

## DEFINITION OF DIPOLE MOMENT

Due to difference in the electronegativity, polarity develops between two adjacent atoms in the molecule (better say bond). The degree of polarity of a bond is called dipole moment ( $\mu$ ). It is a vector quantity and direction is from positive pole to negative pole. Dipole moment of a molecule (polarity) is found by vector addition.

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

(1) Dipole moment depends upon the polarity of bonds as well as shape of the molecule.

(2) Dipole moment of a symmetrical molecule is always zero, e.g.  $\text{CH}_4$ (tetrahedral),  $\text{CCl}_4$ (tetrahedral),  $\text{BF}_3$ (triangular planar),  $\text{BH}_3$ (triangular planar),  $\text{CO}_2$ (linear),  $\text{CS}_2$ (linear),  $\text{XeF}_2$ (linear),  $\text{XeF}_4$ (square planar),  $\text{CH}_2=\text{CH}_2$ (triangular planar),  $\text{CH}\equiv\text{CH}$ (linear).

(3) Dipole moment of an unsymmetrical molecule is always greater than zero ( $\mu \neq 0$ ), e.g.  $\text{H}_2\text{O}$ ,  $\text{CHCl}_3$ . Those molecules where there is one central atom which is bonded with same atoms or groups and has no lone pair are considered as symmetrical.

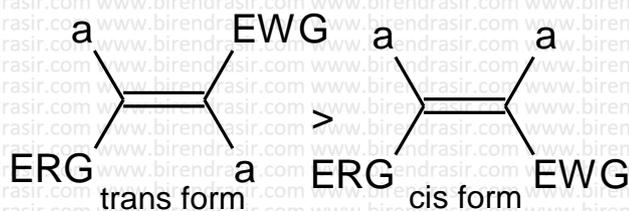
(4) Many times dipole moment is directly proportional to electronegativity of central atom and surrounding atoms.



(5) In geometrical isomers following type, dipole moment of cis form is greater than trans form.



but for following type, dipole moment of trans form is greater than cis form



(6) Dipole moment of trans form is zero only if a and b are atoms. In following example dipole moment is non zero.



(7) Charge separation in acetaldehyde  $\text{CH}_3\text{-CH=O}$  is more than propene  $\text{CH}_3\text{CH=CH}_2$ . Larger charge increases the dipole moment.  $\text{CH}_3\text{-CH=O}$  (2.65D),  $\text{CH}_3\text{CH=CH}_2$  (0.35 D).

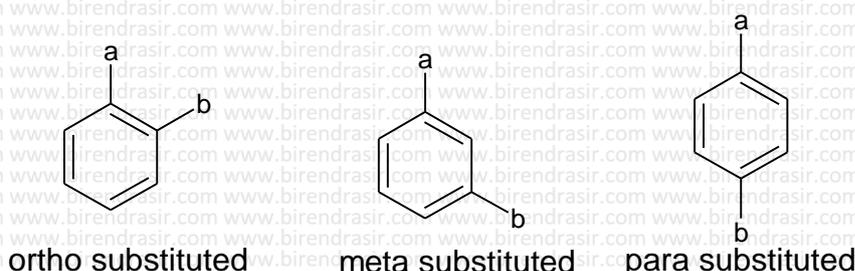
Ozone is polar molecule with dipole moment 0.53 D



Dipole moment charge separation.

due to

(8) Dipole moment of disubstituted benzene



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

$\theta$  for ortho  $60^\circ$ , for meta  $120^\circ$  and para  $180^\circ$ .

(i) when both the groups are either electron withdrawing (e.g. -Cl, -CN, -OH, -NH<sub>2</sub>) or electron releasing (-CH<sub>3</sub>, -O<sup>-</sup>), then dipole moment order ortho > meta > para.

(ii) When one group is electron withdrawing and another is electron releasing then para > meta > ortho.

In hydroquinone (para-hydroxybenzene) oxygen is sp<sup>3</sup> hybridised (non planar), so due to repulsion and other steric factors it simply changes the plane and thus the net dipole moment comes to be non-zero.



