568

RH1=1.09286036

RH2=1.09422654

A=83.4423779

A1=137.13334167

A2=114.51098771

Isobutene, Single bonds trans. C2v symm. B3LYP/6-31G(2df,p) Geometry

0,1

C,0.,0.,-1.4569984546

C,0.,0.,-0.1245699907

H,0.9232491156,0.,-2.0278241905

H,-0.9232491156,0.,-2.0278241905

C,1.2749651379,0.,0.6779468785

H,2.1596895822,0.,0.036454784

H,1.3272264221,0.8783935195,1.3341967356

H,1.3272264221,-0.8783935195,1.3341967356

C,-1.2749651379,0.,0.6779468785

H,-2.1596895822,0.,0.036454784

H,-1.3272264221,-0.8783935195,1.3341967356

H,-1.3272264221,0.8783935195,1.3341967356

n-Butane, B3LYP/6-31G(2df,p) geometry

0,1

C

C,1,dcc1

C,2,dcc2,1,accc

C,3,dcc1,2,accc,1,180.,0

```
H,1,dch1,2,ach1,3,180.,0
H,4,dch1,3,ach1,2,180.,0
H,1,dch2,2,ach2,3,thccc2,0
H,1,dch2,2,ach2,3,-thccc2,0
H,4,dch2,3,ach2,2,thccc2,0
H,4,dch2,3,ach2,2,-thccc2,0
H,2,dch3,3,ach3,4,thccc3,0
H,2,dch3,3,ach3,4,-thccc3,0
H,3,dch3,2,ach3,1,thccc3,0
H,3,dch3,2,ach3,1,-thccc3,0

dcc1=1.5308689
dcc2=1.53257035
accc=113.25595793
dch1=1.09460679
ach1=111.54566525
dch2=1.09586998
ach2=111.17104106
thccc2=59.82111835
dch3=1.09833316
ach3=109.16144001
thccc3=57.66494441


Isobutane, B3LYP/6-31G(2df,p) geometry

0,1
C
H,1,RCH1
C,1,RCC,2,A1
H,3,RCH2,1,A2,2,180.,0
X,3,1.,1,A3,4,180.,0
```

```
H,3,RCH3,5,A4,1,90.,0
H,3,RCH3,5,A4,1,-90.,0
C,1,RCC,2,A1,3,120.,0
H,8,RCH2,1,A2,2,180.,0
X,8,1.,1,A3,9,180.,0
H,8,RCH3,10,A4,1,90.,0
H,8,RCH3,10,A4,1,-90.,0
C,1,RCC,2,A1,3,-120.,0
H,13,RCH2,1,A2,2,180.,0
X,13,1.,1,A3,14,180.,0
H,13,RCH3,15,A4,1,90.,0
H,13,RCH3,15,A4,1,-90.,0

RCC=1.53418012
RCH1=1.09928625
RCH2=1.09690734
RCH3=1.09523299
A1=107.78771059
A2=110.83461306
A3=128.27962037
A4=53.9219933


Spiropentane, D2d symm. B3LYP/6-31G(2df,p) Geometry

0,1
X
C,1,1.
X,2,r,1,90.
X,2,r,1,90.,3,180.,0
C,3,ra,2,90.,1,90.,0
C,3,ra,2,90.,1,-90.,0
```

```
C,4,ra,2,90.,1,0.,0
C,4,ra,2,90.,1,180.,0
H,5,rh,3,ah,2,t1,0
H,5,rh,3,ah,2,-t1,0
H,6,rh,3,ah,2,-t1,0
H,6,rh,3,ah,2,t1,0
H,7,rh,4,ah,2,t1,0
H,7,rh,4,ah,2,-t1,0
H,8,rh,4,ah,2,-t1,0
H,8,rh,4,ah,2,t1,0

r=1.26923506
ra=0.76410145
rh=1.08590598
ah=117.68798133
t1=108.4537837


Benzene, B3LYP/6-31G(2df,p) geometry

0,1
X
C,1,r1
C,1,r1,2,60.
C,1,r1,3,60.,2,180.,0
C,1,r1,4,60.,3,180.,0
C,1,r1,5,60.,4,180.,0
C,1,r1,6,60.,5,180.,0
H,2,r2,3,120.,4,180.,0
H,3,r2,4,120.,5,180.,0
H,4,r2,5,120.,6,180.,0
H,5,r2,6,120.,7,180.,0
```

```
H,6,r2,7,120.,2,180.,0
H,7,r2,2,120.,3,180.,0

r1=1.39356657
r2=1.08518723


CH2F2, C2V B3LYP/6-31G(2df,p) geometry

0,1
C
X,1,1.
F,1,CF,2,XCF
F,1,CF,2,XCF,3,180.,0
H,1,CH,2,XCH,3,90.,0
H,1,CH,2,XCH,3,-90.,0

CF=1.35116413
CH=1.09755107
XCF=54.48411561
XCH=124.07576724


CHF3, TRI-FLUOROMETHANE B3LYP/6-31G(2df,p) geometry

0,1
C
H,1,CH
F,1,CF,2,FCH
F,1,CF,2,FCH,3,120.,0
F,1,CF,2,FCH,3,-120.,0
```

```
CH=1.09540894
CF=1.33357305
FCH=110.34623604


CH2Cl2, C2V B3LYP/6-31G(2df,p) geometry

0,1
C
X,1,1.
Cl,1,CCl,2,HClX
Cl,1,CCl,2,HClX,3,180.,0
H,1,CH,2,HCX,3,90.,0
H,1,CH,2,HCX,3,-90.,0

CCl=1.78534542
CH=1.08633676
HClX=56.48815038
HCX=124.02713411


CHCl3, B3LYP/6-31G(2df,p) geometry

0,1
C
H,1,R
Cl,1,R1,2,A
Cl,1,R1,2,A,3,120.,0
Cl,1,R1,2,A,3,-120.,0

R=1.08454386
R1=1.78080465
```

```
A=107.67546003


Methylamine, B3LYP/6-31G(2df,p) geometry

0,1
C
N,1,AB
H,1,AH3,2,H3AB
X,2,1.,1,ABH78,3,0.,0
H,2,BH7,4,H7BH8,1,90.,0
H,2,BH7,4,H7BH8,1,-90.,0
X,1,1.,2,BAH12,3,180.,0
H,1,AH1,7,H1AH2,2,90.,0
H,1,AH1,7,H1AH2,2,-90.,0

AB=1.46466618
AH1=1.0948822
AH3=1.10260845
BH7=1.01551264
BAH12=123.7159906
H3AB=115.59798696
ABH78=123.87413342
H1AH2=53.58662559
H7BH8=52.86710281


Acetonitrile, CH3-CN. C3v symm. B3LYP/6-31G(2df,p) Geometry

0,1
C
C,1,CC
```

```
X,2,1.,1,90.
N,2,CN,3,90.,1,180.,0
H,1,CH,2,HCC,3,0.,0
H,1,CH,2,HCC,5,120.,0
H,1,CH,2,HCC,5,240.,0

CC=1.45694541
CN=1.15501784
CH=1.09334838
HCC=110.3296525


Nitromethane, ch3no2 B3LYP/6-31G(2df,p) geometry

0,1
C
N,1,rn1
O,2,ro1,1,ao1
O,2,ro2,1,ao2,3,to2,0
H,1,rh1,2,ah1,3,th1,0
H,1,rh2,2,ah2,5,th2,0
H,1,rh3,2,ah3,5,th3,0

rn1=1.49947604
ro1=1.22027025
ao1=116.97787532
ro2=1.22027503
ao2=116.94442212
to2=181.46941032
rh1=1.0915516
ah1=106.80772511
th1=89.86550941
```

```
rh2=1.08778603
ah2=108.0196909
th2=118.68994587
rh3=1.08771661
ah3=108.04470028
th3=-118.77257962


Methylnitrite, CH3-O-N=O. NOCH trans, ONOC cis. Cs symm. B3LYP/6-31G(2df,p) Geom

0,1
C,-0.3002977655,-1.1043691066,0.7324553073
O,-0.3118489985,0.3301264521,0.7610277188
H,-0.6973662558,-1.4049934565,1.7012561318
H,0.7168647712,-1.4824371283,0.5963439072
H,-0.9294727507,-1.4822553908,-0.0783604316
N,0.1607950897,0.9533921894,-0.3920972598
O,0.5101233986,0.2101429591,-1.244689048


Methylsilane, CH3-SiH3. C3v symm. B3LYP/6-31G(2df,p) Geometry

0,1
C
Si,1,SiC
H,1,CH,2,HCSi
H,1,CH,2,HCSi,3,120.,0
H,1,CH,2,HCSi,3,240.,0
H,2,SiH,1,HSiC,3,180.,0
H,2,SiH,1,HSiC,6,120.,0
H,2,SiH,1,HSiC,6,240.,0
```

```
SiC=1.88055604
CH=1.09407086
SiH=1.48615217
HCSi=110.93996132
HSiC=110.77973388


Formic acid, HCOOH. HOCO cis. Cs symm. B3LYP/6-31G(2df,p) Geometry

0,1
O
C,1,RA
X,2,1.,1,A
O,2,RB,3,A,1,180.,0
H,1,R1,2,A1,3,0.,0
H,2,R4,1,A4,4,180.,0

RA=1.34447828
RB=1.19820505
R1=0.97077265
R4=1.10033471
A=62.6515423
A1=106.79341525
A4=109.12185582


Methyl formate, HCOOCH3. Cs symm. B3LYP/6-31G(2df,p) Geometry

0,1
C,-0.9185592322,-0.0601635548,-0.1596058272
O,-0.9033548594,1.1397693859,-0.1566864854
O,0.1393228528,-0.8603211595,0.0240070568
```

H,-1.810937651,-0.6859674558,-0.3147938703

C,1.3884671439,-0.1842955624,0.2411917781

H,2.1317276642,-0.9704119472,0.370145074

H,1.6381278515,0.443976782,-0.617260872

H,1.3338907181,0.4435715125,1.1338293922

Acetamide, ch3cohn2 B3LYP/6-31G(2df,p) geometry

0,1

C

C,1,rc2

O,2,ro1,1,ao1

N,2,rn1,3,an1,1,tn1,0

H,4,rh1,2,ah1,3,th1,0

H,4,rh2,2,ah2,5,th2,0

H,1,rh3,2,ah3,3,th3,0

H,1,rh4,2,ah4,7,th4,0

H,1,rh5,2,ah5,7,th5,0

rc2=1.52260321

ro1=1.21396108

ao1=123.14680963

rn1=1.36936198

an1=122.26829253

tn1=180.05521238

rh1=1.00694763

ah1=117.79591145

th1=7.33544375

rh2=1.00476988

ah2=122.07400395

rh3=1.09402176

ah3=112.16603716

th3=140.3553203

rh4=1.09559437

ah4=109.71398364

th4=119.95617288

rh5=1.08963684

ah5=108.74031152

th5=-121.55541207

th2=164.53384228

Aziridine, (cyclic CH2CH2NH). C2v symm. B3LYP/6-31G(2df,p) Geometry

0,1

C,0.0345609647,0.3971320247,0.7415108991

N,0.0462030276,-0.8737932908,0.

C,0.0345609647,0.3971320247,-0.7415108991

H,-0.8854039011,-1.2800723969,0.

H,0.9493162927,0.6157439331,1.2849230188

H,0.9493162927,0.6157439331,-1.2849230188

H,-0.875690727,0.6997766347,1.2526468406

H,-0.875690727,0.6997766347,-1.2526468406

Cyanogen, NCCN. D*h symm. B3LYP/6-31G(2df,p) Geometry

0,1

N,0.,0.,1.8459106498

C,0.,0.,0.6878682641

C,0.,0.,-0.6878682641

N,0.,0.,-1.8459106498

```
Dimethylamine, B3LYP/6-31G(2df,p) geometry

0,1
C
N,1,RAB
X,2,1.,1,ALPHA
C,2,RAB,3,ALPHA,1,180.,0
X,1,1.,2,90.,3,B16,0
X,4,1.,2,90.,3,-B16,0
H,1,R16,2,A16,5,0.,0
H,1,R27,2,A27,5,B27,0
H,1,R38,2,A38,5,-B38,0
H,2,R4,3,A4,1,90.,0
H,4,R16,2,A16,6,0.,0
H,4,R27,2,A27,6,-B27,0
H,4,R38,2,A38,6,B38,0

RAB=1.45523505
R16=1.10613273
R27=1.09418417
R38=1.09649189
R4=1.01414235
ALPHA=56.45682063
A16=114.32278579
A27=109.79635989
A38=109.38954721
A4=126.774151
B16=54.84744231
B27=121.79275058
B38=120.28404166
```

```
Ethylamine, B3LYP/6-31G(2df,p) geometry

0,1
C
C,1,RA
X,2,1.,1,ALPHA
N,2,RB,3,ALPHA,1,180.,0
X,1,1.,2,90.,3,180.,0
H,1,R1,2,A1,5,0.,0
H,1,R23,2,A23,5,B23,0
H,1,R23,2,A23,5,-B23,0
H,2,R45,3,A45,1,B45,0
H,2,R45,3,A45,1,-B45,0
H,4,R67,2,A67,3,B67,0
H,4,R67,2,A67,3,-B67,0

RA=1.53332363
RB=1.46602785
R1=1.09607286
R23=1.09626072
R45=1.09683946
R67=1.016976
ALPHA=57.96355195
A1=111.46128715
A23=110.96731682
A45=126.95890358
A67=109.45457435
B23=120.15070925
B45=91.35101807
B67=57.61451118
```

```
Ketene, B3LYP/6-31G(2df,p) geometry

0,1
C
C,1,R
H,1,RH,2,A
H,1,RH,2,A,3,180.,0
X,2,1.,1,90.,3,0.,0
O,2,RO,5,90.,1,180.,0

R=1.30834352
RH=1.08044341
RO=1.16342346
A=119.71787024


Oxirane, B3LYP/6-31G(2df,p) geometry

0,1
X
C,1,XC
O,1,XO,2,90.
C,1,XC,3,90.,2,180.,0
X,2,1.,1,YCX,3,180.,0
H,2,CH,5,HCY,1,90.,0
H,2,CH,5,HCY,1,-90.,0
X,4,1.,1,YCX,3,180.,0
H,4,CH,8,HCY,1,90.,0
H,4,CH,8,HCY,1,-90.,0

XC=0.73355333
```

```
XO=1.22214317
YCX=157.42159789
CH=1.08903439
HCY=57.61092752


Acetaldehyde, B3LYP/6-31G(2df,p) geometry

0,1
O
C,1,rco
H,2,rch2,1,aoch
C,2,rcc,1,aocc,3,180.,0
H,4,rch4a,2,accha,1,0.,0
H,4,rch4b,2,acchb,1,t1,0
H,4,rch4b,2,acchb,1,-t1,0

rco=1.20361273
rch2=1.11494784
rcc=1.50762738
rch4a=1.0911166
rch4b=1.09675399
aoch=120.78593222
aocc=124.86200865
accha=110.69798955
acchb=109.6125985
t1=121.67346697


Glyoxal, O=CH-CH=O. Trans, C2h symm. B3LYP/6-31G(2df,p) Geom.

0,1
```

```
C
C,1,rcc
O,1,rco,2,a1
H,1,rch,2,a2,3,180.,0
O,2,rco,1,a1,3,180.,0
H,2,rch,1,a2,3,0.,0

rcc=1.52599374
rco=1.2024143
rch=1.10982629
a1=121.77563107
a2=114.12476354


Ethanol, B3LYP/6-31G(2df,p) geometry

0,1
C
C,1,CC
O,2,CO,1,OCC
H,3,OH,2,HOC,1,180.,0
X,2,1.,1,XCC,3,180.,0
H,2,CH,5,A1,1,90.,0
H,2,CH,5,A1,1,-90.,0
H,1,CH3,2,H3CC,3,180.,0
X,1,1.,2,YCC,3,0.,0
H,1,CH4,9,A2,2,90.,0
H,1,CH4,9,A2,2,-90.,0

CC=1.51988216
CO=1.42065601
OCC=107.90090264
```

```
OH=0.96150494
HOC=108.17560327
XCC=124.83689154
CH=1.10205662
A1=53.54828376
CH3=1.09416486
H3CC=110.62357659
YCC=126.4377202
CH4=1.09388576
A2=54.07670603


Dimethyl ether, B3LYP/6-31G(2df,p) geometry

0,1
C
O,1,RAB
X,2,1.,1,A
C,2,RAB,3,A,1,180.,0
X,1,1.,2,90.,3,180.,0
X,4,1.,2,90.,3,180.,0
H,1,R16,2,A16,5,0.,0
H,1,R2378,2,A2378,5,B2378,0
H,1,R2378,2,A2378,5,-B2378,0
H,4,R16,2,A16,6,0.,0
H,4,R2378,2,A2378,6,B2378,0
H,4,R2378,2,A2378,6,-B2378,0

RAB=1.40607261
R16=1.09286212
R2378=1.1023182
A=56.22446574
```

```
A16=107.49901794
A2378=111.85301198
B2378=119.38319125


Thiirane, (cyclic CH2-S-CH2 ring). C2v symm. B3LYP/6-31G(2df,p) Geom.

0,1
C,0.7407473968,0.8025544365,0.
S,0.,-0.8712700902,0.
C,-0.7407473968,0.8025544365,0.
H,1.2563286559,1.0774170513,-0.9142450158
H,1.2563286559,1.0774170513,0.9142450158
H,-1.2563286559,1.0774170513,0.9142450158
H,-1.2563286559,1.0774170513,-0.9142450158


Dimethylsulfoxide, (CH3)2SO. Cs symm. B3LYP/6-31G(2df,p) Geom.

0,1
S
O,1,so
C,1,cs1,2,cso
C,1,cs2,2,cso2,3,csoc,0
H,3,ch,1,hcs,2,h1cso,0
H,4,ch2,1,h2cs,2,h2cso,0
H,3,ch3,1,h3cs,5,h3csh,0
H,3,ch4,1,h4cs,5,h4csh,0
H,4,ch5,1,h5cs,6,h5csh2,0
H,4,ch6,1,h6cs,6,h6csh2,0

so=1.49013727
```

