Hello students we are going to see a module from;

Program: Bachelor's of Science (Third year)
Subject: Chemistry
Semester: V
Paper code: CHD 105
Paper title: Properties and Processes of Molecular Chemistry
Unit: 1 Electrical properties
Module no: 02
Module name: Determination of dipole moment and its applications

The **outlines** of this module are as follows;

1. Debye Equation
2. Determination of dipole moment There are of two types of methods for determination of dipole moment, Vapor temperature method and Refraction method
3. Applications of dipole moment

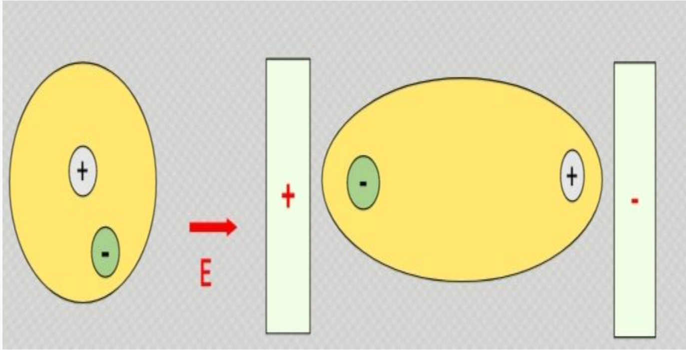
Th **learning outcomes** of this module are,

1. You will be able to recall the term polarizability
2. You will be able to implement or how to use the debye equation to determine dipole moment
3. You will also be able to explain what is vapor temperature method and refraction method and how to use these two methods to find out dipole moment
4. You will also be able to generate various applications of dipole moment

You will be familiar with the module 1 of this unit.

An atom will be having a centrally charged ion that is positively charged proton and there will be negatively charged electrons around this proton. So when an electric field is applied, there will be distortion or polarization taking place. This is **electrical distortion.**

Due to the electric field, there will be polarization taking place, wherein there will be distortion of the two types of ions.The negative ion (electrons) travels towards the positive plate and the positive ion (protons) travels towards the negative plate. This is **polarizability.**



The induced dipole moment will be directly proportional to electric field strength. Higher the electric field strength, more will be the dipole moment induced.

(Induced dipole moment) $\mu_i \propto E$ (Electric field strength)

$$\alpha = \frac{\mu_i}{E}$$

α is a polarizability constant which can be calculated by using the above equation if induced dipole moment and electric field strength is known.

The total molar polarization (P_M) is the sum of the two types of polarization: 1) induced polarization and 2) orientation polarization.

$$\mathbf{P_M = P_i + P_o}$$

Now consider the **Debye equation** which has been derived by considering the theory of orientation polarization.

$$\mathbf{P_M = \frac{4\pi N}{3} \cdot \alpha + \frac{4\pi N \mu^2}{9kT}}$$

where $P_i = \mathbf{\frac{4\pi N}{3} \cdot \alpha}$ and $P_o = \mathbf{\frac{4\pi N \mu^2}{9kT}}$

Here, $\pi = 3.14$
N is Avagadro's number= 6.02×10^{23} per mole
α is polarizability
μ is dipole moment
K is boltzmann constant = 1.38×10^{-16} energy per kelvin
T is temperature

Determination of Dipole moment:

Using this equation we are going to learn how to use it to determine the dipole moment.

1. **Vapor temperature method**

Consider the Debye equation where only T i.e; temperature is written separately as 1/T. Rest everything is the same.

Further this particular equation is being simplified so the first quantity before plus sign is taken as a and the second quantity after plus sign is taken as b except 1/T.

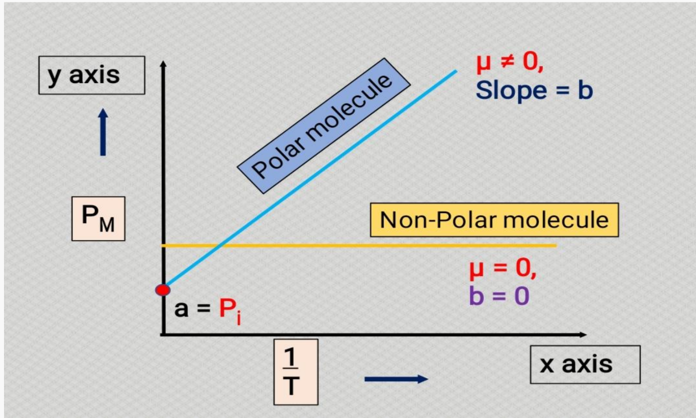
$$P_M = \frac{4\pi N}{3} \cdot \alpha + \frac{4\pi N \mu^2}{9k} \cdot \frac{1}{T}$$

