Gaussian 03 Z-matrices

Although G03 will take cartesian coordinates as input, it can be helpful instead to write a Z-matrix to take advantage of high symmetry. An example is provided here for the case of 3,4-benzothiophene. Note that atomic symbol “x” means a dummy atom. Dummy atoms can often be very helpful in defining symmetry axes.

The sense of the G03 Z-matrix is:

```
Atom   Connect to   Bond Length   Next Connect   Bond Angle   Next Connect   Dihedral Angle
```

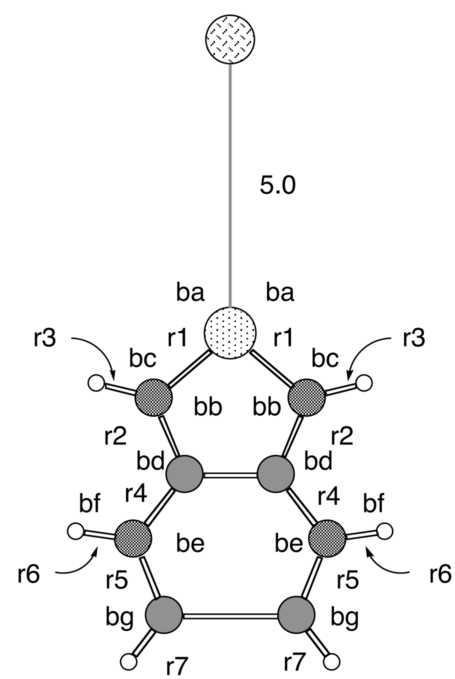
where Bond Length, Bond Angle, and Dihedral angle can either be constant values, or variables to be optimized. Use of a number implies a constant value, use of a name implies a variable. Note that by using the same variable name in different places, symmetry can be assured.

Below is an example for 3,4-benzothiophene in C_{2v} symmetry.

Note that increasingly many chemistry software programs are becoming adept at interfacing between different formats. Chem-3D can read and write G03 input files, for instance. *However*, it is quite rare that these interpreters can output symmetry properly (usually a new variable is assigned to each degree of freedom, with no recognition that symmetry is possible).

The picture of the molecule on the back is directly from the Z-matrix. Note that the base C—C bond looks rather long. That’s because it is not specified, per se, but derives from all the other choices of bond lengths and angles. Fortunately, the optimizer will fix this up quickly. All that matters is that we provide the correct number of degrees of freedom. In this case symmetry reduces $3N-6$ (i.e., 39) degrees of freedom to just 14. G03 will figure out if you have the correct number if you specify the keyword “fopt” and stop if you do not (so as not to waste your time).

```
x
s   1   5.0
c   2   r1   1   ba
c   2   r1   1   ba   3   180.0
c   3   r2   2   bb   1   180.0
c   4   r2   2   bb   1   180.0
h   3   r3   2   bc   1     0.0
h   4   r3   2   bc   1     0.0
c   5   r4   3   bd   2   180.0
c   6   r4   4   bd   2   180.0
c   9   r5   5   be   3   180.0
c  10   r5   6   be   4   180.0
h   9   r6   5   bf   3     0.0
h  10   r6   6   bf   4     0.0
h  11   r7   9   bg   5   180.0
h  12   r7  10   bg   6   180.0
<a blank line ends the Z-matrix and is followed by initial values for variables>
r1=1.7
r2=1.4
r3=1.0
r4=1.4
r5=1.4
r6=1.0
r7=1.0
ba=130.0
bb=108.0
bc=125.0
bd=120.0
be=120.0
bf=120.0
bg=120.0
```



Note that GaussView is able to recognize symmetry and, in favorable cases, adjust nearly symmetric structures to make them fully symmetric. See the “Point Group” command in the Edit menu.

If you cannot draw a fully symmetric molecule, or convince GaussView to successfully generate, you can always create a text Z-matrix input file and read it with GaussView (save it as a .com file) to assess your success.