Major 1

1.

The bond length for O-H is 0.989 A

The angle between H – O – H is 100.020 Degrees

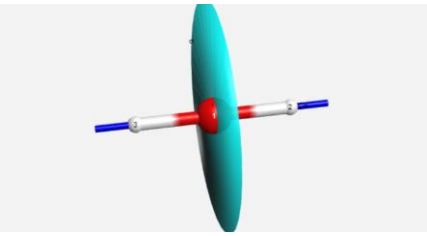
2.

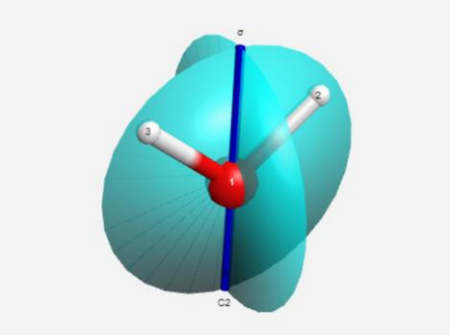
Using Koopman's theorem, the first ionization potential is the energy of the Highest Occupied Molecular Orbital, which equals to -0.393 Hartree

3.

For linear water, the point group symmetry is C_s

For bent water, the point group symmetry is D_{2h}





4.

Angle (Degree)	Energy (Hartree)
180	-74.844633642841
165	-74.856749915940
150	-74.886654542822
135	-74.921364565684
120	-74.949859106285
105	-74.964902268025
90	-74.961203167896
75	-74.934026517279
60	-74.878577565723

5.)

The plot shows exactly what we expected, the lowest energy occurs where HF calculated, around 100 Degrees, the Next plot draws a line exactly at 100.020 and we can see it matches the minimum energy.