

3] Sketch the normal modes of vibration of a)  $H_2O$  (1) and b)  $CO_2$  molecule.

A normal mode vibration is defined as a molecular motion in which all the atoms in the molecule vibrate with same frequency and all the atoms pass through their eqm positions simultaneously.

Normal mode of vibration for a linear molecule }  $= (3N - 5)$

Normal mode of vibration for a non-linear molecule }  $= (3N - 6)$   
internal degrees of freedom

Condition

For a molecule to be Infrared active, it must either possess a permanent dipole moment (or) the dipole moment must change during a ~~vibrati~~ vibration.

$$\frac{d\mu}{dr} \neq 0$$

a)  $H_2O$  molecule:

It is a triatomic non-linear molecule.

$$\begin{aligned} \therefore \text{Normal mode of vibration} &= (3N - 6) \text{ internal degrees of freedom} \\ &= (3 \times 3) - 6 \\ &= 3 \end{aligned}$$

∴ 3 fundamental vibrations

... are all IR-active since each of them is accompanied by a change in dipole moment

- The symmetric stretching frequency is labelled as  $\bar{\nu}_1$
- The symmetric bending frequency is labelled as  $\bar{\nu}_2$
- The asymmetric stretching frequency is labelled as  $\bar{\nu}_3$ .

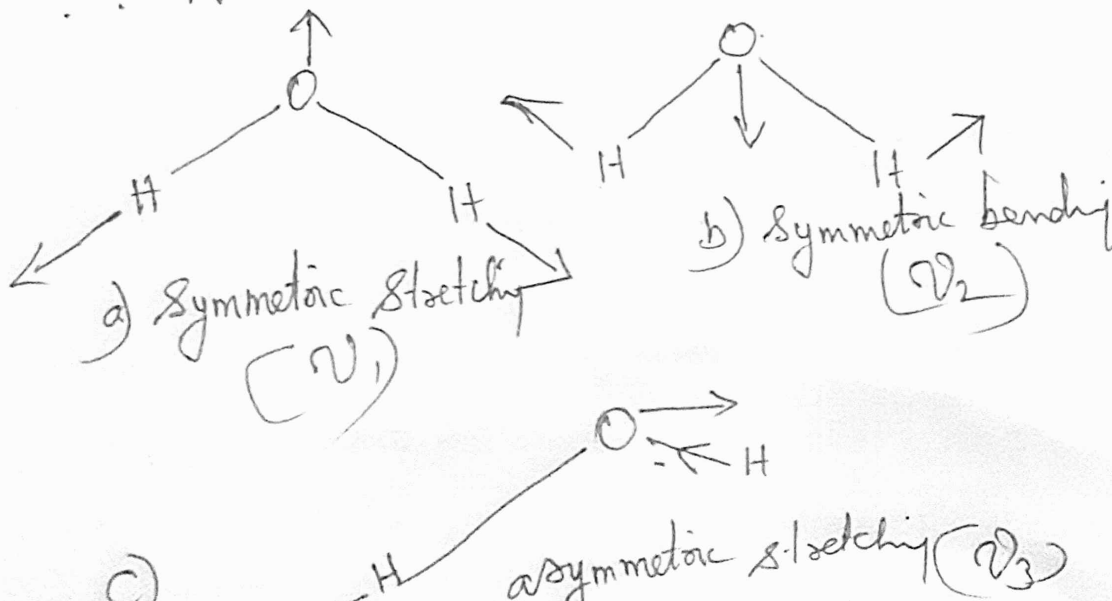
- The ~~two~~ three vibrations are denoted as  $\bar{\nu}_1 = 3651 \text{ cm}^{-1}$ ,  $\bar{\nu}_2 = 1595 \text{ cm}^{-1}$  and  $\bar{\nu}_3 = 3755 \text{ cm}^{-1}$ .

- It is easier to bend a molecule than to stretch it. Hence, the bending frequency is generally lower than stretching frequency

- Also, it is easier to stretch a molecule symmetrically than asymmetrically.

(\*) Hence, symmetric stretching frequency is lower than asymmetric stretching frequency

∴ Normal modes of vibration of water is



\* It is a linear polyatomic molecule:

Normal modes of vibration =  $3N - 5$   
=  $3 \times 3 - 5 = 4$   
= 4 internal degrees of freedom

→ Of the four fundamental vibrations of  $\text{CO}_2$  molecule, two have the same frequency and are said to be degenerate

→ The symmetric stretching frequency  $\bar{\nu}_1$  is not observed in  $\text{CO}_2$ . Since there is no change in dipole moment.

