	H_7	30.30	30.33	30.69	30.72	30.74	30.78	30.84	30.88	30.88
methylcyclopropane	H_1	31.39	31.41	31.76	31.77	31.75	31.81	31.85	31.92	31.90
	H_6	29.92	29.95	30.23	30.25	30.26	30.29	30.36	30.39	30.40
	H_8	30.84	30.87	31.11	31.13	31.16	31.24	31.27	31.36	31.32
	H_9	31.53	31.55	31.83	31.85	31.87	31.94	31.99	32.07	32.05
	H_{10}	31.13	31.16	31.39	31.41	31.43	31.49	31.56	31.61	31.60
2-fluoro-2-methylpropane	H_6	30.30	30.33	30.66	30.69	30.73	30.76	30.82	30.86	30.86
	H_7	29.98	30.01	30.30	30.32	30.38	30.39	30.47	30.49	30.52
N-methylazetidine	H_1	29.67	29.70	30.01	30.03	29.97	30.00	30.04	30.07	30.08
	H_7	29.12	29.15	29.42	29.45	29.49	29.51	29.58	29.59	29.61
	H_9	28.74	28.77	29.05	29.08	29.00	29.11	29.07	29.18	29.12
	H_{10}	28.17	28.20	28.41	28.45	28.37	28.42	28.45	28.50	28.49
	H_{13}	29.89	29.92	30.17	30.19	30.16	30.25	30.25	30.34	30.29
	H_{14}	29.34	29.37	29.65	29.67	29.70	29.76	29.79	29.86	29.83
trimethylaziridine	H_3	29.84	29.86	30.16	30.18	30.14	30.26	30.23	30.35	30.27
	H_6	28.68	28.71	28.95	28.98	29.01	29.05	29.10	29.13	29.13
	H_7	28.84	28.88	29.15	29.18	29.17	29.22	29.26	29.31	29.29
	H_9	29.99	30.02	30.22	30.25	30.29	30.34	30.39	30.44	30.42
	H_{11}	30.69	30.71	30.97	30.99	31.05	31.12	31.15	31.23	31.20
	H_{12}	30.04	30.07	30.38	30.41	30.45	30.45	30.54	30.54	30.58
	H_{13}	30.47	30.49	30.79	30.81	30.86	30.93	30.95	31.03	30.99
	H_{14}	30.89	30.92	31.22	31.24	31.27	31.27	31.37	31.37	31.41
	H_{15}	30.19	30.22	30.54	30.57	30.58	30.57	30.68	30.67	30.72
	H_{16}	30.22	30.25	30.57	30.60	30.68	30.70	30.78	30.80	30.82

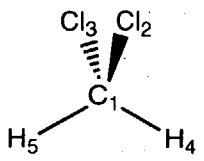
H_{17}	30.11	30.14	30.46	30.49	30.52	30.55	30.61	30.64	30.66

Notes:

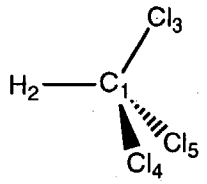
(a) See pages 43-49 of the Supporting Information for atom numbering.

(b) Key:

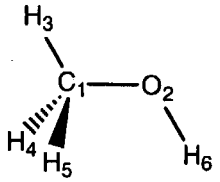
7 = IGAIM/B3P86/6-311++G(2df,p)//MP2/6-31+G(d)
8 = IGAIM/B3PW91/6-311++G(2df,p)//MP2/6-31+G(d)
9 = GIAO/B3P86/6-311++G(2df,p)//MP2/6-31+G(d)
10 = GIAO/B3PW91/6-311++G(2df,p)//MP2/6-31+G(d)
11 = GIAO/B3LYP/6-311++G(2df,p)//B3LYP/6-31+G(d)
12 = GIAO/B3LYP/6-311++G(d,p)//B3LYP/6-31+G(d)
13 = GIAO/B3LYP/6-311++G(2df,p)//B3LYP/6-311++G(d,p)
14 = GIAO/B3LYP/6-311++G(d,p)//B3LYP/6-311++G(d,p)
15 = GIAO/B3LYP/6-311++G(2df,p)//B3LYP/6-311++G(2df,p)



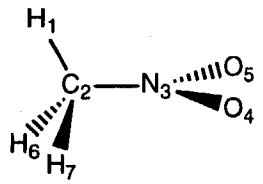
dichloromethane (C_{2V})



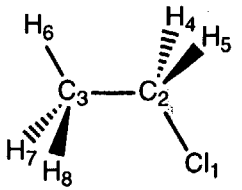
chloroform (C_{3V})



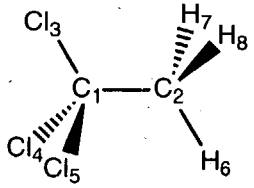
methanol (C_s)



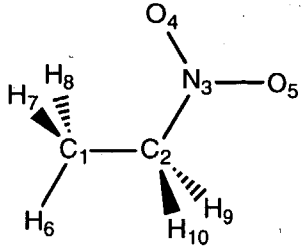
nitromethane (C_s)



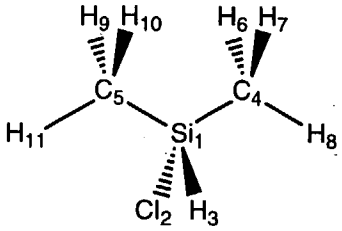
chloroethane (C_s)



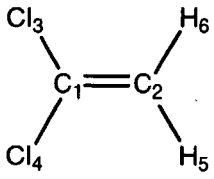
1,1,1-trichloroethane (C_{3v})



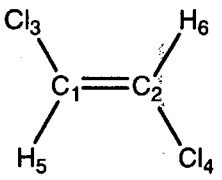
nitroethane (C_s)



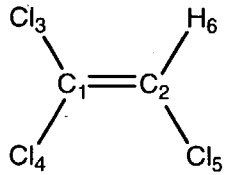
chlorodimethylsilane (C_s)



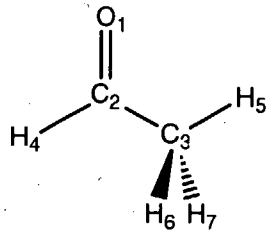
1,1-dichloroethylene (C_{2V})



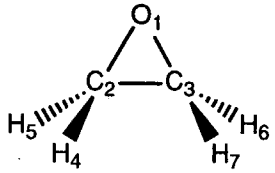
trans-1,2-dichloroethylene (C_{2H})



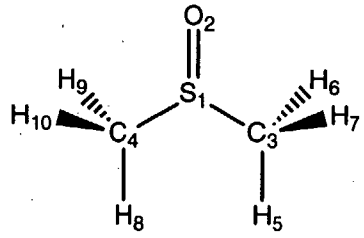
trichloroethylene (C_s)



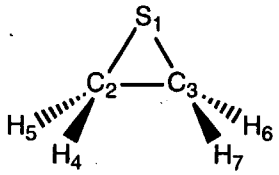
acetaldehyde (C_s)



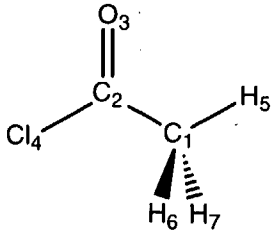
oxirane (C_{2v})



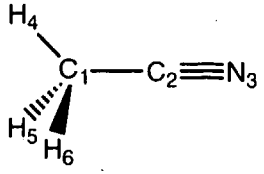
dimethylsulfoxide (C_s)



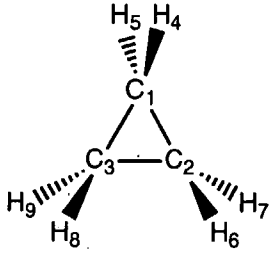
thiirane (C_{2v})



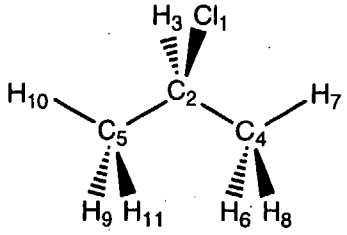
acetyl chloride (C_s)



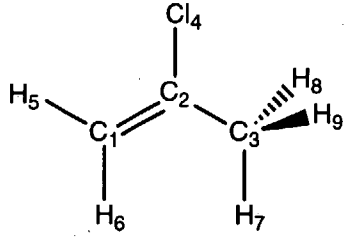
acetonitrile (C_{3V})



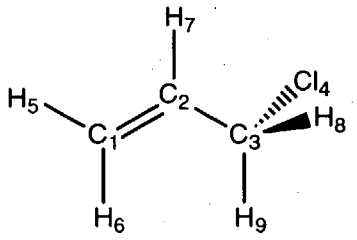
cyclopropane (D_{3H})



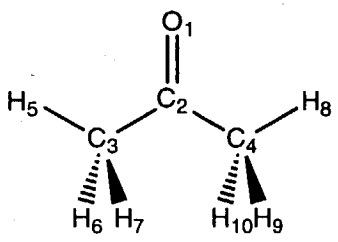
2-chloropropane (C_s)



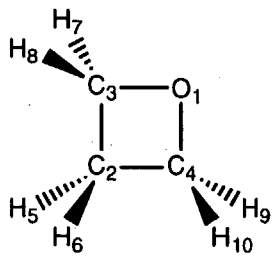
2-chloropropene (C_s)



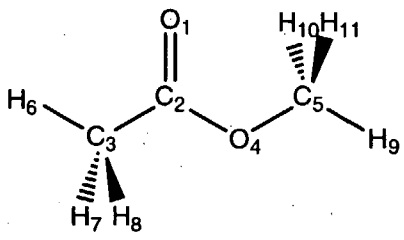
3-chloropropene (C_1)



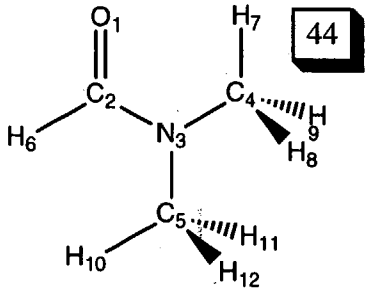
acetone (C_{2V})



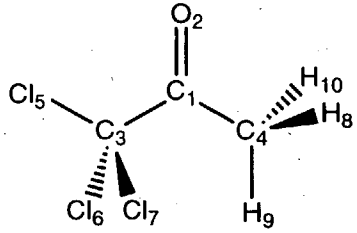
oxetane (C_{2V})