cs1=1.8286297

cs2=1.82862936

ch=1.09280541

ch2=1.09144219

ch3=1.0930432

ch4=1.09144206

ch5=1.09304298

ch6=1.09280552

cso=107.20510948

cso2=107.20483925

hcs=109.21758462

h2cs=106.73465029

h3cs=109.88764417

h4cs=106.7350846

h5cs=109.88743677

h6cs=109.21845529

csoc=102.04092751

h1cso=50.99136532

h2cso=67.7202996

h3csh=122.19342463

h4csh=-118.71205083

h5csh2=119.09411642

h6csh2=-118.71214659

Thioethanol, CH3-CH2-SH. Cs symm. B3LYP/6-31G(2df,p) Geom.

0,1

C,0.0702299923,-1.455492915,0.8251677728

C,0.0704373079,0.0712524028,0.8277003775

S,-0.0768922581,0.6830098111,-0.9035036494

H,-0.0527401924,1.9984610295,-0.6196140347

```
H,-0.7705073525,0.4560813066,1.4090728586
H,0.9975237317,0.4560908144,1.2586125826
H,0.1573729202,-1.8320114857,1.8491445294
H,-0.855233352,-1.8506725304,0.3959217672
H,0.9098565731,-1.8506630384,0.2457117852


CH3SCH3, B3LYP/6-31G(2df,p) geometry

0,1
C
S,1,RAB
X,2,1.,1,A
C,2,RAB,3,A,1,180.,0
X,1,1.,2,90.,3,180.,0
X,4,1.,2,90.,3,180.,0
H,1,R16,2,A16,5,0.,0
H,1,R2378,2,A2378,5,B2378,0
H,1,R2378,2,A2378,5,-B2378,0
H,4,R16,2,A16,6,0.,0
H,4,R2378,2,A2378,6,B2378,0
H,4,R2378,2,A2378,6,-B2378,0

RAB=1.81891268
R16=1.09189194
R2378=1.093183
A=49.82728507
A16=106.97861952
A2378=111.11992584
B2378=118.73003235
```

```
Vinyl fluoride, H2C=CHF. Cs symm. B3LYP/6-31G(2df,p) Geom.

0,1
C
C,1,rcc
F,1,rcf,2,a1
H,1,rhc,2,ahc,3,180.,0
H,2,rha,1,aha,3,0.,0
H,2,rhb,1,ahb,3,180.,0

rcc=1.32149197
rcf=1.33497039
rhc=1.08590139
rha=1.08286528
rhb=1.08188857
a1=122.9078316
ahc=125.21262994
aha=121.67032333
ahb=119.55630955


Ethyl chloride, CH3-CH2-Cl. Cs symm. B3LYP/6-31G(2df,p) Geom.

0,1
C
C,1,cc
Cl,1,ccl,2,cccl
H,1,ch1,2,h1cc,3,h1cccl,0
H,1,ch1,2,h1cc,3,-h1cccl,0
H,2,ch3,1,h3cc,3,180.,0
H,2,ch4,1,h4cc,6,hcch,0
H,2,ch4,1,h4cc,6,-hcch,0
```

```
cc=1.51760842
ccl=1.81605157
ch1=1.09051178
ch3=1.09611278
ch4=1.09278274
cccl=111.4897439
h1cc=112.16058414
h3cc=109.32354468
h4cc=111.11223831
h1cccl=118.4890019
hcch=119.58595505


Vinyl chloride, H2C=CHCl. Cs symm. B3LYP/6-31G(2df,p) Geom.

0,1
C
C,1,rcc
Cl,1,rccl,2,a1
H,1,rhc,2,ahc,3,180.,0
H,2,rha,1,aha,3,0.,0
H,2,rhb,1,ahb,3,180.,0

rcc=1.32361889
rccl=1.74532104
rhc=1.08232981
rha=1.0830947
rhb=1.08442372
a1=123.27461362
ahc=124.55154661
aha=122.46093536
```

```
ahb=119.56298332


Acrylonitrile, H2C=CH-CN, B3LYP/6-31G(2df,p) geometry

0,1
C
C,1,RA
X,2,1.,1,A
C,2,RB,3,A,1,180.,0
H,1,R1,2,A1,3,0.,0
H,1,R2,2,A2,3,180.,0
H,2,R4,1,A4,3,180.,0
X,3,1.,2,A5,1,0.,0
N,3,RN,8,A5,2,180.,0

A5=132.42783859
RN=2.29482104
RA=1.33420764
RB=1.42622361
R1=1.08378793
R2=1.08372811
R4=1.08597034
A=61.60866081
A1=121.79604075
A2=120.7860462
A4=121.20704525


Acetone, B3LYP/6-31G(2df,p) geometry

0,1
```

```
O
C,1,CO
C,2,CC,1,CCO
C,2,CC,1,CCO,3,180.,0
H,3,C-HIN,2,HIN-C-C,1,0.,0
H,4,C-HIN,2,HIN-C-C,1,0.,0
X,3,1.,2,XCC,1,180.,0
X,4,1.,2,XCC,1,180.,0
H,3,CH,7,HHCH,5,90.,0
H,3,CH,7,HHCH,5,270.,0
H,4,CH,8,HHCH,6,90.,0
H,4,CH,8,HHCH,6,270.,0

CO=1.20866085
CC=1.51995489
C-HIN=1.09045852
CH=1.09600335
CCO=121.91946707
HIN-C-C=109.93529343
XCC=125.67969891
HHCH=53.35643288


Acetic acid, single bonds TRANS B3LYP/6-31G(2df,p) geometry

0,1
C
O,1,CDO
O,1,CSO,2,OCO
H,3,OH,1,HOC,2,0.,0
C,1,CC,2,CCO,3,180.,0
H,5,CH,1,HCC,3,180.,0
```

```
X,5,1.,1,XCC,3,0.,0
H,5,CHP,7,HAL,1,90.,0
H,5,CHP,7,HAL,1,-90.,0

CDO=1.20351054
CSO=1.35563612
OCO=122.61470781
OH=0.96896291
HOC=106.03225022
CC=1.50750959
CCO=126.20198604
CH=1.08883192
HCC=109.5482482
XCC=125.07215447
CHP=1.09372151
HAL=53.61327419


Acetyl fluoride, CH3CFO, HCCO CIS B3LYP/6-31G(2df,p) geometry

0,1
C
O,1,co
F,1,cf,2,fco
C,1,cc,2,cco,3,180.,0
H,4,ch1,1,h1cc,2,0.,0
H,4,ch2,1,h2cc,2,hcco,0
H,4,ch2,1,h2cc,2,-hcco,0

co=1.18496916
cf=1.35016387
cc=1.50016634
```

```
ch1=1.0889342
ch2=1.09382953
fco=120.64422979
cco=128.95999802
h1cc=109.91023893
h2cc=109.59603772
hcco=121.29060613


Acetyl chloride, CH3CClO, hcco cis B3LYP/6-31G(2df,p) geometry

0,1
C
C,1,cc
Cl,1,ccl,2,cccl
O,1,co,2,cco,3,180.,0
H,2,ch,1,hcc,4,0.,0
H,2,ch2,1,h2cc,5,hcch,0
H,2,ch2,1,h2cc,5,-hcch,0

cc=1.5012519
ccl=1.83314593
co=1.18027481
ch=1.09103272
ch2=1.09302535
cccl=111.22258382
cco=128.61320303
hcc=109.2437826
h2cc=109.52757364
hcch=121.21446353
```

```
1-Propyl chloride, CH3CH2CH2Cl, B3LYP/6-31G(2df,p) geometry

0,1
C
X,1,1.
C,1,R1,2,THETA1
C,1,R1a,2,theta1a,3,180.,0
H,1,R2,2,THETA2,3,90.,0
H,1,R2,2,THETA2,3,-90.,0
H,3,R3,1,THETA3,2,180.,0
Cl,4,R5,1,theta6,2,180.,0
X,3,1.,1,THETA4,2,0.,0
H,3,R4,9,THETA5,1,90.,0
H,3,R4,9,THETA5,1,-90.,0
X,4,1.,1,THETA4a,2,0.,0
H,4,R4a,12,THETA5a,1,90.,0
H,4,R4a,12,THETA5a,1,-90.,0

R1a=1.52164367
R1=1.53360113
R2=1.09506478
R3=1.09369278
R4=1.09533674
R4a=1.09147887
THETA1=54.61411502
THETA2=126.63134783
theta1a=56.72434445
THETA3=110.66292873
THETA4=128.30524871
THETA5=53.86789025
THETA4a=129.86012997
THETA5a=54.42492941
```

```
R5=1.81432971
theta6=111.79060879


Isopropyl alcohol, (CH3)2CH-OH. Gauche isomer. C1 symm. B3LYP/6-31G(2df,p) Geom.

0,1
O,0.162212311,0.3234743113,-1.3305930225
C,0.1597134661,0.316274466,0.0956179478
H,1.0776436462,0.2847355823,-1.6249172001
H,0.640891374,1.2349708261,0.4727183446
C,-1.3033965182,0.3269402515,0.5218601204
C,0.9194100786,-0.8922871855,0.6448987788
H,-1.8061728689,-0.5810004273,0.1732563915
H,0.4618446777,-1.8218765034,0.2910091914
H,-1.8182957194,1.1892075025,0.0899249298
H,1.9658332135,-0.8804942982,0.3173683505
H,-1.3902254597,0.3777305008,1.6111853046
H,0.9164204896,-0.8966328652,1.7399377855


Methyl ethyl ether, CH3-CH2-O-CH3. Trans. Cs symm. B3LYP/6-31G(2df,p) Geom.

0,1
O
C,1,R2
C,1,R3,2,A3
C,2,R4,1,A4,3,180.,0
H,2,R5,1,A5,3,D5,0
H,2,R5,1,A5,3,-D5,0
H,3,R7,1,A7,2,180.,0
H,3,R8,1,A8,2,D8,0
```

```
H,3,R8,1,A8,2,-D8,0
H,4,R10,2,A10,1,D10,0
H,4,R10,2,A10,1,-D10,0
H,4,R12,2,A12,1,180.,0

R2=1.41191825
R3=1.40549641
R4=1.51928561
R5=1.10406133
R7=1.09295147
R8=1.1022727
R10=1.09370626
R12=1.09412021
A3=112.87004816
A4=108.62391868
A5=110.1859205
A7=107.55054396
A8=111.89724777
A10=110.49971184
A12=110.45136516
D5=-58.77289035
D8=-60.62592591
D10=-59.86903529


Trimethyl amine, (CH3)3N. C3v symm. B3LYP/6-31G(2df,p) Geom.

0,1
X
N,1,1.
C,2,rcn,1,a1
C,2,rcn,1,a1,3,120.,0
```

```
C,2,rcn,1,a1,3,-120.,0
H,3,rha,2,a2,1,180.,0
H,3,rhb,2,a3,1,t1,0
H,3,rhb,2,a3,1,-t1,0
H,4,rha,2,a2,1,180.,0
H,4,rhb,2,a3,1,t1,0
H,4,rhb,2,a3,1,-t1,0
H,5,rha,2,a2,1,180.,0
H,5,rhb,2,a3,1,t1,0
H,5,rhb,2,a3,1,-t1,0

rcn=1.45220669
rha=1.10841687
rhb=1.09481241
a1=107.06704771
a2=113.24796952
a3=109.85440169
t1=59.38962295


Furan, B3LYP/6-31G(2df,p) geometry

0,1
O
X,1,OX
C,2,XC,1,90.
C,2,XC,1,90.,3,180.,0
X,2,XY,3,90.,1,180.,0
C,5,YC,2,90.,3,0.,0
C,5,YC,2,90.,3,180.,0
H,3,CH,1,HCO,2,180.,0
H,4,CH,1,HCO,2,180.,0
```

```
H,6,CHP,5,HCY,2,180.,0
H,7,CHP,5,HCY,2,180.,0

OX=0.80983203
XC=1.09187837
XY=1.30521648
YC=0.71724235
CH=1.07734226
HCO=115.65054261
CHP=1.07855736
HCY=127.43314953


Thiophene, B3LYP/6-31G(2df,p) geometry

0,1
S
C,1,rcs
C,1,rcs,2,a1
C,2,rcdc,1,a2,3,0.,0
C,3,rcdc,1,a2,2,0.,0
H,2,r2h,1,a2h,3,180.,0
H,3,r2h,1,a2h,2,180.,0
H,4,r4h,2,a4h,1,180.,0
H,5,r4h,3,a4h,1,180.,0

rcs=1.72647496
rcdc=1.36565889
r2h=1.07920786
r4h=1.08265147
a1=91.83074246
a2=111.37780401
```

```
a2h=119.97450663
a4h=123.41323883


Pyrrole, PLANAR B3LYP/6-31G(2df,p) geometry

0,1
H
N,1,NH
X,2,1.,1,90.
X,2,NX,3,90.,1,180.,0
C,4,XC,2,90.,3,0.,0
C,4,XC,2,90.,3,180.,0
X,4,XY,5,90.,2,180.,0
C,7,YC,4,90.,5,0.,0
C,7,YC,4,90.,5,180.,0
H,5,CH2,2,H2CC,1,0.,0
H,6,CH2,2,H2CC,1,0.,0
H,8,CH3,5,H3CC,2,180.,0
H,9,CH3,6,H3CC,2,180.,0

NH=1.00442469
NX=0.78833651
XC=1.12298653
XY=1.31239658
YC=0.71169325
CH2=1.07807611
CH3=1.07912772
H2CC=120.98362618
H3CC=125.78250799
```

```
Pyridine, B3LYP/6-31G(2df,p) geometry

0,1
X
X,1,1.
N,2,NXC,1,90.
C,2,NXC,1,90.,3,180.,0
C,2,RC2,1,90.,3,DC2,0
C,2,RC2,1,90.,3,-DC2,0
C,2,RC3,1,90.,4,DC3,0
C,2,RC3,1,90.,4,-DC3,0
X,4,1.,2,90.,1,0.,0
H,4,RH1,9,90.,2,180.,0
H,5,RH2,3,AH2,2,180.,0
H,6,RH2,3,AH2,2,180.,0
H,7,RH3,4,AH3,2,180.,0
H,8,RH3,4,AH3,2,180.,0

NXC=1.39998539
RC2=1.33892643
RC3=1.37979299
RH1=1.08514442
RH2=1.08775968
RH3=1.08444274
AH2=116.03064128
AH3=121.31368972
DC2=58.33146107
DC3=60.05399443


H2, B3LYP/6-31G(2df,p) geometry
```

```
0,1
H
H,1,r

r=0.7427906


SH, B3LYP/6-31G(2df,p) geometry

0,2
S
H,1,R

R=1.35006649


CCH, B3LYP/6-31G(2df,p) geometry nonlinear

0,2
C
C,1,rc2
X,2,1.,1,90.
H,2,rh1,3,90.,1,th1,0

rc2=1.20917316
rh1=1.06423499
th1=-170.5470312


C2H3, CS, 2-A' B3LYP/6-31G(2df,p) geometry

0,2
```

```
C
C,1,RCC
H,1,RCH1,2,ACH1
H,1,RCH2,2,ACH2,3,180.,0
H,2,RCH3,1,ACH3,3,0.,0

RCC=1.30553645
RCH1=1.09426993
RCH2=1.08868086
RCH3=1.0803629
ACH1=122.19867135
ACH2=122.40497655
ACH3=138.66888775


CH3CO, hcco cis 2-a' B3LYP/6-31G(2df,p) geometry

0,2
C
C,1,CC
H,1,CH1,2,H1CC
X,1,1.,2,XCC,3,180.,0
H,1,CH2,4,HCX,2,90.,0
H,1,CH2,4,HCX,2,-90.,0
X,2,1.,1,90.,3,0.,0
O,2,CO,7,OCX,1,180.,0

CC=1.51578632
CH1=1.09548147
CH2=1.09372786
CO=1.18230248
H1CC=111.52725706
```

```
XCC=122.52386783
HCX=53.57816559
OCX=38.29385151


H2COH, C1 B3LYP/6-31G(2df,p) geometry

0,2
C
O,1,CO
H,2,OH,1,HOC
H,1,CH1,2,H1CO,3,PH1,0
H,1,CH2,2,H2CO,3,PH2,0

CO=1.36515416
OH=0.96210661
CH1=1.08676188
CH2=1.0829866
HOC=109.02952554
H1CO=118.70886236
H2CO=113.07068669
PH1=26.09579151
PH2=174.69789674


CH3O, 2A' B3LYP/6-31G(2df,p) geometry

0,2
C
O,1,CO
H,1,CH1,2,A1
X,1,1.,2,X1,3,180.,0
```

```
H,1,CH2,4,HCX,2,90.,0
H,1,CH2,4,HCX,2,-90.,0

CO=1.36200814
CH1=1.11081413
CH2=1.10315148
A1=105.4811589
X1=135.28841955
HCX=55.44888853


CH3CH2O, 2A'' B3LYP/6-31G(2df,p) geometry

0,2
C
C,1,CC
O,2,CO,1,OCC
X,3,0.97,2,107.,1,180.,0
X,2,1.,1,XCC,3,180.,0
H,2,CH,5,A1,1,90.,0
H,2,CH,5,A1,1,-90.,0
H,1,CH3,2,H3CC,3,180.,0
X,1,1.,2,YCC,3,0.,0
H,1,CH4,9,A2,2,90.,0
H,1,CH4,9,A2,2,-90.,0

CC=1.52848375
CO=1.36350194
OCC=115.79238466
XCC=125.67200131
CH=1.11043038
A1=51.28122521
```

```
CH3=1.09512752
H3CC=110.9295453
YCC=126.47601152
CH4=1.09383383
A2=54.08130974


CH3S, 2-A' B3LYP/6-31G(2df,p) geometry

0,2
C
S,1,R
H,1,ch1,2,hcs
X,1,1.,2,alpha,3,180.,0
H,1,ch,4,hch2,3,90.,0
H,1,ch,4,hch2,3,-90.,0

R=1.80425354
ch=1.09203823
hcs=106.33438381
ch1=1.09770659
hch2=55.48193282
alpha=130.59990948


C2H5, staggered Cs 2-A' B3LYP/6-31G(2df,p) geometry

0,2
C
C,1,RCC
H,1,R1,2,A1
X,1,1.,2,X1,3,180.,0
```

```
H,1,R2,4,A2,2,90.,0
H,1,R2,4,A2,2,-90.,0
X,2,1.,1,X2,3,0.,0
H,2,R3,7,A3,1,90.,0
H,2,R3,7,A3,1,-90.,0

RCC=1.4876411
R1=1.10396412
R2=1.09567012
R3=1.08386507
A1=112.09673919
X1=129.43466389
A2=54.03142868
X2=171.93733423
A3=58.73087339


Isobutyl radical, (CH3)2CH, Cs 2A' B3LYP/6-31G(2df,p) geometry

0,2
C
X,1,1.
X,1,1.,2,90.
X,1,1.,3,90.,2,90.,0
C,1,rc2,2,90.,4,tc2,0
C,1,rc2,2,90.,4,-tc2,0
H,1,rh1,3,90.,4,th1,0
H,5,rh2,1,ah2,6,th2,0
H,6,rh2,1,ah2,5,-th2,0
H,5,rh4,1,ah4,8,th4,0
H,5,rh5,1,ah5,8,th5,0
H,6,rh4,1,ah4,9,-th4,0
```

```
H,6,rh5,1,ah5,9,-th5,0

rc2=1.49062324
tc2=119.33243576
rh1=1.08606497
th1=-13.07976343
rh2=1.09459936
ah2=112.02154365
th2=165.36301025
rh4=1.10483515
ah4=112.25232316
th4=119.97567745
rh5=1.09803971
ah5=111.56085965
th5=-121.29160027


t-Butyl radical, C3V B3LYP/6-31G(2df,p) geometry

0,2
C
X,1,1.
C,1,CC,2,CCX
C,1,CC,2,CCX,3,120.,0
C,1,CC,2,CCX,3,-120.,0
X,3,1.,1,XCC,2,0.,0
H,3,CH1,1,H1CC,6,180.,0
H,3,CH2,6,HCX,1,90.,0
H,3,CH2,6,HCX,1,-90.,0
X,4,1.,1,XCC,2,0.,0
H,4,CH1,1,H1CC,10,180.,0
H,4,CH2,10,HCX,1,90.,0
```

```
H,4,CH2,10,HCX,1,-90.,0
X,5,1.,1,XCC,2,0.,0
H,5,CH1,1,H1CC,14,180.,0
H,5,CH2,14,HCX,1,90.,0
H,5,CH2,14,HCX,1,-90.,0

CC=1.49526116
CH1=1.10572352
CH2=1.09623116
XCC=129.22179568
H1CC=112.26270896
HCX=54.09323438
CCX=95.68772503


NO2, 2A1, B3LYP/6-31G(2df,p) geometry

0,2
N
O,1,NO
O,1,NO,2,ONO

NO=1.19568277
ONO=134.31877733


1.2-Butadiene, CH3-CH=C=CH2, C1 symmetry.

0,1
H,0.6085780314,1.9774949502,-1.4712766457
C,0.3785333527,1.6851479095,-0.4398422172
H,1.3193717445,1.5174048891,0.0884898733
```

