SUBJECT - CHEMISTRY
CLASS - B.Sc(Hons) PART-III
PAPER - V
TOPIC - Vibrational energy

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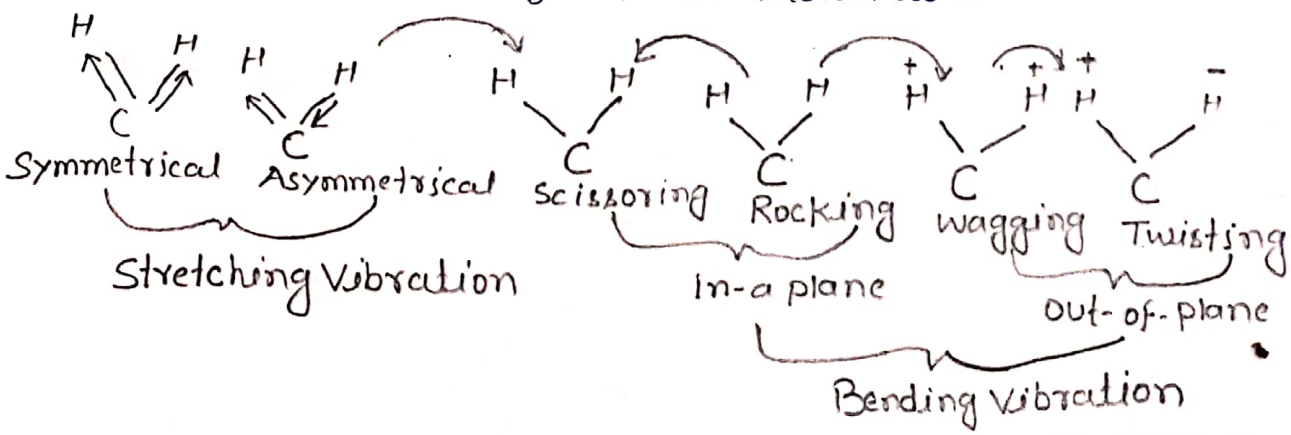
Vibrational energy: In a polyatomic molecule, atoms are taken as balls of varying masses and bonds as flexible spring of varying strengths. Thus balls and springs correspond to atoms and bonds in compounds respectively. If a ball is stretched and left, it undergoes stretching and bending vibrations. In stretching Vibrations, The distance between two atoms changes but atoms remain in the same bond axis without any change in bond angles, while in bending vibrations, positions of atoms change relative to original bond axes. In Symmetrical stretching, atoms move in the same direction but in asymmetrical stretching, one atom approaches while another moves away from the central atom. More energy is required to stretch a bond than that to bend. The energy required to stretch a bond increases with an increase in bond order and the masses of the bonded atoms Non-linear and linear molecules have $3n-6$ and $3n-5$ Vibrational degrees of freedom respectively where n is the number of atoms present in the molecule. The fundamental Vibrations of CH_2 group are shown as -



There are four types of bending vibrations → Scissoring, rocking, wagging and twisting. In Scissoring, two atoms approach opposite to each other while in rocking, atoms move in the same direction. In wagging, atoms move up and below the plane in unison while in twising, one atom moves up and another moves down the plane relative to the central atom. The vibrational energy is given by -

$$E_{vib} = \left(V + \frac{1}{2}\right) h\nu$$

where V = Vibrational quantum number and ν = frequency of radiation.

Electronic energy: The electronic energy in a molecule arises due to the various electronic arrangements. An increase in Kinetic energy and potential energy of its electrons increase the electronic energy of the molecule. The electronic energy is given by

