Dipole Moment

A physical dipole consists of two equal and opposite point charges. In the literal sense, a dipole is that which has two poles (di = two), it is known as a dipole moment. The electric dipole which has a separation of positive and negative charges in a system of electrical charges and is a measure of the electrical polarity of the system. The molecule in which the charge distribution is unsymmetrical is known as a polar molecule and the bond as a polar bond. Since the degree of the polarity of the molecule is generally represented by μ, which is the product of charge q and the distance separating them (bond distance r).

$$\text{Dipole moment } (\mu) = q \times r$$

Key Points

- The dipole moment of a single bond in a polyatomic molecule is known as the bond dipole moment and it is different from the dipole moment of the molecule as a whole.
- It is a vector quantity, i.e. it has magnitude as well as definite directions.
- Being a vector quantity, it can also be zero as the two oppositely acting bond dipoles can cancel each other.
- By convention, it is denoted by a small arrow with its tail on the negative center and its head on the positive center.
- In chemistry, the dipole moment is represented by a slight variation of the arrow symbol. It is denoted by a cross on the positive center and arrowhead on the negative center. This arrow symbolizes the shift of electron density in the molecule.
- In the case of a polyatomic molecule, the dipole moment of the molecule is the vector sum of the all present bond dipoles in the molecule.

Calculation of Dipole Moment

A dipole moment is the product of the magnitude of the charge and the distance between the centers of the positive and negative charges. It is denoted by the Greek letter 'μ'.

Mathematically,

Dipole Moment (μ) = Charge (Q) * distance of separation (r)

It is measured in Debye units denoted by 'D'. 1 D = 3.33564 × 10-30 C.m, where C is Coulomb and m denotes a meter.

The bond dipole moment that arises in a chemical bond between two atoms of different electronegativities can be expressed as follows:

$\mu = \delta.d$

Where: μ is the bond dipole moment,

δ is the magnitude of the partial charges δ+ and δ–,

and d is the distance between δ+ and δ–.

The bond dipole moment (μ) is also a vector quantity, whose direction is parallel to the bond axis. In chemistry, the arrows that are drawn in order to represent dipole moments begin at the positive charge and end at the negative charge.

The unit of a dipole is Debye (D) or Columb meter (Cm). The SI unit Cm is too large to be practical on the molecular scale. So, bond and molecular dipole moment are commonly measured in Debyes 1 Debye results from an electron and a proton separated by 0.208 Å. This is a vector quantity and is represented by an arrow from the positive and negative end.

When two atoms of varying electronegativities interact, the electrons tend to move from their initial positions to come closer to the more electronegative atom. This movement of electrons can be represented via the bond dipole moment.

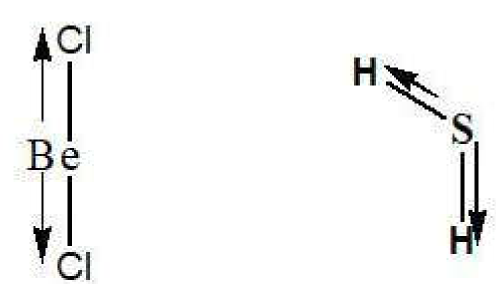
How to Calculate the Dipole Moment of a Molecule?

Carbon dioxide, barium chloride, stannous chloride have zero dipole moment indicating that the molecules have a symmetrical charge distribution between the bond.

In carbon dioxide, one carbon-oxygen cancels the bond moment of the other carbon-oxygen bond. But the bond moment associated with the bond arising from the difference of electronegativity.

The vectorial addition of the ionic bond moments uses to calculate the dipole moment of the molecule.

For example, water and hydrogen sulfide non-polar because they have non-linear structures. The bond angle can be calculated from the polarity of the molecules.



Application of Dipole Moment

Application of dipole moment use for calculation of ionic character, bond angle, polarization, and polarity of molecules in chemistry. For example, the homonuclear diatomic molecule has zero dipole moment but the bond polarity of carbon monoxide, water, methane, ammonia use to calculate the dipole moment of such molecules. When a covalent chemical bond is formed between two identical atoms, the bonding electrons equally sharing by two atoms. Thus the centers of gravity of the two electrons and nuclei therefore coincide.

