IMPROPER AXIS OF ROTATION

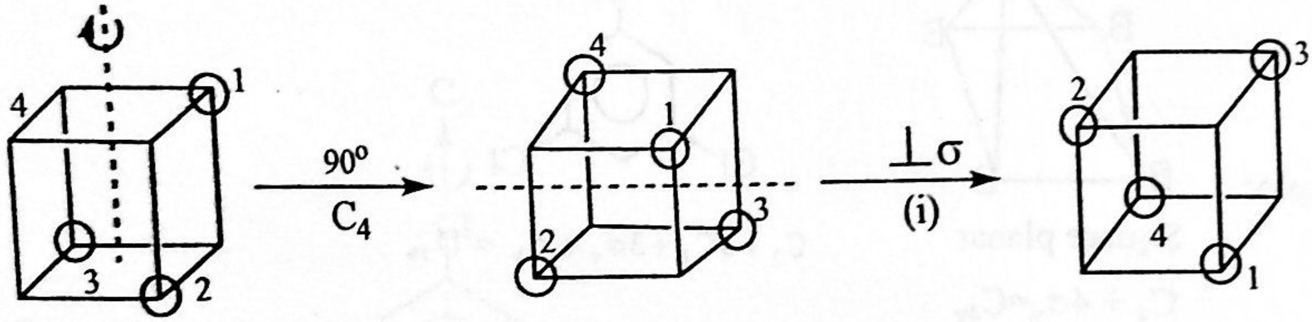
Roto Reflection Axis(Sn) :

$$\text{Initial} \xrightarrow{\theta^\circ \text{ rotation}} \xrightarrow{\perp \sigma} \text{equivalent orientation}$$

CH_4 has, S_4 axis of rotation.

$$\text{Initial} \xrightarrow{90^\circ} \xrightarrow{\perp \sigma} \text{Equivalent}$$

CH_4 has tetrahedral structure. If we place CH_4 molecule in a cube then the four atom t four corners of the cube. CH_4 having S_4 it doesn't mean that C_4 must also be there.



$$\eta = \frac{360^\circ}{90^\circ} = 4$$

So S_4

$$\begin{cases} Cn \rightarrow (n-1) & \text{operation} \\ C_2 \rightarrow 1 & \text{operation} \\ C_3 \rightarrow 2 & \text{operation} \\ C_4 \rightarrow 3 & \text{operation} \\ C_5 \rightarrow 4 & \text{operation} \end{cases}$$

Number of Operation in Sn Axis :

$S_2 \quad C_2 \perp \sigma$

$S_3 \quad C_3 \perp \sigma$

$S_4 \quad C_4 \perp \sigma$

$S_5 \quad C_5 \perp \sigma$

$\sigma_{odd} = \sigma$

$\sigma_{even} = E$

$$C_2^1 \times \sigma^1 = C_2^1$$
$$C_2^2 \times \sigma^2 = E$$
$$C_3^1 \times \sigma^1 = S_3^1$$
$$C_3^2 \times \sigma^2 = C_3^2 \times E = C_3^2$$
$$C_3^3 \times \sigma^3 = \sigma$$
$$C_3^4 \times \sigma^4 = C_3^1$$
$$C_3^5 \times \sigma^5 = C_3^5 \times \sigma = S_3^5 = S_3^2$$
$$C_3^6 \times \sigma^6 = E \times E = E$$

S_5 :

$C_5^1 \times \sigma^1 = S_5^1$
$C_5^2 \times \sigma^2 = C_5^2$
$C_5^3 \times \sigma^3 = S_5^3$
$C_5^4 \times \sigma^4 = C_5^4$
$C_5^5 \times \sigma^5 = \sigma = E \times \sigma = \sigma$ $\quad S_5^1\ S_5^2\ S_5^3\ S_5^4$
$C_5^6 \times \sigma^6 = C_5^1$
$C_5^7 \times \sigma^7 = C_5^2 \times \sigma = S_5^2$
$C_5^8 \times \sigma^8 = C_5^3$
$C_5^9 \times \sigma^9 = C_5^4 \times \sigma = S_5^4$
$C_5^{10} \times \sigma^{10} = E$

$\sigma^2 = \sigma^4 = \sigma^6 = E$
$C_2^2 = C_3^3 = C_4^4 = E$
$E \times X = X$
$\sigma^5 = \sigma^4 \times \sigma$
$= E \times \sigma = \sigma$

S_6 :

$C_6^1 \times \sigma^1 = S_6^1$
$C_6^2 \times \sigma^2 = C_6^2$
$C_6^3 \times \sigma^3 = S_6^3$
$C_6^4 \times \sigma^4 = C_6^4$
$C_6^5 \times \sigma^5 = S_6^5$
$C_6^6 \times \sigma^6 = E$

$\boxed{S_6^1\ S_6^3\ S_6^5}$

Some Imperical Points :

Case : I. If n is even then $C_{n/2}$ axis will exist.