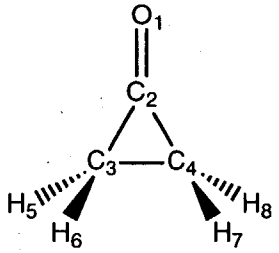
methyl acetate (C_s)



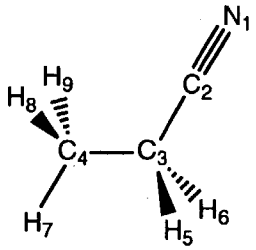
dimethylformamide (C_s)



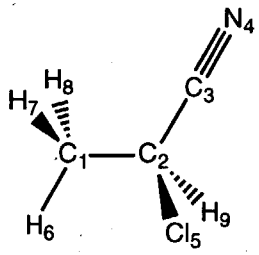
trichloroacetone (C_1)



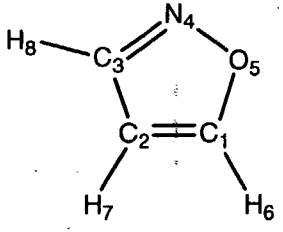
cyclopropanone (C_{2V})



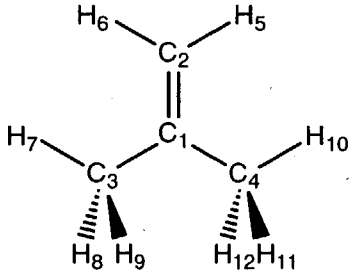
propionitrile (C_s)



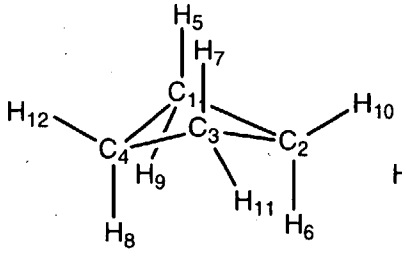
2-chloropropionitrile (C_1)



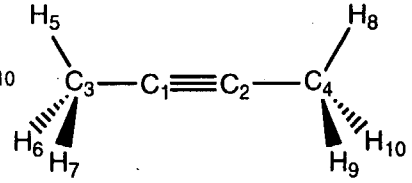
isoxazole (C_s)



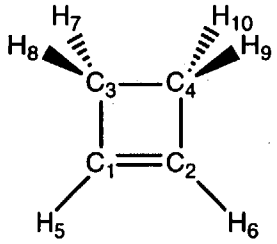
isobutylene (C_{2V})



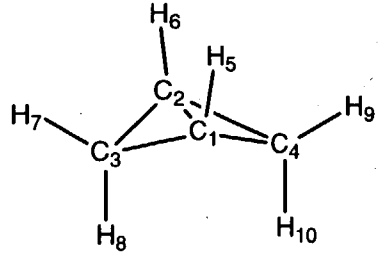
cyclobutane (D_{2D})



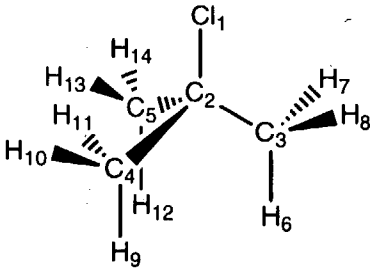
2-butyne (C_{3V})



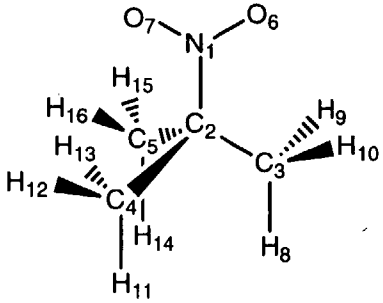
cyclobutene (C_{2V})



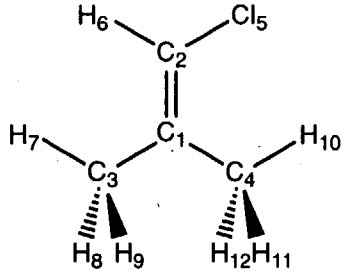
bicyclobutane (C_{2V})



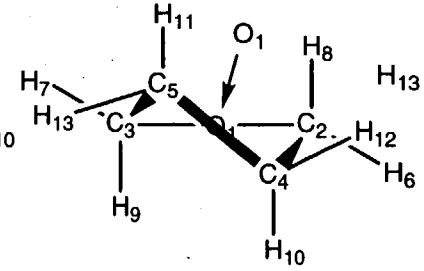
2-chloro-2-methylpropane (C_{3V})



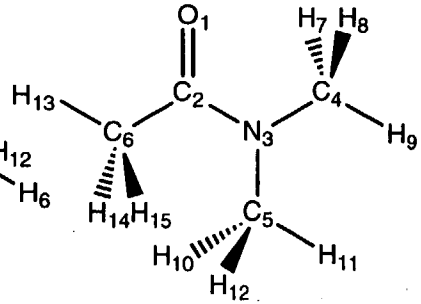
2-methyl-2-nitropropane (C_s)



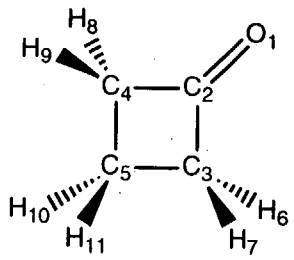
1-chloro-2-methylpropene (C_s)



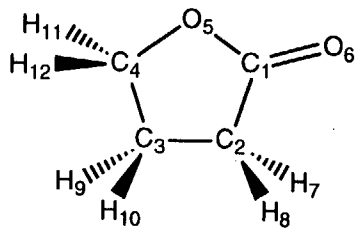
tetrahydrofuran (C_2)



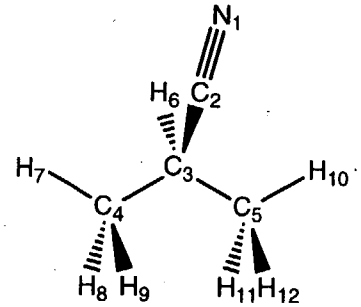
dimethylacetamide (C_1)



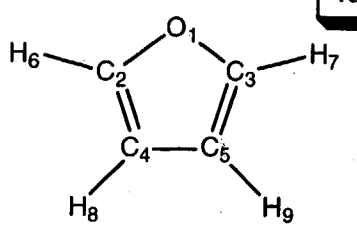
cyclobutanone (C_{2V})



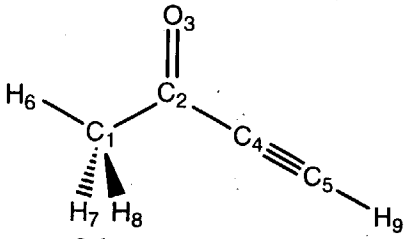
butyrolactone (C_1)



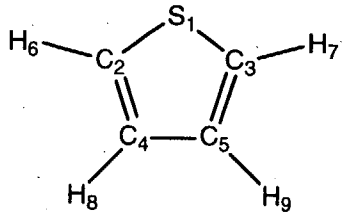
2-methylpropionitrile (C_s)



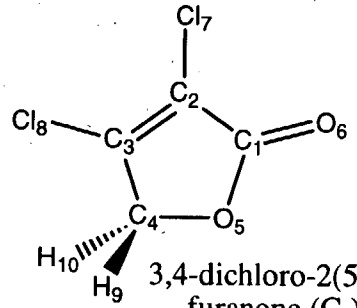
furan (C_{2V})



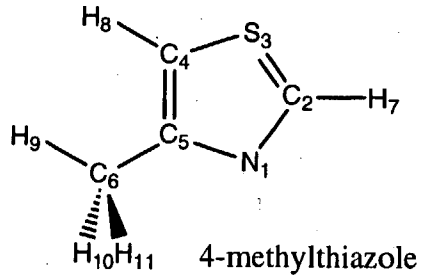
3-butyn-2-one (C_s)



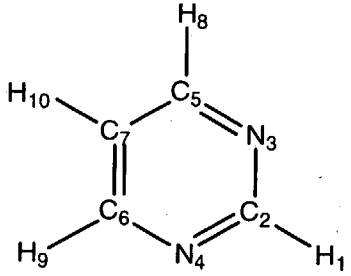
thiophene (C_{2V})



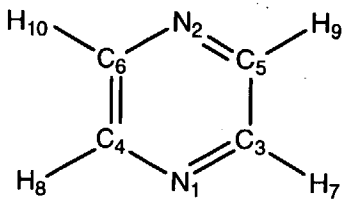
3,4-dichloro-2(5H)-furanone (C_s)



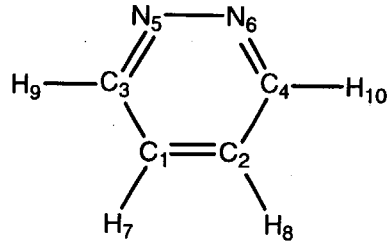
4-methylthiazole (C_s)



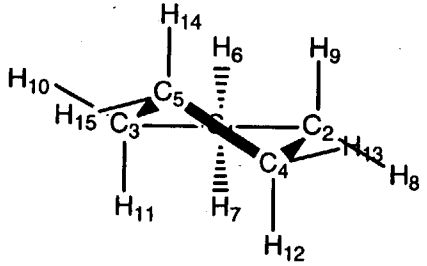
pyrimidine (C_{2V})



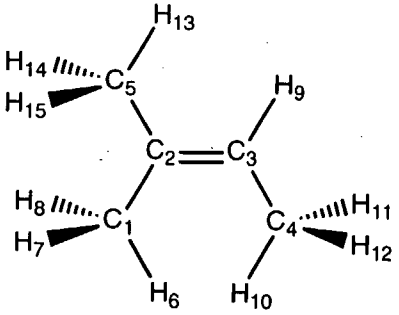
1,4-pyrazine (D_{2H})



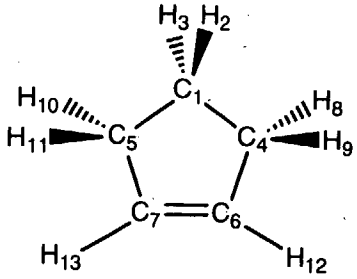
1,2-pyrazine (C_{2V})



