Chemistry 888   Fall 2010   Laboratory Exercise 3

In this exercise you will determine the geometry, dipole moment and charge distribution in CH_3OH using the Hartree-Fock, MP2 and DFT(B3LYP) methods as implemented in MOLPRO. Also compare the time required for each step in the calculation. For example, the time to calculate the integrals, optimize the geometry, etc. Comment on the differences for each method.