Updated 11-5-2024

Chem 106

Name_____ Lab Section_____ Date_____

Pre-Lab: Crystal Violet and Quantum Theory

For this lab you will need a **calculator**, plus:

1. **Computer**. Any desktop or laptop with an Internet connection can be used to complete this lab. Bring your laptop to lab if you wish. Laptops will also be available in lab.

> Using a **mouse** is recommended for technical computing.

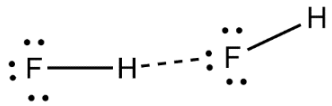
2. **Internet connection**. If you are using your laptop in the Reichardt Bldg, check the **wifi** settings.
3. **UA username and password**. These are required to log in to the UAF WebMO website.
4. **Chem106 group password.** Your TA or professor will announce this in class or online.

To do:

1. Read and study the lab handout and worksheet.

2. Review in your textbook some topics from C105 and C106 such as: electromagnetic spectrum (Sect. 3.2 in Burdge, 4th Ed.), atomic spectroscopy (Sect. 3.4), electronegativity (6.2), Lewis formulas (6.3), resonance (6.5), hydrogen bonds (7.3), molecular orbitals (7.7), visible spectroscopy (9.5), enthalpy (10.3), energy of activation (14.6), and transition states (14.7).
Also **google** "khan academy representing endothermic and exothermic processes"

3. The Lewis structure of a hydrogen fluoride dimer [FH···FH] is shown below. The dashed line represents a hydrogen bond, which is a weak connection between the electron-rich F atom and the partially-positive H atom.



In a similar manner, OH^- ion is stabilized in water by hydrogen bonds. A small model would be a OH^- ion stuck to a water molecule: HOH···OH^-. Draw a Lewis structure for this complex containing one hydrogen bond. Make it look about like the HF dimer.

4. Write a balanced chemical equation for formation of the hydroxide ion-water-complex ($H_3O_2^-$) from H_2O and OH^-. Do not include Lewis formulas.

5. The table on the right lists hypothetical energy values (E) for the above species. Use these to calculate ΔE for formation of $H_3O_2^-$ from water and OH^-.

Note that molecule energies calculated by quantum chemistry programs are **negative** because forming a molecule from the separate particles – a nucleus and several electrons – is extremely exothermic.

	E (kcal/mol)
H_2O	– 47,937.8
HO^-	– 47,599.3
$HOH\cdots OH^-$	– 95,556.4

ΔE = kcal/mol

$$\Delta E = \Sigma E_{\text{products}} - \Sigma E_{\text{reactants}}$$

$$\Delta E = E_{HOH-OH} - \left(E_{OH} + E_{H2O}\right)$$

(c) Is this reaction exothermic_____ or endothermic_____? Check one. (**Hint**: Check the **sign of ΔE.**)

6. Peruse the Wikipedia article on "Computational chemistry". Read about Nobel prizes in the History section. Follow links to "activation energy" in the Catalysis section and "HOMO and LUMO" in the Drug Development section.

7. Log in to WebMO (chem106 group) as described in the Appendix of the lab handout. Calculate the energy of **a single carbon atom** using the default settings invoked when you log in:

Under the **New Job** menu, select **Create New Job**. Left click once on the workspace to insert a C atom. **Continue** (right arrow at the bottom of the screen). **Continue**. **Continue**.

The WebMO Job Manager page should now be displayed.
Record the **Number** of **your** C job here: _____ (No need to report the energy value.)