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Infrared Spectroscopy

* It used for detection of functional groups
* Infrared Spectroscopy deals with the recording of the absorption of radiation in the infrared region of electromagnetic radiation
* Infrared radiations does not have sufficient amount of energy to cause excitation of electrons, however it causes atoms and groups of atoms of organic compounds to vibrate faster about the covalent bonds which connect them.

The vibrations are quantised and as they occur the compound absorbs infrared energy in particular regions of the spectrum.

The position of infrared absorption band is specified in frequency units by its wavenumber $\bar{\nu}$ measured in reciprocal cm (cm^{-1}) or by its wavelength λ, measured in micrometers

The ordinary infrared region (4000 - 667 cm^{-1}) is of greatest practical use to organic Chemist.

* Infrared technique provides a spectrum containing a large number of absorption bands from which a wealth of information can be derived about structure of Organic Compound. Different bands observed in an IR Spectrum corresponds to various functional groups and bonds present in the molecule. Thus IR Spectroscopy is most widely used for the detection of functional groups & identification of Organic Compounds.

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The absorption of infrared radiation cause an excitation of molecule from a lower to the higher vibrational level. Each vibrational level is associated with a number of closely spaced rotational levels. Thus IR spectra often called as Vibrational-rotational spectra.

(IR absorption spectra originate from transitions in rotational & vibrational energy levels in a molecule.

* All the bonds in a molecule are not capable of absorbing infrared energy but only those bonds which are accompanied by a change in dipole moment will absorp in the IR region. Such transitions are IR active transitions - These are responsible for absorption of energy in IR regions

(In general, molecular vibrations which lead to change in dople moment of the molecule will give rise to absorption bands in the infrared. Otherwise they are said to be IR inactive and will show no absorption)

* Symmetrical alkenes and alkynes are IR inactive because no change in dipole moment.
* vibrational transitions of C=O, N-H, O-H bands are accompanied by change in dipole moment and thus absorb strongly in IR region.
* A large change in dipole moment will usually give rise to strong absorption.

* When a molecule absorbs IR radiation below 100 cm^{-1} the absorbed radiation causes transitions in its rotational energy levels. Since these energy levels are quantized, a molecular rotational spectrum consists of discrete lines. When a molecule absorbs IR radiation in the range 100 - 10000 cm^{-1} the absorbed radiation causes transitions in its vibrational energy levels. These energy levels are also quantized, but vibrational spectra appear as bands rather than discrete lines. The energy differences between various rotational energy levels of a molecule are far less than that between its vibrational energy levels. Thus a single transition in vibrational energy levels is accompanied by a large number of transitions in

rotational energy levels and so the vibrational spectra appear as vibrational-rotational bands instead of discrete lines.

In IR Spectroscopy the absorbed energy brings about predominant Change in the vib energy which depends upon

(1) Masses of the atoms present in the molecule
(2) Strength of bonds
(3) The arrangements of atoms within molecule

Molecular Vibrations:-

Various atoms in a molecule may be regarded as balls of different masses and the Covalent bonds between them as weightless tiny Springs holding both balls together. Atoms in a molecule are not still but they vibrate.

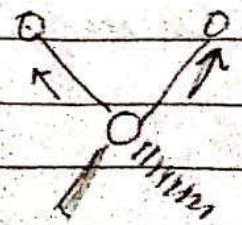
Two types of fundamental Vibrations

(a) Stretching Vibrations
(b) Bending Vibrations

(a) Stretching Vibrations

In these Vibrations, the distance between two atom increases or decreases, but the atoms remain on the same bond axis. Stretching Vibrations are of two types.

(1) Symmetrical Stretching



In this mode of Vibration, the movement of atoms with respect to the Common atom is simultaneously in the same direction along the same bond axis.

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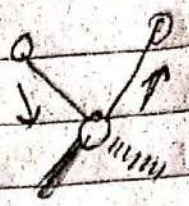
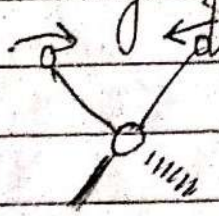
(2) Asymmetrical Stretching:
In this vibration, one atom approaches the common atom while other departs from it.



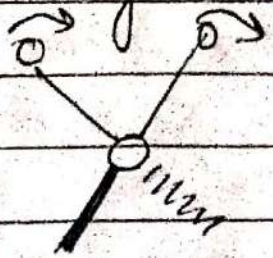
(B) Bending Vibrations
In such vibrations, the positions of the atoms change with respect to their original bond axis. Bending vibrations are of four types:-

(a) Scissoring:-
In this mode of vibration, the movement of atoms is in the opposite direction with change in their bond axis as well as in the bond angle they form with the central atom.



(b) Rocking:-
In this vibration, the movement of atoms takes place in the same direction with change in their bond axis

Scissoring & Rocking are in-plane bendings

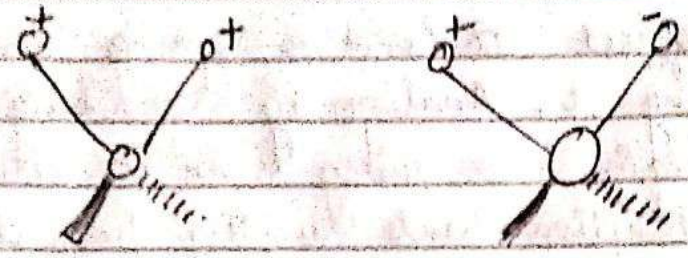


(c) Wagging:-

In this vibration, two atoms simultaneously move above and below the plane with respect to the Common atom.

(d) Twisting:-

In this mode of vibration, one of the atom moves up and the other moves down the plane with respect to the Common atom.



Wagging Twisting

* Infrared radiation is absorbed when oscillating dipole moment, due to a molecular vibration, interacts with the oscillating electric field of the infrared beam. This interaction occurs and hence an absorption band appears only when a molecular vibration produces a change in dipole moment of the molecule. Otherwise, the vibration is said to be Infrared inactive and it will show no absorption band in the infrared spectrum. Usually, larger the change in dipole moment, the higher is intensity of absorption. It is not necessary for a molecule to have a permanent dipole moment for IR absorption.

* Various stretching and bending vibrations of a bond have a definite and quantized frequency of their own. When infrared radiation of the same frequency is incident on the molecule, there is absorption of

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energy resulting in the increase of the amplitude of that particular absorption; now the molecule is in the excited state. Such an absorption gives rise to peak in the IR Spectrum. From the excited state the molecule returns to the ground state by release of extra energy through rotational, collision and translational processes resulting in the increase of temperature of the sample under investigation.

* lesser energy is required to bend a spring than that required for stretching it. Analogously, bending Vibrations of a bond require lesser energy than its stretching Vibrations. Thus, the absorption bands resulting from stretching appear a higher wave number than those resulting from Bending Vibrations of same bond. Stretching vibrations usually cause peaks of high intensity