C,-0.4923226651,0.453834169,-0.4127286108

H,-0.1332664488,2.535158809,0.0268341206

C,-0.176670677,-0.6721013047,0.1627013757

H,-1.4561398634,0.5250932112,-0.9165247142

C,0.1408876639,-1.7962711091,0.7384172961

H,0.6687753997,-2.5820695652,0.2043743279

H,-0.1098849098,-1.9967402824,1.7768159751

Isoprene, H2C=CHC(CH3)=CH2, B3LYP/6-31G(2df,p) geom.

0,1

C

C,1,rc2

C,2,rc3,1,ac3

C,3,rc4,2,ac4,1,tc4,0

C,2,rc5,1,ac5,3,tc5,0

H,1,rh1,2,ah1,3,th1,0

H,1,rh2,2,ah2,6,th2,0

H,3,rh3,2,ah3,1,th3,0

H,4,rh4,3,ah4,2,th4,0

H,4,rh5,3,ah5,9,th5,0

H,5,rh6,2,ah6,3,th6,0

H,5,rh7,2,ah7,11,th7,0

H,5,rh8,2,ah8,11,th8,0

rc2=1.33997853

rc3=1.4649204

ac3=119.84442845

rc4=1.33593282

ac4=126.22556536

tc4=180.00008972

rc5=1.50772317

ac5=121.54556142

tc5=179.9998409

rh1=1.08541296

ah1=121.44119233

th1=0.0000841

rh2=1.08468023

ah2=121.88883855

th2=180.00002298

rh3=1.08876489

ah3=114.97993906

th3=0.0000725

rh4=1.08422177

ah4=121.29373231

th4=179.99989712

rh5=1.08465043

ah5=122.37708856

th5=180.0000487

rh6=1.09619445

ah6=111.16098616

th6=59.41817019

rh7=1.0922659

ah7=111.17130577

th7=120.58035797

rh8=1.09619441

ah8=111.16077284

th8=-118.83962434

Cyclopentane, twist c5h10 C2 symmetry. B3LYP/6-31G(2df,p) geom.

0,1

```
X
X,1,1.
X,1,1.,2,90.
C,1,rc1,2,90.,3,0.,0
C,1,rc2,4,90.,2,-90.,0
C,1,rc2,4,90.,5,180.,0
C,5,rc4,1,ac4,4,tc4,0
C,6,rc4,1,ac4,4,tc4,0
H,4,rh1,7,ah1,5,th1,0
H,4,rh1,8,ah1,6,th1,0
H,5,rh3,6,ah3,7,th3,0
H,6,rh3,5,ah3,8,th3,0
H,5,rh5,6,ah5,11,th5,0
H,6,rh5,5,ah5,12,th5,0
H,7,rh7,5,ah7,4,th7,0
H,8,rh7,6,ah7,4,th7,0
H,7,rh9,5,ah9,15,th9,0
H,8,rh9,6,ah9,16,th9,0

rc1=2.33800386
rc2=0.76795885
rc4=1.54066182
ac4=103.32516469
tc4=20.74716379
rh1=1.09387619
ah1=110.83406592
th1=133.80843881
rh3=1.0940724
ah3=113.48239601
th3=122.72214602
rh5=1.09761179
ah5=109.60272227
```

```
th5=119.85047425
rh7=1.09585309
ah7=109.44268818
th7=118.16837117
rh9=1.0936087
ah9=112.75071981
th9=118.62824669


n-Pentane, c5h12 B3LYP/6-31G(2df,p) geom.

0,1
C
X,1,1.
X,1,1.,2,90.
X,1,1.,3,90.,2,-90.,0
C,1,rc2,4,90.,2,tc2,0
C,1,rc2,4,90.,2,-tc2,0
C,5,rc4,1,ac4,6,180.,0
C,6,rc4,1,ac4,5,180.,0
H,1,rh1,3,90.,2,th1,0
H,1,rh1,3,90.,2,-th1,0
H,5,rh3,1,ah3,6,th3,0
H,5,rh3,1,ah3,6,-th3,0
H,6,rh3,1,ah3,5,th3,0
H,6,rh3,1,ah3,5,-th3,0
H,7,rh7,5,ah7,1,th7,0
H,7,rh7,5,ah7,1,-th7,0
H,8,rh7,6,ah7,1,th7,0
H,8,rh7,6,ah7,1,-th7,0
H,7,rh11,5,ah11,1,180.,0
H,8,rh11,6,ah11,1,180.,0
```

```
rc2=1.53226714
tc2=123.18962145
rc4=1.53107892
ac4=113.24234401
rh1=1.09937156
th1=52.9090133
rh3=1.09824049
ah3=109.20930002
th3=57.70288599
rh7=1.09583819
ah7=111.17499498
th7=59.8254896
rh11=1.09462221
ah11=111.51795415


Neopentane, C(CH3)4, Td symmetry

0,1
C
C,1,R1
C,1,R1,2,109.47122063
C,1,R1,2,109.47122063,3,120.,0
C,1,R1,2,109.47122063,3,-120.,0
H,2,RH,1,A1,3,180.,0
H,2,RH,1,A1,6,120.,0
H,2,RH,1,A1,6,-120.,0
H,3,RH,1,A1,2,180.,0
H,3,RH,1,A1,9,120.,0
H,3,RH,1,A1,9,-120.,0
H,4,RH,1,A1,2,180.,0
```

```
H,4,RH,1,A1,12,120.,0
H,4,RH,1,A1,12,-120.,0
H,5,RH,1,A1,2,180.,0
H,5,RH,1,A1,15,120.,0
H,5,RH,1,A1,15,-120.,0

R1=1.53909339
RH=1.09572611
A1=111.16732438
```

1.3-Cyclohexadiene, C6H8. C2 symmetry.

```
0,1
H,1.2617437136,0.2641459985,-2.0334784675
C,0.7408641056,-0.2072456549,-1.1936719404
C,0.7197647686,0.1354325452,1.2573496907
C,-1.4185281465,-0.1249278632,0.1149334681
C,-0.7197647686,-0.1354325452,1.2573496907
C,-0.7408641056,0.2072456549,-1.1936719404
C,1.4185281465,0.1249278632,0.1149334681
H,1.2107168619,0.3258720198,2.207014208
H,-2.4916168807,-0.2915454328,0.1155482269
H,-1.2107168619,-0.3258720198,2.207014208
H,-0.8205940797,1.2940482011,-1.3607512779
H,2.4916168807,0.2915454328,0.1155482269
H,0.8205940797,-1.2940482011,-1.3607512779
H,-1.2617437136,-0.2641459985,-2.0334784675
```

1.4-Cyclohexadiene, C6H8. D2h symmetry

```
0,1
H,0.,0.8687589169,-2.1757135057
C,0.,0.,-1.4977027979
C,1.253121084,0.,0.6654000845
C,-1.253121084,0.,0.6654000845
C,0.,0.,1.4977027979
C,-1.253121084,0.,-0.6654000845
C,1.253121084,0.,-0.6654000845
H,2.1966373748,0.,1.2060303512
H,2.1966373748,0.,-1.2060303512
H,0.,0.8687589169,2.1757135057
H,-2.1966373748,0.,-1.2060303512
H,-2.1966373748,0.,1.2060303512
H,0.,-0.8687589169,-2.1757135057
H,0.,-0.8687589169,2.1757135057
```

```
Cyclohexane, (chair). D3d symmetry

0,1
X
C,1,xc
C,1,xc,2,120.
C,1,xc,2,120.,3,180.,0
X,1,xx,2,90.,3,90.,0
C,5,xc,1,90.,2,60.,0
C,5,xc,6,120.,1,90.,0
C,5,xc,6,120.,7,180.,0
H,2,cha,1,xcha,3,90.,0
H,2,chb,1,xchb,3,-90.,0
H,3,cha,1,xcha,4,90.,0
H,3,chb,1,xchb,4,-90.,0
```

```
H,4,cha,1,xcha,2,90.,0
H,4,chb,1,xchb,2,-90.,0
H,6,cha,5,xcha,7,-90.,0
H,6,chb,5,xchb,7,90.,0
H,7,cha,5,xcha,8,-90.,0
H,7,chb,5,xchb,8,90.,0
H,8,cha,5,xcha,6,-90.,0
H,8,chb,5,xchb,6,90.,0

xc=1.46567268
cha=1.09925977
chb=1.096102
xchb=160.12344643
xcha=93.45761795
xx=0.45975588


n-Hexane, c6h14 B3LYP/6-31G(2df,p) geom.

0,1
X
X,1,1.
C,1,rc1,2,90.
C,1,rc1,2,90.,3,180.,0
C,3,rc3,1,ac3,2,-90.,0
C,4,rc3,1,ac3,2,-90.,0
C,5,rc5,3,ac5,4,180.,0
C,6,rc5,4,ac5,3,180.,0
H,3,rh1,4,ah1,5,th1,0
H,3,rh1,4,ah1,5,-th1,0
H,4,rh1,3,ah1,6,th1,0
H,4,rh1,3,ah1,6,-th1,0
```

H,5,rh5,3,ah5,4,th5,0

H,5,rh5,3,ah5,4,-th5,0

H,6,rh5,4,ah5,3,th5,0

H,6,rh5,4,ah5,3,-th5,0

H,7,rh9,5,ah9,3,th9,0

H,7,rh9,5,ah9,3,-th9,0

H,8,rh9,6,ah9,4,th9,0

H,8,rh9,6,ah9,4,-th9,0

H,7,rh13,5,ah13,3,180.,0

H,8,rh13,6,ah13,4,180.,0

rc1=0.76599279

rc3=1.53248398

ac3=113.59826964

rc5=1.5310779

ac5=113.24030388

rh1=1.09927448

ah1=109.32679187

th1=122.28209359

rh5=1.09821414

ah5=109.20963104

th5=57.70191868

rh9=1.09584579

ah9=111.17737648

th9=59.82727818

rh13=1.09462962

ah13=111.51118341

3-Methyl pentane, C6H14 B3LYP/6-31G(2df,p) geom.

