Experiments 1 and 2: Structure Calculations

Using your experience making Lewis Dot structures and more sophisticated models in Spartan answer the following questions. Use figures from your lab exercises to support your answers.

1. The Lewis Dot structures for H₂, HF, and LiF all look the same. What do the Spartan electron density surfaces (as well as calculated dipoles/bond lengths) tell you about the bonding in H₂, HF, and LiF? Are those surfaces consistent with what you might expect? Why or why not? Why do we teach you both models (Lewis Dot, and MO)?

2. 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?

3. Consider the molecular orbital surfaces and occupancy for H₂. 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?

4. Consider the molecular orbital surfaces for O₂. Are these consistent with what you expected? Why or why not?

5. Consider the molecular orbital energies (the ordering) for O₂. Are these consistent with what you expected? Why or why not?

6. 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 O₂ and NO? Why do you think these differences arise?

7. Rank the bond energies of H₂, HF, LiF, O₂ and NO and provide a reasonable explanation for the ranking.

Attachments:

Labeled electron density surfaces and molecular orbitals pictures