$$E_{ele} = 2.18 \times 10^{-18} \times \frac{Z^2}{n^2} \text{ Joules}$$

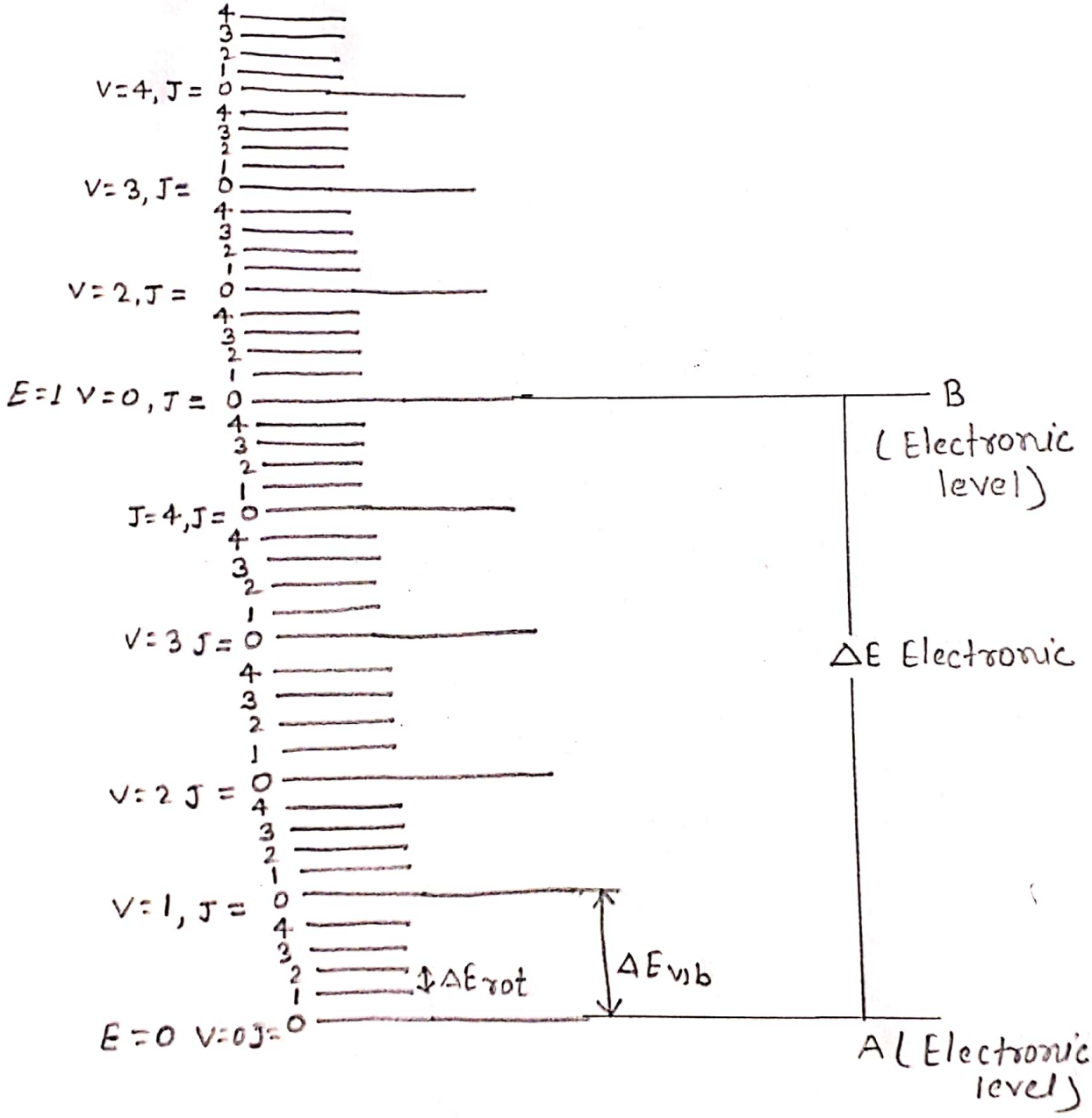
where terms have usual meanings. The order of energy gap between two Successive molecular levels is given as -

Electronic
Vibrational
Rotational
Translational

↓ Decreases

The absorption or emission of radiation by molecule results in the transition of electron from one to another energy levels. All molecular energies are quantised. So, the molecule can exist only in distinct states which correspond to discrete energy values. Therefore, there are few widely separated electronic energy levels.

Each electronic level has many more closely spaced vibrational levels and each vibrational level has a series of very closely spaced rotational levels. Hence any single electronic transition in a molecule has a multitude of lines i.e band.



The absorption of light by a compound occurs only when it is impinged by supplied radiation of exact amount of energy. Each state is characterised by one or more quantum numbers and energy-gap (ΔE) is given by

$$\Delta E = h\bar{\nu}c = \frac{hc}{\lambda}$$