Nature of Bonding In Organic Compounds

The organic compounds are carbon compounds consisting of one or more carbon atoms. Carbon must form only covalent bonds, i.e., it should share its valence electrons with other atoms.

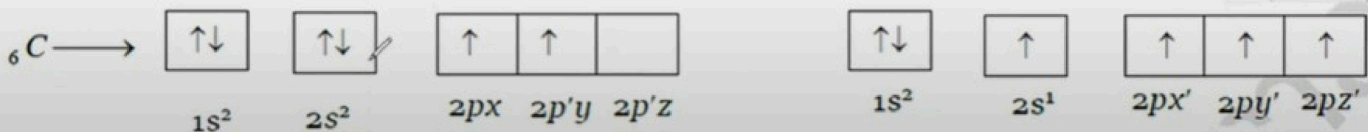
According to the modern concept, a covalent bond is formed between two atoms if there is an overlapping of an atomic orbital of one atom with an atomic orbital of another atom. The overlapping is possible by two ways,

(1) **End to end overlapping:** This type of overlapping is possible between s-s, s-p^x and p^x-p^x atomic orbital's. The molecular bond formed is termed as sigma bond.

(2) **Sidewise or parallel or lateral overlapping:** Such overlapping is possible between p^y-p^y & p^z-p^z atomic orbital's. The molecular bond formed is termed as pi bond.

Introduction

The chemical properties of an element depend on the electronic configuration of the outershell. Carbon has four electrons in its outershell. According to the ground state electronic configuration of carbon, carbon is divalent. Tetravalency of carbon can be explained by promoting one 2s - electron to a 2pz orbital. Some energy must be supplied to the system in order to effect this promotion. This promotion requires energy about 96 kcal/mol, but this energy is more than regained by the concurrent formation of chemical bonds.



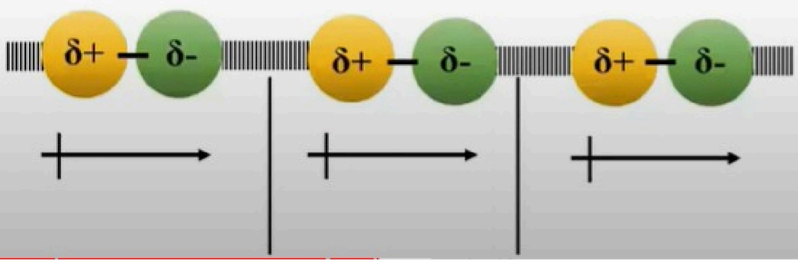
Carbon in ground state

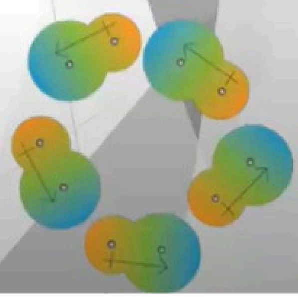
Carbon in excited state

Physical Effects

(1) Dipole-dipole Interactions

- These forces operate between molecules contains polar covalent bonds.
- The Positive end of one polar molecules attract with negative end of another molecules.