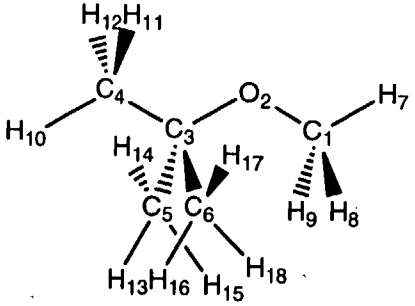
cyclopentane (C_2)



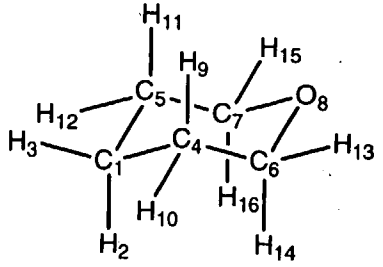
2-methyl-2-butene (C_s)



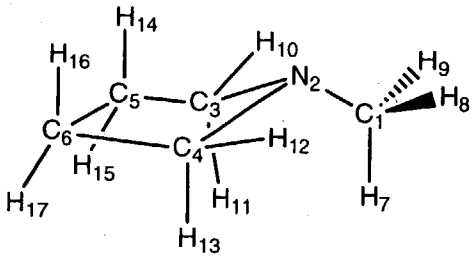
cyclopentene (C_s)



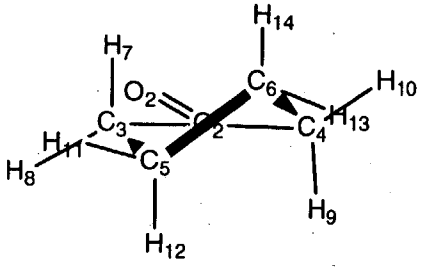
methyl t-butyl ether (C_s)



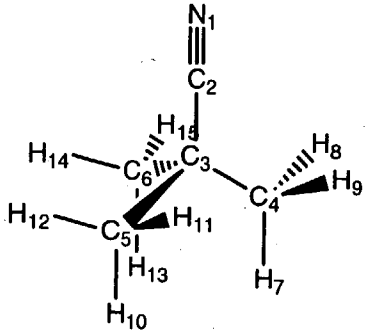
tetrahydropyran (C_s)



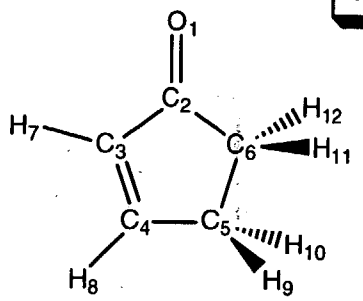
N-methylpyrrolidine (C_s)



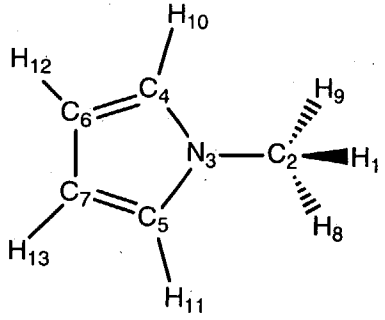
cyclopentanone (C_2)



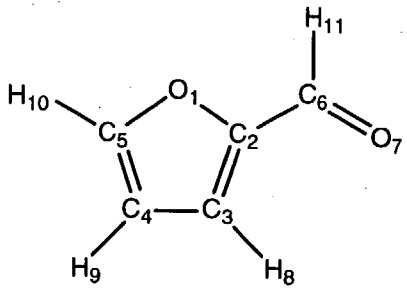
2,2-dimethylpropionitrile (C_{3V})



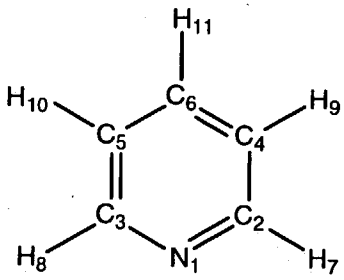
2-cyclopenten-1-one (C_s)



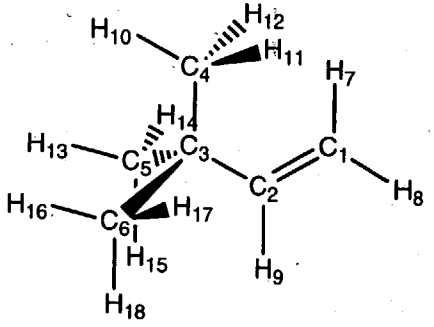
N-methylpyrrole (C_s)



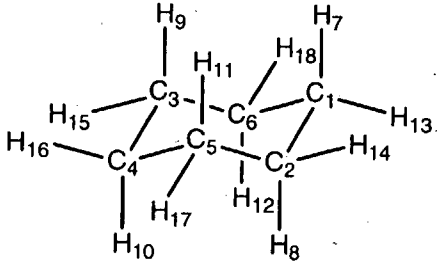
furfural (C_s)



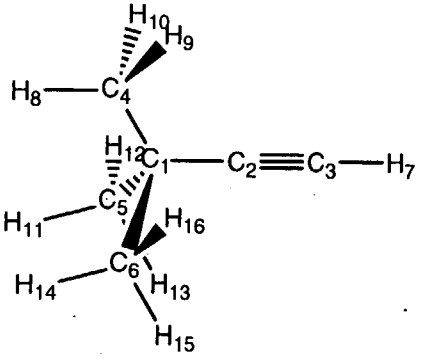
pyridine (C_{2V})



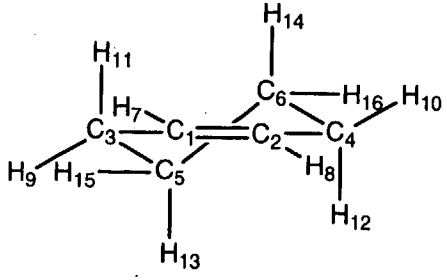
t-butylethylene (C_s)



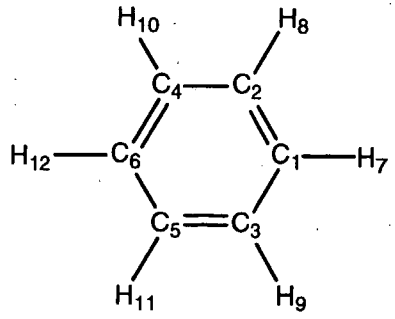
cyclohexane (D_{3D})



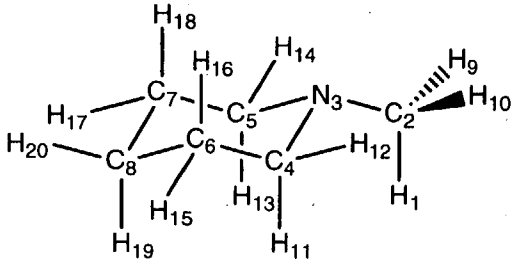
t-butylacetylene (C_{3V})



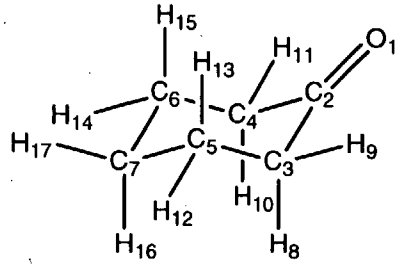
cyclohexene (C_2)



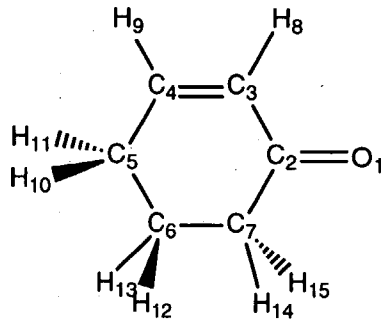
benzene (D_{6H})



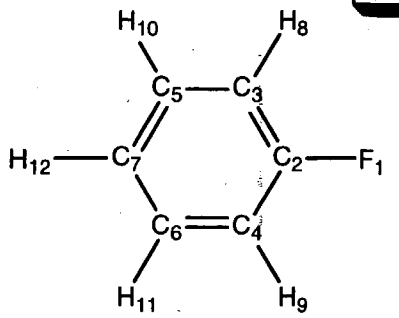
N-methylpiperidine (C_s)



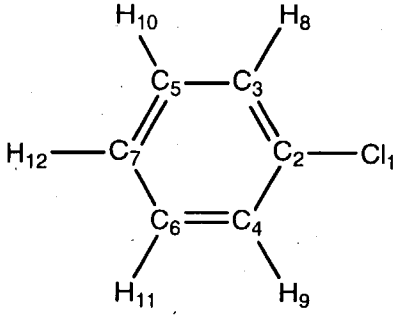
cyclohexanone (C_s)



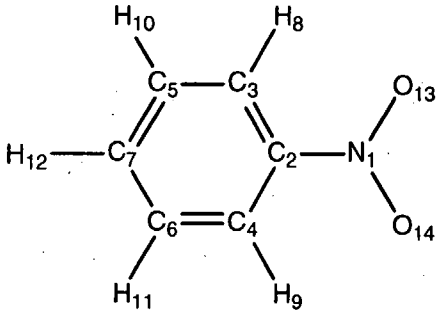
2-cyclohexen-1-one (C_1)



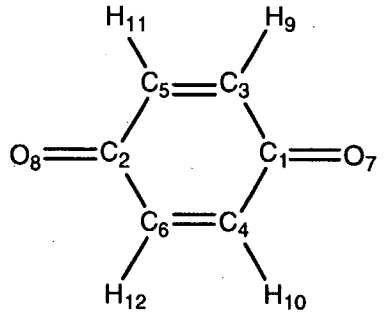
fluorobenzene (C_{2V})



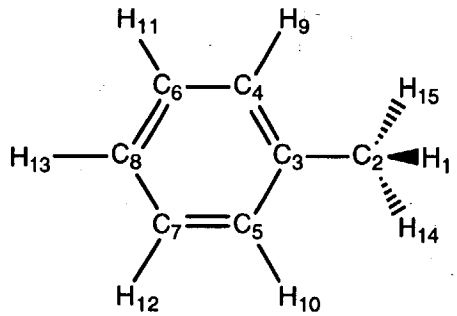
chlorobenzene (C_{2V})