CN

CN



NO<sub>2</sub>

NO<sub>2</sub>



OH

OH



NH<sub>2</sub>

NH<sub>2</sub>

dipole moment = 0

dipole moment = 0

dipole moment nonzero

dipole moment nonzero

Toluene



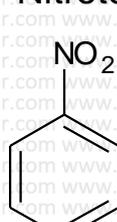
0.43 D

Nitrobenzene



3.93 D

Nitrotoluene

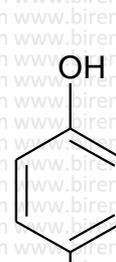


4.39 D

Phenol



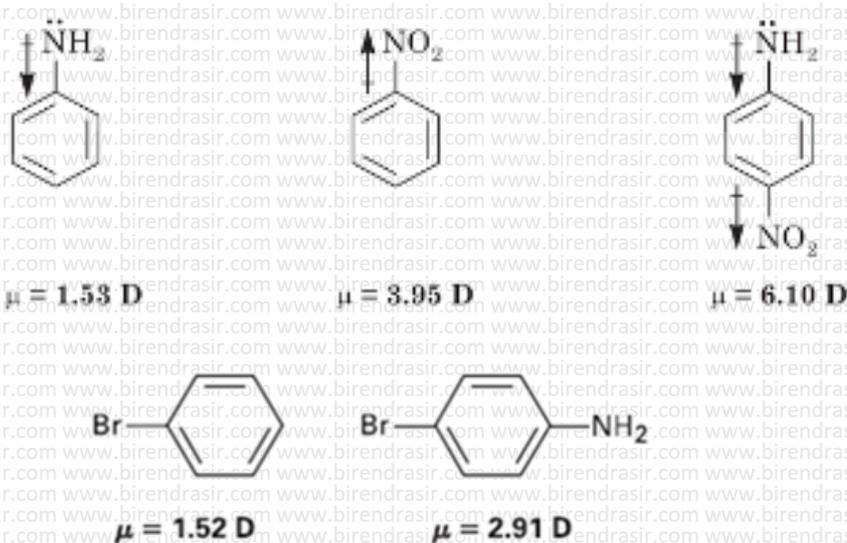
1.54 D



1.57 D

Dipole moment can be defined as the property of the molecule that results from charge separation. It is not possible to measure the dipole moment of individual bonds within the molecule, we can only measure the total moment of the molecule (i.e. the vectorial sum of the individual dipole moments). Individual dipole moments are roughly same from

molecule to molecule (but this constancy is by no means universal). On the basis of dipole moments of toluene and nitrobenzene the expected dipole moment of nitrotoluene was 4.36 D while actual 4.39 roughly same but in a similar manner we expected dipole moment of p cresol 1.11 D but actual is 1.57 D.



The dipole moment values for nitrobenzene and aniline show that  $\text{NH}_2$  and  $\text{NO}_2$  groups induce dipole moments in opposite directions with respect to benzene ring. In paranitrobenzene the dipole moments of these groups reinforce each other to increase the net value.

## Dipole moments of some common bonds of common occurrence

Bond	H-C	H-O	H-N	C-O	C-N	C-F	C-Cl	C-Br	C=O	$\text{C}\equiv\text{N}$
Dipole moment	0.3	1.5	1.3	0.7	0.2	1.4	1.5	1.4	2.4	3.6

Dipole moment of HF (1.91 D) > H<sub>2</sub>O (1.85 D) > NH<sub>3</sub> (1.47 D) > NF<sub>3</sub> (0.24 D). More lone pair more dipole moment. Dipole moment for CCl<sub>4</sub>(0.0D) <CHCl<sub>3</sub> (1.02D)< CH<sub>2</sub>Cl<sub>2</sub> (1.55D) < CH<sub>3</sub>Cl (1.87D). Dipole moment of CH<sub>3</sub>I < CH<sub>3</sub>Br < CH<sub>3</sub>F < CH<sub>3</sub>Cl because of shorter bond length C-F.