Where $\mathbf{a} = \frac{4\pi N}{3} \cdot \alpha$ and $\mathbf{b} = \frac{4\pi N \mu^2}{9k}$

Thus, $$P_M = \mathbf{a} + \mathbf{b} \cdot \frac{1}{T}$$

This equation looks familiar to a straight line equation **y = mx + c**
Thus y axis is P_M, x axis is 1/T, c is the intercept = a = P_i and m is the slope = b.

Hence with respect to this graph is plotted.



Consider a non-polar molecule for which the graph will be straight line and μ will be equal to zero and the slope will also be equal to zero

Consider a polar molecule for which the μ will not be equal to zero and slope will be equal to b and the intercept will be equal to a which is P_i . From this slope i.e; b can be calculated.

We know that **b** = $\frac{4 \pi N \mu^2}{9k}$

Using this formula we can calculate dipole moment (μ). So we have to take μ on one side by rearranging the formula.

$$\mu = \frac{\sqrt{9k}}{\sqrt{4\pi N}} \cdot \sqrt{b}$$

Now by substituting the values of K, π and N the equation will become as follows;

$$\mu = 0.0128 \sqrt{\text{Slope}} \quad \text{Debye}$$

Further the value of dipole moment can be calculated by substituting the value of slope.

Another way is that we can calculate $(P_M)_1$ and $(P_M)_2$ at two different temperatures T_1 and T_2 respectively.

$$(P_M)_1 = a + \frac{b}{T_1} \quad \text{and} \quad (P_M)_2 = a + \frac{b}{T_2}$$

These two equations can be subtracted from one another and you will get,

$$(P_M)_1 - (P_M)_2 = b \ (1/T_1 - 1/T_2)$$

Now we need to rearrange the equation by keeping the value of b on one side.

$$b = [\,(P_M)_1 - (P_M)_2\,] \ \frac{(T_1 T_2)}{(T_2 - T_1)}$$

If we know the value of b from the above equation, then we can further use the value of b to find out the value of dipole moment.

2. **Refraction method.**

In this method the measurement is done by considering dielectric constant in terms of refractive index. This method can be used only at one temperature.

Here also the Debye equation is being considered.

$$P_M = P_i + \frac{4 \pi N \mu^2}{9kT}$$

$$\mu = \frac{\sqrt{(9k)}}{\sqrt{4\pi N}} \cdot \sqrt{(P_M - P_i)} \cdot \sqrt{T}$$

Now by substituting the values of K, π and N the equation will become as follows;

$$\mu = 0.0128 \sqrt{(P_M - P_i)} . \sqrt{T}$$

Where $P_i = \frac{4 \pi N}{3} . \alpha$ can be calculated if α value is known.

Now to determine P_i, let us consider **Clausius-Mossotti equation**

$$P_M = \frac{\varepsilon - 1}{\varepsilon + 2} . \frac{M}{\rho}$$

This equation gives a relationship between dielectric constant and total polarization

Consider Maxwell equation,

$$\varepsilon = n^2$$

Where ε is dielectric constant, M is Molecular weight, ρ is density and n is refractive index

Refractive index is measured with visible light that is at a lower wavelength but actually dielectric constant is measured at the higher wavelength that is why there was a need for some correction factor. The following formula is used to measure refractive index at a higher wavelength.

$$n = n_\lambda + \frac{a}{\lambda^2}$$

Where n_λ is refractive index for long wavelength (λ), a is a constant

This corrected value of n can be substituted in above Clausius-Mossotti equation to determine total molar polarisation as follows,

$$P_M = \frac{n^2 - 1}{n^2 + 2} . \frac{M}{\rho}$$

Further, the value of dipole moment can be calculated once the value of P_M is known.

Applications of dipole moment:

1.To determine percentage ionic character (%P):

This shows us to how much extent the bond is either ionic or covalent.

For example consider HCl, it has calculated dipole moment as 6.14 D and observed dipole moment as 1.03 D

The formula used is as follows,

$$P = \frac{\mu_{obs}}{\mu_{cal}} \times 100$$

$$P = \frac{1.03}{6.14} \times 100$$

Those values are substituted and then the percent is obtained as 17 % ionic. This means it is 83% covalent, indicating H-Cl is a highly covalent bond.

