3.4: Exercise Questions

1. The Molecular Orbitals of HF. For this part please use your knowledge of molecular orbital theory and the results from your calculations performed above to complete the questions.
   A. Please sketch pictures of the molecular orbitals of HF from HOMO-3 to LUMO.
   B. Please use the energy levels next to each of the molecular orbitals in Avogadro to draw the molecular orbital energy diagram for HF. While you should label each of the molecular orbitals, you do not need to sketch pictures of the orbitals.

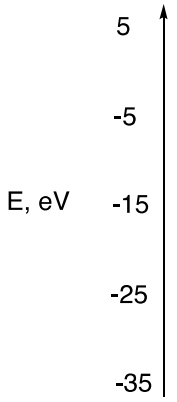
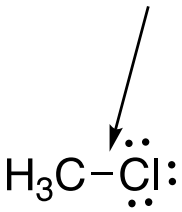
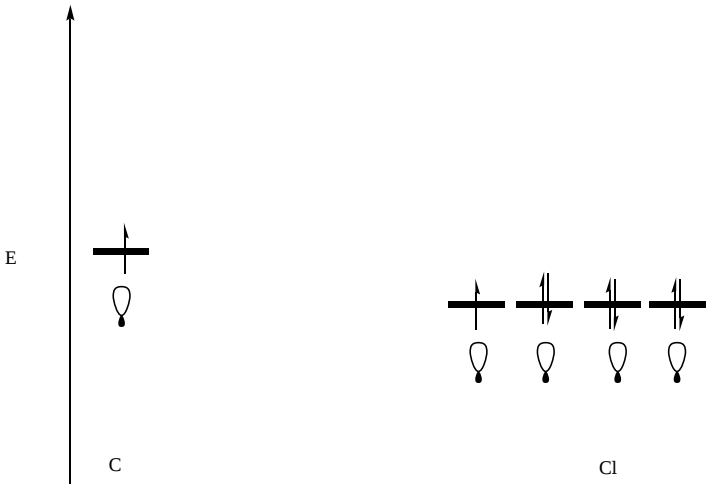


Figure 3.4.1: Copy and Paste Caption here. (Copyright; author via source)

   C. Which orbital corresponds to the σ bonding orbital between hydrogen and fluorine in HF? Does this computer-generated orbital look like sigma bonding orbital generated by visually combining the orbitals of fluorine and hydrogen in and out of phase?
   D. If $H-F$ were to act as an electron pair acceptor (Lewis acid) from a hydroxide anion (OH^-) $H-F$ would accept these electrons into the LUMO. If this occurred, please predict what would happen to the $H-F$ molecule.
2. The Molecular Orbitals of Chloromethane. For this part of the exercise please use your knowledge of molecular orbital theory and the provided calculations.
   A. Using your knowledge of M.O. theory, please construct a molecular orbital diagram for the $C-Cl$ bond in chloromethane.



   You should use an sp^3 orbital from carbon and all 4 sp^3 orbitals from chlorine to do this. Although ORCA models the electrons in the $C-H$ σ bonding orbitals, we don't need to consider them here.



B. In your diagram above, please indicate the identity of the highest occupied molecular orbitals (HOMO) and lowest unoccupied molecular orbital (LUMO).
C. Please open the provided output file for the chloromethane (MeCl.out) to view its molecular orbitals. Please sketch the HOMO and LUMO of chloromethane. How do these orbitals compare those that you sketched in part A?