0,1

```
C
X,1,1.
X,1,1.,2,90.
X,1,1.,3,90.,2,-90.,0
C,1,rc2,4,90.,2,tc2,0
C,1,rc2,4,90.,2,-tc2,0
C,5,rc4,1,ac4,6,tc4,0
C,6,rc4,1,ac4,5,-tc4,0
C,1,rc6,3,90.,2,tc6,0
H,1,rh1,3,90.,2,th1,0
H,5,rh2,1,ah2,7,th2,0
H,6,rh2,1,ah2,8,-th2,0
H,5,rh4,1,ah4,7,th4,0
H,6,rh4,1,ah4,8,-th4,0
H,7,rh6,5,ah6,1,th6,0
H,8,rh6,6,ah6,1,-th6,0
H,7,rh8,5,ah8,15,th8,0
H,8,rh8,6,ah8,16,-th8,0
H,7,rh10,5,ah10,15,th10,0
H,8,rh10,6,ah10,16,-th10,0
H,9,rh12,1,ah12,10,180.,0
H,9,rh13,1,ah13,21,th13,0
H,9,rh13,1,ah13,21,-th13,0

rc2=1.54106665
tc2=124.99163827
rc4=1.53222665
ac4=115.10268158
tc4=171.3598619
rc6=1.53572696
tc6=-49.47626118
rh1=1.10139882
```

th1=58.43062575

rh2=1.09769065

ah2=108.38028015

th2=-121.89521115

rh4=1.09922983

ah4=108.92121018

th4=123.34528828

rh6=1.09470044

ah6=110.87548921

th6=184.27278067

rh8=1.09612238

ah8=111.1163512

th8=119.56815033

rh10=1.0941748

ah10=112.16624719

th10=-119.93227493

rh12=1.09728409

ah12=110.68659875

rh13=1.09363361

ah13=111.74574682

th13=119.99347017

Toluene, C6H5-CH3 (Cs)

0,1

C,-0.003513937,0.9114223543,0.

C,-0.006919749,0.1937986058,1.1997932684

C,-0.006919749,0.1937986058,-1.1997932684

C,-0.006986185,-1.1985539034,1.2027148697

C,-0.006986185,-1.1985539034,-1.2027148697

C,-0.0062424623,-1.9009363035,0.

```
C,0.0266411907,2.4205188575,0.
H,1.0569617756,2.7977749606,0.
H,-0.4674307892,2.8309685821,-0.8855584566
H,-0.4674307892,2.8309685821,0.8855584566
H,-0.0119674841,-1.7350327767,2.146197971
H,-0.0119674841,-1.7350327767,-2.146197971
H,-0.0095640509,-2.9858279819,0.
H,-0.0115193589,0.7336077659,2.1425392074
H,-0.0115193589,0.7336077659,-2.1425392074


n-Heptane, C7H16, B3LYP/6-31G(2df,p) geom.

0,1
C
X,1,1.
X,1,1.,2,90.
X,1,1.,3,90.,2,-90.,0
C,1,rc2,4,90.,2,tc2,0
C,1,rc2,4,90.,2,-tc2,0
C,5,rc4,1,ac4,6,180.,0
C,6,rc4,1,ac4,5,180.,0
C,7,rc6,5,ac6,1,180.,0
C,8,rc6,6,ac6,1,180.,0
H,1,rh1,3,90.,2,th1,0
H,1,rh1,3,90.,2,-th1,0
H,5,rh3,1,ah3,6,th3,0
H,5,rh3,1,ah3,6,-th3,0
H,6,rh3,1,ah3,5,th3,0
H,6,rh3,1,ah3,5,-th3,0
H,7,rh7,5,ah7,1,th7,0
H,7,rh7,5,ah7,1,-th7,0
```

```
H,8,rh7,6,ah7,1,th7,0
H,8,rh7,6,ah7,1,-th7,0
H,9,rh11,7,ah11,5,th11,0
H,9,rh11,7,ah11,5,-th11,0
H,10,rh11,8,ah11,6,th11,0
H,10,rh11,8,ah11,6,-th11,0
H,9,rh15,7,ah15,5,180.,0
H,10,rh15,8,ah15,6,180.,0

rc2=1.53222214
tc2=123.21054515
rc4=1.53250063
ac4=113.59283456
rc6=1.53109134
ac6=113.23870831
rh1=1.09917065
th1=52.93132943
rh3=1.09924509
ah3=109.32734601
th3=57.71906834
rh7=1.09822144
ah7=109.21083946
th7=57.70271591
rh11=1.095844
ah11=111.17614916
th11=59.8264021
rh15=1.09462996
ah15=111.51184665


Cyclooctatetraene, C8H8, B3LYP/6-31G(2df,p) geom.
```

```
0,1
X
X,1,1.
X,1,rx3,2,90.
X,1,rx3,2,90.,3,180.,0
X,1,rx5,2,ax5,4,90.,0
X,1,rx5,2,ax5,4,-90.,0
C,3,rc1,1,90.,2,90.,0
C,3,rc1,1,90.,7,180.,0
C,4,rc1,1,90.,2,90.,0
C,4,rc1,1,90.,9,180.,0
C,5,rc5,1,90.,2,90.,0
C,5,rc5,1,90.,11,180.,0
C,6,rc5,1,90.,2,90.,0
C,6,rc5,1,90.,13,180.,0
H,7,rh1,3,ah1,1,th1,0
H,8,rh1,3,ah1,1,-th1,0
H,9,rh1,4,ah1,1,th1,0
H,10,rh1,4,ah1,1,-th1,0
H,11,rh5,5,ah5,1,th5,0
H,12,rh5,5,ah5,1,-th5,0
H,13,rh5,6,ah5,1,th5,0
H,14,rh5,6,ah5,1,-th5,0

rx3=1.56909091
rx5=1.73328107
ax5=115.14071829
rc1=0.66888601
rc5=0.66888609
rh1=1.09000564
ah1=117.41071108
th1=214.42493168
```

```
rh5=1.09000621
ah5=117.4105089
th5=170.7148702


n-Octane, B3LYP/6-31G(2df,p) geom.

0,1
X
X,1,1.
C,1,rc1,2,90.
C,1,rc1,2,90.,3,180.,0
C,3,rc3,1,ac3,2,-90.,0
C,4,rc3,1,ac3,2,-90.,0
C,5,rc5,3,ac5,4,180.,0
C,6,rc5,4,ac5,3,180.,0
C,7,rc7,5,ac7,3,180.,0
C,8,rc7,6,ac7,4,180.,0
H,3,rh1,4,ah1,5,th1,0
H,3,rh1,4,ah1,5,-th1,0
H,4,rh1,3,ah1,6,th1,0
H,4,rh1,3,ah1,6,-th1,0
H,5,rh5,3,ah5,4,th5,0
H,5,rh5,3,ah5,4,-th5,0
H,6,rh5,4,ah5,3,th5,0
H,6,rh5,4,ah5,3,-th5,0
H,7,rh9,5,ah9,3,th9,0
H,7,rh9,5,ah9,3,-th9,0
H,8,rh9,6,ah9,4,th9,0
H,8,rh9,6,ah9,4,-th9,0
H,9,rh13,7,ah13,5,th13,0
H,9,rh13,7,ah13,5,-th13,0
```

```
H,10,rh13,8,ah13,6,th13,0
H,10,rh13,8,ah13,6,-th13,0
H,9,rh17,7,ah17,5,180.,0
H,10,rh17,8,ah17,6,180.,0

rc1=0.76622363
rc3=1.532223
ac3=113.58199581
rc5=1.53249893
ac5=113.58602445
rc7=1.53108983
ac7=113.24441304
rh1=1.09914739
ah1=109.27868893
th1=122.29587946
rh5=1.09925098
ah5=109.32935376
th5=57.71952204
rh9=1.09822454
ah9=109.20946182
th9=57.70099813
rh13=1.09584708
ah13=111.17737015
th13=59.82704921
rh17=1.09463199
ah17=111.51038917


Naphthalene, C10H8

0,1
C,0.,0.,0.715601602
```

```
C,0.,0.,-0.715601602
C,0.,1.2425631623,1.3992484654
C,0.,-1.2425631623,1.3992484654
C,0.,1.2425631623,-1.3992484654
C,0.,-1.2425631623,-1.3992484654
C,0.,-2.4284098237,0.7070800686
C,0.,2.4284098237,0.7070800686
H,0.,1.2388047555,2.4853108352
H,0.,-1.2388047555,2.4853108352
C,0.,-2.4284098237,-0.7070800686
C,0.,2.4284098237,-0.7070800686
H,0.,1.2388047555,-2.4853108352
H,0.,-1.2388047555,-2.4853108352
H,0.,-3.3719049849,1.2428995005
H,0.,3.3719049849,1.2428995005
H,0.,-3.3719049849,-1.2428995005
H,0.,3.3719049849,-1.2428995005
```

```
Azulene, C10H8
```

```
0,1
C
C,1,rc2
C,1,rc3,2,ac3
C,2,rc4,1,ac4,3,0.,0
C,3,rc5,1,ac5,2,0.,0
C,4,rc6,5,ac6,3,180.,0
C,5,rc7,4,ac7,2,180.,0
C,6,rc8,4,ac8,5,0.,0
C,7,rc9,5,ac9,4,0.,0
C,8,rc10,6,ac10,4,0.,0
```

```
H,1,rh1,2,ah1,4,180.,0
H,2,rh2,4,ah2,5,180.,0
H,3,rh3,5,ah3,4,180.,0
H,6,rh4,4,ah4,5,180.,0
H,7,rh5,5,ah5,4,180.,0
H,8,rh6,6,ah6,4,180.,0
H,9,rh7,7,ah7,5,180.,0
H,10,rh8,8,ah8,6,180.,0

rc2=1.40211493
rc3=1.40214002
ac3=109.91380019
rc4=1.4027714
ac4=108.53504584
rc5=1.40277796
ac5=108.53454548
rc6=1.38803108
ac6=127.26796257
rc7=1.3880543
ac7=127.26178357
rc8=1.39409192
ac8=129.15896123
rc9=1.39408301
ac9=129.15888394
rc10=1.39403577
ac10=128.65924774
rh1=1.08308547
ah1=125.0438146
rh2=1.08139236
ah2=125.11585889
rh3=1.08138971
ah3=125.11757453
```

```
rh4=1.08913578
ah4=115.18117797
rh5=1.08913694
ah5=115.18144314
rh6=1.08653041
ah6=115.69053138
rh7=1.08653012
ah7=115.68928853
rh8=1.08791117
ah8=115.08488741


Methyl acetate, CH3-C(=O)-OCH3, trans C-C-O-C

0,1
C
O,1,O2C1
O,1,O3C1,2,O3C1O2
C,1,C4C1,2,C4C1O2,3,180.,0
C,3,C5O3,1,C5O3C1,2,0.,0
H,4,H6C4,1,H6C4C1,2,0.,0
H,4,H7C4,1,H7C4C1,6,DIH1,0
H,4,H7C4,1,H7C4C1,6,-DIH1,0
H,5,H9C5,3,H9C5O3,1,180.,0
H,5,H10C5,3,H10C5O3,9,DIH2,0
H,5,H10C5,3,H10C5O3,9,-DIH2,0

O2C1=1.20461767
O3C1=1.35076325
C4C1=1.5097116
C5O3=1.43253393
H6C4=1.08917222
```

```
H7C4=1.09365721
H9C5=1.09014942
H10C5=1.09304082
O3C1O2=123.50468223
C4C1O2=125.86860461
C5O3C1=115.22455141
H6C4C1=109.43745249
H7C4C1=110.06936211
H9C5O3=105.8207019
H10C5O3=110.7265913
DIH1=120.99557524
DIH2=119.74255912


t-Butanol, (CH3)3C-OH. Cs symm.

0,1
C
O,1,r1
C,1,r2,2,tha1
C,1,r3,2,tha2,3,dih1,0
C,1,r3,2,tha2,3,-dih1,0
H,2,r4,1,tha3,3,180.,0
H,3,r5,1,tha4,2,180.,0
H,3,r6,1,tha5,2,dih2,0
H,3,r6,1,tha5,2,-dih2,0
H,4,r7,1,tha6,2,dih3,0
H,4,r8,1,tha7,2,dih4,0
H,4,r9,1,tha8,2,-dih5,0
H,5,r7,1,tha6,2,-dih3,0
H,5,r8,1,tha7,2,-dih4,0
H,5,r9,1,tha8,2,dih5,0
```

r1=1.43371461

r2=1.53034516

r3=1.5356681

r4=0.96318272

r5=1.093893

r6=1.09368056

r7=1.09497845

r8=1.0967188

r9=1.0937197

tha1=104.88911769

tha2=109.68259966

tha3=107.66560195

tha4=110.91630684

tha5=110.26054809

tha6=111.47966373

tha7=110.74050816

tha8=110.25734691

dih1=119.03329893

dih2=59.66476387

dih3=182.87981501

dih4=63.15195731

dih5=56.4888576

Aniline, C6H5-NH2 (Cs)

0,1

C,-0.0023340073,0.9367830053,0.

C,0.0016276843,0.2206820227,1.2052433963

C,0.0016276843,0.2206820227,-1.2052433963

C,0.0116098112,-1.1692799768,1.1999137257

C,0.0116098112,-1.1692799768,-1.1999137257

C,0.0166424818,-1.8776293498,0.

N,0.0494250224,2.3333082132,0.

H,-0.3201527884,2.7680978627,-0.8331169983

H,-0.3201527884,2.7680978627,0.8331169983

H,0.0128964575,-1.702361603,2.1455148132

H,0.0128964575,-1.702361603,-2.1455148132

H,0.0230854883,-2.9616243568,0.

H,0.000375612,0.7626239302,2.146773645

H,0.000375612,0.7626239302,-2.146773645

Phenol, C6H5-OH (Planar Cs)

0,1

C,0.0022940814,0.9403596016,0.

C,-1.2020905026,0.2346174786,0.

C,-1.1887526923,-1.1580158746,0.

C,0.0170227174,-1.8535456736,0.

C,1.215504819,-1.1401402042,0.

C,1.2158017658,0.2497336216,0.

O,0.0542741314,2.3031548913,0.

H,-0.8433461961,2.651200063,0.

H,-2.1456081733,0.7746765859,0.

H,-2.1300561206,-1.6979427218,0.

H,0.0242228929,-2.9375643594,0.

H,2.1623311342,-1.6704637061,0.

H,2.1395822792,0.8168013114,0.