2. To determine the polarity of a bond:

The extent of polarity of a particular bond can be determined.

Consider HF, HCl, HBr and HI which are hydrogen halides.

HF = **1.92 D**
HCl = **1.04 D**
HBr = **0.83 D**
HI = **0.78 D**

Electronegativity**: F > Cl > Br > I**

From fluorine, chlorine, bromine and iodine the polarity of HX bond decreases. This is because fluorine is having more electronegativity as compared to remaining. Thus HF is having more dipole moment value as compared to HI.

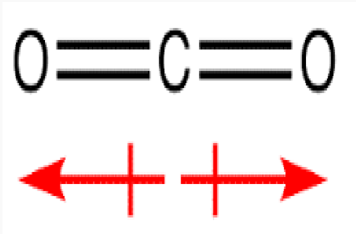
3. To determine the structure of the molecule:

Consider diatomic molecules of the type A_2 such as N_2, Cl_2, H_2; they will be having dipole moments equal to zero. This is because they are similar atoms and they will be having the same electronegativity. The difference of electronegativity will be zero and dipole moment will also be zero.

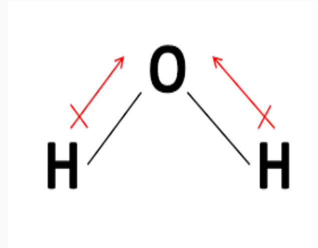
Consider diatomic molecule of the type AB such as HF, HCl, CO; they will be having some value of dipole moment

Consider triatomic molecules of the type AB_2 with linear structure such as CO_2, CS_2, $HgCl_2$. They will be having dipole moments equal to zero whereas now consider triatomic molecules of the types A_2B or AB_2 with triangular bent structure such as H_2O, H_2S, SO_2. They will be having some dipole moments.

Carbon dioxide has a linear structure and two dipole moments which are shown in the opposite direction, they will cancel each other and that is why the dipole moment of carbon dioxide will be zero whereas incase of water it is a triangular bent structure and the overall dipole moment is going upwards and hence it will be having some dipole moment.



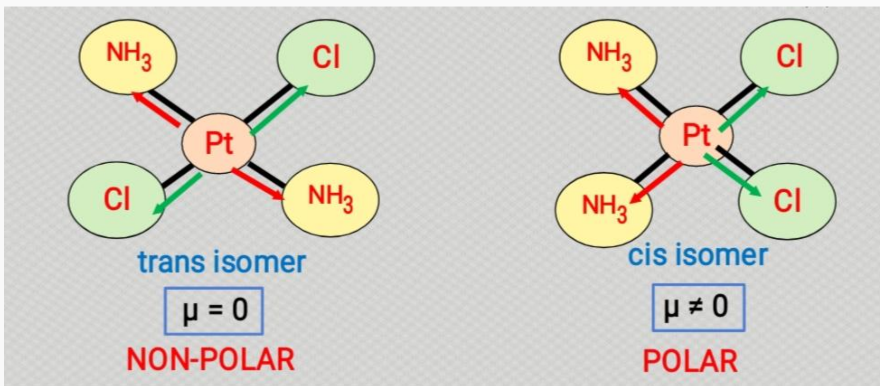
Linear structure



Triangular Bent structure

4. To distinguish between cis and trans isomers:

For Example; consider square planar complex of dichloro diammine platinum



The first structure is a trans isomer and the second structure is a cis isomer.

Considering trans structure, there axis of symmetry in the structure, the dipole moment around Pt-Cl bonds will cancel each other and around Pt-NH_3 bonds also the dipole moment cancel each other. Thus the dipole moment of the trans isomer will be zero.

Now consider cis isomer, the two Pt-Cl bonds are not in a symmetry and the dipole moment around these two bonds will not cancel each other. Same way in case of Pt-NH_3 bonds also the dipole moment will not cancel each other. Thus the dipole moment will not be equal to zero.

Hence we can say that the trans isomer will be non-polar and the cis isomer will be polar.

With the use of this idea of dipole moment we can guess which molecule would be non-polar or polar molecule as we know that the non-polar molecule is having dipole moment equal to zero whereas polar molecule will always have some value of dipole moment.

At the end, you all can go through the glossary given which contains certain terms used in this module. Aso there are offline references and online references given.

Thank you students.