

n -fold proper axis OR Rotation OR Proper rotation.

A circular rotation through $360/n$ about an imaginary axis passing through the molecule to take it from one configuration to another equivalent configuration is called n -fold (or order) proper axis of rotation C_n . By convention, the order of rotation is a clockwise, i.e. from right to left and the rotation from y to x is positive direction and x to y as negative direction.

Several symmetry operations can be carried out around a single rotation axis. The order of the axis (n) is obtained by dividing 360° with an angle of rotation necessary to get indistinguishable configuration.

When $n=1$, the circular rotation is through 360° i.e. doing nothing to the molecule. \therefore It is an identity operation (E)

$$\frac{360^\circ}{1} = 360 \rightarrow C_1 \text{ or one fold axis of symmetry}$$

$$\frac{360^\circ}{2} = 180^\circ \rightarrow C_2 \text{ or two fold axis of symmetry}$$

$$\frac{360^\circ}{3} = 120^\circ \rightarrow C_3 \text{ or three fold axis of symmetry}$$

$$\frac{360^\circ}{4} = 90^\circ \rightarrow C_4 \text{ or four fold axis of symmetry}$$

$$\frac{360^\circ}{5} = 72^\circ \rightarrow C_5 \text{ or five fold axis of symmetry}$$

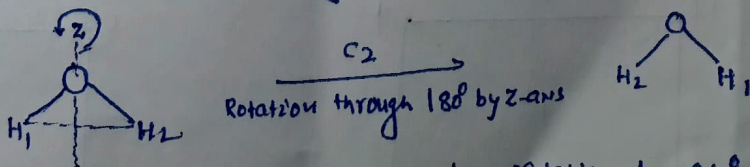
$$\frac{360^\circ}{6} = 60^\circ \rightarrow C_6 \text{ or six fold axis of symmetry}$$

Linear molecules like, H_2 , HeI etc have an 'infinite' fold axis of symmetry i.e. C_∞ , because the appearance of the molecule is not changed by circular rotation through an angle (infinite number) about the molecular axis.

The symmetry axis of linear molecules coincides with the molecular axis.

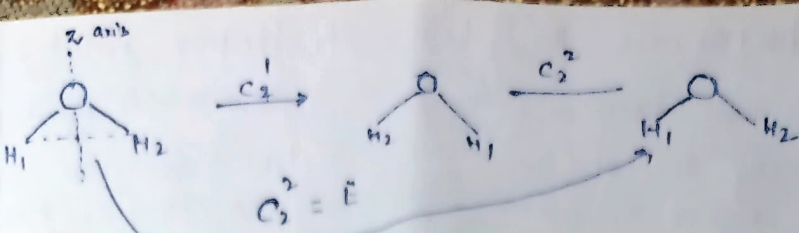
The angular H_2O molecule has C_2 axis which passes through O-atom and bisects the angle between two OH bonds.

A circular rotation through 180° about Z-axis is called C_2 operation.



If C_2 is applied in succession i.e. rotation by 360° in H_2O molecule, we will get identity operation (E) because it will bring back to the original configuration.

It may be depicted as follows:

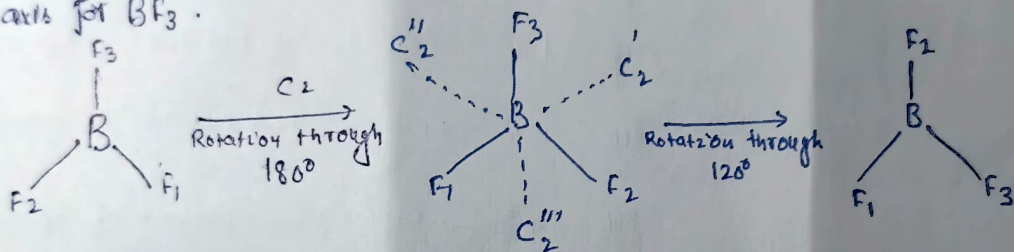


$$\therefore C_2 \cdot C_2 = C_2^2 = E$$

the C_2 operation a rotation of 180° around a C_2 axis.

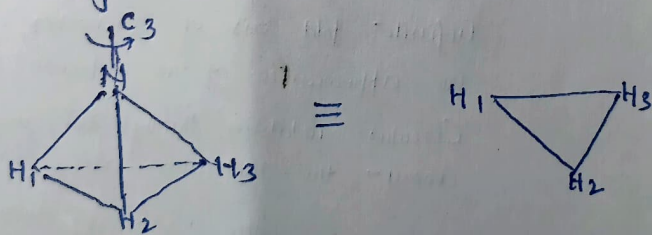
The trigonal planar BF_3 molecule has C_3 axis perpendicular to the triangle i.e. the molecular plane containing all three F-atoms and passing through the centre of B-atom. BF_3 molecule has three C_2 -axis in addition to C_3 axis.

Each C_2 axis passes through the centre of B-atom and falls on each B-F bond and these are in the plane of the molecule C_3 being the highest fold axis, is the principal axis for BF_3 .

