Z matrix

Prepare a table/excel file of a dipeptide (one of the amino acids can be Gly)

Use the format given below.

A sample for hydrogen peroxide is given.

Column 1: Atom identifier

Column 2: Atom type

Column 3: Bond connectivity – Atom id of connected bond e.g

Column 4: Bond distance

Column 5: Angle connectivity – Atom id of connected angle along with column 3 e.g. Angle 3-2-1 is 105^0

Column 6: Angle

Column 7: Dihedral connectivity – Atom id of connected atoms e.g. 4-3-2-1 dihedral 120^0

Column 8: Dihedral angle

Atom id	Atom type	Bond connectivity	Bond distance	Angle connectivity	Angle	Dihedral connectivity	Dihedral angle
1	H						
2	O	1	0.9				
3	O	2	1.4	1	105.0		
4	H	3	0.9	2	105.0	1	120.0