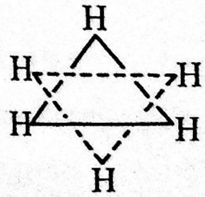
Case : II. n is odd then C_n will exist.

e.g.: S_4 CH_4 C_2 will exist
S_{10} C_5H_5 C_5 will exist

Q. **A molecule have C_2 axis and a perpendicular plane what will be the point group. The possibility is for C_{nh} and D_{nh}.**
- **If molecule having only one C_2 then ans is C_{2h}.**
- **There is not given how many C_2 in this given molecule, so the point group may be D_{2h}.**

Example: STAGGERED ETHANE :

$1C_3$ axis, $3C_2$ axis, $3\sigma_d$
$C_3 + 3C_2 + 3\sigma_d = D_{3d}$

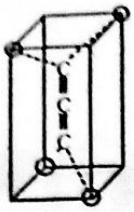


Ethane having H_2O_2 like structure, so having $3C_2$ axis.

Example:

ALLENES : Allenes are elongated tetrahedran.

$C_2 + 2\,C_2 + 2\,\sigma_d = D_{2d}$



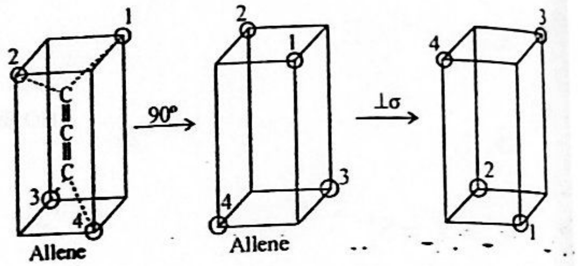
both C_2 having 90° angle and both dihedral plane having 90° angle.

Number of operation in D_{2d} point group:

Total no. of operation = 4 n = 4 × 2 = 8

So, it having

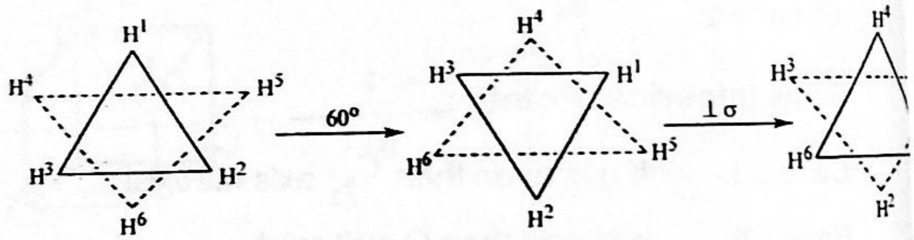
$3C_2$	→	3
$2\sigma d$	→	2
E	→	1
S_4	→	2
		8



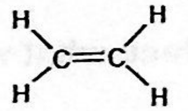
Number of operation in D_{3d} :

$4n = 4 \times 3 = 12$

$1\,C_3$	→	2
$3\,C_2$	→	3
$3\,\sigma_d$	→	3
E	→	1
S_6	→	3
		12



ECLIPSED DOUBLE BOND SYSTEM :

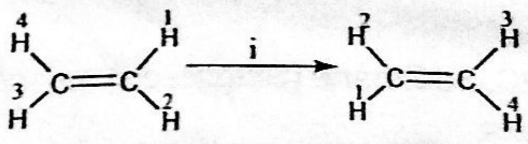


$C_2 + 2C_2 + 2\sigma_v + \sigma_h = D_{2h}$

No. of total operation = 4 × n = 4 × 2 = 8

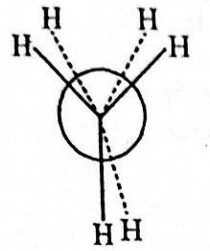
Explanation :

$1\,C_2$	→	1
$2\,C_2$	→	2
$2\sigma_v$	→	2
σ_h	→	1
E	→	1
i	→	1



ECLIPSED ETHANE : $C_3 + 3C_2 + 3\sigma_v + \sigma_h = D_{3h}$

No. of total operation = 4n = 4 × 3 = 12

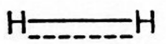


Explanation :

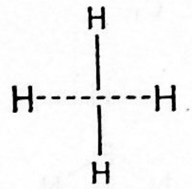
$1C_3$	→	2
$3C_2$	→	3
$3\sigma_v$	→	3
σ_h	→	1
E	→	1
S_3	→	2
		12