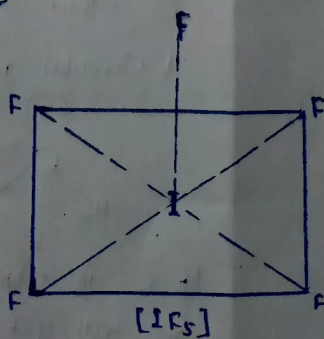
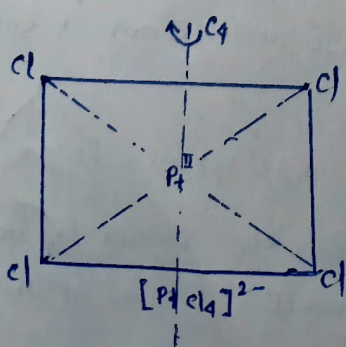


The Pyramidal NH_3 molecule has a C_3 axis which passes through N-atom and the geometrical centre of equilateral triangle describe by three H-atoms.

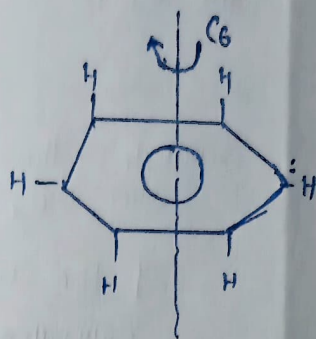
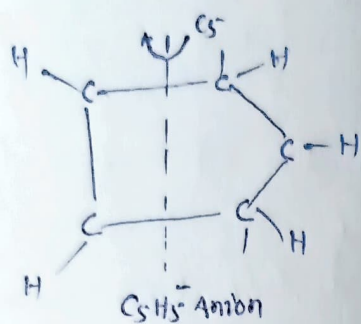
In simplified form, NH_3 molecule is shown by the figure on R.H.S.



A Square planar $[Ni(CN)_4]^{2-}$, $[PtCl_4]^{2-}$ etc. molecules and IF_5 have a C_4 passing through the central atom and perpendicular to the molecular plane

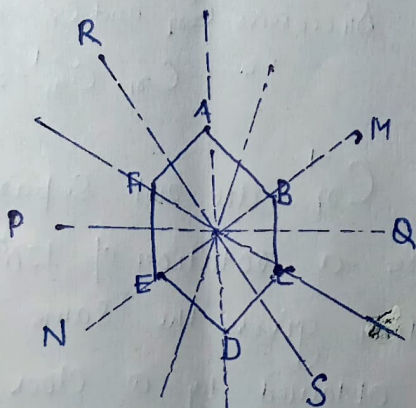


Cyclopentadienyl anion $C_5H_5^-$ has a C_5 and benzene has a C_6 axis which passes through the centre and perpendicular to the plane. i.e. Z axis of the molecule.



H_2O and NH_3 have only one axis of rotation while BF_3 , $[Ni(CN)_6]^{2-}$ and Benzene have many axes of rotation.

In Benzene molecule there are six C_2 axes lying in molecular plane such as AD , BE , CF & PQ , MN & RS respectively. Three passes through the centre of the Benzene and pairs of two opposite C -atoms and other three passes through the centre of the Benzene and centres of $C-C$ bonds.



C_6 being the highest fold axis, is the Principal axis for Benzene molecule.

We can perform rotation many times, if we perform

C_n operations n times, we call it or write it as C_n^m Operation

The possible number of C_n operation is $n-1$

The n th rotation brings back to the original configuration. i.e. identity (E)

$$\therefore C_n^n = E \quad \text{for any value of } n$$

$$\text{for example } C_2^2 = E, C_3^3 = E, C_6^6 = E$$

The successive operation of the same symmetry operation

gives a new symmetry operation

$$\text{For example } C_6^2 = C_3$$

The only operation is possible on C_2 is C_2^1 , i.e. rotation operation
and C_2^2 brings about E

The operations are possible on C_3
(i) C_3^1 (120°)
(ii) C_3^2 (240°)

Similarly Three, four and five operations are possible
over, C_4 , C_5 , and C_6 , since there is a rotation
of 180° in C_2 , C_4^2 , & C_6^3 hence these are
equivalent operations. -

$$C_2^1 = C_4^2 = C_6^3$$

Similarly $C_3^1 \equiv C_6^2$ and $C_3^2 \equiv C_6^4$
because they involve rotation of 120° each

The rotation by $\frac{360^\circ}{n}$ in a clockwise direction is C_n and

rotation by the same angle in anticlockwise direction is C_n^{-1}

The successive C_n and C_n^{-1} operations gives identity (E)

$$\text{i.e. } C_n \cdot C_n^{-1} = E$$

C_n & C_n^{-1} are not separable operations
because a rotation of 120° in anticlockwise
direction gives the same configuration
as obtained by a clockwise rotation
of 240° in BF_3 molecule.

