

CH 107 2020-21

Tutorial 6

A1. Justify or contradict the following statements about sp^3 hybridization:

Contribution of

- | | |
|-----------------------------------------------------------------|-----------------------------|
| (A) each of p_x , p_y and p_z orbitals is necessarily 25% | (B) s orbital is 25% |
| (C) all p orbitals combined is 75% | (D) p_z orbital may be 0% |

A2. If bond angle is 105° , then what is the hybridization of the orbitals?

A3. For a sp^x hybrid orbital, $\psi = 0.625\phi_{2s} + 0.312\phi_{2p_x} + 0.417\phi_{2p_y} + 0.625\phi_{2p_z}$. What is the percentage p-contribution in this orbital?

A4. For BeH_2 molecule aligned along x-axis,

- (A) Write the expression for the appropriate hybrid orbitals.
- (B) Write the Heitler London wavefunction using the constructed hybrid orbital for the two bonds,
- (C) Predict if the overlap integral for the 1s orbital of H with the $2p_x$ orbital or with the hybrid orbital will be greater.

A4. Verify $H_{11} = -1 + J$ and $H_{12} = -S^2 + K$.