

Problem set 7

1. Sketch sp , sp^2 , and sp^3 hybrid orbitals. Indicate the nucleus and node(s).
2. Using a similar approach to that taught in class for N_2 (where the differences between hybrid and full MO model was discussed), construct an MO diagram for F_2 assuming that (i) the two fluorine atoms are sp hybridized and (ii) the two fluorine atoms are sp^3 hybridized. State which orbitals are occupied and compare the resulting descriptions of the bonding with that from the full MO picture for F_2 (that has been discussed during the chemical bonding classes).
3. Use a similar approach (as in question 2) to construct an MO diagram for NO using sp hybrids on both atoms; remember to place the oxygen AOs and HAOs somewhat lower in energy than the corresponding orbitals on nitrogen. What does your diagram predict about the form of the HOMO and the LUMO? Compare your predictions about the MOs with those computed using only atomic orbitals (i.e. without using hybrid orbitals).
4. (a) Construct the MO diagram for Be_2 and use it to explain why, although the bond order is zero, s-p mixing results in the molecule having a weak bond.
(b) Explain the following observations: the bond strength of Li_2 is 100 kJ mol^{-1} , a value much greater than that for Be_2