POLARITY IN COVALENT COMPOUNDS

In each covalent bond, the discrepancy in electronegativity prompts the shared electron cloud between the two nuclei to shift towards the nucleus with higher electronegativity. This asymmetrical distribution of electrons results in charge separation within the molecule. Exemplary instances include H-F and H-Cl molecules.

Molecules formed through such asymmetric electron sharing are referred to as polar molecules. The polar covalent bond, inherent in these molecules, exhibits a partial ionic character. This partial ionic character gives rise to two oppositely charged poles within the molecule, referred to as molecular dipoles.

To gauge the ionic character in a covalent bond, two key metrics are often employed:

1. **Electronegativity Difference:**

   The disparity in electronegativity values between two atoms involved in a covalent bond is a critical factor in determining the ionic character.

   Electronegativity is a measure of an atom's ability to attract shared electrons in a chemical bond.

   When there is a significant difference in electronegativity between the two atoms, it implies an uneven sharing of electrons, leading to an ionic character in the covalent bond.

   Various scales, such as the Pauling scale, quantify electronegativity, providing a numerical representation of the atom's tendency to attract electrons. The greater the electronegativity difference, the higher the degree of ionic character in the covalent bond.

2. **Dipole Moment and Percentage Ionic Character**

   Dipole Moment:

   The dipole moment of a molecule is a crucial measure in determining the extent of ionic character in a covalent bond.

   It quantifies the polarity of the molecule by considering both the magnitude and direction of the charge separation within the molecular structure.

   A higher dipole moment indicates a more polar bond, suggesting a greater ionic character in the covalent interaction.

   Percentage Ionic Character:

   The percentage ionic character is another parameter used to gauge the extent of ionic character in a covalent bond.

   It provides a quantitative measure of how much the actual dipole moment of a bond deviates from the dipole moment expected purely from electronegativity differences.

   The formula for calculating the percentage ionic character involves comparing the observed dipole moment with the dipole moment expected based on electronegativity values. This percentage reflects the proportion of ionic character present in the covalent bond.

Applications

Molecular Shape Analysis:

When the experimental dipole moment value is known, such as $^{u}CO_2$ being zero and $^{u}H_2O$ being non-zero, it indicates the direction of charge pulling in CO_2 molecule is opposite, resulting in a linear structure. Conversely, in the case of a water (H_2O) molecule, where u is non-zero, the shape must be angular.

Differentiating between Non-Polar and Polar Molecules:

Homoatomic molecules like H_2, N_2, O_2, F_2, Cl_2, etc., exhibit zero dipole moment.

Polyatomic molecules such as CO_2, BF_3, CCl_4, CH_4, para-dichlorobenzene, etc., also have zero dipole moment.

Species like HCl, HF, H_2O, NH_3, NF_3, ortho and meta-dichlorobenzene demonstrate a specific, non-zero value of dipole moment (u).

Ionic Character of Bonds in a Molecule:

The percentage ionic character of a bond in a molecule can be determined using the dipole moment (u) with the formula % ionic character of bond = ^{u}observed/ ^{u}calc × 100.
This formula allows for the quantification of the degree of ionic character in a bond based on the observed and calculated dipole moments.

Example: Calculate the percentage covalent character of the A-B bond, given a bond length of 1.62 Å and an observed dipole moment of 0.4 D.

Solution: The calculated dipole moment, assuming a 100% ionic bond, is obtained using the formula: Calculated dipole moment = ^{u}ionic = 4.8×10^{-10} esu cm × 1.62×10^{-8} cm = 7.776×10^{-18} esu cm = 7.776 D
The percentage ionic character is then determined by the observed dipole moment:
Percentage ionic character = 0.47/7.776 × 100 ≈ 5.144%
Therefore, the percentage covalent character is calculated as:
Percentage covalent character = 100 − 5.144 ≈ 94.85%
This calculation yields the percentage of covalent character in the A-B bond based on the observed dipole moment and the calculated dipole moment for a 100% ionic bond.