SOME USEFUL INFORMATION ABOUT G03

- gjf input
- log output
- chk checkpoint (binary)
- fchk formatted checkpoint file
- rwf read-write file (binary)

- Build or open structure
- Choose calculate
  - choose options
    - job type (energy, opt, scan, frequency)
    - method (method, basis set, spin, charge)
    - additional keywords
  - save input file
  - submit
- Results
  - charges
  - vibrations

  - surfaces

MAIN INPUT LINE KEYWORD OPTIONS

```
#    HF/3-21G  test pop=reg
#    HF/3-21G  guess=read  test
#    HF/3-21G  guess=read  gfprint test
#    HF/3-21G  guess=(read, alter, only) test
#    HF/3-21G  opt test

          opt = (restart, maxcycle = 20)
          opt = readfc
          opt = (calchffc, ts, maxcycle = 20)
          Lots of other options
```

COORDINATES

- cartesian
- z - matrix (bond lengths, angles, dihedrals)
- redundant internal coordinates (default)

CONSTRAINTS

If initial structure has symmetry constraints, these are often automatically preserved.

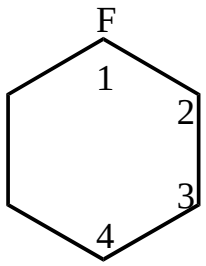
- Build H_2O, with equal OH bond lengths

  C_{2V} symmetry should be recognized

  symmetry speeds up calculations
  facilitates interpretation

- Consider fluorobenzene

  The C_2H_2, C_3H_3, and C_4H_4 bond lengths differ.



Even though your initial geometry may have these CH bond lengths equal, they will become unequal in optimization.

Suppose you wanted them to be equal.
Can add constraints either with Z-matrix or red. int. coordinates

CH_3CN z-matrix example

```
%chk=nccsp
%mem=12000000
# qcisd(TQ) gen SCF=Tight test


CH3CN  MP2 aug-cc-pvdz geometry

0 1
N1
C2 N1 RCN
X C2 1.0 N1 90.0
C3 C2 RCC X 90.0 N1 180.0
H4 C3 RCH C2 ALPHA X 0.0
H5 C3 RCH C2 ALPHA X 120.0
H6 C3 RCH C2 ALPHA X -120.0

RCN=1.185461
RCC=1.471094
RCH=1.099058
ALPHA=109.842

  1 0
 S    9 1.00
   .9046000000D+04   .7000000000D-03
   .1357000000D+04   .5389000000D-02
   .3093000000D+03   .2740600000D-01
   .8773000000D+02   .1032070000D+00
   .2856000000D+02   .2787230000D+00
   .1021000000D+02   .4485400000D+00
   .3838000000D+01   .2782380000D+00
   .7466000000D+00   .1544000000D-01
   .2248000000D+00  -.2864000000D-02
```

Benzene z-matrix

```
%mem=3000000
%chk=benz.chk
# HF/3-21G test pop=reg

 Benzene HF single point

0 1
X1
C1 X1 R1
C2 X1 R1 C1 60.
C3 X1 R1 C2 120. C1 0.
C4 X1 R1 C3 120. C2 180.
C5 X1 R1 C4 60. C2 0.
C6 X1 R1 C3 60. C2 180.
H1 X1 R2 C2 60. C3 180.
H2 X1 R2 C5 60. C1 180.
H3 X1 R2 C1 60. C2 180.
H4 X1 R2 C4 60. C2 180.
H5 X1 R2 C3 60. C4 180.
H6 X1 R2 C5 60. C6 180.

R1=1.3968
R2=2.4843
```

Silicon Cluster model

```
%mem=10000000
%chk=mono
#p pw91pw91/gen test 5d guess=read units=au

monohydride

0 1
h -3.830206 -9.655231  6.853310
h  3.837141 -9.642195  6.766617
h  -3.809799  9.619873  6.797052
h   3.803823  9.620123  6.790977
h  -6.108435 -7.009998  3.806901
h   6.108435 -7.009998  3.806901
h  -6.212115  0.000000  3.950539
h   6.212115  0.000000  3.950539
h  -6.108435  7.009998  3.806901
h   6.108435  7.009998  3.806901
h   0.000000 -9.615137  0.821608
h   0.000000  9.615137  0.821608
h  -2.284973 -3.761431 -1.679292
h   2.284973 -3.761431 -1.679292
h  -2.284973  3.761431 -1.679292
h   2.284973  3.761431 -1.679292
si  -1.841121 -3.663114  6.934265
si   2.437508 -3.697709  7.743857
si  -2.293556  3.725529  7.607578
si 2.362225  3.675376  7.580646
si -3.626050 -7.358906  5.219972
si  3.602057 -7.266590  5.242196
si -3.584353  0.086160  5.320377
si 3.551944 -0.034471  5.321944
si -3.609370  7.286190  5.206803
si 3.611210  7.278029  5.210813
si 0.000000 -7.368053  2.605000
si 0.000000  0.000000  2.605000
si 0.000000  7.368053  2.605000
si 0.000000 -3.684026  0.000000
si 0.000000  3.684026  0.000000
h 3.276947  3.705008 10.292528
h -3.288665  3.688545 10.290079

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 0
3-21g
****
17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 0
6-311G(d,p)
****
```