Divinyl ether, H2C=CH-O-CH=CH2, B3LYP/6-31G(2df,p) geom.

```
0,1
O
C,1,rc1
C,1,rc1,2,ac2
C,2,rc3,1,ac3,3,180.,0
C,3,rc3,1,ac3,2,180.,0
H,2,rh1,1,ah1,3,0.,0
H,3,rh1,1,ah1,2,0.,0
H,4,rh3,2,ah3,1,180.,0
H,5,rh3,3,ah3,1,180.,0
H,4,rh5,2,ah5,8,180.,0
H,5,rh5,3,ah5,9,180.,0

rc1=1.3627484
ac2=118.34931885
rc3=1.3267056
ac3=122.14912195
rh1=1.08835596
ah1=114.8806449
rh3=1.08130029
ah3=119.72653137
rh5=1.08275077
ah5=121.65575537


Tetrahydrofuran, C4H8O, C2 symmetry, B3LYP/6-31G(2df,p) geom.

0,1
O
X,1,1.
X,1,rx2,2,90.
C,1,rc1,2,90.,3,tc1,0
```

```
C,1,rc1,2,90.,3,-tc1,0
C,3,rc3,1,90.,2,tc3,0
C,3,rc3,1,90.,6,180.,0
H,4,rh1,1,ah1,6,th1,0
H,4,rh2,1,ah2,8,th2,0
H,5,rh1,1,ah1,7,th1,0
H,5,rh2,1,ah2,10,th2,0
H,6,rh5,4,ah5,7,th5,0
H,6,rh6,4,ah6,12,th6,0
H,7,rh5,5,ah5,6,th5,0
H,7,rh6,5,ah6,14,th6,0

rx2=2.24574867
rc1=1.42727199
tc1=55.09111863
rc3=0.76810298
tc3=66.65150218
rh1=1.09586998
ah1=108.83705008
th1=122.24675445
rh2=1.10084605
ah2=109.54337227
th2=117.64990307
rh5=1.09543648
ah5=110.43089667
th5=117.02937582
rh6=1.09263899
ah6=112.80529954
th6=120.98458724


Cyclopentanone, C5H8O C2 symmetry, B3LYP/6-31G(2df,p) geom.
```

```
0,1
C
X,1,1.
X,1,rx2,2,90.
O,1,ro1,2,90.,3,180.,0
C,1,rc2,2,90.,4,tc2,0
C,1,rc2,2,90.,4,-tc2,0
C,3,rc4,1,90.,2,tc4,0
C,3,rc4,1,90.,7,180.,0
H,5,rh1,1,ah1,8,th1,0
H,6,rh1,1,ah1,7,th1,0
H,5,rh3,1,ah3,8,th3,0
H,6,rh3,1,ah3,7,th3,0
H,7,rh5,8,ah5,6,th5,0
H,8,rh5,7,ah5,5,th5,0
H,7,rh7,8,ah7,6,th7,0
H,8,rh7,7,ah7,5,th7,0

rx2=2.31010149
ro1=1.2034554
rc2=1.53474506
tc2=125.91730553
rc4=0.77321479
tc4=67.11235546
rh1=1.09848787
ah1=107.05961401
th1=-118.14416577
rh3=1.09240968
ah3=111.00466812
th3=125.5108708
rh5=1.09651394
```

```
ah5=109.69345978
th5=-117.51083449
rh7=1.09260529
ah7=112.70944189
th7=123.0964272


1.4-Benzoquinone, C6H4O2 B3LYP/6-31G(2df,p) geom.

0,1
C
C,1,rc2
X,1,1.,2,90.
X,2,1.,1,90.,3,0.,0
O,1,ro1,3,90.,2,180.,0
O,2,ro1,4,90.,1,180.,0
C,1,rc3,3,90.,5,tc3,0
C,1,rc3,3,90.,5,-tc3,0
C,2,rc3,4,90.,6,tc3,0
C,2,rc3,4,90.,6,-tc3,0
H,7,rh1,1,ah1,5,0.,0
H,8,rh1,1,ah1,5,0.,0
H,9,rh1,2,ah1,6,0.,0
H,10,rh1,2,ah1,6,0.,0

rc2=2.89017261
ro1=1.21793983
rc3=1.48534909
tc3=121.47924443
rh1=1.08528449
ah1=115.64030745
```

```
Pyrimidine, C4H4N2 B3LYP/6-31G(2df,p) geom.

0,1
C
X,1,1.
X,1,1.,2,90.
C,1,rc2,2,90.,3,180.,0
X,4,1.,1,90.,2,0.,0
N,1,rn1,2,90.,3,tn1,0
N,1,rn1,2,90.,3,-tn1,0
C,6,rc3,1,ac3,7,0.,0
C,7,rc3,1,ac3,6,0.,0
H,1,rh1,2,90.,3,0.,0
H,4,rh2,5,90.,1,180.,0
H,8,rh3,6,ah3,1,180.,0
H,9,rh3,7,ah3,1,180.,0

rc2=2.65918767
rn1=1.334289
tn1=116.33934651
rc3=1.33548356
ac3=115.73906814
rh1=1.08760546
rh2=1.08356837
rh3=1.08786308
ah3=116.51149117


Dimethyl sulfone, (CH3)2SO2 C2H6O2S B3LYP/6-31G(2df,p) geom.

0,1
```

```
S
X,1,1.
X,1,1.,2,90.
X,1,1.,3,90.,2,90.,0
O,1,ro1,3,90.,4,to1,0
O,1,ro1,3,90.,4,-to1,0
C,1,rc1,2,90.,4,tc1,0
C,1,rc1,2,90.,4,-tc1,0
H,7,rh1,1,ah1,8,180.,0
H,8,rh1,1,ah1,7,180.,0
H,7,rh3,1,ah3,9,th3,0
H,7,rh3,1,ah3,9,-th3,0
H,8,rh3,1,ah3,10,-th3,0
H,8,rh3,1,ah3,10,th3,0

ro1=1.44687334
to1=60.30231995
rc1=1.79809827
tc1=128.37891961
rh1=1.09155192
ah1=105.75513118
rh3=1.09080477
ah3=109.57648302
th3=118.66389216


Chlorobenzene, C6H6Cl B3LYP/6-31G(2df,p) geom.

0,1
C
C,1,rc2
X,1,1.,2,90.
```

```
X,2,1.,1,90.,3,0.,0
Cl,1,rcl1,3,90.,2,180.,0
C,1,rc3,3,90.,5,tc3,0
C,1,rc3,3,90.,5,-tc3,0
H,2,rh1,4,90.,1,180.,0
C,2,rc5,4,90.,8,tc5,0
C,2,rc5,4,90.,8,-tc5,0
H,6,rh2,1,ah2,5,0.,0
H,7,rh2,1,ah2,5,0.,0
H,9,rh4,2,ah4,8,0.,0
H,10,rh4,2,ah4,8,0.,0

rc2=2.77135967
rcl1=1.753362
rc3=1.39121484
tc3=119.25382149
rh1=1.08440375
rc5=1.39298022
tc5=120.1033852
rh2=1.08305484
ah2=119.97920225
rh4=1.08482528
ah4=120.21223128


Succinonitrile, N==C-CH2-CH2-C==N. C2h symmetry.

0,1
C,0.1739759527,0.,1.8775570143
N,-0.1882723757,0.,2.9743053371
C,0.6061254563,0.,0.4826481359
H,1.2304065054,-0.8799734247,0.2995582144
```

H,1.2304065054,0.8799734247,0.2995582144

C,-0.6061254563,0.,-0.4826481359

H,-1.2304065054,-0.8799734247,-0.2995582144

C,-0.1739759527,0.,-1.8775570143

H,-1.2304065054,0.8799734247,-0.2995582144

N,0.1882723757,0.,-2.9743053371

Pyrazine, C4H4N2 (1,4-dipyridine) D2h symmetry.

0,1

H,-2.0641130502,0.,-1.2540407428

N,0.,0.,1.4052642786

N,0.,0.,-1.4052642786

C,-1.1306814969,0.,0.6967716751

C,1.1306814969,0.,0.6967716751

C,1.1306814969,0.,-0.6967716751

C,-1.1306814969,0.,-0.6967716751

H,-2.0641130502,0.,1.2540407428

H,2.0641130502,0.,1.2540407428

H,2.0641130502,0.,-1.2540407428

Acetyl acetylene, CH3-C(=O)-C==CH, Cs symmetry.

0,1

H,1.6115372062,-0.8800482787,1.121323161

C,0.994246348,0.,1.3319384395

H,0.684573032,0.,2.3778454001

C,-0.2290078584,0.,0.4407050072

H,1.6115372062,0.8800482787,1.121323161

O,-1.3631360383,0.,0.8651648415

C,0.0432457101,0.,-0.9899750757

C,0.2794375497,0.,-2.1702795038

H,0.4699103654,0.,-3.216143658

Crotonaldehyde, CH3-CH=CH-CHO. Cs symmetry.

0,1

H,0.1300778686,-0.8777328854,2.9870593437

C,-0.2106183154,0.,2.4239444383

H,-1.3031475416,0.,2.4081447244

C,0.367528031,0.,1.0471232384

H,0.1300778686,0.8777328854,2.9870593437

C,-0.32454725,0.,-0.0978735315

H,1.4567711737,0.,0.9843348381

H,-1.4114263406,0.,-0.1168269867

C,0.35737332,0.,-1.3983342613

O,-0.201402961,0.,-2.4713780878

H,1.4704559457,0.,-1.3279058642

Acetic anhydride, Ch3-C(=O)-O-C(=O)-CH3. C2v -> C2 symmetry.

0,1

O,0.,0.,0.5961330826

C,-0.0185131513,1.210849331,-0.0909867751

O,0.4562887813,1.3580560419,-1.1744433242

C,-0.6607942036,2.2670501784,0.7676722919

C,0.0185131513,-1.210849331,-0.0909867751

O,-0.4562887813,-1.3580560419,-1.1744433242

C,0.6607942036,-2.2670501784,0.7676722919

H,0.5514378993,-3.2406040842,0.2915215038

H,0.2062882951,-2.2751845939,1.7618920971

H,1.7223929082,-2.0339912271,0.8974875616

H,-0.5514378993,3.2406040842,0.2915215038

H,-0.2062882951,2.2751845939,1.7618920971

H,-1.7223929082,2.0339912271,0.8974875616

2.5-Dihydrothiophene, C4H6S. C2v symmetry

0,1

S,0.6240415643,0.9198029976,0.5763077723

C,-0.731053741,0.915423259,-0.6751344413

C,0.7284390271,-0.9192772036,0.6727197304

C,-1.0250427936,-0.5319808519,-0.9466358695

C,-0.3081869695,-1.4331266067,-0.284613327

H,-1.6040297886,1.4453263524,-0.2786284408

H,1.7376747919,-1.2483409563,0.4020507552

H,-0.4051207416,1.4453263524,-1.5768394196

H,0.538765745,-1.2483409563,1.7002617341

H,-1.7993970089,-0.7925122647,-1.6617586727

H,-0.4374911656,-2.5045380694,-0.4040268685

2-Methyl propanenitrile, (CH3)2CH-CN, Cs symmetry.

0,1

H,-0.2615291236,2.1758330974,0.5495280545

C,0.1482388751,1.2786528661,1.0196271828

H,1.2384453073,1.319050265,0.941981669

C,-0.3982338775,0.,0.3561802036

H,-0.1223092556,1.2870933039,2.0793346747

C,-0.101006307,0.,-1.0811247129

H,-1.4916618741,0.,0.4497722754
C,0.1482388751,-1.2786528661,1.0196271828
H,1.2384453073,-1.319050265,0.941981669
H,-0.2615291236,-2.1758330974,0.5495280545
H,-0.1223092556,-1.2870933039,2.0793346747
N,0.1427175177,0.,-2.2110457443

Methyl ethyl ketone, CH3-CO-CH2-CH3. Cs -> C1 symmetry.

0,1
H,1.2257672413,-1.8239829585,0.882500623
C,0.5905666985,-1.930328554,-0.0004776482
H,1.234825811,-1.8207598598,-0.8764702513
C,-0.5156342035,-0.8787558937,-0.0042506979
H,0.1676145523,-2.9388144698,-0.0045014002
C,0.004085278,0.5544050886,0.0010082167
H,-1.1807829126,-0.99721127,0.8626927763
H,-0.5656883778,2.6287866623,0.001798558
H,-1.6999880888,1.5583962867,0.8739962438
H,-1.6913991231,1.5614392031,-0.8851544596
H,-1.1718255486,-0.9940492939,-0.8784178277
O,1.1872251422,0.8061164864,0.0074314613
C,-1.0484052214,1.6508899937,-0.0022625294

Isobutyraldehyde, (CH3)2CH-CHO, Cs symmetry.

0,1
H,-0.4781305979,0.4394700793,2.1751498401
C,-1.0781022583,0.2990194155,1.2711535469
H,-1.5496410121,-0.6889951012,1.3272255201

C,-0.221833506,0.4321093097,0.

H,-1.8760938984,1.0477279749,1.2722717739

C,0.8459235989,-0.6442029758,0.

H,0.2971164059,1.396195919,0.

C,-1.0781022583,0.2990194155,-1.2711535469

H,-1.5496410121,-0.6889951012,-1.3272255201

H,-0.4781305979,0.4394700793,-2.1751498401

H,-1.8760938984,1.0477279749,-1.2722717739

O,2.0339097889,-0.4531446147,0.

H,0.4320228423,-1.6831158964,0.

1.4-dioxane, C4H8O2. cyc-CH2-CH2-O-CH2-CH2-O (para). C2h symmetry.

0,1

H,-1.2589594121,-2.0242953597,0.2496866421

H,-1.2589594121,2.0242953597,0.2496866421

C,0.7382358251,-1.1688899315,0.1916311151

C,0.7382358251,1.1688899315,0.1916311151

H,1.2589594121,2.0242953597,-0.2496866421

C,-0.7382358251,1.1688899315,-0.1916311151

C,-0.7382358251,-1.1688899315,-0.1916311151

H,0.8317525308,-1.2258713037,1.2888663181

H,0.8317525308,1.2258713037,1.2888663181

O,1.3801759659,0.,-0.2947496837

H,-0.8317525308,1.2258713037,-1.2888663181

H,-0.8317525308,-1.2258713037,-1.2888663181

O,-1.3801759659,0.,0.2947496837

H,1.2589594121,-2.0242953597,-0.2496866421

Tetrahydrothiophene, C4H8S. C2 symmetry

0,1

H,0.9920776719,1.8110826578,0.0266120278

S,0.,0.,1.3136382445

C,-0.0011317895,-1.3500136237,0.0530427103

C,0.3424053262,-0.6857180894,-1.2847395749

C,-0.3424053262,0.6857180894,-1.2847395749

C,0.0011317895,1.3500136237,0.0530427103

H,-0.7259523544,2.1095159927,0.346086359

H,-0.9920776719,-1.8110826578,0.0266120278

H,0.7259523544,-2.1095159927,0.346086359

H,1.4278506649,-0.5562002206,-1.3642961778

H,0.0207864524,-1.3069378172,-2.1273269776

H,-1.4278506649,0.5562002206,-1.3642961778

H,-0.0207864524,1.3069378172,-2.1273269776

t-Butyl chloride, (CH3)3C-Cl. C3v symmetry.

0,1

Cl,0.,0.,1.4877394634

C,0.,0.,-0.3674885306

C,0.,1.4602976746,-0.8144379112

C,1.2646548833,-0.7301488373,-0.8144379112

C,-1.2646548833,-0.7301488373,-0.8144379112

H,0.,1.5047593829,-1.9100441723

H,1.3031598522,-0.7523796914,-1.9100441723

H,-1.3031598522,-0.7523796914,-1.9100441723

H,0.8867214367,1.9840064939,-0.4494374626

H,-0.8867214367,1.9840064939,-0.4494374626

H,1.2748393066,-1.7599265372,-0.4494374626

H,2.1615607433,-0.2240799567,-0.4494374626

H,-2.1615607433,-0.2240799567,-0.4494374626
H,-1.2748393066,-1.7599265372,-0.4494374626

n-Butyl chloride, CH3-CH2-CH2-CH2-Cl. Cs symmetry.

0,1
H,-1.1321086088,0.8837695252,2.9716369734
C,-0.4850876891,0.,2.9809042234
H,0.0666464534,0.,3.92575399
C,0.4676780952,0.,1.7820437985
H,-1.1321086088,-0.8837695252,2.9716369734
H,1.1251091527,0.8775654869,1.8356370678
C,-0.2758645184,0.,0.4385260937
H,1.1251091527,-0.8775654869,1.8356370678
H,-0.9270461377,0.8790813369,0.3717298662
H,-0.9270461377,-0.8790813369,0.3717298662
C,0.6877861001,0.,-0.7383727894
H,1.3226457402,0.8876987211,-0.7457355117
Cl,-0.188877569,0.,-2.3276999258
H,1.3226457402,-0.8876987211,-0.7457355117

Tetrahydropyrrole, C4H8NH. Cs symmetry.

