Experiments 8 and 9: Structure Calculations

Use complete sentences. Use the proper number of digits and/or significant figures where appropriate, and include units. Erase all the words in italics and type your answers/information into this template (your text/answers shouldn't be in italics).

Introduction: *2-sentence maximum; state the scientific purpose of the experiment. Describe the method you will use, in a general sense.*

Procedure: *Give a general and brief description of the experimental procedure, and include information about the computational packages (the computer programs) that you used. Reference the experiment handout on the CH141 website. List any changes from the written procedure on the handout (if any).*

Results: *Tabulate your numerical results generated in Spartan. Your images (electron density surfaces and molecular orbitals pictures) can be added as attachments. Make sure to include labels and descriptions for both your table(s) and on your attachments.*

Discussion: *Provide a description of what you were able to accomplish using the computational modeling programs, and also address the following questions/topics:*

- *What do the electron density surfaces (as well as calculated dipoles/bond lengths) tell you about the bonding in H_2, HF, and LiF? Are those surfaces consistent with what you might expect? Why or why not?*
- *What do the electron density surface, bond lengths, and bond angles tell you about the electron distribution in nitrate and acetate? Is that information consistent with what you might expect? Why or why not?*
- *Consider the molecular orbital surfaces and occupancy for H_2. What type(s) of molecular orbitals are these? Are they consistent with what you expected (consider the surfaces [shapes], and relative energies)? Why or why not?*
- *Consider the molecular orbital surfaces for O_2. Are these consistent with what you expected? Why or why not?*
- *Consider the molecular orbital energies (the ordering) for O_2. Are these consistent with what you expected? Why or why not?*
- *Consider the molecular orbital surfaces and energy for NO. Are these consistent with what you expected? Why or why not? Just looking at the shape of the surfaces, are there differences between O_2 and NO? Why do you think these differences arise?*

Attachments:

Labeled electron density surfaces and molecular orbitals pictures