Chemistry Study Materials for Class 11 (NCERT Based Notes of Chapter- 04)

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CHEMICAL BONDING AND MOLECULAR STRUCTURE

Valence bond theory (VBT)

This theory was introduced by Heitler and London and later developed by Linus Pauling in order to explain the shape of molecules theoretically. VBT can be explained by considering the formation of H_2 molecule.

Consider 2 hydrogen atoms A and B with nuclei N_A and N_B and electrons e_A and e_B respectively. When the two atoms are at large distance from each other, there is no interaction between them. So their potential energy is zero. When the two atoms approach each other, new attractive and repulsive forces begin to operate.

Attractive forces arise between nucleus of one atom and electron of other atom i.e., N_A– e_B and N_B– e_A. Similarly repulsive forces arise between electrons of two atoms i.e., e_A – e_B, and the nuclei of two atoms N_A – N_B. Attractive forces bring the two atoms close to each other whereas repulsive forces push them away.

Valence Bond theory assumes that electrons occupy atomic orbitals of individual atoms within a molecule, and that the electrons of one atom are attracted to the nucleus of another atom. This attraction increases as the atoms approach one another until the atoms reach a minimum distance where the electron density begins to cause repulsion between the two atoms. This electron density at the minimum distance between the two atoms is where the lowest potential energy is acquired, and it can be considered to be what holds the two atoms together in a chemical bond.

The overlap of atomic orbitals is given by the following postulates:

- The atoms which unite to form a molecule completely retain their identities in the resulting molecule.
- The formation of a covalent bond is due to overlap of atomic orbitals .
- If the two atoms, each having on unpaired electron, come together, the AO's accommodating these unpaired electrons overlap (i.e, electron waves interact) and the spins of the two electrons get mutually neutralized, resulting in the formation of covalent bond which is localized between the two atoms.
- If the electrons present in the AO's have parallel spins, no bond formation will occur, and no molecule will be formed.
- If the AO's possess more than one unpaired electrons, more than one bond can be formed. Thus, in N_2 molecule there are three bonds, since
- N atom has three unpaired electrons. N = $2s^2$, $2p_x^1$, $2p_y^1$, $2p_z^1$
- Electrons already paired in the valence shell cannot take part in the bond formation. They can only take part in the bond formation if they can be unpaired with the use of lot of energy. This is seen in the case of Phosphorus, which forms PF_5 by sharing 5 electrons (three from the three unpaired P electrons and two from paired s).
- The strength of the covalent bond is related to the extent of overlapping of the atomic orbitals. The more the two bonding orbitals overlap, The more the bonding electrons are concentrated between the nuclei where they can minimize the nuclear repulsion and maximize the attractive forces between themselves and both nuclei jointly.

  Thus, greater the overlap of the atomic orbitals, the greater will be the strength of the resulting covalent bond.

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