0,1
H,-0.741872938,-2.0731556222,-0.3598070466
H,-2.1452253915,0.,-0.0691896736
C,-0.4480941985,1.1616705874,0.1703391122
C,1.0286381681,0.7781770517,-0.0577139581
C,1.0286381681,-0.7781770517,-0.0577139581
C,-0.4480941985,-1.1616705874,0.1703391122

N,-1.1706959923,0.,-0.3501609067

H,-0.626280457,1.3306019325,1.2486783574

H,-0.741872938,2.0731556222,-0.3598070466

H,1.378552481,1.1603963213,-1.0198256393

H,1.6763857649,1.1986457604,0.7153614135

H,1.6763857649,-1.1986457604,0.7153614135

H,1.378552481,-1.1603963213,-1.0198256393

H,-0.626280457,-1.3306019325,1.2486783574

2-Nitrobutane, CH3-CH2-CH(CH3)-NO2, C1 symm.

0,1

H,1.8739109,1.4994116208,-0.0588500368

C,1.3435306476,0.594820471,0.2604689688

C,2.1962208158,-0.642331403,-0.0323142879

C,-0.0128127472,0.6042711337,-0.450948488

H,1.1656353703,0.6925346353,1.3363929601

H,0.106196936,0.4252673956,-1.5210107068

C,-0.8269791406,1.8671816166,-0.1854221239

N,-0.819476817,-0.5981430836,0.0232738173

H,-0.275603838,2.7359054535,-0.5554350465

H,-1.0018289293,1.9899779302,0.8856294457

H,-1.792635576,1.832441449,-0.6973181988

H,3.1602886666,-0.5723799896,0.4790103517

H,2.3914996972,-0.7480321565,-1.1045498575

H,1.7065545883,-1.559113834,0.3099614885

O,-1.1054272435,-1.4475011005,-0.8061728377

O,-1.1192524503,-0.6340816281,1.2077413959

Diethyl ether, CH3-CH2-O-CH2-CH3, C2v symmetry

0,1

H,3.3091787479,0.,-0.1563245092

C,2.3765118877,0.,0.4157848118

H,2.3617839419,-0.8859338386,1.0570216011

C,1.179076672,0.,-0.5198319741

H,2.3617839419,0.8859338386,1.0570216011

H,1.2031724026,-0.8858998467,-1.1781356593

H,1.2031724026,0.8858998467,-1.1781356593

O,0.,0.,0.2557088997

C,-1.179076672,0.,-0.5198319741

C,-2.3765118877,0.,0.4157848118

H,-1.2031724026,-0.8858998467,-1.1781356593

H,-1.2031724026,0.8858998467,-1.1781356593

H,-3.3091787479,0.,-0.1563245092

H,-2.3617839419,0.8859338386,1.0570216011

H,-2.3617839419,-0.8859338386,1.0570216011

1.1-Dimethoxy ethane, CH3-CH(OCH3)2, C1 symmetry. More stable conformer

0,1

H,-1.877231974,-0.0488758335,-1.1469451649

C,-1.8777794346,-0.0630081001,-0.0542583102

C,-0.4559560275,-0.071486033,0.4920186507

H,-0.4661701333,-0.196521116,1.5857901255

H,-2.4169130162,0.8122363763,0.3169940489

H,-2.3994063871,-0.9663930564,0.2705884945

O,0.2414573715,1.1444736501,0.3175607328

O,0.2095984951,-1.1562207219,-0.105727887

C,0.3686932864,1.592522264,-1.0222523799

C,1.4558900152,-1.4613152515,0.4935208486

H,1.1107290569,2.3944095542,-1.0131280276

H,1.8761167741,-2.3073417156,-0.0548432561

H,-0.574895277,1.9957352791,-1.4141043732

H,0.7141617895,0.791227926,-1.6857770438

H,1.3306066248,-1.7469193555,1.5489990535

H,2.149468572,-0.6138587601,0.4435905206

t-Butanethiol, (CH3)3C-SH. Cs symm.

0,1

C,0.005014536,0.,-0.3529188938

S,0.029739024,0.,1.5110540398

C,1.4820980896,0.,-0.7742133336

C,-0.6985930646,-1.2621132327,-0.8672650464

C,-0.6985930646,1.2621132327,-0.8672650464

H,-1.3048314353,0.,1.6924244618

H,1.5523587541,0.,-1.8674748447

H,2.0029957842,-0.8870021505,-0.4017629295

H,2.0029957842,0.8870021505,-0.4017629295

H,-0.6774653675,-1.282992022,-1.9641616272

H,-1.7468791748,-1.2890215265,-0.5539186978

H,-0.2101065822,-2.1665222741,-0.4960769117

H,-0.6774653675,1.282992022,-1.9641616272

H,-1.7468791748,1.2890215265,-0.5539186978

H,-0.2101065822,2.1665222741,-0.4960769117

Diethyl disulfide, CH3-CH2-S-S-CH2-CH3. C2h -> C2 symmetry

0,1

H,0.059074419,3.9082703212,1.3881569242

H,-1.4774795378,3.1924018894,0.8778812872
H,-0.3327807354,3.7899343014,-0.3349345998
C,-0.4154965748,3.2786755125,0.6287519344
H,1.3199149273,1.994948961,0.3339671462
H,0.1774240749,1.4030970871,1.5551893087
C,0.2619645297,1.9095771727,0.5907195431
S,-0.552752825,0.8694981767,-0.6960680582
S,0.552752825,-0.8694981767,-0.6960680582
C,-0.2619645297,-1.9095771727,0.5907195431
C,0.4154965748,-3.2786755125,0.6287519344
H,-1.3199149273,-1.994948961,0.3339671462
H,-0.1774240749,-1.4030970871,1.5551893087
H,-0.059074419,-3.9082703212,1.3881569242
H,1.4774795378,-3.1924018894,0.8778812872
H,0.3327807354,-3.7899343014,-0.3349345998

t-Butylamine, (CH3)3C-NH2. Cs symmetry

0,1
C,0.2033688121,-0.1464015503,1.5136313207
C,-0.0003878616,0.0169625627,0.0003516425
C,-1.48651357,-0.1464015507,-0.3503085135
C,0.8358690872,-1.0338008367,-0.7578143982
N,0.3831985193,1.4002657011,-0.3474148764
H,0.5439985727,-2.0566606426,-0.4931991828
H,1.9016283918,-0.9209208516,-0.5282009309
H,0.7115012771,-0.9209208519,-1.8409108333
H,-2.0867341083,0.6028304149,0.1730558303
H,-1.8487705154,-1.1419111849,-0.0752362176
H,-1.6504668466,-0.0188747791,-1.4268569005
H,-0.1057869425,-1.1419111845,1.8472742165

```
H,-0.3761445948,0.6028304153,2.0598356251
H,1.2587430905,-0.0188747785,1.7820009143
H,1.3723838809,1.5352008926,-0.1498462801
H,0.2832393536,1.5352008924,-1.3511724144


Tetramethylsilane, Si(CH3)4. Td symmetry.

0,1
C
Si,1,rsic
C,2,rsic,1,109.47122063
C,2,rsic,1,109.47122063,3,120.,0
C,2,rsic,1,109.47122063,3,-120.,0
H,1,rch,2,ach,3,180.,0
H,1,rch,2,ach,3,60.,0
H,1,rch,2,ach,3,-60.,0
H,3,rch,2,ach,1,180.,0
H,3,rch,2,ach,1,60.,0
H,3,rch,2,ach,1,-60.,0
H,4,rch,2,ach,1,180.,0
H,4,rch,2,ach,1,60.,0
H,4,rch,2,ach,1,-60.,0
H,5,rch,2,ach,1,180.,0
H,5,rch,2,ach,1,60.,0
H,5,rch,2,ach,1,-60.,0

rsic=1.88738083
rch=1.09547975
ach=111.41554923
```

2-Methyl thiophene, cyc-CH=CH-S-CH(CH3)=CH-. Cs symmetry.

0,1
H,-0.3473196716,0.,-2.7167796127
S,-1.1459785878,0.,-0.3958506368
C,0.1126401922,0.,0.8065791211
H,2.2651433744,0.,0.764127745
H,2.1492845226,0.,-1.8643680988
C,-0.0030117764,0.,-1.693939053
C,1.2765165171,0.,-1.2234976748
C,1.3388217367,0.,0.2017252124
C,-0.2056726166,0.,2.2706192403
H,0.7217548686,0.,2.8499368121
H,-0.7844850038,-0.882184485,2.5658861334
H,-0.7844850038,0.882184485,2.5658861334

N-methyl pyrrole, cyc-CH=CH-N(CH3)-CH=CH-. Cs symmetry.

0,1
H,0.,1.0637246623,-2.432465295
N,0.,-0.0359145799,-0.6233734447
C,1.1175053353,-0.0143652897,0.1745039937
H,0.8855835027,-0.4772838537,-2.4604399873
H,-0.8855835027,-0.4772838537,-2.4604399873
C,-1.1175053353,-0.0143652897,0.1745039937
C,0.,0.0291948027,-2.0688538837
C,0.7108893285,0.0124985343,1.4887419037
H,2.1025359745,-0.0211785019,-0.2653616773
C,-0.7108893285,0.0124985343,1.4887419037
H,-2.1025359745,-0.0211785019,-0.2653616773
H,1.3600037634,0.0159171785,2.3509276357

H,-1.3600037634,0.0159171785,2.3509276357

Tetrahydropyran, C5H10O. Cs symmetry.

0,1
O,-1.4259996922,0.,0.0323998362
C,1.4674840258,0.,0.024501831
C,-0.7248004459,-1.1769688712,-0.3332982821
C,-0.7248004459,1.1769688712,-0.3332982821
C,0.646166884,-1.258011486,0.343107117
C,0.646166884,1.258011486,0.343107117
H,-0.600565513,-1.2145654464,-1.4307178808
H,-1.3642108006,-2.0153357633,-0.0410491235
H,-0.600565513,1.2145654464,-1.4307178808
H,-1.3642108006,2.0153357633,-0.0410491235
H,0.4993646443,-1.3408884676,1.427164434
H,1.1680428155,-2.1641877916,0.0142536888
H,0.4993646443,1.3408884676,1.427164434
H,1.1680428155,2.1641877916,0.0142536888
H,2.4115651515,0.,0.5795227964
H,1.7298686811,0.,-1.0427407276

Diethyl ketone, CH3-CH2-CO-CH2-CH3. C2v symmetry.

0,1
H,-3.4519403748,0.,-0.4912223137
C,-2.5531754434,0.,0.1318623723
H,-2.5803855786,0.8794987513,0.780100326
C,-1.2951861268,0.,-0.7330563821
H,-2.5803855786,-0.8794987513,0.780100326

H,-1.2745183031,0.8707595806,-1.4031349665

H,-1.2745183031,-0.8707595806,-1.4031349665

C,0.,0.,0.07185865

O,0.,0.,1.2822199259

C,1.2951861268,0.,-0.7330563821

C,2.5531754434,0.,0.1318623723

H,1.2745183031,0.8707595806,-1.4031349665

H,1.2745183031,-0.8707595806,-1.4031349665

H,2.5803855786,-0.8794987513,0.780100326

H,2.5803855786,0.8794987513,0.780100326

H,3.4519403748,0.,-0.4912223137

Isopropyl acetate, CH3-C(=O)-O-CH(CH3)2. C5H10O2 isomer. C1 symmetry.

0,1

H,2.3898570907,-0.6935231506,1.5226933061

C,2.4536580709,-0.6551909079,0.4314642453

H,3.369370437,-0.1480490189,0.1301503482

C,1.2608310963,0.0829968311,-0.1302389286

H,2.4607233143,-1.6876394397,0.0709729469

O,1.3147216456,1.0841023083,-0.80094277

O,0.1148829698,-0.5360699541,0.2196672525

C,-1.1270265614,0.0524041883,-0.2529359944

C,-1.5502280575,1.1776950832,0.6855563822

C,-2.1325029033,-1.0874139346,-0.3247801899

H,-0.935488902,0.4621226188,-1.2486320824

H,-0.7988589036,1.9700924441,0.6958545272

H,-1.6851292897,0.7996606237,1.7041375289

H,-2.498720023,1.6092177281,0.3506181726

H,-3.0903745478,-0.719611861,-0.7044446082

H,-2.2991426657,-1.5216909305,0.6660217421

H,-1.7774633037,-1.8777854085,-0.9915608307

Tetrahydrothiopyran, C5H10S. Cs symmetry.

0,1
S,-0.0123223563,1.51615877,0.
C,0.0652459609,-1.7260577601,0.
C,-0.379213922,0.3743030025,1.3827517161
C,-0.379213922,0.3743030025,-1.3827517161
C,0.3888558771,-0.9459948953,1.2828341858
C,0.3888558771,-0.9459948953,-1.2828341858
H,-1.4597309728,0.191914912,1.4138449684
H,-0.1117585861,0.9214357759,2.2905537148
H,-1.4597309728,0.191914912,-1.4138449684
H,-0.1117585861,0.9214357759,-2.2905537148
H,1.4647445596,-0.7389468439,1.3278742316
H,0.1440871415,-1.5633349107,2.1569076912
H,1.4647445596,-0.7389468439,-1.3278742316
H,0.1440871415,-1.5633349107,-2.1569076912
H,0.6169898433,-2.6726781911,0.
H,-1.0016956547,-1.9913507213,0.

Piperidine, cyc-C5H10NH. Cs symmetry.

0,1
H,-1.3104506722,2.0823586546,-0.1555583578
C,-0.7581715539,1.2158182362,0.2241472381
C,-0.7581715539,-1.2158182362,0.2241472381
C,1.4576259714,0.,0.2223847555
C,0.7110527596,-1.2641962564,-0.2295076101

C,0.7110527596,1.2641962564,-0.2295076101

N,-1.4702600839,0.,-0.178217112

H,-0.7982131921,-1.2734792386,1.3215233928

H,1.5326368371,0.,1.3191433475

H,0.7455036167,-1.3384023928,-1.3257617393

H,0.7455036167,1.3384023928,-1.3257617393

H,-1.5779107937,0.,-1.1891689463

H,-0.7982131921,1.2734792386,1.3215233928

H,-1.3104506722,-2.0823586546,-0.1555583578

H,2.4847224973,0.,-0.1590620008

H,1.1991811228,-2.1645826882,0.1631083612

H,1.1991811228,2.1645826882,0.1631083612

t-Butyl methyl ether, (CH3)3C-O-CH3. Cs symmetry.

0,1

H,-0.5499900229,0.,-2.5030453984

H,-1.6712267428,0.8852556827,-1.4457159327

H,-1.6712267428,-0.8852556827,-1.4457159327

H,0.2573686502,2.1594278335,-0.3553791389

H,1.6602703871,1.2775831163,0.2805791956

H,1.368109867,1.3235187486,-1.4573946316

O,-0.7934345736,0.,0.7952223707

C,0.0070616629,0.,-0.3975094828

C,0.8757496055,1.2656480918,-0.4817510769

C,-1.0336884037,0.,-1.5218919103

C,0.8757496055,-1.2656480918,-0.4817510769

H,1.6602703871,-1.2775831163,0.2805791956

H,1.368109867,-1.3235187486,-1.4573946316

H,0.2573686502,-2.1594278335,-0.3553791389

C,-0.1282759081,0.,2.0363854174

H,-0.907686482,0.,2.8034068108

H,0.4982646993,0.8907956626,2.1863947069

H,0.4982646993,-0.8907956626,2.1863947069

1.3-Difluorobenzene, C6H4F2. C2v symmetry.

