Building a Z-Matrix:

The Z-Matrix is a simple, geometrical approximation. It works by identifying each atom in a molecule by a bond distance, bond angle and dihedral angle (the so called internal coordinates) in relation to other atoms in the molecule.

When constructing a Z-matrix, you should follow these steps:

1. Draw the molecule.
2. Assign one atom to be #1.
3. Starting with atom #1, assign all other atoms a sequential number. List the atoms you numbered, in order, down your paper, one right under the other.
4. Place the atom designated as #1 at the origin of your coordinate system. The first atom does not have any defining measurements since it is at the origin.
5. To identify the second atom, you must only define its bond length to the first atom.
6. For the third atom, you must define a bond length to atom #1 and a bond angle between atom #3 and atoms #1 and #2. (Bond angles are the angles between three atoms.)
7. Remember that you can only use previously defined atoms when defining your current atom. This means that you cannot reference atom #7 when defining atom #5.
8. To identify atom #4 and all other atoms, you must include a bond length, bond angle and a dihedral angle. (Dihedral angles are the angles between an atom and the plane created by three other atoms.) This is done by using neighboring atoms to the atom you are describing.
**EXAMPLE 1: Z MATRIX FOR WATER**

O1
H2  1  r2
H3  1  r3  2  a3

Variables:
r2= 0.9687
r3= 0.9687
a3= 104.00

In sequence, this says:
Atom H2 is connected to input atom O1 at a distance r2. Atom H3 is connected to input atom O1 at a distance r3 and is forming with atom O1 and H2 the angle a3.