

Name _____

Pre-lab questions for *Computational Chemistry* experiment

1. What is meant by the term basis set?
+1
2. In semi-empirical methods, which electrons are considered explicitly?
+1
3. What is your username and password for WebMO? Your professor will provide this information in a digital format.
+2
4. After you have drawn a molecule, what is the first calculation that you will select to do? (Molecular Energy is the default in Figure 5.)
+1
5. What basis set do you use for H₂ and N₂?
+1
6. What basis set do you use for N₂O?
+1
7. What are the two theories that you use for ClF₃?
+2
8. How many calculations do you perform on ClF₃?
+1