Normal modes of Vibration :-

Nuclei of molecules do not vibrate with random motion. They exhibit normal vibrations in such a way that all the nuclei in the molecule move in phase and with the same frequency. These vibrations are called fundamental vibrations or normal modes of vibrations. During these vibrations, there is no net translational motion i.e. the centre of mass does not change.

The no. of normal modes of vibrations of a polyatomic molecule is given by —

$N = 3n-6$ (for non-linear molecules)

& $N = 3n-5$ (for linear molecules)

where, n is the no. of atoms or nuclei in the molecule.

Thus, for diatomic molecules ($3\times2-5 = 1$) whether homonuclear or heteronuclear have only one fundamental vibrational frequency.

		Normal modes of Vibration
CO_2	(linear)	$3\times3-5 = 4$
COS	(linear)	$3\times3-5 = 4$
H_2O	(non-linear)	$3\times3-6 = 3$
SO_2	(non-linear)	$3\times3-6 = 3$
CH_4	(non-linear)	$3\times5-6 = 9$
C_6H_6	(non-linear)	$3\times12-6 = 30$

All the theoretically predicted normal modes of vibrations are, in general, not actually observed in the IR-spectrum. This may be due to the fact that some of these may be degenerate or may not involved a change in dipole moment.

All modes of CO_2 are not IR-active –

In the case of CO_2, the four fundamental vibration may be shown as –

(ν_1) O —— C —— O

Symmetric Stretching ($1330\ cm^{-1}$) IR inactive

(ν_2) O —— C —— O

Antisymmetric stretching ($2349.3\ cm^{-1}$)
IR active

(ν_3) O ↑ —— C —— O ↑
↓

Bending Vibrations
(degenerate modes)
($667.3\ cm^{-1}$)

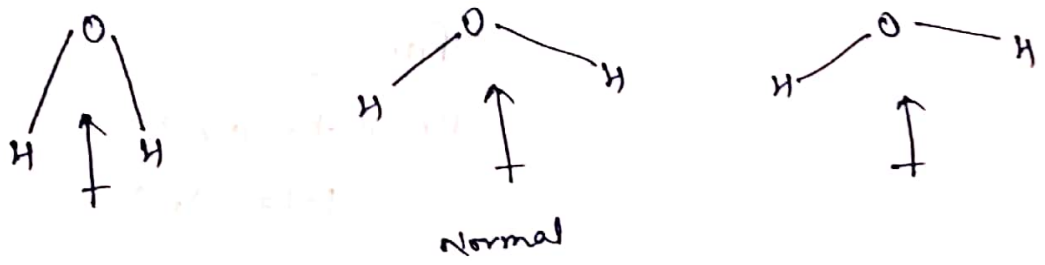
for the CO_2 molecule, there are two different sets of symmetry axis. There is an infinite number of two-fold axes (C_2) passing through the carbon atom at right angles to the bond direction & there is an ∞-fold axis (C_∞) passing through the bond axis itself. These two are symmetric stretching and antisymmetric stretching. Symmetric stretching produces no change in dipole moment. so, this vibration is IR inactive.

for linear triatomic molecule, there should be four vibrational modes. The bending vibration (ν_2) shows two vibrations. one in the plane of the paper and other is which the oxygen atoms move simultaneously into and out of the plane. The two ~~sorts~~ sorts of motions are identical in all respect except directions. So, these are termed as degenerate.

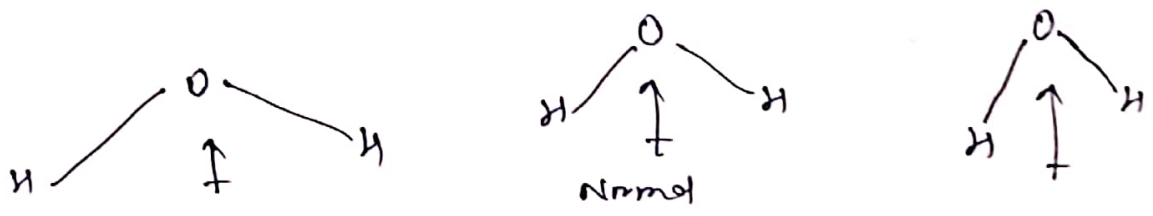
So, only two IR-active vibrations one for anti-symmetric stretching and other for degenerate bending modes are possible for CO_2 molecule.

Modes of Vibrations of H_2O. —

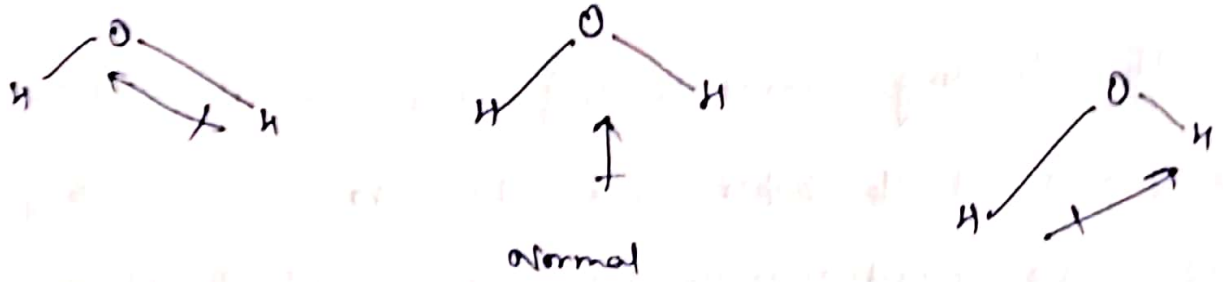
for H_2O, there are three ($3\times3-6=3$) fundamental modes of vibrations which may be sketched as:



(a) ν_1 Symmetric Stretching ($3651.7\ cm^{-1}$)



(b) ν_2 Bending modes ($1595.0\ cm^{-1}$)



(c) ν_3 Asymmetric stretching ($3755.8\ cm^{-1}$)

The direction of displacement vector shows that there, is a dipole change during the vibration for all the three modes of vibration.

Therefore, all the three modes of vibrations for H_2O molecule, are IR-active.

—x—

from.

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(Chemistry)