Eclipsed

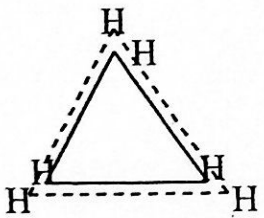
Staggered



D_{2h} (S_2)

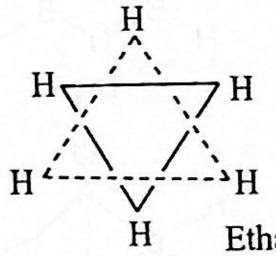


D_{2d} (S_4)



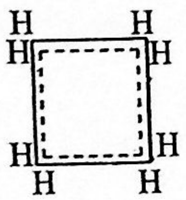
Ethane

D_{3h} (S_3)



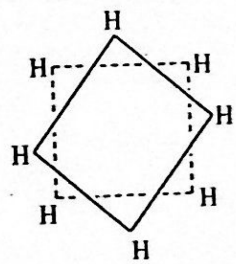
Ethane

D_{3d} (S_6)



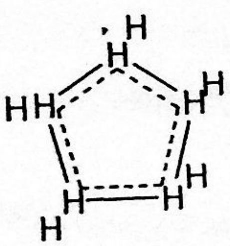
D_{4h} (S_4)

Cyclobutane



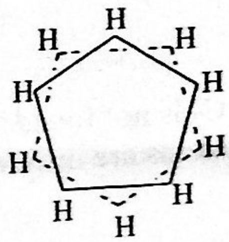
D_{4d} (S_8)

Cyclobutane



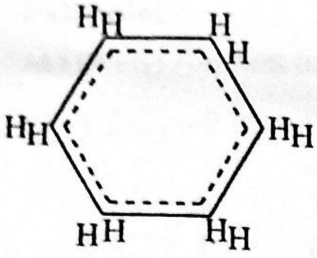
D_{5h} (S_5)

Ferrocene

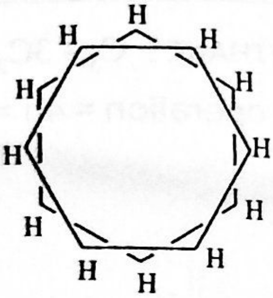


D_{5d} (S_{10})

Ferrocene

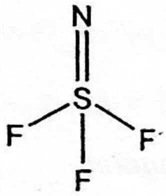


D_{6h} (S_6)
Dibenzene chromium



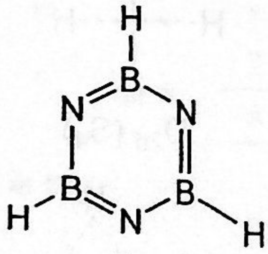
D_{6d} (S_{12})
Dibenzene chromium

NSF_3 : C_{3V} :



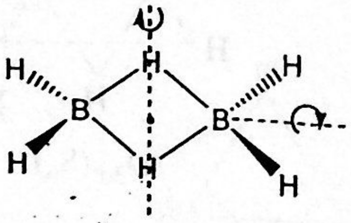
C_{3V}

BORAZINE :



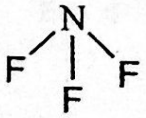
D_{3h}

B_2H_6 :



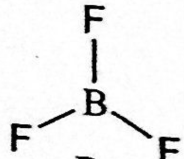
$$D_{2h} = C_2 + 2C_2 + 2\sigma_v + \sigma_h$$

NF_3 :



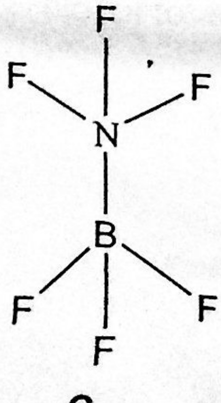
C_{3v}

BF_3:



D_{3h}

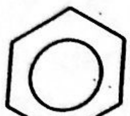
Example:



C_{3V}

C_2 is not found here because both central atoms are different

BENZENE :



D_{6h}

TOTAL OPERATION = 4N = 4 × 6 = 24

C_6	=	5
$6C_2 = 6$		
$6\sigma_v$	=	6
σ_h	=	1
S_6	=	2
S_3	=	2
$S_2 = i$	=	1
E	=	1
		24

$$C_6^1 \times \sigma^1 = S_6^1$$
$$C_6^2 \sigma^2 = C_6^2$$
$$C_6^3 \sigma^3 = S_6^3 = S_2$$
$$C_6^4 \sigma^4 = C_6^4$$
$$C_6^5 \sigma^5 = S_6^5$$
$$C_6^6 \sigma^6 = E$$