General Conventions about Axis of Symmetry.

General Conventions which are followed to specify Co-ordinates

(1) The rotational axis with the highest order is principal axis Generally Z axis is Considered as rotational axis.

(2) If all the rotational axis are of the same order then the axis passing through the largest number of atoms must be considered as principal axis or Z axis. Or an axis passing through a large number of bonds is Considered as Z axis or Principal axis.

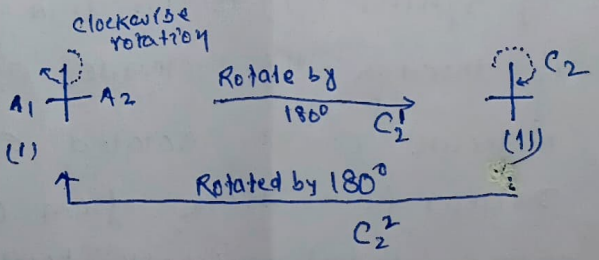
(3) In a planar molecule the rotational axis perpendiculas to the plane of the molecule is taken as Z-axis.

The above facts can be illustrated as follows.

Let us Consider a linear molecule A_2 which is made with two atoms A_1 & A_2

$$A_1 - A_2$$

Let us perform operation about an axis perpendicular to $A_1 - A_2$ bond, in the plane of the paper



Molecule (I) gives an Indistinguishable Image (II) by rotation through 180°.

Hence $\theta = 180^0$

then Order of the axis 'n'

$$n = \frac{360}{\theta}$$

$$= \frac{360}{180} = 2$$

Hence this axis is C_2 axis

If we perform C_2 operation again on (II), then we will get the original Image (I), and it will look as if no operation were performed on A_2 molecule, This is identity E

Hence for the above case

$$C_2^2 = E$$

Where Super Script 2 denotes that Operation has been performed twice.

(a) Axis of Symmetry - Can be clearly understood as follows:

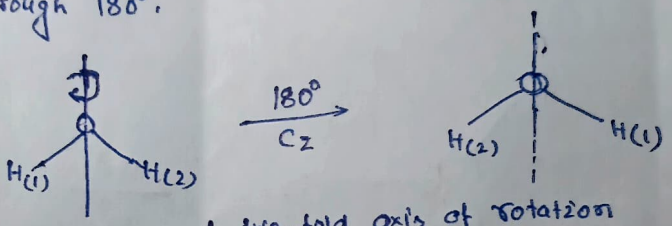
Axis of Symmetry - is defined as an axis around which the rotation of the molecule by an angle $\theta = \frac{2\pi}{n}$ or $\frac{360^\circ}{n}$ gives an equivalent Configuration.

Where n is the Order of the axis

The Order of axis may be two fold (C_2)
three fold (C_3)
and four fold (C_4) etc.

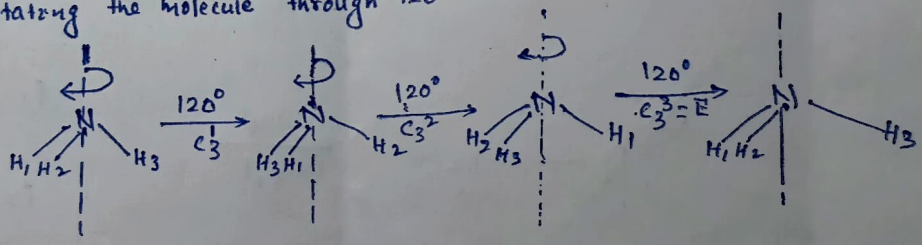
If there are axes of different orders in a molecule, the axis with the highest Order is reffered as Principal axis of rotation

In Water (H_2O) molecule, C_2 (two fold) axis of rotation is present because equivalent Configuration is obtained by rotation through 180°.



A two-fold axis of rotation

Ammonia (NH_3) molecule has a C_3 axis passing throug Nitrogen atom. The identical Configuration is obtained by rotating the molecule through 120°



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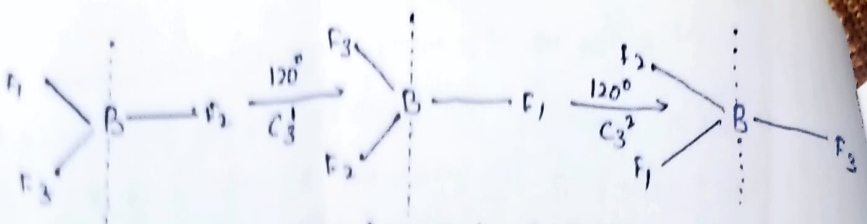
C_3^1 indicate One time rotation by an angle 120°, C_3^2 means two times rotation by an angle 120°. While C_3^3 is the identity - (identity means Original Configuration is obtained.

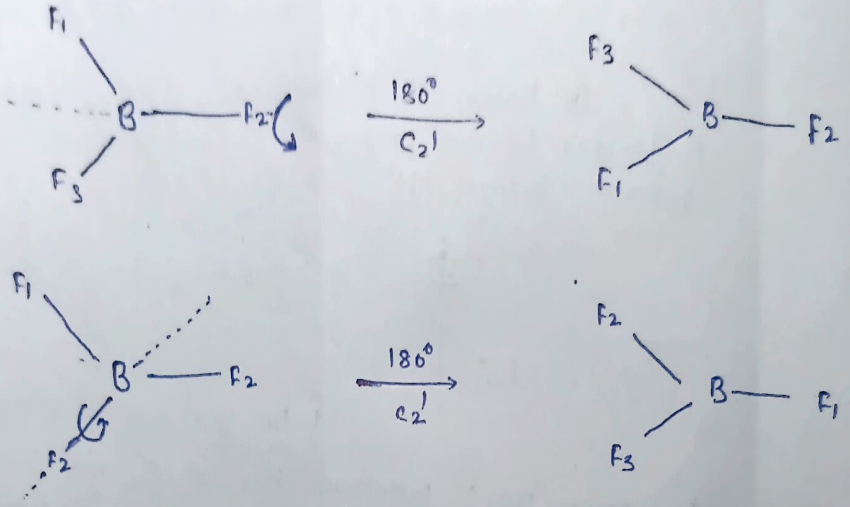
Now we Consider BF_3 molecule (i.e AB_3 type planar molecule) possesses three fold (C_3) axis of rotation passing through B-atom and axis is perpendicular to the plane of molecule.

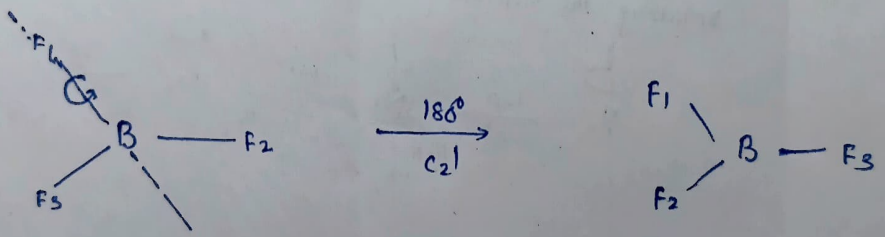
As shown below.



Three fold axis of rotation

In addition to C_3, this type of molecules possess three more two fold (C_2) axes, which are perpendicular to the C_3 axis, passing through Boron or B and each of the fluorine atoms. These axes are in the plane of the molecule.





Two fold axis of rotation

Here,

the C_3 axis is the principal axis of rotation.