But for two dissimilar atoms, two electrons are not symmetrically disposed. Because each atom has a different attraction for electrons.

When chlorine and bromine combine to form covalent HBr, the electrons forming the covalent bond displaced towards the bromine atom without any separation of the nucleus of an atom.

Ionic Character of Molecules

Application of **dipole moment** data uses for the determination of the ionic or covalent character of heteronuclear diatomic molecules in chemistry.

Let us consider compound HBr having the observed dipole moment = μ_{obs} and the bond length l cm. If we consider HBr is a purely ionic compound the charge on H and Br = 4.8×10^{-10} esu. Thus the dipole moment for this ionic compound,

Therefore $\mu_{ionic} = e \times l$

$= (4.8 \times 10^{-10})\, l$ esu cm

Where l = bond length

Therefore the original dipole moment differs from the calculation. This data used to calculate the percentage of ionic character of molecules.

Dipole Moment of Monoatomic Molecules

The dipole moment application provides the structure and bond angle calculation of different molecules in chemistry. Thus for mono-atomic noble gases are non-polar because the charge of the constituent atom is distributed symmetrically.

Polarity of the Diatomic Molecules

Polarity homonuclear diatomic molecules like nitrogen, oxygen, and chlorine are zero because of the symmetrical charge distributions.

Hydrogen bromide and hydrogen iodide have non zero values of dipole moment. This indicates the unsymmetrical charge distribution between two bonding atoms.

$$H^{+} — I^{-}$$

Due to the difference in electronegativity of the constituent atoms in heteronuclear diatomic molecules always polar. Thus the electron pair is not equally shared and shifted to the more electronegative atom.

HCl	1.03 D
HBr	0.79 D
HI	0.38 D
HF	2.00 D

Polarity of Carbon Monoxide

The electronegativity difference between carbon and oxygen in CO is very large but the polarity of carbon monoxide very low. This suggested that the electron charge density in the oxygen atom somehow back-donated to the carbon atom. Thus CO formed a coordinate covalent bond directing towards carbon atom.

Dipole Moment of the Water Molecule

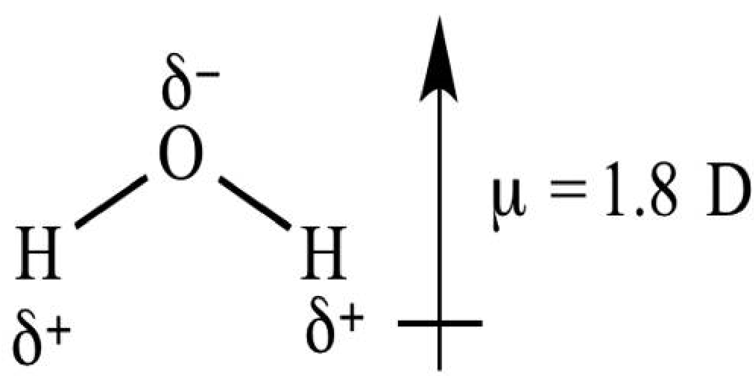
Due to the non-linear structure of the water molecule, we can calculate the net dipole moment from the bond moment, which ≠ 0.

If the dipole moment of water

μ = 1.84 D and

bond moment = 1.60 D.

Thus the contribution of non-bonding electrons towards the total μ included within the bond moment.

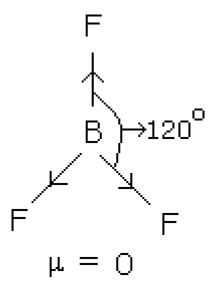


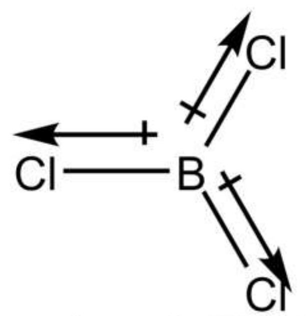
Polarity of Polyatomic Molecules

Boron trifluoride (BF_3)

Boron trichloride, boron trifluoride are the tetratomic compound having dipole moment zero, indicating that they have regular planar structure.

Their halogen atoms are on a plane at the corner of the equilateral triangle and boron atom at the intersection of the molecules. Thus the μ of the above molecules is zero.