0,1

F,2.3407563247,0.,-0.9801766039

C,1.1867681931,0.,-0.3075199211

C,-1.2125252979,0.,1.0807223393

C,0.,0.,-1.0277358219

C,1.2125252979,0.,1.0807223393

C,0.,0.,1.7658048573

C,-1.1867681931,0.,-0.3075199211

H,0.,0.,-2.1098403072

H,2.1636782453,0.,1.5980193211

H,0.,0.,2.8501373026

F,-2.3407563247,0.,-0.9801766039

H,-2.1636782453,0.,1.5980193211

1.4-Difluorobenzene, C6H4F2. D2h symmetry.

0,1

C,0.,0.,1.3720846572

C,1.2125849384,0.,0.6961466765

C,1.2125849384,0.,-0.6961466765

C,0.,0.,-1.3720846572

C,-1.2125849384,0.,-0.6961466765

C,-1.2125849384,0.,0.6961466765

F,0.,0.,2.7103267337

F,0.,0.,-2.7103267337

H,2.1381422579,0.,1.2590989558

H,2.1381422579,0.,-1.2590989558

H,-2.1381422579,0.,-1.2590989558

H,-2.1381422579,0.,1.2590989558

Fluorobenzene, C2v symmetry.

0,1

F,0.,0.,-2.2720428265

C,0.,0.,-0.933634173

C,1.2140241563,0.,-0.260605529

C,-1.2140241563,0.,-0.260605529

C,1.2054895964,0.,1.1322749847

C,-1.2054895964,0.,1.1322749847

C,0.,0.,1.8314044209

H,2.1373929321,0.,-0.8276672562

H,-2.1373929321,0.,-0.8276672562

H,2.1472260604,0.,1.670722947

H,-2.1472260604,0.,1.670722947

H,0.,0.,2.9156191019

Diisopropyl ether, (CH3)2CH-O-CH(CH3)2. C2 symmetry.

0,1

O,0.,0.,0.5235395771

C,1.1992487691,-0.1574856784,-0.2296155791

C,-1.1992487691,0.1574856784,-0.2296155791

C,2.1701302884,-0.9417532069,0.6476611187

C,-2.1701302884,0.9417532069,0.6476611187

```
C,1.7661851584,1.2047308019,-0.6417638273
C,-1.7661851584,-1.2047308019,-0.6417638273
H,0.9909795691,-0.7451687325,-1.1376411546
H,-0.9909795691,0.7451687325,-1.1376411546
H,1.0512464984,1.7687088866,-1.2485616966
H,-1.0512464984,-1.7687088866,-1.2485616966
H,2.6812855376,1.0835263241,-1.2309655974
H,-2.6812855376,-1.0835263241,-1.2309655974
H,2.0014022169,1.7982579509,0.2475341372
H,-2.0014022169,-1.7982579509,0.2475341372
H,1.7485473903,-1.9158427409,0.9094131326
H,-1.7485473903,1.9158427409,0.9094131326
H,2.3643595755,-0.3943608709,1.5756776281
H,-2.3643595755,0.3943608709,1.5756776281
H,3.1229956122,-1.0979105784,0.1326949687
H,-3.1229956122,1.0979105784,0.1326949687


PF5, B3LYP/6-31G(2df,p) geom.

0,1
P
F,1,rf1
F,1,rf2,2,90.
F,1,rf1,3,90.,2,180.,0
F,1,rf2,2,90.,3,120.,0
F,1,rf2,2,90.,3,-120.,0

rf1=1.57861787
rf2=1.54965939
```

```
SF6, octahedral symmetry

0,1
S
F,1,rf1
F,1,rf1,2,90.
F,1,rf1,3,90.,2,180.,0
F,1,rf1,3,90.,2,90.,0
F,1,rf1,3,90.,2,-90.,0
F,1,rf1,2,90.,3,180.,0

rf1=1.57565915


P4 Td, B3LYP/6-31G(2df,p) geometry

0,1
X
P,1,rp1
P,1,rp1,2,109.47122063
P,1,rp1,2,109.47122063,3,109.47122063,1
P,1,rp1,2,109.47122063,3,109.47122063,-1

rp1=1.3540231


SO3 D3h, B3LYP/6-31G(2df,p) geom.

0,1
S
O,1,ro1
O,1,ro1,2,120.
```

```
O,1,ro1,2,120.,3,180.,0

ro1=1.43191338


SCl2, C2v, B3LYP/6-31G(2df,p) geom.

0,1
S
Cl,1,rcl1
Cl,1,rcl1,2,acl2

rcl1=2.04415891
acl2=104.07302392


POCl3, C3v symmetry, B3LYP/6-31G(2df,p) geom.

0,1
P
O,1,ro1
Cl,1,rcl1,2,acl1
Cl,1,rcl1,2,acl1,3,120.,0
Cl,1,rcl1,2,acl1,3,-120.,0

ro1=1.45677999
rcl1=2.02679242
acl1=115.11375237


PCl5, D3h symmetry, B3LYP/6-31G(2df,p) geom.
```

```
0,1
P
Cl,1,rclax
Cl,1,rcleq,2,90.
Cl,1,rclax,3,90.,2,180.,0
Cl,1,rcleq,2,90.,3,120.,0
Cl,1,rcleq,2,90.,3,-120.,0

rclax=2.15653894
rcleq=2.05535709


SO2Cl2, C2v symmetry, B3LYP/6-31G(2df,p) geom.

0,1
S
X,1,1.
X,1,1.,2,90.
X,1,1.,2,90.,3,90.,0
O,1,ro1,2,90.,3,to1,0
O,1,ro1,2,90.,3,-to1,0
X,1,1.,4,90.,3,180.,0
Cl,1,rcl1,4,90.,7,tcl1,0
Cl,1,rcl1,4,90.,7,-tcl1,0

ro1=1.42624581
to1=61.78647338
rcl1=2.06081622
tcl1=50.03750165


PCl3, C3v symmetry, B3LYP/6-31G(2df,p) geom
```

```
0,1
P
X,1,1.
Cl,1,rcl1,2,acl1
Cl,1,rcl1,2,acl1,3,120.,0
Cl,1,rcl1,2,acl1,3,-120.,0

rcl1=2.0777331
acl1=117.20163358


S2Cl2, C2 symmetry, B3LYP/6-31G(2df,p) geom.

0,1
S
S,1,rs2
Cl,1,rcl1,2,acl1
Cl,2,rcl1,1,acl1,3,tcl2,0

rs2=1.96396601
rcl1=2.09810546
acl1=109.15076959
tcl2=87.1366298


SiCl2 (1A1), C2v symmetry, B3LYP/6-31G(2df,p) geom.

0,1
Si
Cl,1,rcl1
Cl,1,rcl1,2,acl2
```

```
rcl1=2.10024884
acl2=101.92837859


CF3Cl, B3LYP/6-31G(2df,p) geom.

0,1
C
Cl,1,rcl1
F,1,rf1,2,af1
F,1,rf1,2,af1,3,120.,0
F,1,rf1,2,af1,3,-120.,0

rcl1=1.78657988
rf1=1.32130204
af1=109.74008562


C2F6, B3LYP/6-31G(2df,p) geom.

0,1
C
C,1,rc2
F,1,rf1,2,af1
F,1,rf1,2,af1,3,120.,0
F,1,rf1,2,af1,3,-120.,0
F,2,rf1,1,af1,3,180.,0
F,2,rf1,1,af1,6,120.,0
F,2,rf1,1,af1,6,-120.,0

rc2=1.54811405
```

```
rf1=1.3291226
af1=109.70543579


CF3 radical, B3LYP/6-31G(2df,p) geom.

0,2
C
X,1,1.
F,1,rf1,2,af1
F,1,rf1,2,af1,3,120.,0
F,1,rf1,2,af1,3,-120.,0

rf1=1.31792101
af1=107.44927521


Phenyl radical, C6H5, C2v symmetry, B3LYP/6-31G(2df,p) geom.

0,2
C
X,1,1.
C,1,rc2,2,90.
X,3,1.,1,90.,2,0.,0
C,1,rc3,2,90.,3,tc3,0
C,1,rc3,2,90.,3,-tc3,0
C,5,rc5,1,ac5,2,-90.,0
C,6,rc5,1,ac5,2,90.,0
H,3,rh1,4,90.,1,180.,0
H,5,rh2,1,ah2,2,90.,0
H,6,rh2,1,ah2,2,-90.,0
H,7,rh4,5,ah4,1,180.,0
```

H,8,rh4,6,ah4,1,180.,0

rc2=2.71609727

rc3=1.3743534

tc3=62.97381644

rc5=1.4019379

ac5=116.51519789

rh1=1.08483579

rh2=1.08475203

ah2=122.49000264

rh4=1.08593272

ah4=119.67363689

Expt. enthalpies of formation of atoms at 0K (kcal/mol)

H: 51.63,

Li: 37.69,

Be: 76.48,

B: 136.2,

C: 169.98,

N: 112.53,

O: 58.99,

F: 18.47,

Na: 25.69,

Mg: 34.87,

Al: 78.23,

Si: 106.6,

P: 75.42,

S: 65.66,

Cl: 28.59

Experimental H_298 - H_0 values for atoms (kcal/mol)

H: 1.01,
Li: 1.10,
Be: 0.46,
B: 0.29,
C: 0.25,
N: 1.04,
O: 1.04,
F: 1.05,
Na: 1.54,
Mg: 1.19,
Al: 1.08,
Si: 0.76,
P: 1.28,
S: 1.05,
Cl: 1.10

Experimental standard enthalpies of formation dHf(298K) (kcal/mol)

LiH: 33.3,
BeH: 81.7,
CH radical: 142.5,
CH2 (3B1): 93.7,
CH2 (1A1): 102.8,
CH3 radical: 35.0,
CH4: -17.9,
NH radical: 85.2,
NH2 (2B1): 45.1,

```
Ammonia: -11.0,
OH radical: 9.4,
H2O: -57.8,
HF: -65.1,
SiH2 (1A1): 65.2,
SiH2 (3B1): 86.2,
SiH3: 47.9,
SiH4: 8.2,
PH2 doublet: 33.1,
PH3: 1.3,
H2S: -4.9,
HCl: -22.1,
Li2: 51.6,
LiF: -80.1,
Acetylene: 54.2,
Ethylene: 12.5,
Ethane: -20.1,
CN radical: 104.9,
HCN: 31.5,
CO: -26.4,
HCO: 10.0,
H2CO: -26.0,
Methanol: -48.0,
Nitrogen N2: 0.0,
H2NNH2: 22.8,
NO radical: 21.6,
Oxygen O2: 0.0,
H2O2: -32.5,
Fluorine F2: 0,
CO2: -94.1,
Na2: 34.0,
Si2 3-SGG: 139.9,
```

P2: 34.3,

S2: 30.7,

Cl2: 0.0,

NaCl: -43.6,

SiO: -24.6,

CS: 66.9,

SO: 1.2,

ClO 2-PI: 24.2,

ClF 1-SG: -13.2,

Si2H6: 19.1,

CH3Cl: -19.6,

CH3SH: -5.5,

HOCl: -17.8,

SO2: -71.0,

BF3 (planar): -271.4,

BCl3 (D3h): -96.3,

AlF3: -289.0,

AlCl3: -139.7,

CF4: -223.0,

CCl4: -22.9,

O=C=S: -33.1,

CS2: 28.0,

COF2: -149.1,

SiF4: -386.0,

SiCl4: -158.4,

N2O: 19.6,

ClNO: 12.4,

NF3: -31.6,

PF3: -229.1,

Ozone O3: 34.1,

F2O: 5.9,

ClF3: -38.0,

CF2=CF2: -157.4,

Cl2C=CCl2: -3.0,

CF3CN: -118.4,

Propyne: 44.2,

Allene: 45.5,

Cyclopropene: 66.2,

Propene: 4.8,

Cyclopropane: 12.7,

Propane: -25.0,

1.3-Butadiene: 26.3,

2-Butyne: 34.8,

Methylene cyclopropane: 47.9,

Bicyclo[1.1.0]butane: 51.9,

Cyclobutene: 37.4,

Cyclobutane: 6.8,

Isobutene: -4.0,

n-Butane: -30.0,

Isobutane: -32.1,

Spiropentane: 44.3,

Benzene: 19.7,

CH2F2: -107.7,

CHF3: -166.6,

CH2Cl2: -22.8,

CHCl3: -24.7,

Methylamine: -5.5,

Acetonitrile: 18.0,

Nitromethane: -17.8,

Methylnitrite: -15.9,

Methylsilane: -7.0,

Formic acid: -90.5,

Methyl formate: -85.0,

Acetamide: -57.0,

Aziridine: 30.2,

Cyanogen: 73.3,

Dimethylamine: -4.4,

Ethylamine: -11.3,

Ketene: -11.4,

Oxirane: -12.6,

Acetaldehyde: -39.7,

Glyoxal: -50.7,

Ethanol: -56.2,

Dimethyl ether: -44.0,

Thiirane: 19.6,

Dimethylsulfoxide: -36.2,

Thioethanol: -11.1,

CH3SCH3: -8.9,

Vinyl fluoride: -33.2,

Ethyl chloride: -26.8,

Vinyl chloride: 8.9,

Acrylonitrile: 43.2,

Acetone: -51.9,

Acetic acid: -103.4,

Acetyl fluoride: -105.7,

Acetyl chloride: -58.0,

1-Propyl chloride: -31.5,

Isopropyl alcohol: -65.2,

Methyl ethyl ether: -51.7,

Trimethyl amine: -5.7,

Furan: -8.3,

Thiophene: 27.5,

Pyrrole: 25.9,

Pyridine: 33.6,

H2: 0.0,

SH: 34.2,

CCH: 135.1,

C2H3: 71.6,

CH3CO: -2.4,

H2COH: -4.1,

CH3O: 4.1,

CH3CH2O: -3.7,

CH3S: 29.8,

C2H5: 28.9,

Isobutyl radical: 21.5,

t-Butyl radical: 12.3,

NO2: 7.9,

1.2-Butadiene: 38.8,

Isoprene: 18.0,

Cyclopentane: -18.3,

n-Pentane: -35.1,

Neopentane: -40.2,

1.3-Cyclohexadiene: 25.4,

1.4-Cyclohexadiene: 25.0,

Cyclohexane: -29.5,

n-Hexane: -39.9,

3-Methyl pentane: -41.1,

Toluene: 12.0,

n-Heptane: -44.9,

Cyclooctatetraene: 70.7,

n-Octane: -49.9,

Naphthalene: 35.9,

Azulene: 69.1,

Methyl acetate: -98.4,

t-Butanol: -74.7,

Aniline: 20.8,

Phenol: -23.0,

Divinyl ether: -3.3,

Tetrahydrofuran: -44.0,

Cyclopentanone: -45.9,

1.4-Benzoquinone: -29.4,

Pyrimidine: 46.8,

Dimethyl sulfone: -89.2,

Chlorobenzene: 12.4,

Succinonitrile: 50.1,

Pyrazine: 46.9,

Acetyl acetylene: 15.6,

Crotonaldehyde: -24.0,

Acetic anhydride: -136.8,

2.5-Dihydrothiophene: 20.8,

2-Methyl propanenitrile: 5.6,

Methyl ethyl ketone: -57.1,

Isobutyraldehyde: -51.6,

1.4-dioxane: -75.5,

Tetrahydrothiophene: -8.2,

t-Butyl chloride: -43.5,

n-Butyl chloride: -37.0,

Tetrahydropyrrole: -0.8,

2-Nitrobutane: -39.1,

Diethyl ether: -60.3,

1.1-Dimethoxy ethane: -93.1,

t-Butanethiol: -26.2,

Diethyl disulfide: -17.9,

t-Butylamine: -28.9,

Tetramethylsilane: -55.7,

2-Methyl thiophene: 20.0,

N-methyl pyrrole: 24.6,

Tetrahydropyran: -53.4,

Diethyl ketone: -61.6,

Isopropyl acetate: -115.1,

Tetrahydrothiopyran: -15.2,

Piperidine: -11.3,

t-Butyl methyl ether: -67.8,

1.3-Difluorobenzene: -73.9,

1.4-Difluorobenzene: -73.3,

Fluorobenzene: -27.7,

Diisopropyl ether: -76.3,

PF5: -381.1,

SF6: -291.7,

P4 Td: 14.1,

SO3 D3h: -94.6,

SCl2: -4.2,

POCl3: -133.8,

PCl5: -86.1,

SO2Cl2: -84.8,

PCl3: -69.0,

S2Cl2: -4.0,

SiCl2 (1A1): -40.3,

CF3Cl: -169.5,

C2F6: -321.3,

CF3 radical: -111.3,

Phenyl radical: 81.2

All following values are in a.u.

