TDC Part 1 chem (Hons)
Topic - Dipolemoment

Shashi Kumar Singh
L.S. College
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Dipole moment → As we know there are two types of diatomic molecule i.e. Homonuclear diatomic (ex - H_2, N_2, F_2, Cl_2, O_2 etc.) (ii) Heteronuclear diatomic molecule (ex - HCl, H_2O, HBr, etc.). In hetronuclear diatomic molecule due to diffrence in electronegativity polarity arises → $H^{+\delta} Cl^{-\delta}$. The difference of Polarity is known as DIPOLE MOMENT denoted by μ, (+→)

$$\mu = e \times d$$

where e = electric charges, d = distance between centre of the Positive and negative charges. This is a Vector quantity

The SI unit for electric dipole moments are coulumb - meter (Cm)

and a commonly used unit is debye (D)

$1D = 10^{-18}$ e.s.u (C.G.S. unit)

electronic charge is range of 10^{-10} e.s.u

and distance is in order of 10^{-8} A°,

So, $10^{-10} \times 10^{-8} = 10^{-18}$ e.s.u

$1D = 3.336 \times 10^{-30}$ coulomb meter

- Dipole moments increases with ionic Character and decreases with covalent Character

Bond dipole moment – The bond dipole moments uses the idea of electric dipole moment to measure a chemical bond's polarity within a molecule. The greater the difference in two electronegativity the larger the dipole.

A symmetrical molecule like Cl_2, has 0 dipole moment.

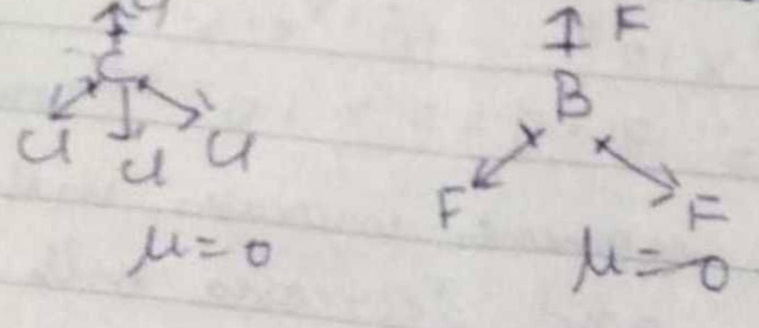
The highly ionic gas KBr, has a dipole moment of 10.5 D

Bond symmetry :– Symmetry is another factor.

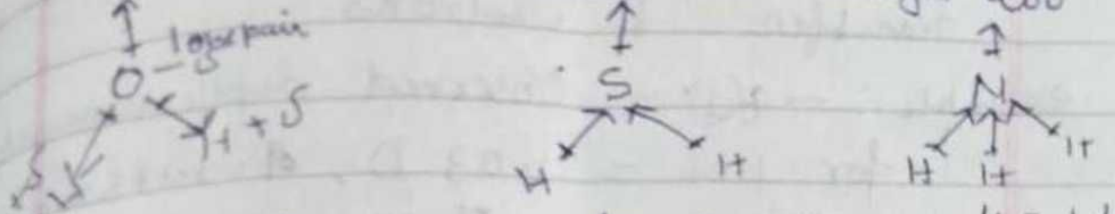
Example – CO_2

$\overset{-\delta}{O}=\overset{+\delta}{C}=\overset{-\delta}{O}$, It has two C – O bonds that are polar due to EN difference, but Dipole moment is zero. The bonds are on exact opposite sides of the central atom, the charges cancelled out.

Dipole moment of CH_4, CCl_4, BF_3 are zero due to symmetry



Molecular Dipole moment :— When a molecule consist more than two atoms, more than one bond is holding the molecule together. μ depends polarity and bond angle too



$\mu = 1.84D$ $\mu = 0.90$ $\mu = 1.49D$

$$\mu = \sqrt{\mu_1^2 + \mu_2^2 + 2\mu_1\mu_2 \cos\theta}$$

$$\mu = \text{total} - \mu \text{ lone pair} + 3\cos\theta \, \mu_{bond}$$

Percentage ionic character $= 16(\Delta x) + 3.5(\Delta x)^2$

where Δx = Electronegativity difference.

Application of dipole moment :—

① In predicting the nature of molecule.
 ⓐ BeF_2 ($\mu = 0$) - nonpolar.
 ⓑ H_2O ($\mu = 1.84D$) - Polar

② Relative polarity of molecules → Greater the value of μ, more in polarity.

