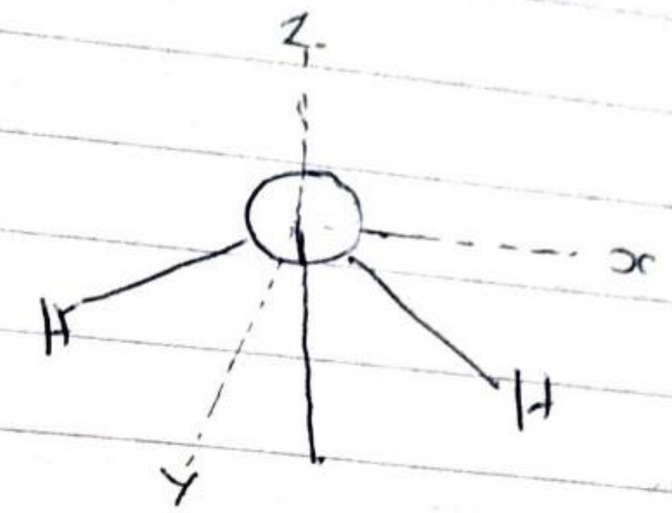
P.G II ; Inorg. chem. ; core course VI

Determination of Point group of some molecules :→

1. For H_2O.



(i) The molecule is not linear and does not contain higher order axes.

(ii) The molecule possess no improper axes. The higher order proper axis is C_2 passing passing through O-atom and deviding the angle between H-atoms. Also there are no other C_2 axis.

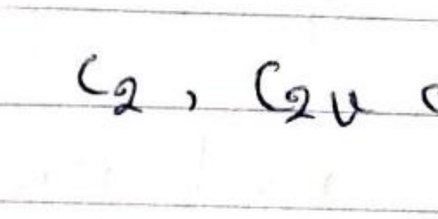
$\therefore H_2O$ belongs to C_2, C_{2v} or C_{2h}.

(iii) Since, it has two vertical plane xz and yz.

xz is the molecular plane

$\therefore$ It belongs ~~to C_2~~ to C_{2v}.

For NH_3



(i) There is no improper axis.

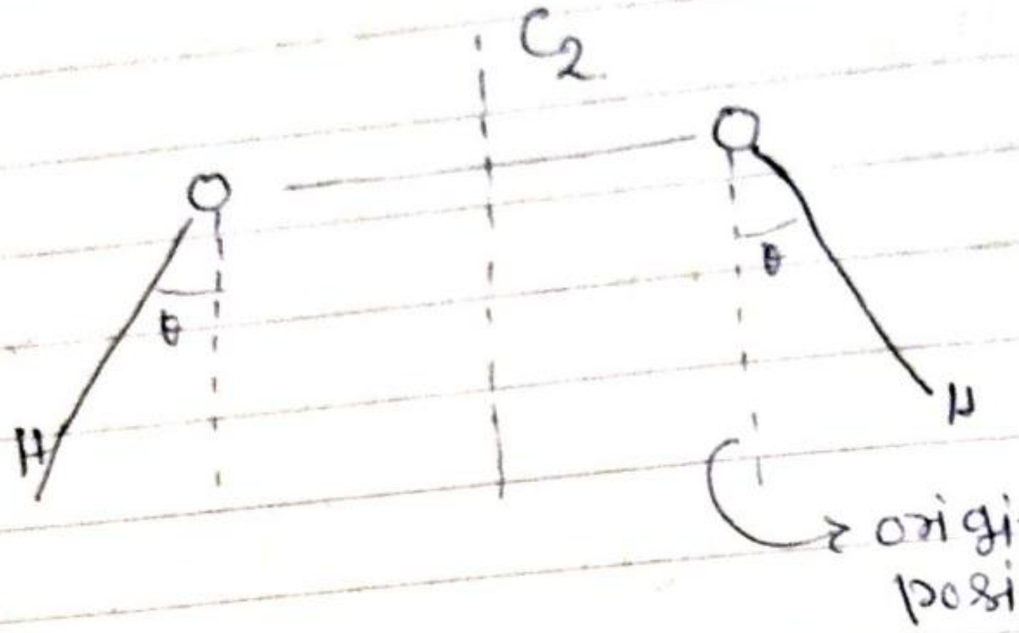
(ii) There is no C_2 axis.