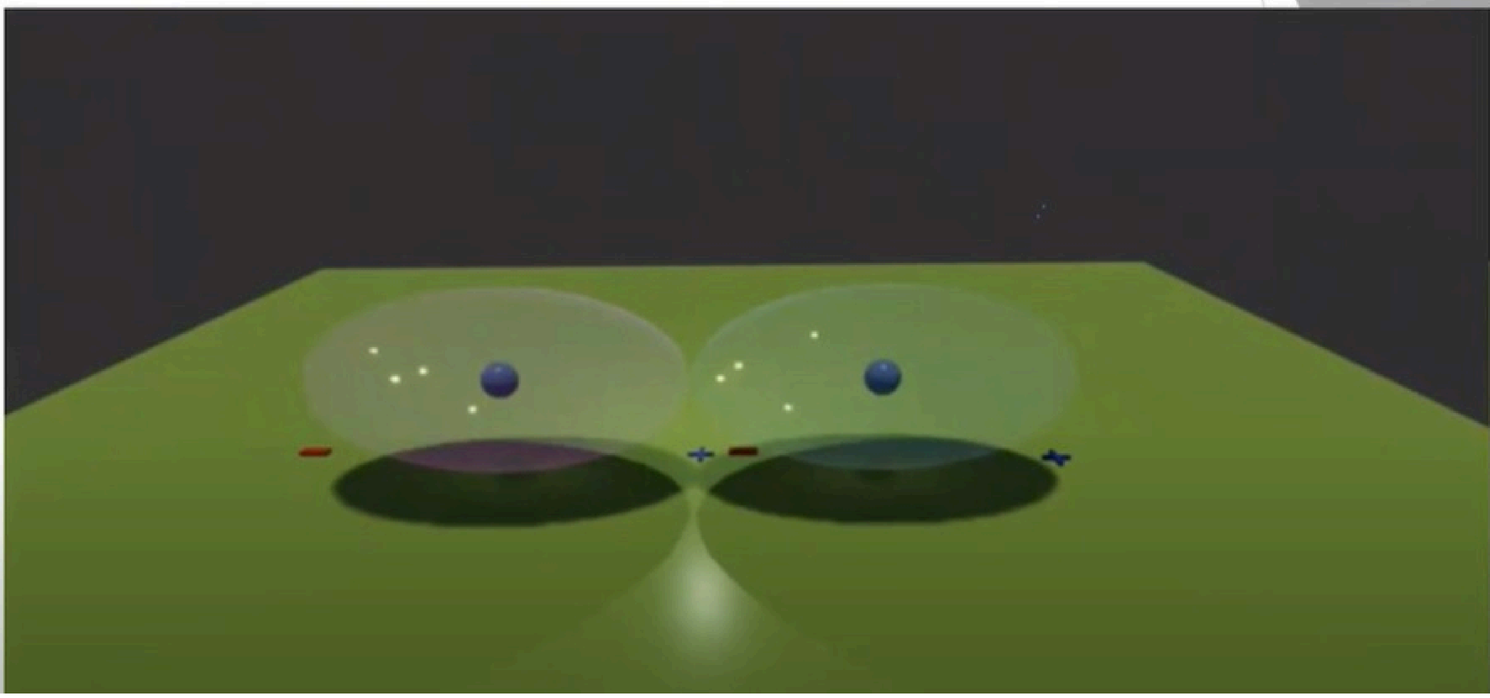




Nature of Bonding In Organic Compounds

∂-Bond	π-Bond
Formed by End to End overlap of AO's	Formed by lateral overlap of p-orbitals
Has cylindrical charge symmetry about bond axis	Has maximum charge density in the cross sectional plane of the orbital's
Has free rotation	No free rotation, i.e., frozen rotation
Low energy	Higher energy
Only one **∂**-bond can exist between two atoms	One or two π bonds can exist between two atoms
Sigma bonds are directional. Thus the geometry of the molecule depends on the **∂**-bonds	π bonds are not directional. Geometry of the molecule not depends on π-bond
Area of overlapping is higher hence bond is Stronger	Area of overlapping is small hence bond is Weaker
∂-bond can have independent existence	π-bond always exist along with a π bond and π-bond is formed after the formation of π-bond

Origin of Van der Waals Forces



Physical Effects

(3) Hydrogen Bonding

An electrostatic attractive force between the covalently bonded hydrogen atom of one molecule and an electronegative atom (such as N,O,F) of the other molecule is known as **hydrogen bonding.**

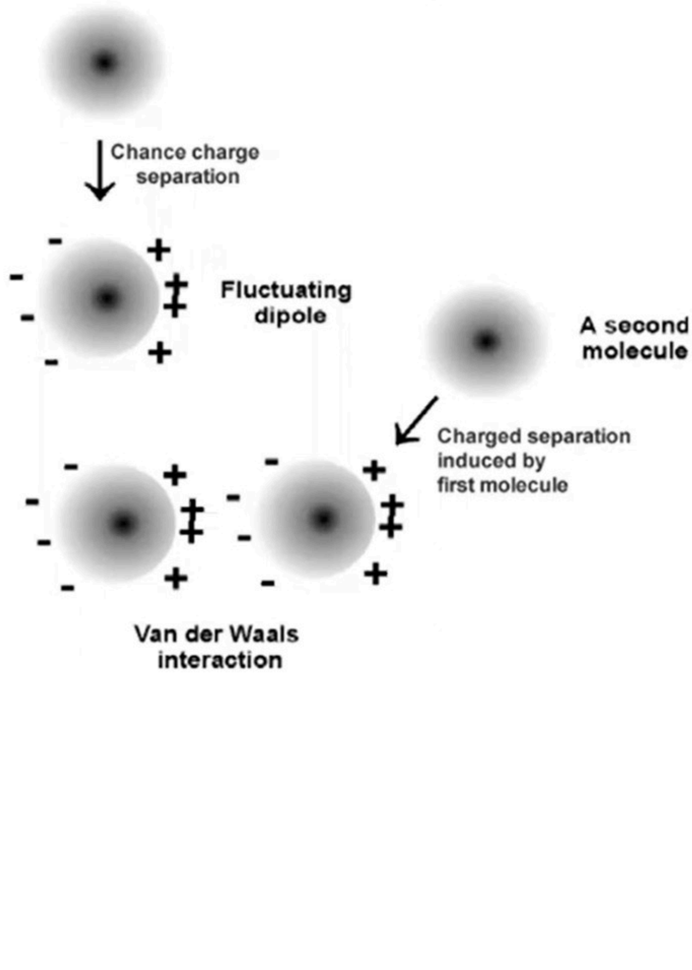
Examples of H-bonding in between the two molecules of same or different compounds are:

$$H^{\delta+}\text{---}X^{\delta-}\cdots\cdots\cdots H^{\delta+}\text{---}X^{\delta-}\cdots\cdots\cdots H^{\delta+}\text{---}X^{\delta-}$$

Hydrogen Bond

Physical Effects

Origin of Van der Waals Forces



Physical Effects

Factors influencing van der Waals forces:

- **Number of electron in the molecules.**
- **Size of the molecules.** CH_4, C_2H_6 and C_3H_8 etc.
- **Shape of the molecules.**

$H_3C-CH_2-CH_2-CH_2-CH_3$

Pentane

$$\begin{array}{c} CH_3 \\ | \\ H_3C-C-CH_3 \\ | \\ CH_3 \end{array}$$

Neopentane

- **Temperature and Pressure.** The van der Waals forces are relatively stronger at low temperature and high pressure.

Physical Effects

Condition for Hydrogen bonding and its strength

1) **High electronegativity of atom**: The atom which is covalently bonded with hydrogen have high electronegativity, so that it can attract shared pair of electron strongly toward itself.

2) **Small size of the atom**: If the atom attached with hydrogen should be small then it will be able to develop strong electrostatics interaction with neighbouring hydrogen.

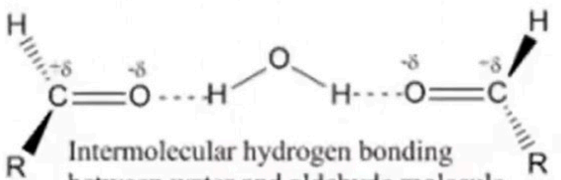
Fluorine, Oxygen and Nitrogen, are three elements which fulfil these conditions and give rise to effective hydrogen bond.

Physical Effects

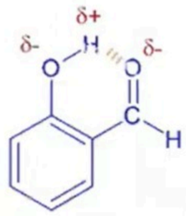
Types of Hydrogen Bonding:

1) Intermolecular Hydrogen Bonding: When hydrogen bond formed between separate molecules of the same or different substance.

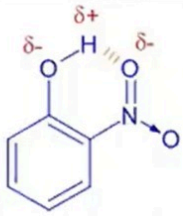
2) Intramolecular Hydrogen Bonding: When hydrogen bond formed between atoms or groups within same molecules.



Intermolecular hydrogen bonding between water and aldehyde molecule



Intramolecular hydrogen bonding in ortho hydroxy benzaldehyde (salicylaldehyde)



Intramolecular hydrogen bonding in ortho nitrophenol

Physical Effects

Nature and Importance of Hydrogen bonding

1) Hydrogen bond is merely an electrostatic force rather than a chemical bond.
2) Hydrogen bond never involves more than two atoms.
3) With the increase of electronegativity of the atom to which hydrogen is covalently linked, the strength of the hydrogen bond increases.
4) All the three atoms in $X^{\delta-}$ - - - $H^{\delta+}$- - - $X^{\delta+}$ lie in a straight line.
5) The bond length of hydrogen bond is of the order of 250 to 275 pm.

The relative order of these intermolecular forces is,

Hydrogen bonding > dipole-dipole forces > Vander waal's forces.

Hybridisation in Organic Compounds

The process of mixing atomic orbital's to form a set of new equivalent orbitals is termed as **hybridisation**.

There are three types of hybridisation encountered in carbon atom. These are:

(i) sp^3 **hybridisation (involved in saturated organic compounds containing only single** covalent bonds),

(ii) sp^2 **hybridisation (involved in organic compounds having carbon linked by double** bonds) and

(iii) sp **hybridisation (involved in organic compounds having carbon linked by a triple** bonds).

Physical Effects

Types of van der Waals interaction:

1. **Dipole-dipole attraction**: These forces operate between molecules which are permanently polar in nature, i.e. HCl, NH_3, SO_2 and acetone etc.
2. **Dipole-induced dipole attraction**: These forces operate between molecules which one is polar and another is non-polar in nature.