ENGINEERING CHEMISTRY

Department of Science and Humanities

Class content:

- *Introduction to rotational spectroscopy*
- *Expression for rotational energy levels of a diatomic molecule*

Rotational spectroscopy

- A molecule undergoing rotation absorbs in the **microwave region**
- For a molecule to be rotationally active or microwave active the molecule has to possess a **permanent dipole moment**
- Rotations of a molecule having permanent dipole moment will cause changes in **electric dipoles** that will interact with the **electrical component** of the electromagnetic radiation

Module I- Molecular Spectroscopy

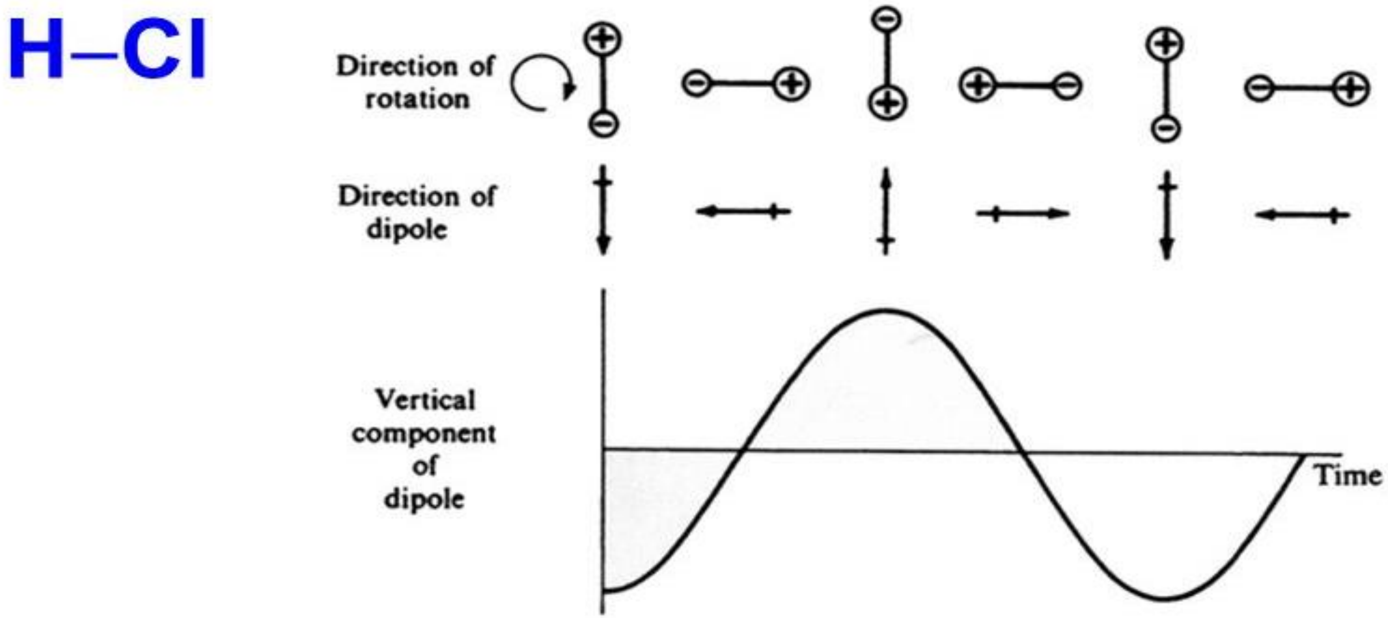


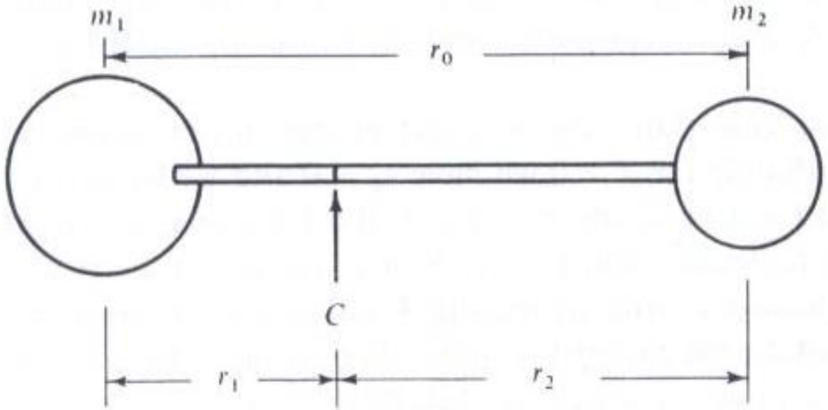
Fig. The rotation of a polar diatomic molecule, showing the fluctuation in the dipole moment measured in a particular direction

Source: Fundamentals of Molecular Spectroscopy: C. N. Banwell and Elaine M McCash, Fifth Edition, MCGRAW-HILL Education (India) Private Ltd.

- When the frequencies match, **resonance occurs** and the molecule absorbs energy and goes to the higher rotational levels and a **rotational spectrum** can be recorded
- Molecules such as **HCl and CO** show rotational spectra as they possess permanent dipole moment while **H_2, Cl_2 and CO_2** do not

Expressions for rotational energy levels for a diatomic molecule

- **Derivation of Moment of Inertia** for a heteronuclear diatomic molecule- **rigid rotor model**



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A rigid diatomic molecule with masses m_1 and m_2 joined by a thin rod of length $\mathbf{r_0 = r_1 + r_2}$ .The centre of mass is at C

Module I- Molecular Spectroscopy

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The molecule rotates end- over- end about a point C, the centre of gravity , this is defined by the moment, or balancing, equation:

$$m_1 r_1 = m_2 r_2$$

The **moment of inertia** about C is defined by

$$I = m_1 r_1^2 + m_2 r_2^2$$

$$I = m_2 r_2 r_1 + m_1 r_1 r_2$$

$$I = r_1 r_2 (m_1 + m_2)$$

Since $m_1 r_1 = m_2 r_2 = m_2 (r_o - r_1)$, $r_1 = \frac{m_2 r_o}{m_1 + m_2}$

Since $m_1 r_1 = m_2 r_2 = m_1 (r_o - r_2)$, $r_2 = \frac{m_1 r_o}{m_1 + m_2}$

Therefore $I = \frac{m_1 m_2}{m_1 + m_2} r_o^{\ 2} = \mu r_o^{\ 2}$

Where μ is the reduced mass given by $\mu = \frac{m_1 m_2}{m_1 + m_2}$

Rotational energy $E_r = \frac{1}{2} I\omega^2 = \frac{L^2}{2I}$; Since L=Iω

Solving the Schrodinger equation for a rigid rotor shows that angular momentum is quantised and is given by,

$$L = \frac{\sqrt{J(J+1)}}{2\pi} h$$

where J is the rotational quantum number.

The quantity J **, rotational quantum number**, which can take integral values from zero upwards; **J=0,1,2,3......**

Hence the rotational energy levels are quantised and given by the expression,

$$E_J = \frac{h^2}{8\pi^2 I} J(J+1) Joules$$

h= Planck's constant=6.626×10^{-34} Js and I is the moment of inertia

THANK YOU

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