(iii) It has C_3 axis as proper axis. Hence, point group may be, C_3, C_{3v} or C_{3h}.

(iv) There are three vertical planes passing through N and each H-atoms.

$\therefore$ group is C_{2v}

For H_2O_2, F_2O_2 :→



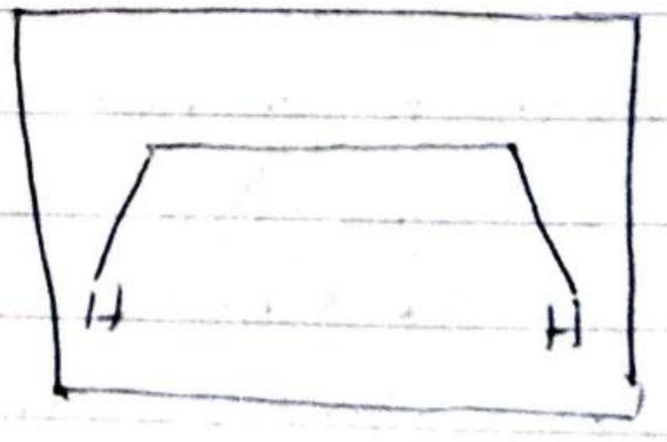
It is a non planar molecule. The planes $H-O-O$, $O-O-H$ are inclined at 110 C_2 bisects the O-O bond

(i) There is no improper axis.
(ii) There is one C_2 axis and no other proper axis.
(iii) There is no Symmetry plane
(iv) The group is therefore C_2. And E and C_2 are the elements.

Cis planer configuration (cis-H_2O_2 ; F

$\theta = 0°$

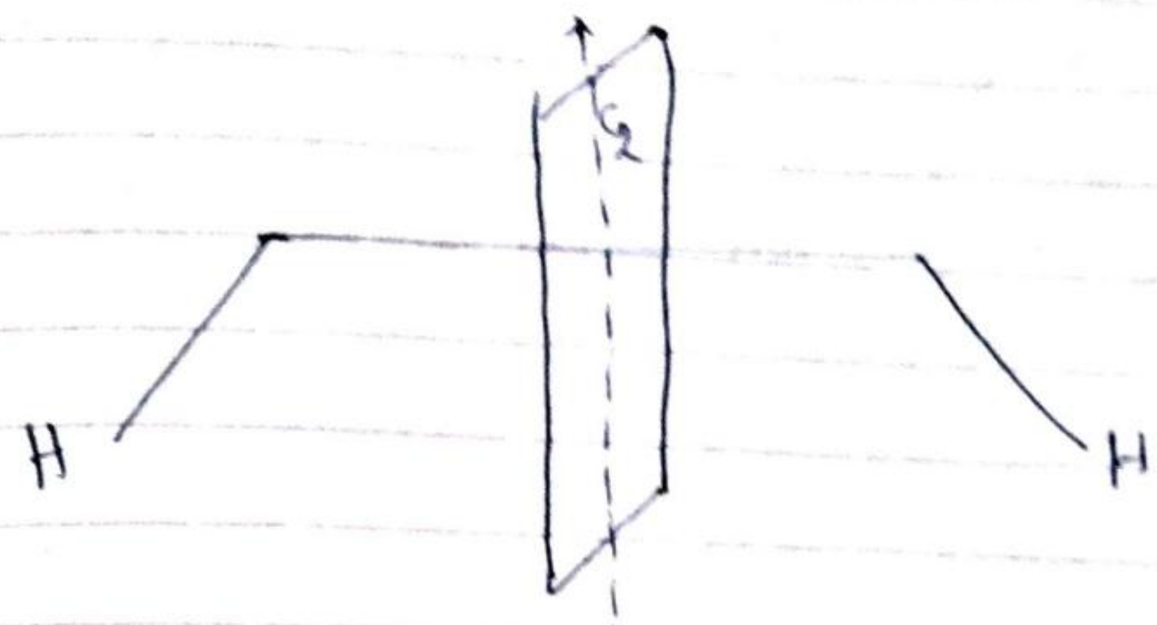
(i) There is no even order S_n axis.
(ii) There is a C_2 axis. There is no other proper axis.
(iii) The molecule has a planer Symm.



