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Q3 Q4 Unit V — II (1)

Qs Write a note on Infra red Spectroscopy?

OR

Qs Dicuss Vibrational, Rotational spectroscopy?

OR

Qs Give an Introduction of I.R. spectroscopy?

Ans When the molecule or a compound absorbs Infra red radiations from wavelength 25um – 2.5 um then vibrational level or vibrational energy of the molecule changes also there is simultaneo change of rotational level of a molecule. further from the emitted radiations we (from the molecule) we obtain a spectrum called as Infra red spectrum or Vibrational-rotational spectrum.

Conditions for I.R spectrum :—

All the molecules did not give out I.R spectrum only those molecule interact with I.R radiations & give I.R spectrum which show change in there dipole moment during a vibration.

Thus homonuc diatomic molecules like H_2, O_2, N_2, Cl_2 did not show change in dipole moment during there vibration show they not give out I.R spectrum.

As we know that when I.R radiations are absorbed by a molecule then rotational and Vibrational level or energy of a molecule changes.

Now the various Vibrational level ($v=0, v=1$, etc) of a molecule have some Vibrational energies values, and the vibrational energies of different levels can be calculated by using Schrodinger equation.

Energy associated with any vibrational level is given by:

$$E_{vib} = h\nu_0 \left(v + \tfrac{1}{2}\right) \text{ joules}$$

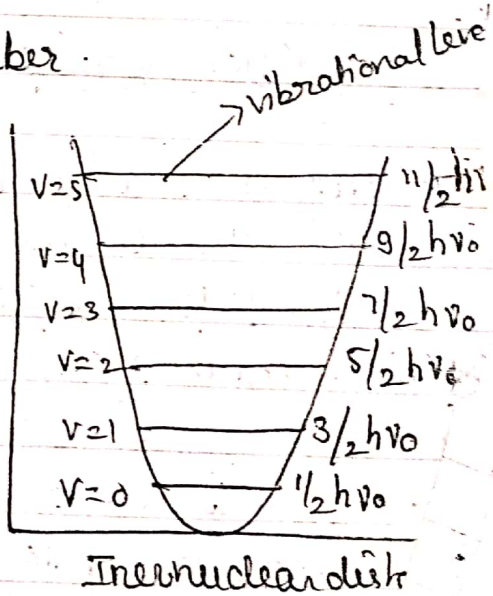
v = vibrational quantum number.
ν_0 = fundamental frequency.

for $v = 0$

$$E_{vib} = \tfrac{1}{2} h\nu_0$$

$v = 1$

$$E_{vib} = \tfrac{3}{2} h\nu_0$$



So we can see that in ground vibrational ~~state or~~ level also molecule has the vibral energy $= \tfrac{1}{2} h\nu_0$ it is called Zero point Energy, it r

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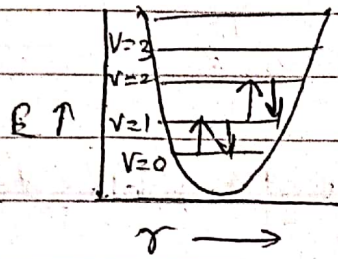
molecule always vibrate and is never at rest

MVI

Selection Rule for harmonic vibrational transition :—

$$\Delta V = \pm 1$$

it means increase or ~~deck~~ decrease in vibrational quantum number is by one unit only.



Calculation of Number of modes of Vibration of a Molecule

For linear molecule

We calculate it by formula $(3n-5)$

For non linear molecule

We calculate it by formula $(3n-6)$

example → CH_4 $(3\times5-6) = 9$

C_2H_5 $(3\times7-6) = 18$

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Frequency of Simple harmonic motion

$$\boxed{\nu = \frac{1}{2\pi}\sqrt{k/\mu}\ s^{-1}}$$

k = force constant

μ = reduced mass

Dividing by 'c' (velocity)

$$\bar{\nu} = \frac{\nu}{c} = \frac{1}{2\pi c}\sqrt{\frac{k}{\mu}}\ cm^{-1}$$

Qs. What are the various Vibrational modes of a molecule?

OR

Qs Discuss various types of vibrations of a molecule?

Ans The 2 kinds of fundamental vibrations in a molecule are

1) Streching Vibrations 2) Bending Vibrations

1) Streching Vibrations :- In this type of vibrations, the distance beween the 2 atoms increases and decreases, but atoms remain in the same bond axis

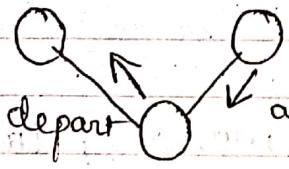
Types of Streching Vibrations: (stretching change in Bond length)

a) Symmetric streching :-

In this type the movement of the atoms, with respect to a particular atom in a molecule is in the same direction.