ZPE: B3LYP/6-31G(2df,p) frequency scale factor: 0.9854

LiH: 0.003211,

BeH: 0.004633,

CH radical: 0.006320,

CH2 (3B1): 0.017044,

CH2 (1A1): 0.016322,

CH3 radical: 0.029224,

CH4: 0.044102,

NH radical: 0.007289,

NH2 (2B1): 0.018712,

Ammonia: 0.033858,

OH radical: 0.008293,

H2O: 0.021064,

HF: 0.009242,

SiH2 (1A1): 0.011454,

SiH2 (3B1): 0.011825,

SiH3: 0.020860,

SiH4: 0.030703,

PH2 doublet: 0.013183,

PH3: 0.023567,

H2S: 0.014841,

HCl: 0.006641,

Li2: 0.000771,

LiF: 0.002234,

Acetylene: 0.026454,

Ethylene: 0.050241,

Ethane: 0.073457,

CN radical: 0.004810,

HCN: 0.016359,

CO: 0.004950,

HCO: 0.012795,

H2CO: 0.026215,

Methanol: 0.050459,

Nitrogen N2: 0.005457,

H2NNH2: 0.052542,

NO radical: 0.004458,

Oxygen O2: 0.003736,

H2O2: 0.026148,

Fluorine F2: 0.002419,

CO2: 0.011654,

Na2: 0.000358,

Si2 3-SGG: 0.001120,

P2: 0.001810,

S2: 0.001606,

Cl2: 0.001233,

NaCl: 0.000821,

SiO: 0.002846,

CS: 0.002907,

SO: 0.002575,

ClO 2-PI: 0.001900,

ClF 1-SG: 0.001771,

Si2H6: 0.048169,

CH3Cl: 0.037133,

CH3SH: 0.045254,

HOCl: 0.012994,

SO2: 0.006891,

BF3 (planar): 0.012471,

BCl3 (D3h): 0.007416,

AlF3: 0.007752,

AlCl3: 0.004731,

CF4: 0.016892,

CCl4: 0.009156,

O=C=S: 0.009196,

CS2: 0.006913,

COF2: 0.014058,

SiF4: 0.012553,

SiCl4: 0.007075,

N2O: 0.011115,

ClNO: 0.006473,

NF3: 0.010275,

PF3: 0.008443,

Ozone O3: 0.007359,

F2O: 0.005476,

ClF3: 0.006840,

CF2=CF2: 0.021373,

Cl2C=CCl2: 0.015080,

CF3CN: 0.022473,

Propyne: 0.054599,

Allene: 0.054372,

Cyclopropene: 0.055394,

Propene: 0.078379,

Cyclopropane: 0.080018,

Propane: 0.101673,

1.3-Butadiene: 0.083867,

2-Butyne: 0.082665,

Methylene cyclopropane: 0.083860,

Bicyclo[1.1.0]butane: 0.085023,

Cyclobutene: 0.085115,

Cyclobutane: 0.108893,

Isobutene: 0.106085,

n-Butane: 0.129716,

Isobutane: 0.129249,

Spiropentane: 0.113140,

Benzene: 0.098684,

CH2F2: 0.032313,

CHF3: 0.025031,

CH2Cl2: 0.028833,

CHCl3: 0.019438,

Methylamine: 0.063042,

Acetonitrile: 0.044621,

Nitromethane: 0.049014,

Methylnitrite: 0.047732,

Methylsilane: 0.060016,

Formic acid: 0.033390,

Methyl formate: 0.061039,

Acetamide: 0.072121,

Aziridine: 0.069119,

Cyanogen: 0.016305,

Dimethylamine: 0.090881,

Ethylamine: 0.091221,

Ketene: 0.031232,

Oxirane: 0.056446,

Acetaldehyde: 0.054547,

Glyoxal: 0.036402,

Ethanol: 0.078576,

Dimethyl ether: 0.078391,

Thiirane: 0.054100,

Dimethylsulfoxide: 0.077844,

Thioethanol: 0.073558,

CH3SCH3: 0.074383,

Vinyl fluoride: 0.043471,

Ethyl chloride: 0.065447,

Vinyl chloride: 0.042000,

Acrylonitrile: 0.050052,

Acetone: 0.082164,

Acetic acid: 0.060823,

Acetyl fluoride: 0.048245,

Acetyl chloride: 0.046510,

1-Propyl chloride: 0.093496,

Isopropyl alcohol: 0.106072,

Methyl ethyl ether: 0.106283,

Trimethyl amine: 0.118179,

Furan: 0.068862,

Thiophene: 0.065661,

Pyrrole: 0.081224,

Pyridine: 0.087366,

H2: 0.010025,

SH: 0.005996,

CCH: 0.012515,

C2H3: 0.035975,

CH3CO: 0.042401,

H2COH: 0.036859,

CH3O: 0.035731,

CH3CH2O: 0.062858,

CH3S: 0.034966,

C2H5: 0.058274,

Isobutyl radical: 0.086521,

t-Butyl radical: 0.114394,

NO2: 0.008706,

1.2-Butadiene: 0.082675,

Isoprene: 0.111738,

Cyclopentane: 0.138187,

n-Pentane: 0.157727,

Neopentane: 0.156434,

1.3-Cyclohexadiene: 0.120256,

1.4-Cyclohexadiene: 0.120035,

Cyclohexane: 0.167327,

n-Hexane: 0.185690,

3-Methyl pentane: 0.185364,

Toluene: 0.125537,

n-Heptane: 0.213656,

Cyclooctatetraene: 0.130342,

n-Octane: 0.241593,

Naphthalene: 0.144756,

Azulene: 0.143673,

Methyl acetate: 0.088130,

t-Butanol: 0.133058,

Aniline: 0.115142,

Phenol: 0.102947,

Divinyl ether: 0.087801,

Tetrahydrofuran: 0.114654,

Cyclopentanone: 0.119128,

1.4-Benzoquinone: 0.083675,

Pyrimidine: 0.075807,

Dimethyl sulfone: 0.083606,

Chlorobenzene: 0.089430,

Succinonitrile: 0.072297,

Pyrazine: 0.075609,

Acetyl acetylene: 0.064206,

Crotonaldehyde: 0.088104,

Acetic anhydride: 0.096609,

2.5-Dihydrothiophene: 0.087930,

2-Methyl propanenitrile: 0.100808,

Methyl ethyl ketone: 0.110353,

Isobutyraldehyde: 0.110612,

1.4-dioxane: 0.120260,

Tetrahydrothiophene: 0.111864,

t-Butyl chloride: 0.120184,

n-Butyl chloride: 0.121539,

Tetrahydropyrrole: 0.127414,

2-Nitrobutane: 0.132928,

Diethyl ether: 0.134129,

1.1-Dimethoxy ethane: 0.138739,

t-Butanethiol: 0.128408,

Diethyl disulfide: 0.132306,

t-Butylamine: 0.145801,

Tetramethylsilane: 0.144898,

2-Methyl thiophene: 0.092873,

N-methyl pyrrole: 0.108392,

Tetrahydropyran: 0.143814,

Diethyl ketone: 0.138475,

Isopropyl acetate: 0.143412,

Tetrahydrothiopyran: 0.140335,

Piperidine: 0.156298,

t-Butyl methyl ether: 0.160776,

1.3-Difluorobenzene: 0.082818,

1.4-Difluorobenzene: 0.082785,

Fluorobenzene: 0.090772,

Diisopropyl ether: 0.188864,

PF5: 0.016668,

SF6: 0.020587,

P4 Td: 0.006119,

SO3 D3h: 0.012072,

SCl2: 0.002739,

POCl3: 0.009414,

PCl5: 0.008341,

SO2Cl2: 0.011883,

PCl3: 0.004663,

S2Cl2: 0.004407,

SiCl2 (1A1): 0.002674,

CF3Cl: 0.014907,

C2F6: 0.029002,

CF3 radical: 0.012048,

Phenyl radical: 0.085879

Thermal enthalpy corrections (including ZPE)

LiH: 0.006523,

BeH: 0.007938,

CH radical: 0.009625,

CH2 (3B1): 0.020849,

CH2 (1A1): 0.020106,

CH3 radical: 0.033269,

CH4: 0.047917,

NH radical: 0.010594,

NH2 (2B1): 0.022493,

Ammonia: 0.037666,

OH radical: 0.011598,

H2O: 0.024844,

HF: 0.012546,

SiH2 (1A1): 0.015267,

SiH2 (3B1): 0.015662,

SiH3: 0.024830,

SiH4: 0.034724,

PH2 doublet: 0.016983,

PH3: 0.027424,

H2S: 0.018635,

HCl: 0.009946,

Li2: 0.004450,

LiF: 0.005579,

Acetylene: 0.030315,

Ethylene: 0.054241,

Ethane: 0.077905,

CN radical: 0.008115,

HCN: 0.019828,

CO: 0.008255,

HCO: 0.016598,

H2CO: 0.030028,

Methanol: 0.054735,

Nitrogen N2: 0.008761,

H2NNH2: 0.056770,

NO radical: 0.007764,

Oxygen O2: 0.007043,

H2O2: 0.030328,

Fluorine F2: 0.005752,

CO2: 0.015211,

Na2: 0.004294,

Si2 3-SGG: 0.004655,

P2: 0.005194,

S2: 0.005022,

Cl2: 0.004733,

NaCl: 0.004476,

SiO: 0.006164,

CS: 0.006224,

SO: 0.005902,

ClO 2-PI: 0.005274,

ClF 1-SG: 0.005161,

Si2H6: 0.054213,

CH3Cl: 0.041110,

CH3SH: 0.049826,

HOCl: 0.016885,

SO2: 0.010914,

BF3 (planar): 0.016916,

BCl3 (D3h): 0.012791,

AlF3: 0.013168,

AlCl3: 0.011020,

CF4: 0.021787,

CCl4: 0.015810,

O=C=S: 0.012967,

CS2: 0.010949,

COF2: 0.018300,

SiF4: 0.018458,

SiCl4: 0.014594,

N2O: 0.014734,

ClNO: 0.010782,

NF3: 0.014785,

PF3: 0.013429,

Ozone O3: 0.011260,

F2O: 0.009579,

ClF3: 0.012145,

CF2=CF2: 0.027594,

Cl2C=CCl2: 0.022591,

CF3CN: 0.028528,

Propyne: 0.059570,

Allene: 0.059112,

Cyclopropene: 0.059659,

Propene: 0.083435,

Cyclopropane: 0.084364,

Propane: 0.107192,

1.3-Butadiene: 0.089499,

2-Butyne: 0.089413,

Methylene cyclopropane: 0.089100,

Bicyclo[1.1.0]butane: 0.089746,

Cyclobutene: 0.089913,

Cyclobutane: 0.114042,

Isobutene: 0.112379,

n-Butane: 0.136510,

Isobutane: 0.135987,

Spiropentane: 0.119060,

Benzene: 0.104084,

CH2F2: 0.036385,

CHF3: 0.029448,

CH2Cl2: 0.033379,

CHCl3: 0.024898,

Methylamine: 0.067413,

Acetonitrile: 0.049171,

Nitromethane: 0.053458,

Methylnitrite: 0.053093,

Methylsilane: 0.065193,

Formic acid: 0.037510,

Methyl formate: 0.066573,

Acetamide: 0.078386,

Aziridine: 0.073326,

Cyanogen: 0.020980,

Dimethylamine: 0.096261,

Ethylamine: 0.096588,

Ketene: 0.035706,

Oxirane: 0.060560,

Acetaldehyde: 0.059396,

Glyoxal: 0.041584,

Ethanol: 0.083875,

Dimethyl ether: 0.083672,

Thiirane: 0.058449,

Dimethylsulfoxide: 0.084522,

Thioethanol: 0.079279,

CH3SCH3: 0.080268,

Vinyl fluoride: 0.047780,

Ethyl chloride: 0.070465,

Vinyl chloride: 0.046505,

Acrylonitrile: 0.055157,

Acetone: 0.088519,

Acetic acid: 0.066364,

Acetyl fluoride: 0.053524,

Acetyl chloride: 0.052125,

1-Propyl chloride: 0.099852,

Isopropyl alcohol: 0.112563,

Methyl ethyl ether: 0.112826,

Trimethyl amine: 0.124654,

Furan: 0.073560,

Thiophene: 0.070713,

Pyrrole: 0.086189,

Pyridine: 0.092626,

H2: 0.013330,

SH: 0.009301,

CCH: 0.016950,

C2H3: 0.040036,

CH3CO: 0.047316,

H2COH: 0.041118,

CH3O: 0.039710,

CH3CH2O: 0.067664,

CH3S: 0.039118,

C2H5: 0.063205,

Isobutyl radical: 0.092646,

t-Butyl radical: 0.121830,

NO2: 0.012589,

1.2-Butadiene: 0.088679,

Isoprene: 0.118579,

Cyclopentane: 0.143505,

n-Pentane: 0.165841,

Neopentane: 0.164450,

1.3-Cyclohexadiene: 0.126460,

1.4-Cyclohexadiene: 0.126282,

Cyclohexane: 0.174087,

n-Hexane: 0.195160,

3-Methyl pentane: 0.194805,

Toluene: 0.132806,

n-Heptane: 0.224490,

Cyclooctatetraene: 0.138117,

n-Octane: 0.253803,

Naphthalene: 0.152633,

Azulene: 0.151817,

Methyl acetate: 0.095340,

t-Butanol: 0.140894,

Aniline: 0.121947,

Phenol: 0.109458,

Divinyl ether: 0.094626,

Tetrahydrofuran: 0.120630,

Cyclopentanone: 0.125714,

1.4-Benzoquinone: 0.090935,

Pyrimidine: 0.080976,

Dimethyl sulfone: 0.090863,

Chlorobenzene: 0.095940,

Succinonitrile: 0.079441,

Pyrazine: 0.080765,

Acetyl acetylene: 0.070859,

Crotonaldehyde: 0.094894,

Acetic anhydride: 0.105722,

2.5-Dihydrothiophene: 0.093786,

2-Methyl propanenitrile: 0.107774,

Methyl ethyl ketone: 0.117983,

Isobutyraldehyde: 0.118011,

1.4-dioxane: 0.126480,

Tetrahydrothiophene: 0.118028,

t-Butyl chloride: 0.127814,

n-Butyl chloride: 0.129225,

Tetrahydropyrrole: 0.133393,

2-Nitrobutane: 0.142081,

Diethyl ether: 0.141989,

1.1-Dimethoxy ethane: 0.147598,

t-Butanethiol: 0.136665,

Diethyl disulfide: 0.142546,

t-Butylamine: 0.153687,

Tetramethylsilane: 0.155259,

2-Methyl thiophene: 0.099688,

N-methyl pyrrole: 0.114986,

Tetrahydropyran: 0.150305,

Diethyl ketone: 0.147431,

Isopropyl acetate: 0.153198,

Tetrahydrothiopyran: 0.147412,

Piperidine: 0.162939,

t-Butyl methyl ether: 0.170022,

1.3-Difluorobenzene: 0.089742,

1.4-Difluorobenzene: 0.089721,

Fluorobenzene: 0.096915,

Diisopropyl ether: 0.199402,

PF5: 0.023079,

SF6: 0.027233,

P4 Td: 0.011532,

SO3 D3h: 0.016568,

SCl2: 0.007527,

POCl3: 0.016295,

PCl5: 0.017443,

SO2Cl2: 0.018173,

PCl3: 0.010843,

S2Cl2: 0.010754,

SiCl2 (1A1): 0.007489,

CF3Cl: 0.020221,

C2F6: 0.036779,

CF3 radical: 0.016446,

Phenyl radical: 0.091253