σ_v'.

(iv) Also the molecule has another plan of Symm. which is a vertical plane

containing C_2 axis and bisecting the molecular plane.



(v) The group is therefore C_{2v}.

Trans H_2O_2 :→

$\theta = 90°$

(i) There is no even order S_n axis.
(ii) There is a C_2 axis.
(iii) There are no other proper axis.
(iv) There is a σ_h plane $\perp^r$ C_2 axis. which is a molecular plane. As n is even the is a centre of symm.

∴ The gr. is C_{2h}.

The elements are → E, C_2, σ_h & i a Other examples are N_2F_2 and tran dichloroethylene.

C_{nh} group

These contain 'n' rotational operators and contain '2n' elements. All the elements commute. Hence the group is a "Albian"

C_{nh} (n = odd) → elements are - E, C_n, σ_h.

C_{nh} (n = even) → elements are - E, C_n, σ_h, i.

Thus, C_{1h} group has the elements —

E, C_1, σ_h.

But $C_1 = E$

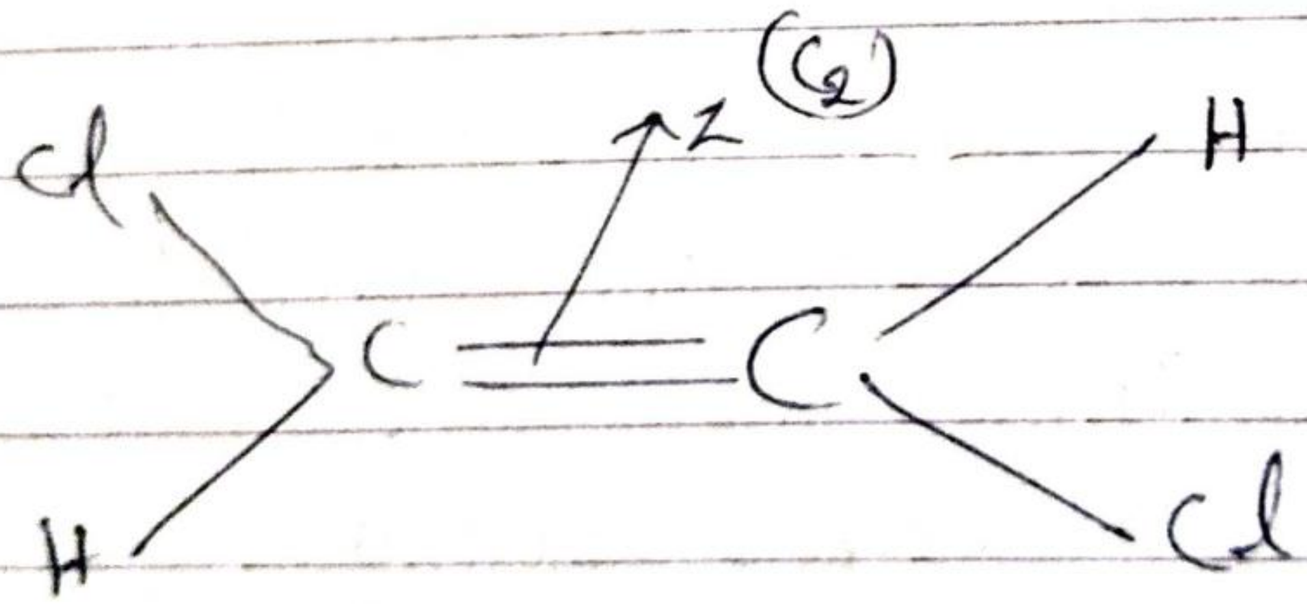
∴ elements are = E & σ_h.

C_{2h} gr. has the elements —

E, C_2, σ_h, & i.

Example — Trans-dichloroethylene

Trans - dichloroethylene :→



Elements — E, C_2, $\sigma_h(xy)$, i

z-axis ⊥ σ_h → molecular plan

Hence the group is C_{2h}.