CH-107 Tutorial - 5

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. **The binding energy of N_2^+ is less than that of N_2 whereas the binding energy of O_2^+ is greater than that of O_2. Explain on the basis of M.O. configurations.**

3. **Draw the π and π^* MOs for N_2 and CO. Qualitatively show the difference.**

4. **Write down the Hamiltonian for a linear H_3^+ molecular ion (*hypothetical*, with equal H – H bond lengths). Write the complete expression for the lowest energy MO (include spin). Draw a qualitative sketch of bonding and antibonding MOs using 1s AOs.**

5. **Draw a qualitative contour sketch of a sp hybridized orbital oriented along -y direction showing the position of the nucleus, and the nodal plane/surface.**

6. **What are the coefficients of the AOs in the hybrid orbitals sp, sp^2 and sp^3. Rationalize the values of the coefficients of the above hybrid orbitals. Using the coefficients, compute the angles between the hybrid orbitals.**