Problem Set I: CHEM302

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Think of a neutral molecule with 4-8 heavy atoms (i.e., atoms other than hydrogen) that you would like to get to know a little better. (It can be the same molecule you used in you first WebMO experience if you want.) By 4PM on Wednesday, 2010-03-03, turn in a brief report on you molecule containing the following information.

1. The IUPAC name of your molecule and its molecular formula.
2. A line drawing of your molecule. (Like Figure 1)
3. A color, ball and stick, representation of your molecule. (Like Figure 2)
4. The convergence of at least three interesting geometric parameters as a function of basis set size at the Hartree-Fock level of theory. Your largest geometry optimization calculation must use a basis set of at least triple-zeta quality.
5. The convergence of the energy of the molecule as a function of basis set size at the Hartree-Fock level of theory. Your largest energy calculation should involve a single point calcualtion using your best geometry and a basis set substantially larger than that used for your largest geometry optimization. Include the electronic energy, ZPCE, internal energy, enthalpy, and free energy in your results (computed at 1 atm and 298 K for the last three quantities).
6. The convergence of the vibrational (IR) spectrum of the molecule as a function of basis set size at the Hartree-Fock level of theory.
7. A depiction of an electrostaic potential map for your molecule at your highest model chemistry.
8. The convergence of the first non-zero multipole moment of the molecule as a function of basis set size at the Hartree-Fock level of theory.
9. A comparision of the Mulliken and one other set of charges (Merz-Singh-Kollman, CHelp, NPA, etc.) with various model chemistries.
10. The convergence of the polarizability of the molecule as a function of basis set size at the Hartree-Fock level of theory up through at least a triple-zeta basis set.

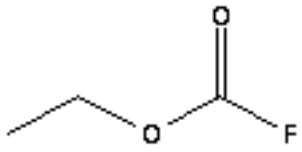

Figure 1: Ethyl fluoroformate

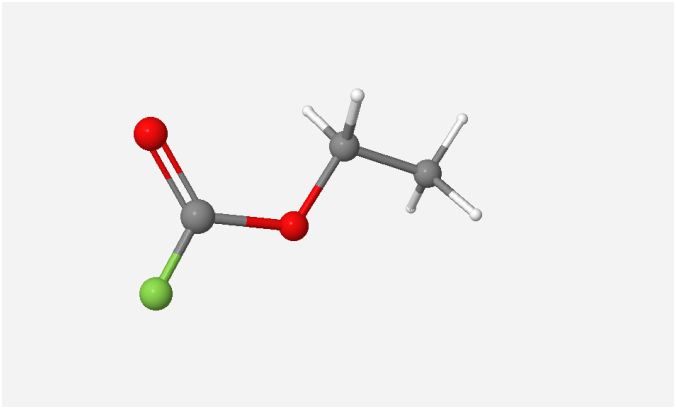

Figure 2: Ethyl fluoroformate. Gray atoms are carbon, red oxygen, white hydrogen, and green fluorine.