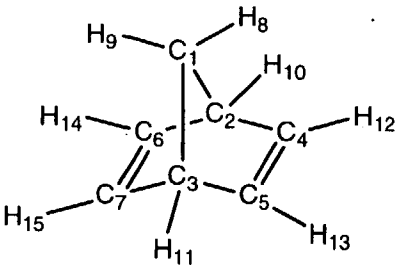
nitrobenzene (C_{2V})



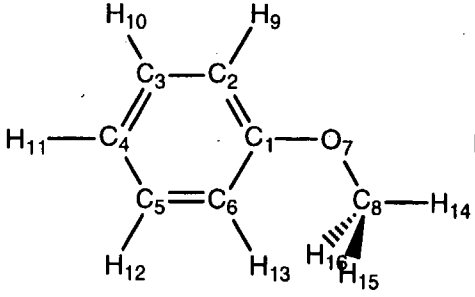
p-benzoquinone (D_{2H})



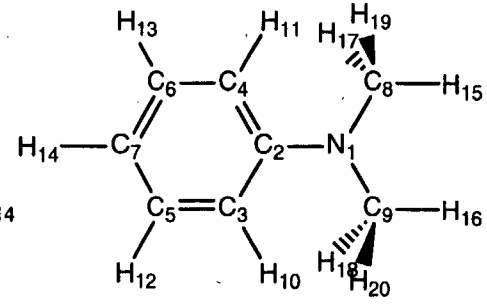
toluene (C_s)



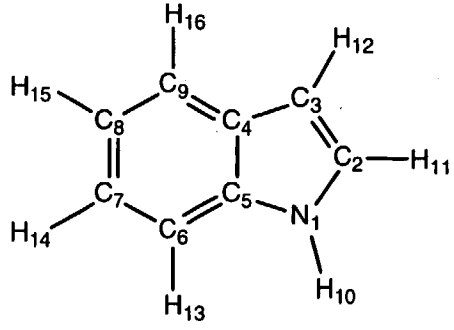
norbornadiene (C_{2V})



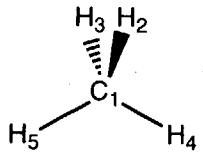
anisole (C_s)



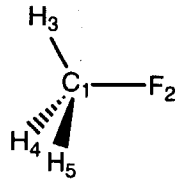
N,N-dimethylaniline (C_s)



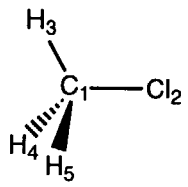
indole (C_s)



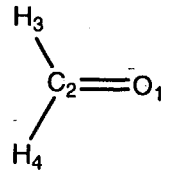
methane (T_d)



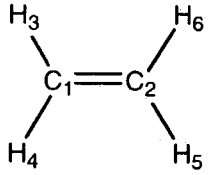
fluoromethane (C_{3V})



chloromethane (C_{3V})

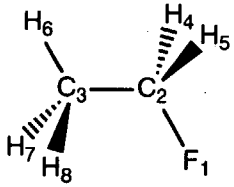


formaldehyde (C_{2V})

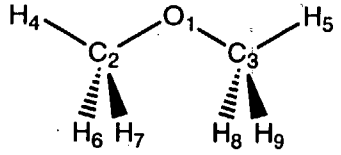


ethylene (D_{2H})

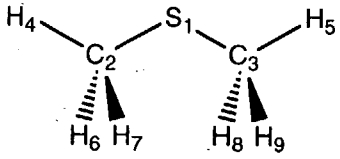
acetylene ($D_{\infty H}$)



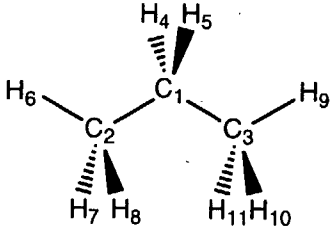
fluoroethane (C_s)



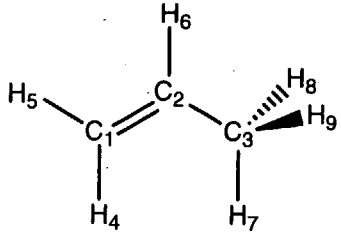
dimethyl ether (C_{2V})



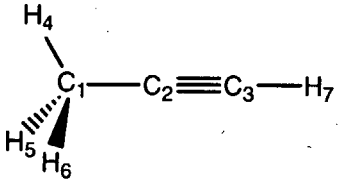
dimethyl sulfide (C_{2V})



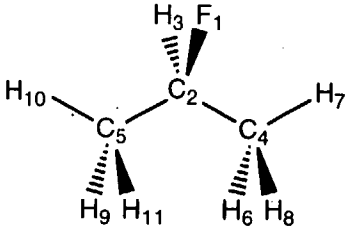
propane (C_{2V})



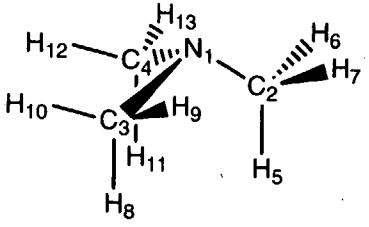
propene (C_s)



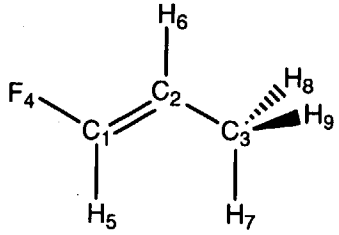
propyne (C_{3V})



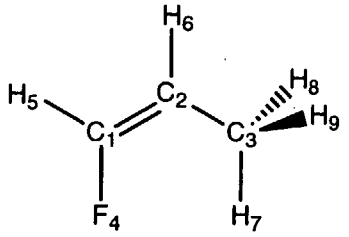
2-fluoropropane (C_s)



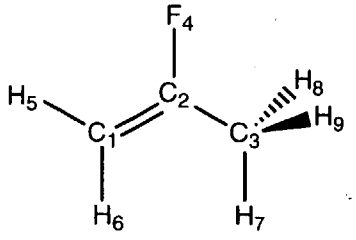
trimethylamine (C_{3V})



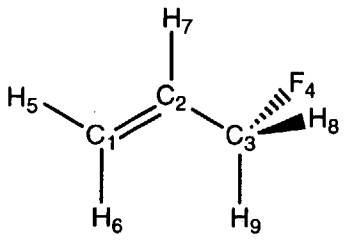
trans-1-fluoropropene (C_s)



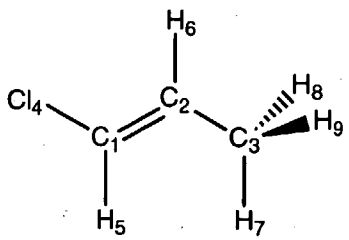
cis-1-fluoropropene (C_s)



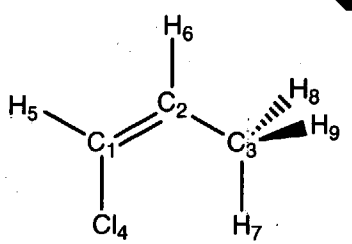
2-fluoropropene (C_s)



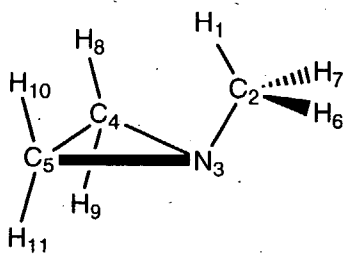
3-fluoropropene (C_1)



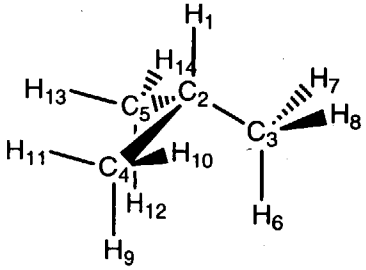
trans-1-chloropropene (C_s)



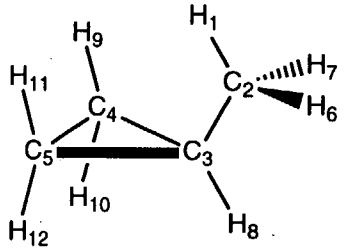
cis-1-chloropropene (C_s)



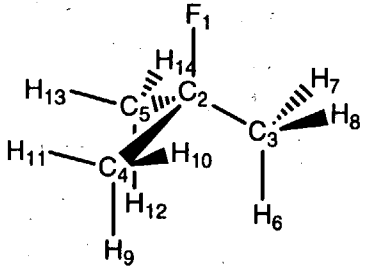
N-methylaziridine (C_s)



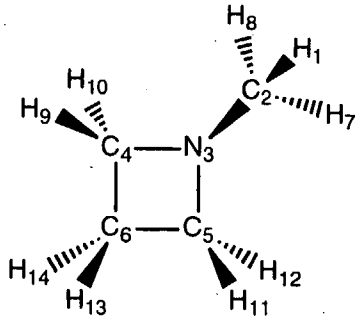
isobutane (C_{3V})



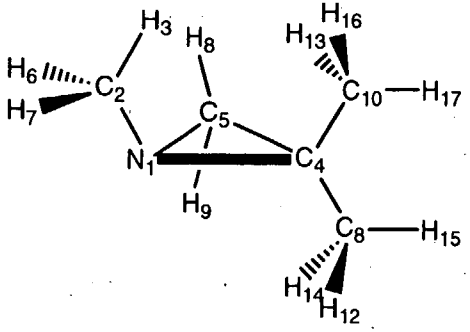
methylcyclopropane (C_s)



2-fluoro-2-methylpropane (C_{3V})



N-methylazetidine (C_s)



1,2,2-trimethylaziridine (C_1)

Z-Matrices for MP2/6-31+G* Optimizations:

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-------------------------------------
 Dichloromethane C2V MP2/6-31+G* fopt
-------------------------------------

Molecule:
---------
Stoichiometry    = CH2Cl2
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 21
Beta Electrons   = 21

Z-matrix:
--------------------------------------------------------------------------

0        1
C
X        1         1.
Cl       1         r1        2         a1
Cl       1         r1        2         a1        3         180.      0
H        1         r2        2         a2        3         90.       0
H        1         r2        2         a2        3         -90.      0

r1 = 1.769794
r2 = 1.087298
a1 = 56.458320
a2 = 124.489449
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
--------------------------------
 Chloroform C3V MP2/6-31+G* fopt
--------------------------------

