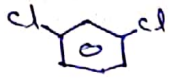
Symmetry Point Group

The group of symmetry operations of a molecule is called point group. Several molecules have the same set of operations, belongs to same point group.

for examples- H_2O, $HCHO$, $CH_3-CH=CH-CH_3$ (cis)



etc belongs to same point group. C_{2V}.

We have only constructing here to point group.

→ Identity (E) is omnipresent and it is redundant.

→ C_1 → E and C_1 is present only.

→ C_2 → E and C_2 is present only.

→ C_S → E and σ (molecular plane) is present.

→ C_i → E and i (inversion centre) is present.

→ If molecule has only proper axis of rotation.

(a). E and C_2 present — C_2

(b) E and C_3 present — C_3

(c) E and C_3^2 present — C_3^2

(d) E and C_4 present — C_4

(e) E and C_4^2 " — C_2

(f) E and C_4^3 " — C_4^3

→ If molecules has proper axis of rotation and plane of symmetry.

σ → σ_v, σ_h, σ_d.

(a). E, C_2 & σ_v present → C_{2V}.

(b) E, C_3 & σ_v " → C_{3V}.

(c) E, C_2 & σ_h present → C_{2h}.

(d) E, C_3 & σ_h " → C_{3h}.

(e). E, C_2, C_3, σ_h present and $C_2 \perp C_3$ then – D_{3h}.

→ for linear molecule which does not consists of equivalent halves, the only symmetry operations are the rotation about C_∞ and reflection in the vertical plane – called $C_{\infty v}$.

→ <u>special group.–</u>

T, O, I
Th, Oh, Ih
Td

} These seven groups containing multiple higher order axis. These are pure rotational group.

(a). $C_{\infty v}$ → a linear molecule having C_n with $n = \infty$ and σ_v but no σ_h. eg: S=C=O

(b) $D_{\infty h}$ → a linear molecule having C_n with $n = \infty$ and σ_h.

eg: O=C=O

(c) Td → a molecule having tetrahedral symmetry. (CH_4)

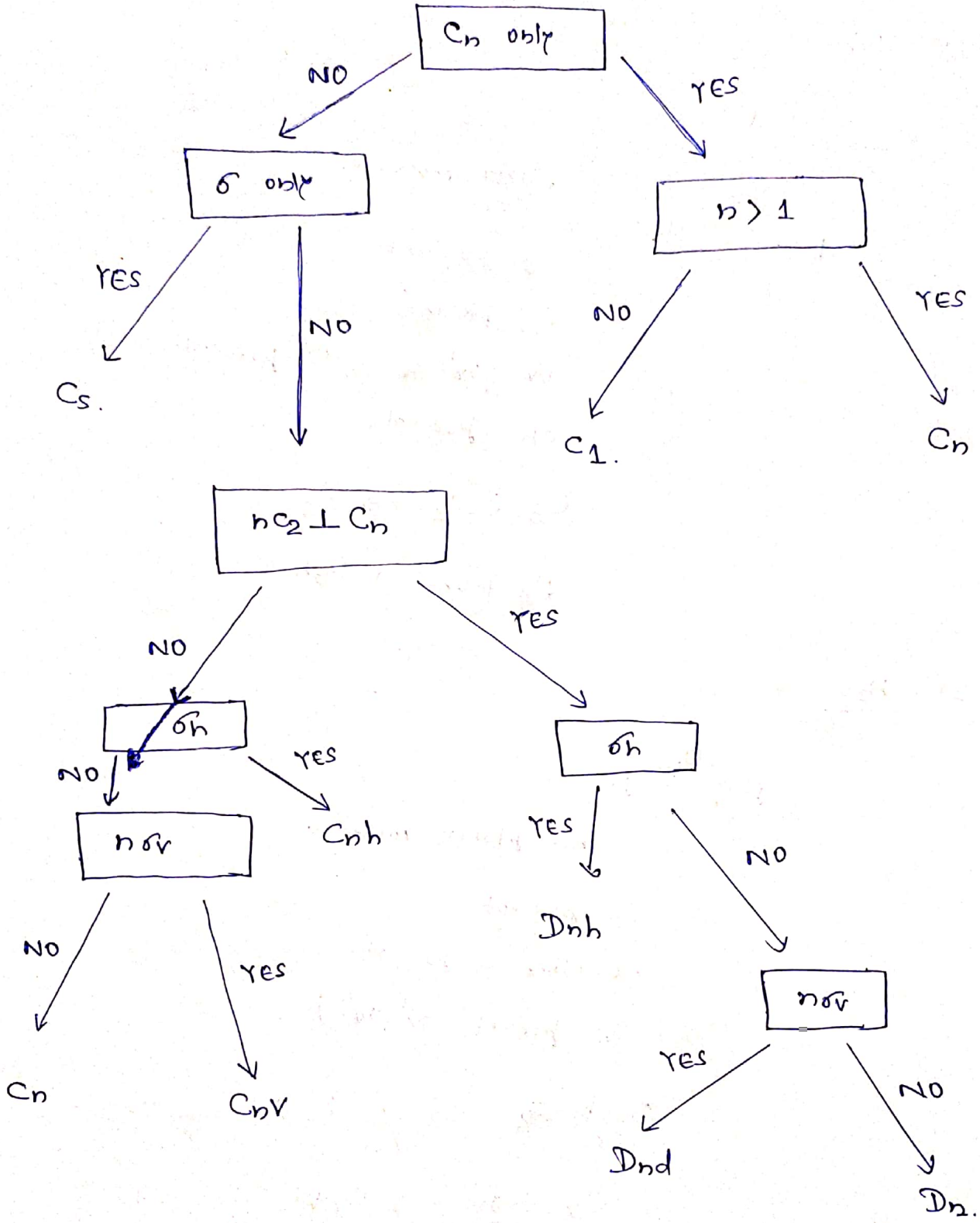
(d) Th → a molecule having tetrahedral symmetry with i (inversion centre).

(e) Oh → a molecule having Octahedral symmetry

eg: $[Co(NH_3)_6]^{a+}$

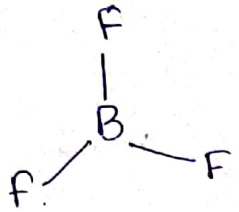
(f) Ih → a molecule having dodecahedral or icosahedral symmetry.

FLOW CHART (Point group)



Q. Assign the Point group of the following molecules. ?

(1) BF_3.



planer molecule.

C_3 present

C_2 present.

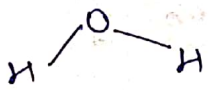
σ_v (σ_v^1, σ_v^2, σ_v^3) present

σ_h present.

$C_3 \perp C_2 \rightarrow D_3$

$D_3 + \sigma_h \rightarrow D_{3h}$.

(2) H_2O.



non-planer molecule.

C_2 present.

no other C_2 present.

σ_v present (σ_v^1, σ_v^2)

$C_2 \neq \perp C_2 \rightarrow C_2$.

$C_2 + \sigma_v \rightarrow C_{2v}$.

for yourself

Other molecules.

$HCHO$, $CH_3-CH=CH-CH_3$ (cis & trans), H_2O_2, C_6H_6, CH_4, CH_2Cl_2, $CH_2=C=CH_2$., HF, CO_2, HCN, H_2, $CHCl=CHCl$ (cis & trans) $[Pt(Cl)_4]^{2+}$, $[Co(NH_3)_6]^{2+}$, PCl_3, PCl_5, SF_4 etc.