Dipole moment.

"The product of magnitude of negative or positive charge (q) and the distance (d) between the centres of positive and negative charges is called dipole moment".

It is usually denoted by μ. Mathematically, it can be expressed as follows :

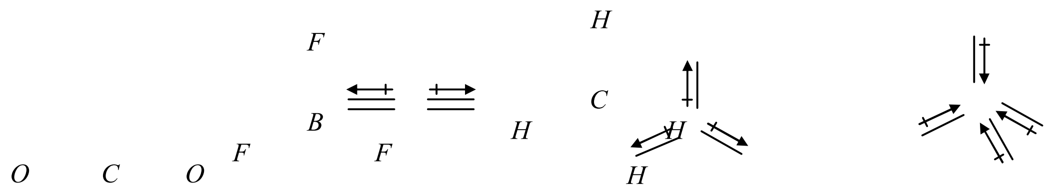
μ = Electric charge × bond length

As q is in the order of 10–10 esu and d is in the order of 10–8 cm, μ is in the order of 10–18 esu cm. Dipole moment is measured in "Debye" (D) unit. $1D = 10^{-18}$ esu cm = 3.33×10^{-30} coulomb metre.

Generally, as electronegativity difference increases in diatomic molecules, the value of dipole moment increases. Greater the value of dipole moment of a molecule, greater the polarity of the bond between the atoms.

Dipole moment is indicated by an arrow having a symbol (⟶) pointing towards the negative end. Dipole moment has both magnitude and direction and therefore it is a vector quantity.

Symmetrical polyatomic molecules are not polar so they do not have any value of dipole moment.



μ = 0 due to symmetry

Some other examples are – CCl4,CS2 , $PbCl_4, SF_6, SO_3, C_6H_6$, naphthalene and all homonuclear molecules (H2, O2, Cl2 etc)

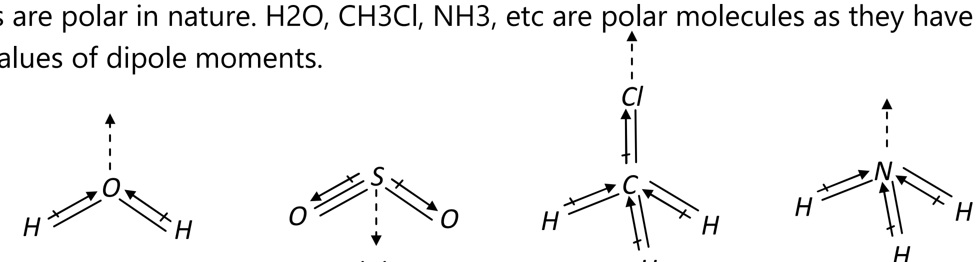
Note : ❑ Benzene, Naphthalene have zero dipole moment due to planar structure.

❑ Amongst isomeric dihalobenzenes, the dipole moment decreases in the order : o > m > p.

❑ A molecule of the type MX4, MX3 has zero dipole moment, because the σ-bonding orbitals used by M(Z < 21) must be sp3, sp2 hybridization respectively (e.g. CH4, CCl4, SiF4 , SnCl4, BF3 , AlCl3 etc.)

sp^3 sp^2

Unsymmetrical polyatomic molecules always have net value of dipole moment, thus such molecules are polar in nature. H2O, CH3Cl, NH3, etc are polar molecules as they have some positive values of dipole moments.



Water $\mu = 1.84D$ | Sulphur dioxide | Methyl chloride | Ammonia

μ≠ 0 due to unsymmetry

Some other examples are – CH3Cl, CH2Cl2, CHCl3, SnCl2, ICl, C6H5CH3 , H2O2, O3, Freon etc.

Applications of dipole moment

(i) In determining the symmetry (or shape) of the molecules : Dipole moment is an important factor in determining the shape of molecules containing three or more atoms. For instance, if any molecule possesses two or more polar bonds, it will not be symmetrical if it possesses some molecular dipole moment as in case of water $(\mu = 1.84\,D)$ and ammonia $(\mu = 1.49\,D).$ But if a molecule contains a number of similar atoms linked to the central atom and the overall dipole moment of the molecule is found to be zero, this will imply that the molecule is symmetrical, e.g., in case of BF_3, CH_4, CCl_4 etc.,

(ii) In determining percentage ionic character : Every ionic compound having some percentage of covalent character according to Fajan's rule. The percentage of ionic character in a compound having some covalent character can be calculated by the following equation.

The percent ionic character $= \dfrac{\text{Observed dipole moment}}{\text{Calculated dipole moment assuming 100\% ionic bond}} \times 100$

(iii) In determining the polarity of bonds as bond moment : As $\mu = q \times d$, obviously, greater is the magnitude of dipole moment, higher will be the polarity of the bond. The contribution of individual bond in the dipole moment of a polyatomic molecule is termed as bond moment. The measured dipole moment of water molecule is 1.84 D. This dipole moment is the vectorial sum of the individual bond moments of two O-H bonds having bond angle 104.5o.

Thus, $\mu_{obs} = 2\mu_{O-H} \cos 52.25$ or 1.84 = 2μO – H × 0.6129 ;μO – H = 1. 50 D

Note :❑ $\Delta EN \propto$ dipole moment, so HF > HCl > HBr > HI , } Where, ΔEN = Electronegativity difference

❑ $\Delta EN \propto$ bond polarity, so HF > H2O > NH3 > H2S.

❑ If the electronegativity of surrounding atom decreases, then dipole moment increases.
$NCl_3 < NBr_3 < NI_3$

(iv) To distinguish cis and trans forms : The trans isomer usually possesses either zero dipole moment or very low value in comparision to cis–form

$$\begin{matrix} H & - & C & - & Cl \\ & & \| & & \\ H & - & C & - & Cl \end{matrix} \qquad \begin{matrix} H & - & C & - & Cl \\ & & \| & & \\ Cl & - & C & - & H \end{matrix}$$

Cis – 1, 2 – dichloro ethene $\mu = 1.9\ D$ Trans – 1, 2 –dichloro ethene, $\mu = 0$

Example: Calculate the % of ionic character of a bond having length = 0.92 Å and 1.91 D as its observed dipole moment.

(a) 43.25 (b) 86.5 (c) 8.65 (d) 43.5

Solution: (a) Calculated μ considering 100% ionic bond [When we consider a compound ionic, then each ionic sphere should have one electron charge on it of $4.80 \times 10^{-10}\ esu$ (in CGS unit) or $1.60 \times 10^{-19}\ C$ (in SI unit)]

= 4.8 × 10–10 × 0.92 × 10–8 esu cm = 4.416 D

% Ionic character $= \frac{1.91}{4.416} \times 100 = 43.25.$

Important Tips

The dipole moment of CO molecule is greater than expected. This is due to the presence of a dative (co-ordinate) bond.

Critical temperature of water is higher than that of O2 because H2O molecule has dipole moment.

Liquid is not deflected by a non uniform electrostatic field in hexane because of μ = 0
