

SOME USEFUL INFORMATION ABOUT G03

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

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- 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.

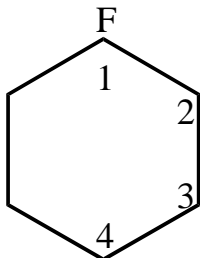
- Build H_2O , with equal OH bond lengths

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

CH₃CN 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)
