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TITLE

Date : Mo Tu We Th Fr Sa Su

* Normal modes of vibration :-

Let us consider a molecule containg N - atoms. The position of each atom contains three co-ordinates (x, y, z). Thus the total no. of co-ordinates value is 3N. Thus ~~we can say~~ a molecules has 3N degree of freedom. where N is the no. of atoms in the molecule.

This 3N molecules contains translational, vibration & rotational degree of freedom.

$\therefore$ 3N = Translational + vibrational + Rotational. —— (1)

Since, all the molecule has three co-ordinate in space.

$\therefore$ molecules has always 3 translational degree of freedom.

There are 2 rotational degree of freedom for linear molecules.

and there are 3 rotational degree of freedom for non-linear molecule.

$\therefore$ from eqn —(1)

$$3N = 3 + \text{vibrational} + 2$$

or vibrational degree of freedom

$= 3N - 3 - 2$ (for linear molecules)

$= 3N - 5$

and

$$3N = 3 + \text{vibrational} + 3$$

⇒ vibrational degree of freedom $= 3N-6$
(Non-linear molecules)

eg —

(b) CO_2 molecule –

O = C = O   linear

vibrational degree of freedom $= 3N-5$
$= 3\times3-5$
$= 4.$

(a) symmetric stretching

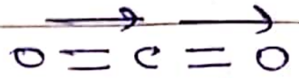
O = C = O   O == C == O
$\mu = 0.$

or

O = C = O   O = C = O
$\mu = 0.$

IR inactive

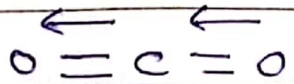
(b) Assymmetric stretching -



$O=C\text{===}O$

$\mu \neq 0.$

or

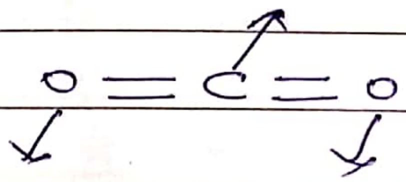


$O\text{---}C=O$

$\mu \neq 0.$

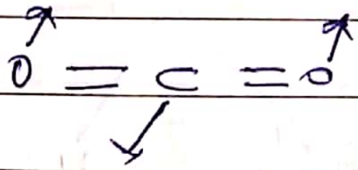
IR active.

(c) Bending -



$\mu \neq 0$

or

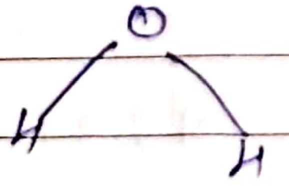


$\mu \neq 0$

IR. active.

There are three I.R active modes of vibration in case of CO_2 molecule. Out of which ~~also~~ two Assymmetric stretching and bending modes give two bands in IR spectra.