Molecule:
---------
Stoichiometry    = CHCl3
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 29
Beta Electrons   = 29

Z-matrix:
--------------------------------------------------------------------------

0        1
C
H        1         r1
Cl       1         r2        2         a1
Cl       1         r2        2         a1        3         120.      0
Cl       1         r2        2         a1        3         -120.     0

r1 = 1.086816
r2 = 1.766515
a1 = 107.689174
```

++

Methanol Cs MP2/6-31+G* fopt

Molecule:

Stoichiometry = CH4O
Charge = 0
Multiplicity = 1
Alpha Electrons = 9
Beta Electrons = 9

Z-matrix:

0	1						
C							
O	1	r1					
H	1	r2	2	a1			
H	1	r3	2	a2	3	t1	0
H	1	r3	2	a2	3	-t1	0
H	2	r4	1	a3	3	180.	0

r1 = 1.432310
r2 = 1.089279
r3 = 1.095607
r4 = 0.971731
a1 = 105.859857
a2 = 111.628880
a3 = 108.648742
t1 = 118.535119

++

Nitromethane Cs MP2/6-31+G* fopt

Molecule:

Stoichiometry = CH3NO2
Charge = 0
Multiplicity = 1
Alpha Electrons = 16
Beta Electrons = 16

Z-matrix:

0	1						
H							
C	1	rch1					
N	2	rcn	1	a1			
O	3	rno	2	a2	1	t1	0
O	3	rno	2	a2	1	-t1	0
H	2	rch2	3	a3	1	t2	0
H	2	rch2	3	a3	1	-t2	0

```
rch1 = 1.090963
rcn = 1.489602
rno = 1.243762
rch2 = 1.087923
a1 = 107.011424
a2 = 117.285265
a3 = 107.727129
t1 = 88.923176
t2 = 119.014019
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
---------------------------------
 Chloroethane Cs MP2/6-31+G* fopt
---------------------------------

Molecule:
---------
Stoichiometry    = C2H5Cl
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 17
Beta Electrons   = 17

Z-matrix:
--------------------------------------------------------------------------------

0        1
Cl
C        1         r1
C        2         r2        1         a1
H        2         r3        3         a2        1         t1        0
H        2         r3        3         a2        1         -t1       0
H        3         r4        2         a3        1         180.      0
H        3         r5        2         a4        6         t2        0
H        3         r5        2         a4        6         -t2       0

r1 = 1.791227
r2 = 1.516211
r3 = 1.091098
r4 = 1.095411
r5 = 1.092682
a1 = 111.289936
a2 = 111.443369
a3 = 109.383661
a4 = 110.927528
t1 = 119.141102
t2 = 119.682460
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-------------------------------------------
 1,1,1-Trichloroethane C3V MP2/6-31+G* fopt
-------------------------------------------

Molecule:
---------
Stoichiometry    = C2H3Cl3
Charge           = 0
```

```
Multiplicity     = 1
Alpha Electrons  = 33
Beta Electrons   = 33

Z-matrix:
--------------------------------------------------------------------------

0        1
C
C        1         r1
Cl       1         r2        2         a1
Cl       1         r2        2         a1        3         120.      0
Cl       1         r2        2         a1        3         -120.     0
H        2         r3        1         a2        3         180.      0
H        2         r3        1         a2        6         120.      0
H        2         r3        1         a2        6         -120.     0

r1 = 1.516441
r2 = 1.780639
r3 = 1.092174
a1 = 109.810906
a2 = 109.496811
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
---------------------------------
 Nitroethane Cs MP2/6-31+G* fopt
---------------------------------

Molecule:
---------
Stoichiometry    = C2H5NO2
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 20
Beta Electrons   = 20

Z-matrix:
--------------------------------------------------------------------------

0        1
C
C        1         r1
N        2         r2        1         a1
O        3         r3        2         a2        1         0.        0
O        3         r4        2         a3        1         180.      0
H        1         r5        2         a4        3         180.      0
H        1         r6        2         a5        6         t1        0
H        1         r6        2         a5        6         -t1       0
H        2         r7        3         a6        1         t2        0
H        2         r7        3         a6        1         -t2       0

r1 = 1.512413
r2 = 1.505304
r3 = 1.243521
r4 = 1.243487
r5 = 1.094604
r6 = 1.091379
r7 = 1.092626
```

```
a1 = 112.872195
a2 = 118.778734
a3 = 116.005734
a4 = 108.364392
a5 = 111.351025
a6 = 104.606988
t1 = 119.416829
t2 = 123.312531
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
------------------------------------------------------
 Chlorodimethylsilane ((CH3)2SiHCl) Cs MP2/6-31+G* fopt
------------------------------------------------------

Molecule:
---------
Stoichiometry    = C2H7ClSi
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 25
Beta Electrons   = 25

Z-matrix:
--------------------------------------------------------------------------

O        1
Si
Cl       1         r1
H        1         r2        2         a1
C        1         r3        2         a2        3         t1        0
C        1         r3        2         a2        3         -t1       0
H        4         r4        1         a3        2         t2        0
H        4         r5        1         a4        6         t3        0
H        4         r6        1         a5        6         t4        0
H        5         r4        1         a3        2         -t2       0
H        5         r5        1         a4        9         -t3       0
H        5         r6        1         a5        9         -t4       0

r1 = 2.077158
r2 = 1.484308
r3 = 1.870624
r4 = 1.094783
r5 = 1.096001
r6 = 1.094244
a1 = 106.551067
a2 = 108.207708
a3 = 110.917410
a4 = 110.498869
a5 = 111.326763
t1 = 119.076717
t2 = 61.232762
t3 = 119.790631
t4 = -120.201541
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
------------------------------------------
 1,1--Dichloroethylene C2V MP2/6-31+G* fopt
------------------------------------------
```

```
Molecule:
---------
Stoichiometry    = C2H2Cl2
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 24
Beta Electrons   = 24

Z-matrix:
--------------------------------------------------------------------------

0        1
C
C        1         r1
Cl       1         r2        2         a1
Cl       1         r2        2         a1        3         180.      0
H        2         r3        1         a2        3         180.      0
H        2         r3        1         a2        5         180.      0

r1 = 1.337417
r2 = 1.726977
r3 = 1.083312
a1 = 122.581331
a2 = 120.377112
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
------------------------------------------------
 trans-1,2-Dichloroethylene C2H MP2/6-31+G* fopt
------------------------------------------------

Molecule:
---------
Stoichiometry    = C2H2Cl2
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 24
Beta Electrons   = 24

Z-matrix:
--------------------------------------------------------------------------

0        1
C
C        1         r1
Cl       1         r2        2         a1
Cl       2         r2        1         a1        3         180.      0
H        1         r3        2         a2        3         180.      0
H        2         r3        1         a2        4         180.      0

r1 = 1.337074
r2 = 1.725518
r3 = 1.083994
a1 = 121.505970
a2 = 123.535510
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
--------------------------------------
```

```
 Trichloroethylene Cs MP2/6-31+G* fopt
---------------------------------------

Molecule:
---------
Stoichiometry    = C2HCl3
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 32
Beta Electrons   = 32

Z-matrix:
--------------------------------------------------------------------------

0        1
C
C        1         r1
Cl       1         r2        2         a1
Cl       1         r3        2         a2        3         180.      0
Cl       2         r4        1         a3        3         180.      0
H        2         r5        1         a4        5         180.      0

r1 = 1.343749
r2 = 1.724790
r3 = 1.713363
r4 = 1.713703
r5 = 1.083366
a1 = 119.833582
a2 = 124.076616
a3 = 123.940207
a4 = 120.724935
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
---------------------------------
 Acetaldehyde Cs MP2/6-31+G* fopt
---------------------------------

Molecule:
---------
Stoichiometry    = C2H4O
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 12
Beta Electrons   = 12

Z-matrix:
--------------------------------------------------------------------------

0        1
O
C        1         rco
C        2         rcc       1         a1
H        2         rch1      1         a2        3         180.      0
H        3         rch2      2         a3        1         0.        0
H        3         rch3      2         a4        5         t1        0
H        3         rch3      2         a4        5         -t1       0

rco = 1.227305
```

```
rcc = 1.501015
rch1 = 1.108052
rch2 = 1.091316
rch3 = 1.096047
a1 = 124.405444
a2 = 119.671910
a3 = 110.283366
a4 = 109.626356
t1 = 121.318952
------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
------------------------------
 Oxirane C2V MP2/6-31+G* fopt
------------------------------

Molecule:
---------
Stoichiometry    = C2H4O
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 12
Beta Electrons   = 12

Z-matrix:
------------------------------------------------------------------------

O        1
O
C        1         r1
C        1         r1        2         a1
H        2         r2        1         a2        3         t1        0
H        2         r2        1         a2        3         -t1       0
H        3         r2        1         a2        2         t1        0
H        3         r2        1         a2        2         -t1       0

r1 = 1.445275
r2 = 1.087034
a1 = 60.955531
a2 = 114.604538
t1 = 111.121688
------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
---------------------------------------
 Dimethylsulfoxide Cs MP2/6-31+G* fopt
---------------------------------------

Molecule:
---------
Stoichiometry    = C2H6OS
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 21
Beta Electrons   = 21

Z-matrix:
------------------------------------------------------------------------

0        1
```

```
S
O       1       rso
X       1       1.      2       90.
C       1       rsc     2       a1      3       t1      0
C       1       rsc     2       a1      3       -t1     0
H       4       rch1    1       a2      2       t2      0
H       4       rch2    1       a3      6       t3      0
H       4       rch3    1       a4      6       t4      0
H       5       rch1    1       a2      2       -t2     0
H       5       rch2    1       a3      9       -t3     0
H       5       rch3    1       a4      9       -t4     0

rso = 1.521568
rsc = 1.808629
rch1 = 1.094007
rch2 = 1.091805
rch3 = 1.093853
a1 = 106.731325
a2 = 110.118976
a3 = 107.330415
a4 = 108.865811
t1 = 128.917320
t2 = 172.619467
t3 = 119.478593
t4 = -122.092382
-------------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
------------------------------
 Thiirane C2V MP2/6-31+G* fopt
------------------------------

Molecule:
---------
Stoichiometry    = C2H4S
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 16
Beta Electrons   = 16

Z-matrix:
-------------------------------------------------------------------------

