This experiment will be written up with 2 sections (Data and Discussion):

**Data Section:**

(A) Record the bond angle and bond length parameters for methane, ethane, ethylene, acetylene, 1-butanol, and 2-butanone.

(B) Record the single point energies for 2-bromopentane as a function of dihedral angle. Generate an EXCEL plot depicting the variation of energy as the dihedral angle is changed. Be sure to label energy minima and maxima.

(C) Record the energies of the bonding and antibonding molecular orbitals for the sigma bond in H$_2$. Likewise, record the energies for the bonding and antibonding molecular orbitals for the pi bond in ethylene. Print and insert pictures of the orbitals. Label each orbital as BONDING or ANTIBONDING. Indicate any nodes.

(D) Arrange the 4 alcohols (from prelaboratory question #2) in order of increasing electron density surfaces. Also, record the dipole moment of each alcohol (show direction and magnitude -- you may have to draw this in).

(E) Record the energies for each of the alkene isomers (from prelaboratory question #4) and arrange them in order of increasing stability.

(F) Record the dipole moment values and hydrogen bonding capabilities for the compounds selected in prelaboratory question #3.

(G) Record the atomic charges and results of electrostatic potential maps that you collected for the various ions.

(H) Record the energies for each cyclic hydrocarbon (cyclopropane through cyclohexane) as $\Delta H_f$ per CH$_2$. See Table 5.1 on page 200 of the Jones text.

(I) Record the energy values for each of the chair conformations for cis-1-isopropyl-2-methylcyclohexane as well as for trans-1-isopropyl-2-methylcyclohexane.

**Discussion Section:**

1. How well do the calculated values in (A) above compare with the values that you looked up in the Jones text or via any other source (please indicate your source!!)? Discuss any deviations between the two data sets.

2. Interpret the energy vs. dihedral angle graph. Be sure to include Newman projections for each dihedral angle and to discuss contributions of torsional and steric strain relating to your results and drawings.
3. Compare and contrast the orbital pictures and energy values for both the H\textsubscript{2} sigma bond and the ethylene pi bond. You should compare your results with the representations in Figures 1.37 and 3.12 of the Jones text.

4. Compare the shapes and charge distribution of the 4 alcohols being sure to comment on how well these factors correlate to the boiling point trend (that you looked up in your prelab exercise). Does there seem to be a clear-cut trend? Provide any alternative explanations that may better describe the observed trend in boiling point.

5. Compare the results of part (E) above with the answer that you proposed for question #4 of the prelab exercises. Explain why the alkenes are ordered as observed (with respect to stability). You may want to consult Section 3.6 of your Jones text.

6. Compare and contrast the polarity (in terms of measured dipole moment) for the compounds in question #3 of the prelab exercises. Given this information, rank them in order of increasing solubility in water (a polar solvent). What evidence have you uncovered in your molecular models that suggests polarity?

7. If we also consider that hydrogen bonding is an important intermolecular force in determining solubility, determine the solubility of each compound from question #3 of the prelab exercises in water (insoluble, partially soluble, soluble). Be sure to indicate whether the compounds are likely to accept a hydrogen bond from the solvent (water), donate a hydrogen bond to the solvent, or both. What evidence have you uncovered in your molecular models that suggests hydrogen bonding capability?

8. In light of your answers to #6 and #7, what do you think the order of water solubility should be for the entire series of compounds. You'll need to consider the contributions of polarity AND hydrogen bonding. Compare with literature solubility data for each compound in water. Be sure to cite your source!!!

9. Describe how the modeled ions demonstrate the hybrid structure or weighted average of the resonance structures that you drew as part of the prelaboratory exercises.

10. How well do your calculated (experimental) heats of formation per CH\textsubscript{2} for the series of cyclic hydrocarbons cyclic hydrocarbon (cyclopropane through cyclohexane) agree with the data in Table 5.1 on page 200 of the Jones text? Explain.

11. Calculate the energy difference between the two chair conformations of cis-1-isopropyl-2-methylcyclohexane. How well does this number agree with the prediction from Worked Problem #5.20 from the Jones text? Explain.

12. Calculate the energy difference between the two chair conformations of trans-1-isopropyl-2-methylcyclohexane. How well does this number agree with the prediction from Worked Problem #5.20 from the Jones text? Explain.