CH107: Week 7

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3^{rd} February 2023

1 Homonuclear Diatomic Molecules

We then studied the MOs of homonuclear diatomic molecules of the first romw and mainly the second row. Here the main point to note is that till N_2 the normal Energy diagrams were not matching with the experiments. Here we observe the **sp minxing**. The s and p orbital in these atoms are **nearly degenrate** so in the MOs the energy of σ BO becomes more than the π. After N_2 the energy difference s and p becomes more so no sp mixing.

2 Heteronuclear Diatomic molecules

We studies the MO energy diagrams of HF, HCl, HBr. In HF since the energy gap between H-1s and F-2s is very much , F-2p combines with H-1s. 4 electrons are left and they remain in the pi - non boding orbital of F. IN HCl the Cl-3p is very close to H-1s so they form MOs and the 3s and other 2 3p orbitals remain in the non bonding orbitals. in HBr, the Br-4s is slightly more in enrgy than the H1s .

3 Hybridisation

Linear combination of atomic orbitals within the atoms can lead to more effective bonding. $\phi_{hy} = \alpha\psi_1 + \beta\psi 2 + \gamma\psi 3$. Here thes ecoefficients depend on the field strenght. The square of the coefficients represent the contribtion of AO to the hybrid orbital. Hybrid orbitals are ortho-normal to each other. We then indiviaully studied indiviual the eaxct expressions of sp, sp2, sp3 orbitals. We mathematically derived the expression of each of the coeffecients by apllying ortho-normality , percentage of orbitals and usinf symmetry arguments. We also studied the contour plots of spefically sp orbital. We also studied the sp3 orbitals in H_2O . Two of the orbitals have 20-80 sp ratio and the other two have 30-70 sp ratio.

4 Hybridisation v/s MOT

- Hybridization represents highly directional and localized orbitals
- MOT represents delocalized orbitals .
- MOT can also be used to explain the tetrahedral structure of methane. Only AOs with proper symmtery can be combined .Here 1 MO with no nodes ,lower energy and 3 MOs with 1 node, higher energy were formed.
- This fact was helpful in explaining the photoelectron-intesity vs ionozation energy graph which cannot be explained with the hybridisation theory.