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# Spectroscopy as a Tool to Elucidate the Structure of Compounds

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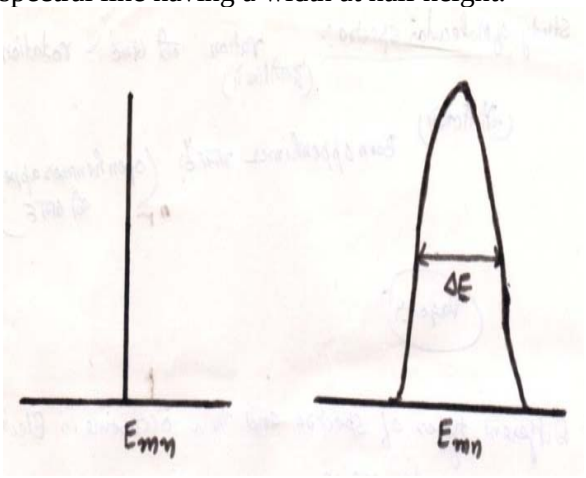
**Abstract**:-
In Modern Period spectroscopy is a powerful tool to determine the atomic and molecular structure. There are so many types of spectroscopic techniques have been occurs between the electromagnetic radiation and molecules under consideration. When a molecule absorbs the suitable radiation it shows the transition from lower energy level to higher energy level upon absorption molecule shows absorption spectrum on the other hand when molecule falls from higher energy level to lower energy level it shows emission spectrum. The molecular spectra are governed by the so called selection rules of Quantum Mechanics. Present topic related with the details of spectroscopic technique used for structure determination.

**Key Words**:-Spectroscopy, Spectrum, Quantum Mechanics, Radiation, Emission, Absorption.

**Introduction**:-Spectroscopy is the branch of science that deals with the transitions between electromagnetic radiation and molecules. When a molecule absorbs a suitable radiation this result in the transition between rotational and vibrational energy levels in addition to electronic transitions. According to Quantum Mechanics the ground state of a Molecule is that state in which molecule has lowest energy and the other states are called excite states. Depending upon the absorption and emission of radiations molecules shows absorption spectra or emission spectra respectively. The spectra of molecules are much more complicated than those of atoms. So molecular spectroscopy is of great importance now days, because the number of molecules is extremely large as compared with free atoms. The molecular spectrum is governed by the selection rules. These rules are obtained from the Quantum Theory of interaction of radiation with molecule.

The spectral transitions with obey a given selection rules are termed as allowed transition while those which violate a selection rule are termed as forbidden transitions. In general allowed transitions are stronger than the forbidden transitions.

When the spectrum of a molecule is analyzed the first thing to know is how sharp and how strong is the spectral line i.e. to know the width and intensity of a spectral transitions, these two quantities are common to all branches of spectroscopy. The fig(i) shows a sharp spectral line having no width while fig.(ii) shows a spectral line having a width at half height.




**Study of Molecular spectra**:- Molecular spectra arise from three types of energy changes such as molecular rotation, Molecular vibration and electronic transition. The total energy of a molecule, according to Born oppenhimer approximation is given as.

$$E=E_{tr}+E_{rot}+E_{vib}+E_{el}.$$

Where $E_{tr}$= translational energy $E_{rot}$ is rotational energy. $E_{vib}$= Vibrational energy and $E_{el}$ electronic energy.

The Translational energy does not quantize while all other energies get quantized.

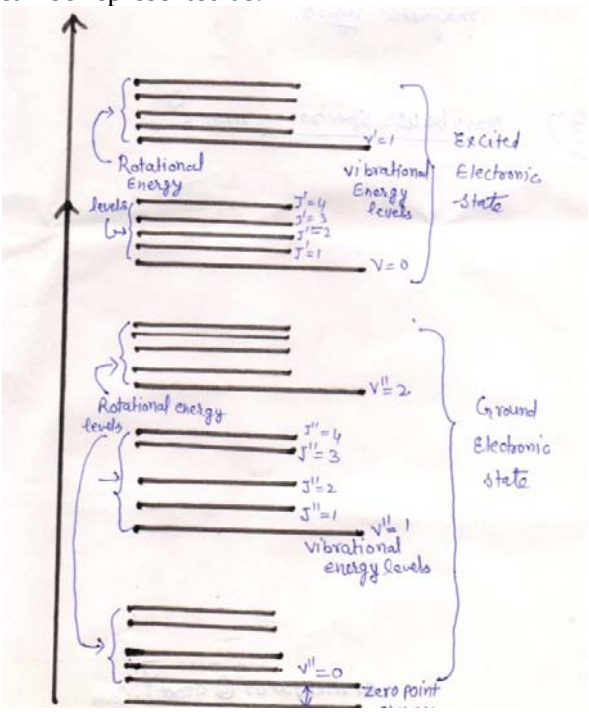
$$E_{el}>>E_{vib}>>E_{rot}>>E_{tr}.$$

Translational energy is negligibly very small so Born oppenhirner approximation can be written as.

$$E=E_{rot}+E_{vib}+E_{cl}$$

For a diatomic molecule these types of energy can be explained as Due to motion its centre of gravity change and molecule shows translational energy. Rotational energy of molecule due to rotation of molecule about an axis perpendicular to the inter nuclear axis and passes through the centre of gravity of the molecule. Vibrational energy of the molecule is due to its to and fro motion of the nuclei of the molecule in which centre of gravity of molecule does not change and the electronic energy of the molecule due to the transition of an electron from the ground state to and excited state by the absorption of suitable light radiation.

The diagrammatically energy levels of molecule can be represented as.




**Different types of spectra and their occurrence in Electromagnetic Mossbauer spectra:-**

1- Nuclear Magnetic Resonance or NMR spectroscopy shows the transitions of nuclear spin energy levels of a molecule in the external field. It occurs in the radio frequency region 5-10 MHZ.

2- ESR or EPR or electron spin Resonance spectroscopy- it shows the transition arises between the electron spin energy levels of a molecule in the external magnetic field. It occurs in the microwave region 2000-9600MHZ.

3- Moss baver Spectra:- In NMR spectrascopy absorption of how energy photons of frequency about to 60 MHZ are used while in the spectroscopy absorption of high energy Y-photon of frequency around $10^{13}$ MHZ are used.

4- Microwave of Rotational spectra:- when a molecule having permanent dipole moment absorbs radiation in the micro wave region, shows pure rotational spectra. 1-100$cm^{-1}$

5- Vibrational and vibrational Rotational spectra:- this type of spectra occurs in the Infra red region. Molecule having permanent dipole moment absorbs I.R radiations and shows vibrational rotational spectra. 500-400$cm^{-1}$

6- Raman spectra:- In this spectra scattering of the light is measured, these spectra occurs in visible region 12500-25000$cm^{-1}$

7- Electronic spectra:- The Electronic spectra of a molecule would be highly complex it occurs in visible regions 12500-25000$cm^{-1}$ and in UV regions 25000-70,000$cm^{-1}$

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