0       1
S
C       1       r1
C       1       r1      2       a1
H       2       r2      1       a2      3       t1      0
H       2       r2      1       a2      3       -t1     0
H       3       r2      1       a2      2       t1      0
H       3       r2      1       a2      2       -t1     0

r1 = 1.817166
r2 = 1.085977
a1 = 48.185729
a2 = 115.521624
t1 = 110.903925
-------------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

```
-------------------------------------
 Acetyl chloride Cs MP2/6-31+G* fopt
-------------------------------------

Molecule:
---------
Stoichiometry    = C2H3ClO
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 20
Beta Electrons   = 20

Z-matrix:
--------------------------------------------------------------------------

0        1
C
C        1         r1
O        2         r2        1         a1
Cl       2         r3        1         a2        3         180.      0
H        1         r4        2         a3        3         0.        0
H        1         r5        2         a4        5         t1        0
H        1         r5        2         a4        5         -t1       0

r1 = 1.499889
r2 = 1.204480
r3 = 1.793248
r4 = 1.090826
r5 = 1.093231
a1 = 127.168158
a2 = 112.452226
a3 = 108.877526
a4 = 109.630559
t1 = 120.959164
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------
 Acetonitrile C3V MP2/6-31+G* fopt
-----------------------------------

Molecule:
---------
Stoichiometry    = C2H3N
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 11
Beta Electrons   = 11

Z-matrix:
--------------------------------------------------------------------------

0        1
C
C        1         r1
X        2         1.        1         90.
N        2         r2        3         90.       1         180.      0
H        1         r3        2         a1        3         0.        0
H        1         r3        2         a1        3         120.      0
```

```
H       1       r3      2       a1      3       -120.   0

r1 = 1.464078
r2 = 1.180831
r3 = 1.092256
a1 = 109.967333
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------
 Cyclopropane D3H MP2/6-31+G* fopt
-----------------------------------

Molecule:
---------
Stoichiometry    = C3H6
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 12
Beta Electrons   = 12

Z-matrix:
--------------------------------------------------------------------------------

0       1
X
X       1       1.
C       1       r1      2       90.
C       1       r1      2       90.     3       120.    0
C       1       r1      2       90.     3       -120.   0
H       3       r2      1       a1      2       0.      0
H       3       r2      1       a1      2       180.    0
H       4       r2      1       a1      2       0.      0
H       4       r2      1       a1      2       180.    0
H       5       r2      1       a1      2       0.      0
H       5       r2      1       a1      2       180.    0

r1 = 0.869702
r2 = 1.085196
a1 = 122.779494
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------
 2-Chloropropane Cs MP2/6-31+G* fopt
-----------------------------------

Molecule:
---------
Stoichiometry    = C3H7Cl
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 21
Beta Electrons   = 21

Z-matrix:
--------------------------------------------------------------------------------

0       1
Cl
```

```
C         1         r1
H         2         r2        1         a1
C         2         r3        1         a2        3         t1        0
C         2         r3        1         a2        3         -t1       0
H         4         r4        2         a3        1         t2        0
H         4         r5        2         a4        6         t3        0
H         4         r6        2         a5        6         t4        0
H         5         r4        2         a3        1         -t2       0
H         5         r5        2         a4        9         -t3       0
H         5         r6        2         a5        9         -t4       0

r1 = 1.803216
r2 = 1.093556
r3 = 1.518503
r4 = 1.095703
r5 = 1.092816
r6 = 1.094207
a1 = 105.060954
a2 = 109.350481
a3 = 109.353017
a4 = 111.262594
a5 = 110.498715
t1 = 117.926523
t2 = 182.336677
t3 = 119.947513
t4 = -119.450353
-------------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------
 2-Chloropropene Cs MP2/6-31+G* fopt
-----------------------------------

Molecule:
---------
Stoichiometry    = C3H5Cl
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 20
Beta Electrons   = 20

Z-matrix:
-------------------------------------------------------------------------

0         1
C
C         1         r1
C         2         r2        1         a1
Cl        2         r3        1         a2        3         180.      0
H         1         r4        2         a3        3         180.      0
H         1         r5        2         a4        5         180.      0
H         3         r6        2         a5        4         180.      0
H         3         r7        2         a6        7         t1        0
H         3         r7        2         a6        7         -t1       0

r1 = 1.339193
r2 = 1.496375
r3 = 1.749236
r4 = 1.083826
```

```
r5 = 1.085338
r6 = 1.093388
r7 = 1.094479
a1 = 125.964784
a2 = 119.911401
a3 = 122.178622
a4 = 119.605102
a5 = 109.856717
a6 = 110.658632
t1 = 120.348834
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------
 Allyl chloride C1 MP2/6-31+G* fopt
-----------------------------------

Molecule:
---------
Stoichiometry    = C3H5Cl
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 20
Beta Electrons   = 20

Z-matrix:
--------------------------------------------------------------------------------

0        1
C
C        1         r1
C        2         r2        1         a1
Cl       3         r3        2         a2        1         t1        0
H        1         r4        2         a3        3         t2        0
H        1         r5        2         a4        5         t3        0
H        2         r6        1         a5        3         t4        0
H        3         r7        2         a6        4         t5        0
H        3         r8        2         a7        4         t6        0

r1 = 1.341501
r2 = 1.491400
r3 = 1.798965
r4 = 1.085277
r5 = 1.087128
r6 = 1.088717
r7 = 1.092160
r8 = 1.091713
a1 = 123.014271
a2 = 110.995705
a3 = 121.378488
a4 = 121.576751
a5 = 120.422278
a6 = 111.675134
a7 = 111.088374
t1 = 118.629215
t2 = 178.736308
t3 = 179.977279
t4 = 180.471294
t5 = 118.256949
```

```
t6 = -119.502086
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
------------------------------
 Acetone C2V MP2/6-31+G* fopt
------------------------------

Molecule:
---------
Stoichiometry    = C3H6O
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 16
Beta Electrons   = 16

Z-matrix:
--------------------------------------------------------------------------------

0        1
O
C        1         rco
C        2         rcc       1         a1
C        2         rcc       1         a1        3         180.      0
H        3         rch1      2         a2        1         0.        0
H        3         rch2      2         a3        5         t1        0
H        3         rch2      2         a3        5         -t1       0
H        4         rch1      2         a2        1         0.        0
H        4         rch2      2         a3        8         t1        0
H        4         rch2      2         a3        8         -t1       0

rco = 1.231701
rcc = 1.512011
rch1 = 1.090991
rch2 = 1.095719
a1 = 121.642183
a2 = 109.750447
a3 = 110.143940
t1 = 121.012156
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
------------------------------
 Oxetane C2V MP2/6-31+G* fopt
------------------------------

Molecule:
---------
Stoichiometry    = C3H6O
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 16
Beta Electrons   = 16

Z-matrix:
--------------------------------------------------------------------------------

0        1
O
C        1         r1
```

```
C          1          r2         2          a1
C          1          r2         2          a1         3          180.       0
H          2          r3         1          a2         3          90.        0
H          2          r3         1          a2         3          -90.       0
H          3          r4         2          a3         1          t1         0
H          3          r4         2          a3         1          -t1        0
H          4          r4         2          a3         1          -t1        0
H          4          r4         2          a3         1          t1         0

r1 = 2.155002
r2 = 1.458052
r3 = 1.092058
r4 = 1.094953
a1 = 45.477631
a2 = 125.344990
a3 = 116.005257
t1 = 114.634912
-------------------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
--------------------------------------
 Methyl acetate Z Cs MP2/6-31+G* fopt
--------------------------------------

Molecule:
---------
Stoichiometry    = C3H6O2
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 20
Beta Electrons   = 20

Z-matrix:
-------------------------------------------------------------------------------

O          1
O
C          1          rco1
C          2          rcc        1          a1
O          2          rco2       1          a2         3          180.       0
C          4          rco3       2          a3         1          0.         0
H          3          rch1       2          a4         1          0.         0
H          3          rch2       2          a5         6          t1         0
H          3          rch2       2          a5         6          -t1        0
H          5          rch3       4          a6         2          180.       0
H          5          rch4       4          a7         9          t2         0
H          5          rch4       4          a7         9          -t2        0

rco1 = 1.223233
rcc = 1.503152
rco2 = 1.359125
rco3 = 1.445224
rch1 = 1.089789
rch2 = 1.093195
rch3 = 1.088346
rch4 = 1.091261
a1 = 125.985509
a2 = 123.256741
a3 = 114.696934
```

```
a4 = 109.198457
a5 = 109.816404
a6 = 104.896903
a7 = 110.165580
t1 = 120.844397
t2 = 119.535388
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
------------------------------------------
 N,N-Dimethylformamide Cs MP2/6-31+G* fopt
------------------------------------------

Molecule:
---------
Stoichiometry    = C3H7NO
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 20
Beta Electrons   = 20

Z-matrix:
--------------------------------------------------------------------------------

0        1
O
C        1         r1
N        2         r2        1         a1
C        3         r3        2         a2        1         0.        0
C        3         r4        2         a3        1         180.      0
H        2         r5        1         a4        4         180.      0
H        4         r6        3         a5        2         0.        0
H        4         r7        3         a6        7         t1        0
H        4         r7        3         a6        7         -t1       0
H        5         r8        3         a7        7         180.      0
H        5         r9        3         a8        10        t2        0
H        5         r9        3         a8        10        -t2       0

r1 = 1.234917
r2 = 1.362372
r3 = 1.452970
r4 = 1.450423
r5 = 1.104083
r6 = 1.090278
r7 = 1.095740
r8 = 1.092518
r9 = 1.096017
a1 = 125.614500
a2 = 120.556358
a3 = 121.765417
a4 = 121.805790
a5 = 108.272778
a6 = 110.161547
a7 = 109.482314
a8 = 110.541238
t1 = 119.942805
t2 = 119.849806
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

1,1,1-Trichloroacetone C1 MP2/6-31+G* fopt

Molecule:

Stoichiometry = C3H3Cl3O
Charge = 0
Multiplicity = 1
Alpha Electrons = 40
Beta Electrons = 40

Z-matrix:

O	1						
C							
O	1	r1					
C	1	r2	2	a1			
C	1	r3	2	a2	3	t1	0
Cl	3	r4	1	a3	2	t2	0
Cl	3	r5	1	a4	5	t3	0
Cl	3	r6	1	a5	5	t4	0
H	4	r7	1	a6	2	t5	0
H	4	r8	1	a7	8	t6	0
H	4	r9	1	a8	8	t7	0

r1 = 1.219464
r2 = 1.561044
r3 = 1.507848
r4 = 1.755824
r5 = 1.778467
r6 = 1.781717
r7 = 1.091811
r8 = 1.090477
r9 = 1.094889
a1 = 119.904928
a2 = 122.967624
a3 = 111.001880
a4 = 108.659681
a5 = 106.847085
a6 = 107.755160
a7 = 113.195102
a8 = 108.543686
t1 = 179.490098
t2 = 7.867109
t3 = 121.138565
t4 = -120.090193
t5 = 31.923910
t6 = 122.267548
t7 = -117.297165

++

Cyclopropanone C2V MP2/6-31+G* fopt

Molecule:

```
---------
Stoichiometry    = C3H4O
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 15
Beta Electrons   = 15

Z-matrix:
--------------------------------------------------------------------------

O        1
O
C        1         r1
C        2         r2        1         a1
C        2         r2        1         a1        3         180.      0
H        3         r3        2         a2        1         t1        0
H        3         r3        2         a2        1         -t1       0
H        4         r3        2         a2        1         t1        0
H        4         r3        2         a2        1         -t1       0

r1 = 1.216919
r2 = 1.468636
r3 = 1.087738
a1 = 147.564916
a2 = 118.891701
t1 = 74.319017
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
---------------------------------
 Ethanitrile Cs MP2/6-31+G* fopt
---------------------------------

Molecule:
---------
Stoichiometry    = C3H5N
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 15
Beta Electrons   = 15

Z-matrix:
--------------------------------------------------------------------------

0        1
N
C        1         r1
X        2         1.        1         90.
C        2         r2        3         a1        1         180.      0
C        4         r3        2         a2        3         180.      0
H        4         r4        2         a3        3         t1        0
H        4         r4        2         a3        3         -t1       0
H        5         r5        4         a4        2         180.      0
H        5         r6        4         a5        8         t2        0
H        5         r6        4         a5        8         -t2       0

r1 = 1.181967
r2 = 1.467640
r3 = 1.532625
```

```
r4 = 1.095089
r5 = 1.093467
r6 = 1.092601
a1 = 91.234098
a2 = 111.968209
a3 = 108.109334
a4 = 109.765908
a5 = 110.776136
t1 = 57.828844
t2 = 119.825160
-------------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------------
 2-Chloropropanitrile C1 MP2/6-31+G* fopt
-----------------------------------------

Molecule:
---------
Stoichiometry    = C3H4ClN
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 23
Beta Electrons   = 23

Z-matrix:
-------------------------------------------------------------------------

0        1
C
C        1         r1
C        2         r2        1         a1
X        3         1.        2         90.       1         180.      0
N        3         r3        4         a2        2         t1        0
Cl       2         r4        1         a3        3         t2        0
H        1         r5        2         a4        3         t3        0
H        1         r6        2         a5        7         t4        0
H        1         r7        2         a6        7         t5        0
H        2         r8        1         a7        3         t6        0

r1 = 1.523323
r2 = 1.465889
r3 = 1.182612
r4 = 1.793415
r5 = 1.092476
r6 = 1.092228
r7 = 1.094057
r8 = 1.093435
a1 = 111.723883
a2 = 91.646320
a3 = 110.800845
a4 = 109.615771
a5 = 110.503237
a6 = 109.479070
a7 = 110.572359
t1 = 181.869736
t2 = 122.200545
t3 = 178.724630
t4 = 120.175915
```

```
t5 = -119.668757
t6 = -120.460508
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-------------------------------
 Isoxazole Cs MP2/6-31+G* fopt
-------------------------------

Molecule:
---------
Stoichiometry    = C3H3NO
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 18
Beta Electrons   = 18

Z-matrix:
--------------------------------------------------------------------------------

0        1
C
C        1         r1
C        2         r2        1         a1
N        3         r3        2         a2        1         0.        0
O        4         r4        3         a3        2         0.        0
H        1         r5        2         a4        5         180.      0
H        2         r6        3         a5        1         180.      0
H        3         r7        4         a6        2         180.      0

r1 = 1.366203
r2 = 1.415993
r3 = 1.330050
r4 = 1.395041
r5 = 1.081044
r6 = 1.080615
r7 = 1.082753
a1 = 103.573385
a2 = 112.206841
a3 = 105.128500
a4 = 134.617127
a5 = 128.578804
a6 = 118.353071
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
--------------------------------
 Isobutylene Cs MP2/6-31+G* fopt
--------------------------------

Molecule:
---------
Stoichiometry    = C4H8
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 16
Beta Electrons   = 16

Z-matrix:
--------------------------------------------------------------------------------
```

```
0        1
C
C        1         r1
C        1         r2        2         a1
C        1         r2        2         a1        3         180.      0
H        2         r3        1         a2        3         180.      0
H        2         r3        1         a2        5         180.      0
H        3         r4        1         a3        2         0.        0
H        3         r5        1         a4        7         t1        0
H        3         r5        1         a4        7         -t1       0
H        4         r4        1         a3        2         0.        0
H        4         r5        1         a4        10        t1        0
H        4         r5        1         a4        10        -t1       0

r1 = 1.344390
r2 = 1.504994
r3 = 1.086832
r4 = 1.093820
r5 = 1.096862
a1 = 122.145138
a2 = 121.574111
a3 = 111.544165
a4 = 110.679408
t1 = 120.806520
-------------------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
--------------------------------
 Cyclobutane D2D MP2/6-31+G* fopt
--------------------------------

Molecule:
---------
Stoichiometry    = C4H8
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 16
Beta Electrons   = 16

Z-matrix:
-------------------------------------------------------------------------

0        1
X
X        1         r1
C        1         r2        2         90.
C        2         r2        1         90.       3         90.       0
C        1         r2        2         90.       3         180.      0
C        2         r2        1         90.       3         270.      0
H        3         r3        1         a1        2         180.      0
H        4         r3        2         a1        1         180.      0
H        5         r3        1         a1        2         180.      0
H        6         r3        2         a1        1         180.      0
H        3         r4        1         a2        7         180.      0
H        4         r4        2         a2        8         180.      0
H        5         r4        1         a2        9         180.      0
H        6         r4        2         a2        10        180.      0
```

```
r1 = 0.295219
r2 = 1.073590
r3 = 1.095485
r4 = 1.094753
a1 = 104.595934
a2 = 146.632704
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-------------------------------
 2-Butyne D3H MP2/6-31+G* fopt
-------------------------------

Molecule:
---------
Stoichiometry    = C4H6
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 15
Beta Electrons   = 15

Z-matrix:
--------------------------------------------------------------------------------

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
C        2         r2        5         90.       1         180.      0
H        4         r3        1         a1        3         0.        0
H        4         r3        1         a1        7         120.      0
H        4         r3        1         a1        7         -120.     0
H        6         r3        2         a1        5         0.        0
H        6         r3        2         a1        10        120.      0
H        6         r3        2         a1        10        -120.     0

r1 = 1.223823
r2 = 1.465672
r3 = 1.094316
a1 = 110.903606
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
---------------------------------
 Cyclobutene C2V MP2/6-31+G* fopt
---------------------------------

Molecule:
---------
Stoichiometry    = C4H6
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 15
Beta Electrons   = 15

Z-matrix:
--------------------------------------------------------------------------------
```

```
0        1
C
C        1         r1
C        1         r2        2         a1
C        2         r2        1         a1        3         0.        0
H        1         r3        2         a2        3         180.      0
H        2         r3        1         a2        4         180.      0
H        3         r4        1         a3        2         t1        0
H        3         r4        1         a3        2         -t1       0
H        4         r4        2         a3        1         t1        0
H        4         r4        2         a3        1         -t1       0

r1 = 1.350451
r2 = 1.515406
r3 = 1.087663
r4 = 1.095793
a1 = 94.111903
a2 = 133.537503
a3 = 115.785639
t1 = 115.447455
-------------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------
 Bicyclobutane C2V MP2/6-31+G* fopt
-----------------------------------

Molecule:
---------
Stoichiometry    = C4H6
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 15
Beta Electrons   = 15

Z-matrix:
-------------------------------------------------------------------------

0        1
X
X        1         1.
C        2         r1        1         90.
C        2         r1        1         90.       3         180.      0
C        2         r2        1         a1        3         90.       0
C        2         r2        1         a1        4         90.       0
H        3         r3        2         a2        1         0.        0
H        4         r3        2         a2        1         0.        0
H        5         r4        2         a3        1         0.        0
H        5         r5        2         a4        1         180.      0
H        6         r4        2         a3        1         0.        0
H        6         r5        2         a4        1         180.      0

r1 = 0.753411
r2 = 1.292403
r3 = 1.081153
r4 = 1.089121
r5 = 1.092709
a1 = 118.578099
a2 = 126.839375
```

```
a3 = 121.710621
a4 = 124.029533
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
--------------------------------------
 t-Butyl chloride C3V MP2/6-31+G* fopt
--------------------------------------

Molecule:
---------
Stoichiometry    = C4H9Cl
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 25
Beta Electrons   = 25

Z-matrix:
--------------------------------------------------------------------------

0        1
Cl
C        1         r1
C        2         r2        1         a1
C        2         r2        1         a1        3         120.      0
C        2         r2        1         a1        3         -120.     0
H        3         r3        2         a2        1         180.      0
H        3         r4        2         a3        6         t1        0
H        3         r4        2         a3        6         -t1       0
H        4         r3        2         a2        1         180.      0
H        4         r4        2         a3        9         t1        0
H        4         r4        2         a3        9         -t1       0
H        5         r3        2         a2        1         180.      0
H        5         r4        2         a3        12        t1        0
H        5         r4        2         a3        12        -t1       0

r1 = 1.817245
r2 = 1.522772
r3 = 1.096319
r4 = 1.093822
a1 = 107.591795
a2 = 109.231954
a3 = 110.923407
t1 = 119.646689
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
--------------------------------------------
 2-Methyl-2-nitropropane Cs MP2/6-31+G* fopt
--------------------------------------------

Molecule:
---------
Stoichiometry    = C4H9NO2
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 28
Beta Electrons   = 28

