

Normalised VB wave function and MO wave function for H₂ molecules: -

H₂ molecules contains two electrons labelled 1 and 2 and two Hydrogen nuclei labelled A and B. The pairing of electrons leads to the formation of a covalent bond.

In the VB approach, if electron 1 is on nucleus A then electron 2 would be on nucleus B and vice-versa. Since however the two electrons are indistinguishable, therefore the VB wave function for H₂ molecule can be written as,

$$\Psi_{VB} = \left(\frac{1}{\sqrt{2}}\right) [\Phi_A(1) \Phi_B(2) + \Phi_A(2) \Phi_B(1)] \quad \text{--- (1)}$$

Where $\frac{1}{\sqrt{2}}$ is the normalization constant obtained by normalizing Ψ_{VB} .

In MO theory, the MO wave function for H₂ molecule is given by

$$\Psi_{MO} = \Psi_1 \Psi_2 \quad \text{--- (2)}$$

where Ψ_1 and Ψ_2 are the normalized wave functions for MO's of H₂ given by

$$\Psi_1 = \left(\frac{1}{\sqrt{2}}\right) [\Phi_A(1) + \Phi_B(1)] \quad \text{--- (3)}$$

$$\Psi_2 = \left(\frac{1}{\sqrt{2}}\right) [\Phi_A(2) + \Phi_B(2)] \quad \text{--- (4)}$$

Multiplying Ψ_1 and Ψ_2 we get Ψ_{MO} as

$$\Psi_{MO} = \frac{1}{2} [\Phi_A(1) + \Phi_B(1)] [\Phi_A(2) + \Phi_B(2)] \quad \text{--- (5)}$$

$$= \frac{1}{2} [\Phi_A(1) \Phi_A(2) + \Phi_B(1) \Phi_B(2)] + \frac{1}{2} [\Phi_A(1) \Phi_B(2) + \Phi_B(1) \Phi_A(2)]$$

In eqn (6) the first two terms represent the probability of finding both the electrons on the same atom at the same time.

In other words, these terms represent the ionic structure of H₂ molecule which may be written as $H_A^- H_B^+$ and $H_A^+ H_B^-$.

The last two terms represent the covalent structure of H₂ molecule.

Comparing Ψ_{VB} and Ψ_{MO} . We observe that while the wavefunction in VBT does not give any weightage to ionic structures, the MOT gives equal weightage to covalent and ionic structures.