Moment of Inertia (I)

The moment of inertia of a molecule may be defined as the product of mass of each atom and the square of its distance from the rotational axis through the centre of mass of the molecule. Mathematically, it may be written as

$$I = \sum_i m_i r_i^2$$

The moment of inertia of a molecule may be resolved into rotational components about three mutually perpendicular directions through the centre of gravity. Thus, a molecule has three principal moments of inertia, usually designated as I_A (it is also written as $I_{\parallel}$), I_B and I_C (I_B and I_C are also written as $I_{\perp}$). The three principal moments of inertia may be taken as –

I_A for rotation about the bond axis

I_B for end-over-end rotation in the plane of the paper and

I_C for end-over-end rotation at right angles to the plane of the paper

Based on the values of I_A, I_B and I_C, molecules may be classified into several groups as –

(i) **Linear molecule**: In case of this type of molecules,

$$I_A = 0 \text{ while } I_B = I_C$$

Examples of this type of molecules are CO_2,HCl, OCS etc.

(ii) **Symmetric top molecule**: In case of this type of molecules, two moments of inertia are equal but the third one is different i.e.

$$I_B = I_C \neq I_A$$

Unlike linear molecules the values of I_A is not negligible in this case i.e. here

$$I_A \neq 0$$

This type of molecules can be further sub-divided into two categories –

(a) If $I_B = I_C > I_A$, then the molecule is called a **prolate symmetric top molecule**. eg. CH_3Cl

(b) If $I_B = I_C < I_A$, then the molecule is called an **oblate symmetric top molecule**. eg. BCl_3.

(iii) **Spherical top molecule:** In case of this type of molecules, all the three moments of inertia are equal i.e.

$$I_A = I_B = I_C$$

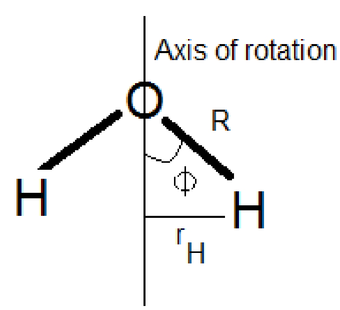
Examples of this type of molecules are CH_4, SF_6 etc.

(iv) **Asymmetric top molecule:** In case of this type of molecules, all the three moments of inertia are different i.e.

$$I_A \neq I_B \neq I_C$$

Examples of this type of molecules are H_2O, CH_2= CHCl etc.

Problem 1.10: Calculate the moment of inertia of a H_2O molecule around its two-fold axis. The HOH bond angle is 104.5^0 and the bond length is 95.7 pm. [**GU 2014**]



Solution:

Given,

Bond length, R = 95.7 pm = 95.7×10^{-12} m

Bond angle, $2\phi = 104.5^0$

Mass of H, $m_H = 1.67 \times 10^{-27}$ kg

As the O atom is immobile while the H-atoms circulate around it, so it makes no contribution to the moment of inertia for this mode of rotation. Thus, we have

$$I = m_H r_H^2 + m_H r_H^2$$

or, $$I = 2\, m_H r_H^2$$

Again from trigonometric ratios, we have,

$$r_H = R \sin \phi$$

Hence, $$I = 2\, m_H R^2 \sin^2 \phi$$

or, $$I = 2 \times 1.67 \times 10^{-27}\ \text{kg} \times (95.7 \times 10^{-12}\ \text{m})^2 \times \sin^2 52.25$$

or, $$I = 1.91 \times 10^{-47}\ \text{kg m}^2$$