Asymmetric stretch.

b) In these vibrations the movement of the atoms, with respect to a particular atom in a molecule is not in the same direction, that is one atom approaches the central atom while the other atom departs from it

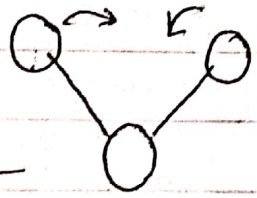


Bending Vibrations :- (change in Bond angle)

In this type of Vibration position of atom's changes with respect to the original bond axis

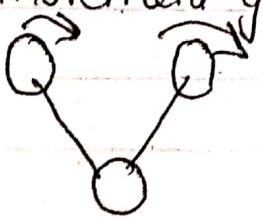
Types of Bending Vibration's :-

a) Scissoring :- In this vibration 2 atoms approach each other



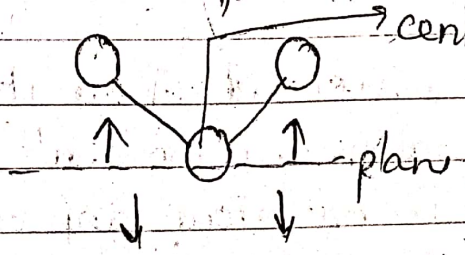
b) Rocking :-

In this type of vibration, movement of the atoms take place in same direction



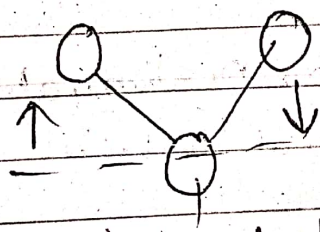
c) Wagging.

In this type of Vibration, 2 atoms move up & below the plane with respect to the central atom.



d) Twisting.

In this type, one atom moves up the plane and other moves down the plane with respect to the central atom.



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Discuss

Q: Application of I.R Spectroscopy:— Date (7)

Ans

1) Determination of Purity :—

Infrared spectroscopy is helpful in conforming the purity of compound, Whenever a compound contains impurity then in its IR spectrum extra bands or peaks are seen and also the sharpness of the individual band or peak decreases.

So Impurities are easily detected out in a compound, when that impurity gives strong bands (peak) in IR spectrum, which are absent in the IR spectra of the pure compound.

So IR spectra of impure sample will show some extra absorbtion bands, By comparing it with IR spectra of pure compound presence of impurity can be detected.

Example :— Hydrocarbon pure form do not contain carbonyl group, but if small quantity of ketone is present in hydrocarbon then we get a peak or Band at 1720 cm^{-1}, which is due to carbonyl group

Date 10

2> Determination of Symmetry of a Molecule :-

By the help of IR spectroscopy we can detect or deduce the shape or symmetry of a molecule

Example → NO_2 (Nitrogendioxide).

If NO_2 is linear then it IR spectrum should contain 2 active Bands (peaks)

If NO_2 is Bent shaped then its IR spectrum should contain 3 active Bands (peak) at 750 cm^{-1}, 1323 cm^{-1} & 1616 cm^{-1}

And it was seen that IR spectrum of NO_2 molecule contained 3 peaks at 750, 1323 & 1616 cm^{-1} which show it is Bent & not linear molecule

3> Presence of water in a sample :-

With the help of IR spectroscopy we can detect (find) the presence of water in a sample, if water is present then 3 bands are present one at 3600 – 3200 cm^{-1}

Second band (peak) at — 1650 cm^{-1}

Third " " → 600 cm^{-1}

Date (9)

If water is coordinated to a metal ion then additional band in 850-650 cm^{-1} is region is observed

Example :- With the help of IR spectroscopy water molecule was detected in clathrate compound.

$Ni(CN)_2 \cdot NH_3 \cdot C_6H_6 \cdot xH_2O$

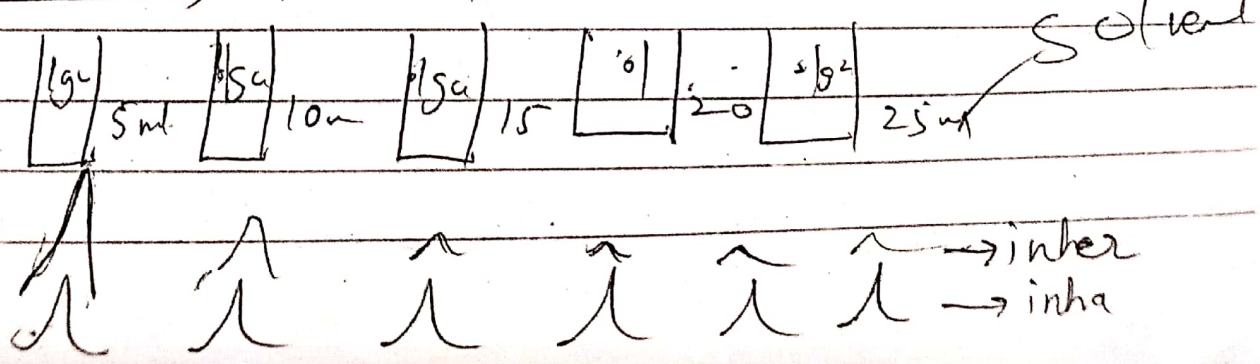
4) Presence of or Detection of inter and intra-molecular hydrogen bonding in a compound

