**ChE 2110/2111**

**WebMO Challenge Problem**

**Motivation:** In Chapter 6, we have been mentioning intermolecular forces and how they impact phase change behavior. In this assignment, you will estimate the intermolecular forces between two identical molecules. Your classmates will do the same, with each of the 32 teams in the class studying a different pair of identical molecules. As a class, you will then attempt to correlate the intermolecular forces with various physical properties related to phase change behavior.

**For questions about the computational chemistry software:** Please talk to Cameron Bodenschatz or Felipe Polo Garzón, who are our computational chemistry experts.

**To prepare for this activity:**

1. Work with Cameron Bodenschatz, Christine Duval, and Felipe Polo Garzón to select a molecule to study. Only one team per molecule, please.
2. Reference your General Chemistry book or another resource (e.g., a physical chemistry text, the Internet) and brush up on intermolecular forces. Think about the types of intermolecular forces that you expect to be present in a pair of your molecules. Don’t forget the Coulomb contributions for molecules with partial charge distributions and dipoles! Are the interactions in your molecule relatively short-ranged or relatively long-ranged? How do you know?
3. Think about the other molecules that have been assigned to other teams. What do you expect the intermolecular forces for your molecule are like compared with the others? How do you think the intermolecular forces will impact the phase change properties such as vapor pressure, boiling point, melting point, etc.?

**Carrying out the activity:**

1. Use the WebMO software to compute the energy of interaction in your pair of molecules as a function of the distance between the two molecules. You can access the WebMO software at: [http://user.palmetto.clemson.edu/~webmo/cgi-bin/login.cgi](http://user.palmetto.clemson.edu/~webmo/cgi-bin/login.cgi). Please configure your Java security options to “trust” these pages, and note that you must either be on campus or use the VPN to access the software. Login information for WebMO will be provided in class, and Cameron Bodenschatz will show you how to do the calculations. You can also view job numbers 539, 541 – 544, 546, 559 – 564 in the WebMO Job Manager, which are jobs associated with calculating the interactions between two propane molecules at distances of 2.5 – 5.0 Å from the centers of mass.
2. Plot the interaction energy in units of kJ/mol versus the distance between molecules in units of Å. (What is an Å?) Your plot should look similar to a “Lennard-Jones potential,” which is often used to describe physical bonding. Do a Google Images search to see what your plot should look like. Note: In WebMO, distances are given in Å, but energies are given in Hartrees, so you’ll need to convert!
3. Assess the minimum interaction energy and optimal molecule-molecule distance. The minimum energy can be read directly off of your plot, and the optimal distance is the associated distance between molecules. Let’s call the minimum energy $\varepsilon$ and the optimal distance $\sigma$. 
4. Use Perry’s Handbook to obtain phase change properties for your molecule. *You are required to use Perry’s Handbook here, even if you could obtain the data from Felder & Rousseau.* (Why? To practice with information literacy.) Record the edition of Perry’s that you’re using as well as the table and/or figure #’s that you used to obtain the data. Obtain at least 3 different properties related to phase changes. Note: If you absolutely cannot find data for your molecule in Perry’s Handbook (which should only happen in extreme cases), you may look the information up in the academic literature. But be sure to cite your sources.

5. Get together with 4 or more other teams, and compare your results: ε, σ, phase change properties. Can you correlate ε and/or σ with any of these properties? What about other properties that we haven’t considered, yet? Be creative.

**Turn in the following:**

Team # ____________________

Team members:

Molecule studied: _____________________________________________________________

Describe the intermolecular forces for your molecule, and compare and contrast them with those expected for other molecules in this assignment:

Calculated value for $\varepsilon =$ ____________________________  $\sigma =$ ____________________________
List the phase change properties that you looked up. State the property (e.g., p*), its value, and the table or figure where you located it:

1.

2.

3.
What version of Perry’s Handbook are you using? ________________________________

Discuss the relationships between $\varepsilon$, $\sigma$, and phase change properties for the 5+ molecules you considered in #5 under Carrying out the activity. Make sure to state the other molecules that you compared with and the properties that you considered!

Attach the following items:
1. Your plot of interaction energy versus molecule-molecule distance
2. Any plots that you created which illustrate the correlations that you found in #5 under Carrying out the activity.