Z-matrix:
```

```
---------------------------------------------------------------------

0        1
N
C        1         r1
C        2         r2        1         a1
C        2         r3        1         a2        3         t1        0
C        2         r3        1         a2        3         -t1       0
O        1         r4        2         a3        3         0.        0
O        1         r5        2         a4        3         180.      0
H        3         r6        2         a5        1         180.      0
H        3         r7        2         a6        8         t2        0
H        3         r7        2         a6        8         -t2       0
H        4         r8        2         a7        1         t3        0
H        4         r9        2         a8        11        t4        0
H        4         r10       2         a9        11        t5        0
H        5         r8        2         a7        1         -t3       0
H        5         r9        2         a8        14        -t4       0
H        5         r10       2         a9        14        -t5       0

r1 = 1.525954
r2 = 1.519620
r3 = 1.526348
r4 = 1.245456
r5 = 1.244947
r6 = 1.094996
r7 = 1.092497
r8 = 1.094768
r9 = 1.095098
r10 = 1.092386
a1 = 109.228458
a2 = 106.317388
a3 = 119.034250
a4 = 116.577961
a5 = 108.141097
a6 = 111.447198
a7 = 108.885520
a8 = 110.733785
a9 = 110.901740
t1 = 120.503435
t2 = 119.364069
t3 = 180.251959
t4 = 119.006103
t5 = -119.776888
---------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-------------------------------------------------
 1-Chloro-2-methyl-1-propene Cs MP2/6-31+G* fopt
-------------------------------------------------

Molecule:
---------
Stoichiometry    = C4H7Cl
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 24
Beta Electrons   = 24
```

```
Z-matrix:
--------------------------------------------------------------------------

0        1
C
C        1         r1
C        2         r2        1         a1
C        2         r3        1         a2        3         180.      0
Cl       1         r4        2         a3        3         180.      0
H        1         r5        2         a4        5         180.      0
H        3         r6        2         a5        1         0.        0
H        3         r7        2         a6        7         t1        0
H        3         r7        2         a6        7         -t1       0
H        4         r8        2         a7        1         0.        0
H        4         r9        2         a8        10        t2        0
H        4         r9        2         a8        10        -t2       0

r1 = 1.342717
r2 = 1.505494
r3 = 1.500118
r4 = 1.737097
r5 = 1.084723
r6 = 1.094007
r7 = 1.096522
r8 = 1.091094
r9 = 1.096646
a1 = 119.028172
a2 = 124.750175
a3 = 124.847541
a4 = 122.738339
a5 = 111.926235
a6 = 110.462553
a7 = 112.168401
a8 = 110.140226
t1 = 120.799767
t2 = 121.060314
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-------------------------
 THF C2 MP2/6-31+G* fopt
-------------------------

Molecule:
---------
Stoichiometry    = C4H8O
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 20
Beta Electrons   = 20

Z-matrix:
--------------------------------------------------------------------------

0        1
O
C        1         r1
C        1         r1        2         a1
C        2         r2        1         a2        3         t1        0
```

```
C       3       r2      1       a2      2       t1      0
H       2       r3      1       a3      4       t2      0
H       3       r3      1       a3      5       t2      0
H       2       r4      1       a4      4       t3      0
H       3       r4      1       a4      5       t3      0
H       4       r5      2       a5      5       t4      0
H       5       r5      3       a5      4       t4      0
H       4       r6      2       a6      5       t5      0
H       5       r6      3       a6      4       t5      0

r1 = 1.443139
r2 = 1.525145
r3 = 1.093942
r4 = 1.098412
r5 = 1.096041
r6 = 1.094508
a1 = 109.372733
a2 = 105.890306
a3 = 107.922729
a4 = 108.826121
a5 = 110.488019
a6 = 112.660044
t1 = 12.846539
t2 = 122.347447
t3 = -119.759831
t4 = 116.900737
t5 = -121.756404
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
--------------------------------------------------------
 N,N-Dimethylacetamide ((Me)2NCOCH3)) C1 MP2/6-31+G* fopt
--------------------------------------------------------

Molecule:
---------
Stoichiometry    = C4H9NO
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 24
Beta Electrons   = 24

Z-matrix:
--------------------------------------------------------------------------

0       1
O
C       1       r1
N       2       r2      1       a1
C       3       r3      2       a2      1       t1      0
C       3       r4      2       a3      1       t2      0
C       2       r5      1       a4      3       t3      0
H       4       r6      3       a5      2       t4      0
H       4       r7      3       a6      7       t5      0
H       4       r8      3       a7      7       t6      0
H       5       r9      3       a8      7       t7      0
H       5       r10     3       a9      10      t8      0
H       5       r11     3       a10     10      t9      0
H       6       r12     2       a11     1       t10     0
```

```
H        6          r13        2          a12        13         t11        0
H        6          r14        2          a13        13         t12        0

r1 = 1.240729
r2 = 1.376055
r3 = 1.458454
r4 = 1.456391
r5 = 1.516139
r6 = 1.088827
r7 = 1.098561
r8 = 1.093133
r9 = 1.089036
r10 = 1.093319
r11 = 1.099595
r12 = 1.090096
r13 = 1.094494
r14 = 1.094815
a1 = 121.698471
a2 = 117.494902
a3 = 122.481838
a4 = 120.945486
a5 = 108.946115
a6 = 111.343228
a7 = 108.755859
a8 = 110.912638
a9 = 108.562574
a10 = 111.810275
a11 = 107.135694
a12 = 111.826880
a13 = 111.471458
t1 = 8.685303
t2 = 163.561023
t3 = 181.879622
t4 = -33.677779
t5 = 119.937774
t6 = -119.848528
t7 = 202.576313
t8 = 118.552007
t9 = -121.983945
t10 = 2.562333
t11 = 119.583892
t12 = -119.180022
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------
 Cyclobutanone C2V MP2/6-31+G* fopt
-----------------------------------

Molecule:
---------
Stoichiometry    = C4H6O
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 19
Beta Electrons   = 19

Z-matrix:
--------------------------------------------------------------------------
```

```
0        1
O
C        1         r1
X        2         1.        1         90.
C        2         r2        1         a1        3         90.       0
C        2         r2        1         a1        3         -90.      0
C        2         r3        3         90.       1         180.      0
H        4         r4        2         a3        6         t1        0
H        4         r4        2         a3        6         -t1       0
H        5         r4        2         a3        6         -t1       0
H        5         r4        2         a3        6         t1        0
H        6         r5        2         a4        3         0.        0
H        6         r5        2         a4        3         180.      0

r1 = 1.218193
r2 = 1.531576
r3 = 2.144330
r4 = 1.095592
r5 = 1.092420
a1 = 133.538322
a3 = 113.493290
a4 = 125.662724
t1 = 117.773649
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
--------------------------------------------
 gamma-Butyrolactone (C4H6O2) MP2/6-31+G* fopt
--------------------------------------------

Molecule:
---------
Stoichiometry    = C4H6O2
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 23
Beta Electrons   = 23

Z-matrix:
--------------------------------------------------------------------------------

0        1
C
C        1         r1
C        2         r2        1         a1
C        3         r3        2         a2        1         t1        0
O        4         r4        3         a3        2         t2        0
O        1         r5        2         a4        5         t3        0
H        2         r6        1         a5        3         t4        0
H        2         r7        1         a6        3         t5        0
H        3         r8        2         a7        4         t6        0
H        3         r9        2         a8        4         t7        0
H        4         r10       3         a9        5         t8        0
H        4         r11       3         a10       5         t9        0

r1 = 1.519650
r2 = 1.525320
r3 = 1.527875
```

```
r4 = 1.451853
r5 = 1.214315
r6 = 1.097482
r7 = 1.091776
r8 = 1.093525
r9 = 1.094886
r10 = 1.095878
r11 = 1.090841
a1 = 103.132027
a2 = 101.416800
a3 = 105.050627
a4 = 128.595742
a5 = 108.009734
a6 = 110.052226
a7 = 114.022640
a8 = 110.444625
a9 = 112.185771
a10 = 114.696481
t1 = 30.673743
t2 = -33.042136
t3 = 180.288890
t4 = 118.597850
t5 = -123.770309
t6 = 121.018676
t7 = -116.664822
t8 = 117.201030
t9 = -117.116996
-------------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-------------------------------------
 2-Chloropropane Cs MP2/6-31+G* fopt
-------------------------------------

Molecule:
---------
Stoichiometry    = C3H7Cl
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 21
Beta Electrons   = 21

Z-matrix:
-------------------------------------------------------------------------

0        1
Cl
C        1         r1
H        2         r2        1         a1
C        2         r3        1         a2        3         t1        0
C        2         r3        1         a2        3         -t1       0
H        4         r4        2         a3        1         t2        0
H        4         r5        2         a4        6         t3        0
H        4         r6        2         a5        6         t4        0
H        5         r4        2         a3        1         -t2       0
H        5         r5        2         a4        9         -t3       0
H        5         r6        2         a5        9         -t4       0

r1 = 1.803216
```

```
r2 = 1.093556
r3 = 1.518503
r4 = 1.095703
r5 = 1.092816
r6 = 1.094207
a1 = 105.060954
a2 = 109.350481
a3 = 109.353017
a4 = 111.262594
a5 = 110.498715
t1 = 117.926523
t2 = 182.336677
t3 = 119.947513
t4 = -119.450353
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
----------------------------
 Furan C2V MP2/6-31+G* fopt
----------------------------

Molecule:
---------
Stoichiometry    = C4H4O
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 18
Beta Electrons   = 18

Z-matrix:
--------------------------------------------------------------------------------

0        1
O
X        1         1.
C        1         r1       2        a1
C        1         r1       2        a1       3        180.      0
C        3         r2       1        a2       2        180.      0
C        4         r2       1        a2       2        180.      0
H        3         r3       1        a3       2        0.        0
H        4         r3       1        a3       2        0.        0
H        5         r4       3        a4       1        180.      0
H        6         r4       4        a4       1        180.      0

r1 = 1.369029
r2 = 1.368622
r3 = 1.080213
r4 = 1.082155
a1 = 126.615330
a2 = 110.323780
a3 = 115.562505
a4 = 126.153505
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
----------------------------------
 3-Butyn-2-one Cs MP2/6-31+G* fopt
----------------------------------

Molecule:
```