Name_____KEY_____ 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.

> For technical computing, use of a mouse is recommended.

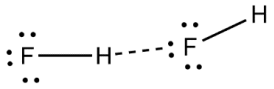
2. **Internet connection**. If you are using your laptop in the Reichardt Bldg, check the **wifi** settings.
3. **UA username and password**. These are required to log in to the UAF WebMO website.
4. **Chem106 group password.** Your TA or professor will announce this in class or online.

To do:

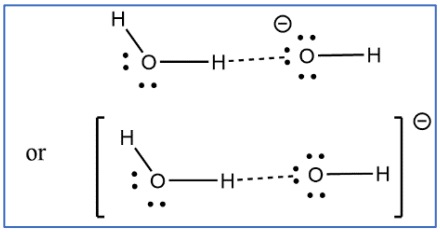
1. Read and study the lab handout and worksheet.

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), heat of formation (10.7), energy of activation (14.6), and transition states (14.7).

3. The Lewis structure of a hydrogen fluoride (HF) dimer is shown on the right. The dashed line represents a hydrogen bond (H-bond), which is a weak connection between the electron-rich F atom and the partially-positive H atom.



In a similar manner, OH^- ion in water is stabilized by hydrogen bonds. Draw a Lewis structure for the smallest such complex [HOH···OH^-] (with just one H-bond). Make it look about like the HF dimer.



4. (a) Write a balanced chemical equation for formation of the water-hydroxide ion complex [HOH···OH^-] from water and OH^-. .

$H_2O(aq) + OH^-(aq) \rightarrow H_3O_2^-(aq)$ or $H_2O(aq) + OH^-(aq) \rightarrow H_2O\text{-}OH^-(aq)$

(b) Calculate $\Delta H_{rxn}°$ for this reaction. This number is a good estimate for the strength of a (strong) hydrogen bond.

	$\Delta H_f°$ kcal/mol *
H_2O	-61.309
HO^-	-133.188
[HOH···OH^-]	-204.833
*calculated by PM6 quantum theory.	

$\Delta H_{rxn}° = \Sigma\Delta H_f°(products) - \Sigma\Delta H_f°(reactants) = -204.833 –(-61.309 + (-133.188))$ kcal/mol

$\Delta H_{rxn}° = -10.336$ kcal/mol

(c) (Check one.) This reaction is exothermic_____✓_____ endothermic_____ .

5. 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.

6. 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 blank space 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.)