③ Shape of molecule -
 $O=C=O$ — linear $\mu = 0$
 H_2O — angular, or bend $\mu = 1.84D$

(4) Calculating % ionic character.
It is the ratio of observed or experimental dipole moment to the dipole moments for complete transfer of electrons

example :— Q(1) – Observed dipole moment for HCl = 1.03 D, $d = 1.275 \times 10^{-8}$ cm
$\mu = q \times d$, % ionic character = ?

$$\% \text{ ionic} = \frac{\mu \text{ observed}}{\mu \text{ (100\% ionic)}} \times 100$$

μ obsb. — 1.03 D. (C.G.S. unit)

$\mu = q \times d$

μ for 100%. $= 4.8 \times 10^{-10}$ e.s.u. $\times 1.275 \times 10^{-8}$ cm

$= 6.12 \times 10^{-18}$ e.su cm

$= 6.12$ D

$$\mu = \frac{\mu \text{ observe} = 1.03\text{ D}}{\mu \text{ for } 100\% = 6.12\text{ D}} \times 100$$

$= 16.83\%$.

Q.2. The dipole moment of LiH is 1.964×10^{-29} [illegible] and interatomic distance between Li and H in the mol is 1.596 A°. Calculate the % ionic character of LiH.

For 100% ionic character = $e = 1.602 \times 10^{-19}$ C $\times d$

i.e. $= 1.602 \times 10^{-19}$ C $\times 1.596 \times 10^{-10}$ m

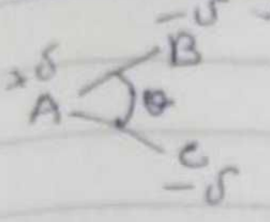
$= 2.557 \times 10^{-29}$ C.m

% ionic character = $\frac{\mu \text{ obs.}}{\mu \text{ for } 100\% \text{ ionic}} \times 100$

$= \frac{1.964 \times 10^{-2}}{2.557 \times 10^{-29}} \times 100$

$= 66.8\%$

(3) calculating of resultant bond moment



$\mu_R = \sqrt{\mu_1^2 + \mu_2^2 + 2\mu_1\mu_2 \cos\theta}$

If $\theta = 0$, $\cos 0 = 1$

$\mu_R = \sqrt{\mu_1^2 + \mu_2^2 + 2\mu_1\mu_2 \cdot 1}$ = maximum value

if $\theta = 180°$. $\cos 180 = -1$

$\mu_R = \sqrt{\mu_1^2 + \mu_2^2 - 2\mu_1\mu_2}$

$= \sqrt{(\mu_1 - \mu_2)^2}$

$\cos 0 = 1$

$\cos 45 = \frac{1}{\sqrt{2}}$

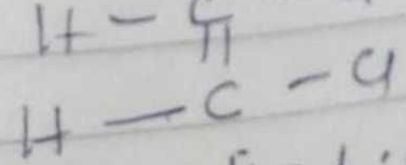
$\cos 60 = \sqrt{3}/2$

$\cos 90 = 0$

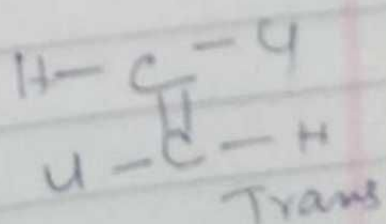
$\cos 180 = -1$

$\cos 120 = -1/2$

Geometry of the molecule can also be determined :



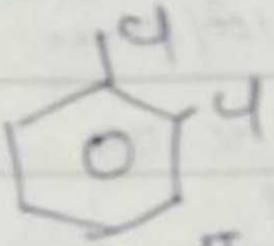
$\mu = 1.9 D$



Trans

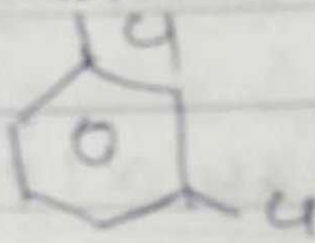
$\mu = 0$

(1) Orientation in Benzene



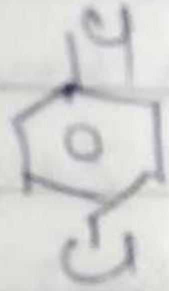
ortho

$\mu = 2.54\,D$



Meta

$\mu = 1.48$



Para

$\mu = 0$.