H_2O - molecule -



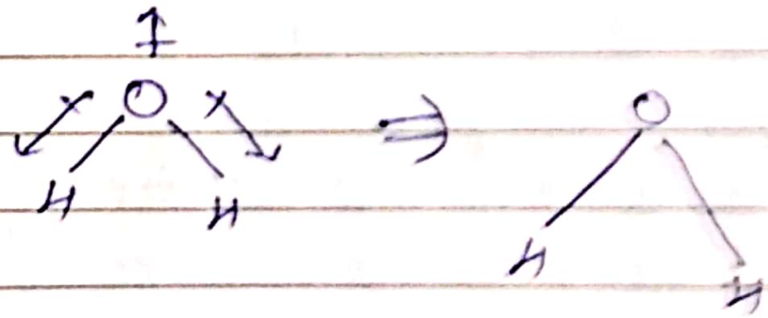
Non linear

$= 3N - 6$

$= 3 \times 3 - 6$

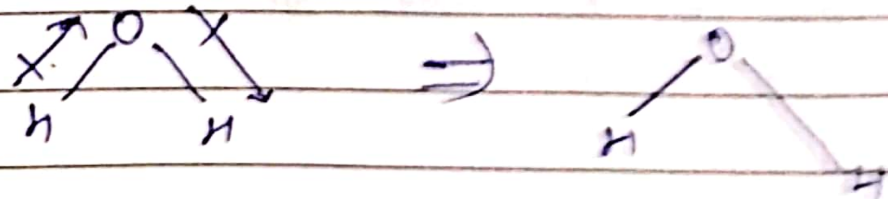
$= 3.$

ⓐ Symmetric streching -



$\mu \neq 0.$

ⓑ Asymmetric streching —



or

$\mu \neq 0.$

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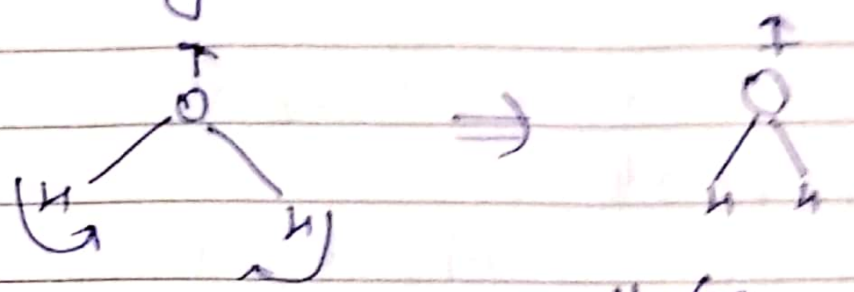
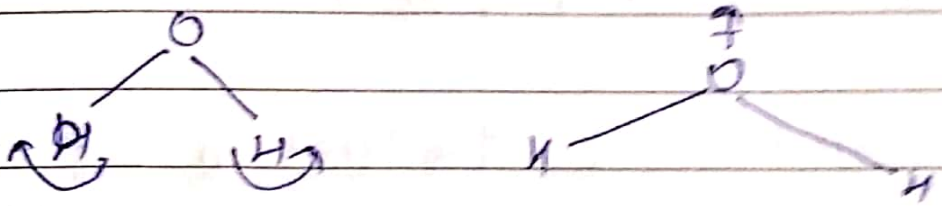
(c) Bending —



$\mu \neq 0$.

or



$\mu \neq 0$.

There are three vibrational degree of freedom in case of H_2O molecule. All of these are IR active and thus gives three bands in IR spectra.

Q. Calculate the no. of fundamental vibration in case of CH_4, C_6H_6, C_2H_4, C_2H_2 ~~molecule~~. C_2H_6, etc.

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Q. Calculate the wave no. of stretching vibration of C=C double bond.
Given force constant $K = 10 \times 10^{5}$ dyne cm^{-1}.

We know that —

$$\text{wave no. } \bar{\nu} = \frac{1}{2\pi c}\sqrt{\frac{K}{\mu}}\ cm^{-1}.$$

$$\mu = \frac{m_1 \times m_2}{m_1 + m_2} = \frac{12 \times 12}{12+12}\ amu.$$

$$= \frac{144}{24} = 6\ amu$$

$$1\ amu = 1.66 \times 10^{-24}\ g.$$

$$6\ amu = 1.66 \times 6 \times 10^{-24}\ g.$$

$$\mu = 9.97 \times 10^{-24}\ g.$$

$$\bar{\nu} = \frac{1}{2 \times 3.14 \times 3 \times 10^{10}\ cm\ sec^{-1}}\sqrt{\frac{10 \times 10^{5}\ dyn\ cm^{-1}}{9.97 \times 10^{-24}\ g}}$$

$$= \frac{1}{18.852 \times 10^{10}\ cm\ sec^{-1}}\sqrt{10.03 \times 10^{28}}$$

$$= 0.1680 \times 10^{4}\ cm^{-1}.$$

$$\bar{\nu} = 1680\ cm^{-1}.$$

1 dyne = gm cm sec^{-2}.

Neelgagan

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