The presence of Inter and intra hydrogen bonding in a compound can be known by help of IR spectroscopy. For this IR spectrum of a compound at different dilution is taken out ~~as the di~~

If intermolecular hydrogen Bonding is present in a compound then in the (different dilution) spectrum of different dilution of a compound the bands or peaks diminishes,

An when intramolecular hydrogen bonding is present then in the IR spectrum of different dilution / compound the bands remains unchanged.

increase dilution



5) Distinguishing Between the Geometrical isomers of a compound (means out of 2 Geometrical isomers of a compound which one is trans & cis can be found out)

By the help of IR spectroscopy we can distinguish geometrical isomers by there IR spectrum.

Example → 2 isomers of bipyridyl cobalt chloride was prepared, which had different colories, violet & pink.,

By IR spectrum it was found that violet coumpound is a trans isomer & pink form is cis form

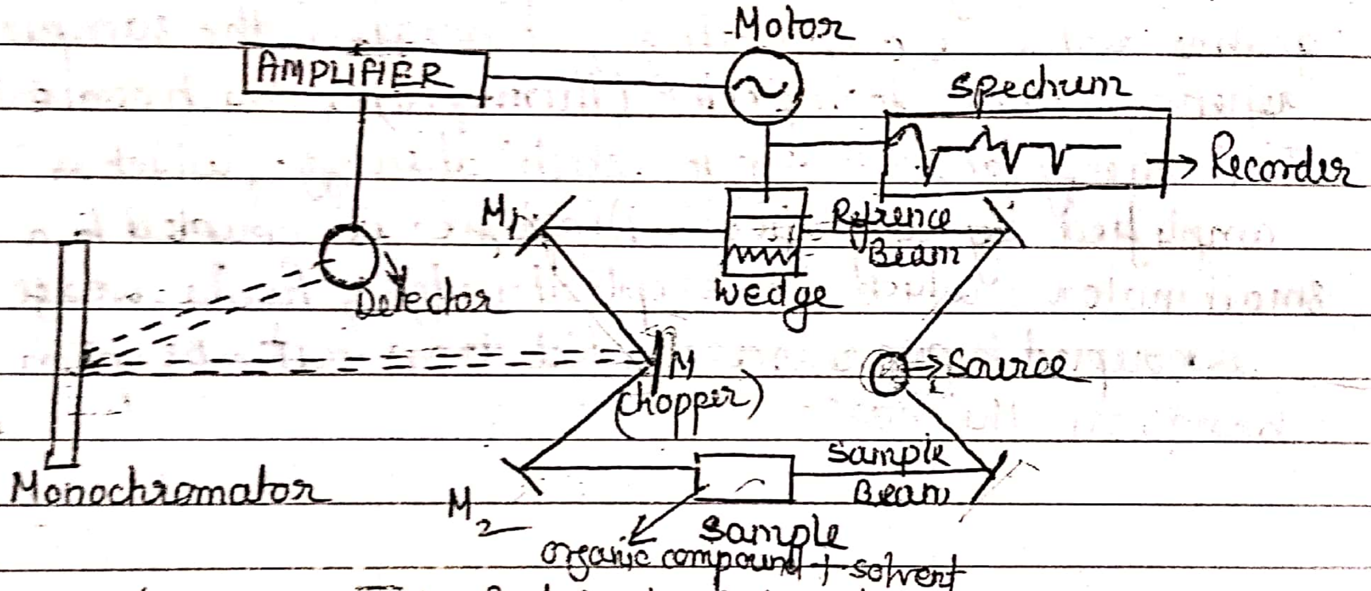
6) IR spectra is useful for quantitative analysis of a mixture of compounds, in pollution detection, in milk analysis etc.

Bipy CoCl

Date ....

Qs Discuss I.R Spechophotometre or I.R spechophotomet

By help of it we obtain IR spectrum of a compound or molecule



Infra Red Spechophotometer

Light from the source split into 2 beams, One beam pass through sample, it is called sample beam. The other beam is called Refrence beam.

When one of the beam passes through sample, then it becomes less intense due to absorption by sample, So there is difference in intensity of beam obtained or emitted from sample and refrence beam.

The two beams, i.e from Sample Beam & refrence Beam are made to fall on segmented Mirror M (chopper) with the help of 2 mirrors M_1 & M_2, further chopper reflect the sample and the refrence beam on to monochromator grating. Then grating or monochromator grating as it is slowly rotating, it transfers the sample & refrence beam to detector (Thermopile), which convert I.R energy or radiation to electrical energy, which is amplified by amplifier. Amplifier is coupled to a small motor which drives optical wedge, further wedge is coupled to pen recorder which draw out absorption bands on the chart.