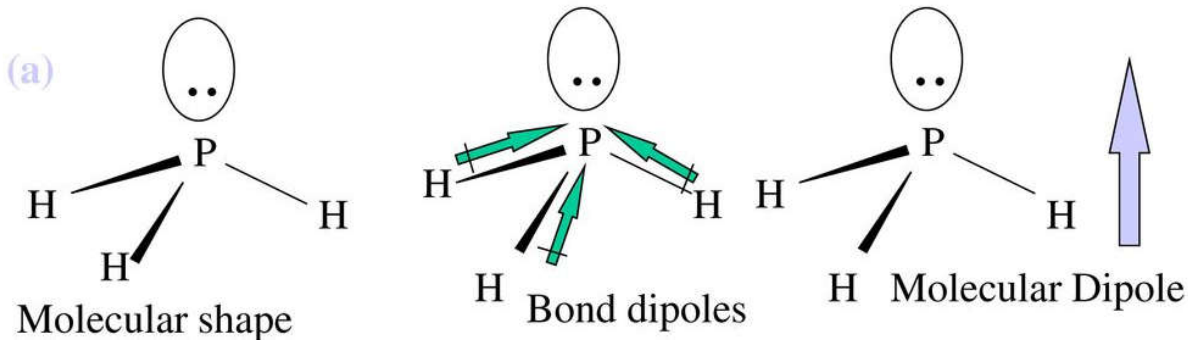


Ammonia and Phosphine

Other types of the molecule such as ammonia and phosphine are polar, where $\mu \neq 0$ indicated that the molecule has a pyramidal structure.

Hence three hydrogen atoms on a plane and nitrogen atom at the apex of the pyramid in ammonia and phosphine.

But NF_3 shows a very small bond moment although there is a great difference of electronegativity between nitrogen and fluorine atoms and similar structure of NH_3.



Thus this low value of μ in NF_3 explained by the fact that the resultant bond moment of the three nitrogen – fluorine bonds are acting in the opposite direction to that of the lone pair placed at the nitrogen-atom.

But in NH_3, the resultant bond moment is acting in the same direction as that of the lone pair electrons.

Dipole Moment Pent atomic Molecule

Methane, carbon tetrachloride, platinum chloride are examples of Penta-atomic molecules having zero dipole moment.

This suggests that the molecules either regular tetrahedral or square planer structure. But polar molecules of this type have pyramidal structures.

Dipole Moment of Methane Molecule

For calculating bond polarity, let us discuss the structure of methane that has regular tetrahedral structure and the angle of each H-C-H = 109°28. Therefore the application group moment of methane provides the arrangement of the bonds. Where the difference of the electronegativity of the constituent atoms forming the bonds in the group.

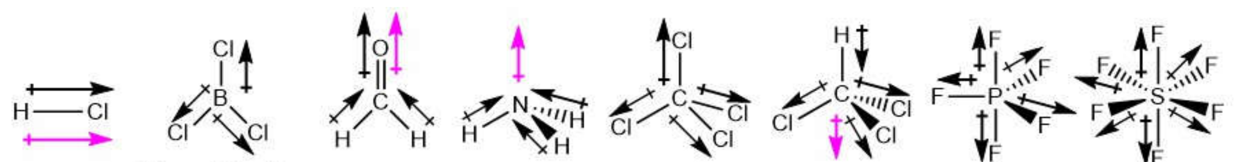
But it can be shown that the group moment of methyl group identical to the bond moment of a carbon hydrogen bond.

Therefore two bond moments cancel each other and use for calculation of dipole moment of methane molecules.

Dipole Moment of CH_3Cl and $CHCl_3$

A similar calculation is done for μ of C_2H_4, C_3H_7, C_4H_9, etc in organic chemistry. Thus the group moment equal to the μ_{CH} or carbon-hydrogen.

But the application of dipole moment gives identical and homologous alcohol and saturated hydrocarbon in chemistry



Net dipole	No net dipole	Net dipole	Net dipole	No net dipole	Net dipole	No net dipole	No net dipole
HCl	BCl_3	CH_2O	NH_3	CCl_4	$CHCl_3$	PF_5	SF_6