NAME/TEAM: _____

Computational Chemistry Prelab
Last modified: June 17, 2014

Recommended reading:

<u>AirUCI Manual</u>: Computational Chemistry Lab (Spartan)
<u>Environmental Chemistry Text</u>: Pages: 175–179, 184–187 and 193–196
                                                                          on Molecular Vibrations

Prelab Questions:

1) What is the overall goal of this lab?

2) What computer program will be used for the computations?

3) What region of the electromagnetic spectrum can induce molecular vibrations:

4) Convert the wavenumber (similar to a "frequency") 1000 cm^{-1} to a wavelength in μm.

5) What is a dipole?

6) What is the model chemistry (i.e., theoretical model and basis set) that will be used for the calculations in this lab:

7) What do the terms HOMO and LUMO stand for?