

CH 107 Tutorial 6

Please solve these problems BEFORE the tutorial session

1. Photoelectron spectrum of a second-row homonuclear-diatomic molecule was recorded using 21.21 eV photons. It is observed that KE_{Max} of ejected electrons from the top three HOMOs were 10.01, 8.23 and 5.22 eV, having intensity ratios of 1:2:1. Sketch the MO energy level diagram and hence identify the molecule.
2. Qualitatively draw the bonding and antibonding MOs formed due to overlap of (i) two $2s$ and (ii) two $3p_z$ AOs. Assume the internuclear axis to be in z -direction. Show nodes and signs of MOs. *Hint: Draw the wavefunctions centered on the two nuclei along $\pm z$ to find nodes!*
3. Write the expressions for the delocalized σ bonding MOs of BeH_2^+ as linear combinations of valence AOs of appropriate symmetry. *Do not invoke s - p mixing and consider $+z$ to be the internuclear axis for this linear molecule.*
 - a) Sketch the bonding MOs, show signs and nodes (if any), and assign symmetries (g/u).
 - b) How many lines/bands are expected in the *entire* photoelectron (PE) spectrum?
 - c) What are their relative intensities? (note that the molecule has $+1$ charge)
4. Draw a qualitative contour sketch of a $2s$ - $2p$ hybridized orbital oriented along $-y$ direction carefully showing the position of the nucleus, and the nodal plane/surface.
5. For water, it is experimentally determined that the H-O-H bond angle is 104.5° . Determine the coefficients of atomic orbitals of O that participate in hybridization (see schematic, lone pairs are in xz plane, not relevant).

