P.G Sem - IV
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GROUP THEORY

Symmetry Elements & Symmetry operation :-

Symmetry arises when the molecule possesses identical atoms in certain part of it. These identical atoms are mutually equivalent.

In a molecule possessing a number of identical atom in a suitable positions. It is possible to perform on them specific geometrical operations like rotation, reflection, inversion etc. so that the resulting geometrical configuration is indistinguishable from the original geometrical configuration. Such operations are reffered to as symmetry operation.

Thus,

"Symmetry operation is the geometrical operation such as rotation, reflection, inversion etc. which leads to a configuration indistinguishable from the original configuration."

In a molecule, there are five types of symmetry operations. These are —

1). Identity — denoted by 'E'.
2). Proper axis of rotation — denoted by 'C_n'.
3). Reflection — denoted by 'σ'.
4). Improper axis of rotation — denoted by 'S_n'.
5). Inversion — denoted by '$\dot{2}$'.

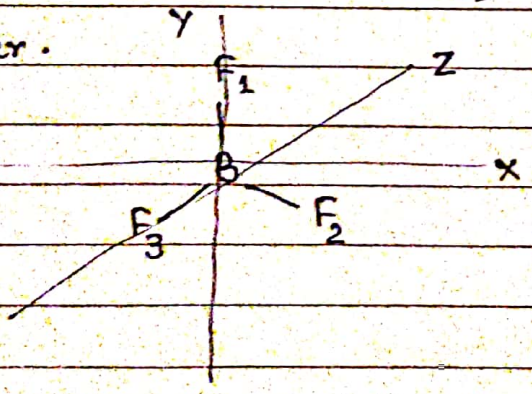
"The geometrical entity such as a line, a point, a plane etc. on which symmetry operation is carried out, is called symmetry elements."

	Symmetry operation	symbol	Symmetry elements
1).	Identity	E	Doing nothing.
2).	Proper axis of rotation	C_n	rotation arises through a line. (axis)
3).	Reflection	σ	reflection axies through a plane. (xy, xz & yz).
4).	Improper axis of rotation	S_n	rotation arises through a line and reflection wrt the plane ⊥ to the rotational axis (Principal axis).
5).	Inversion	i	Centre of symmetry (inversion centre arises through a point)

for Example-

Let us Consider a molecule BF_3.

It is planer.



1). Identity operation :- E.

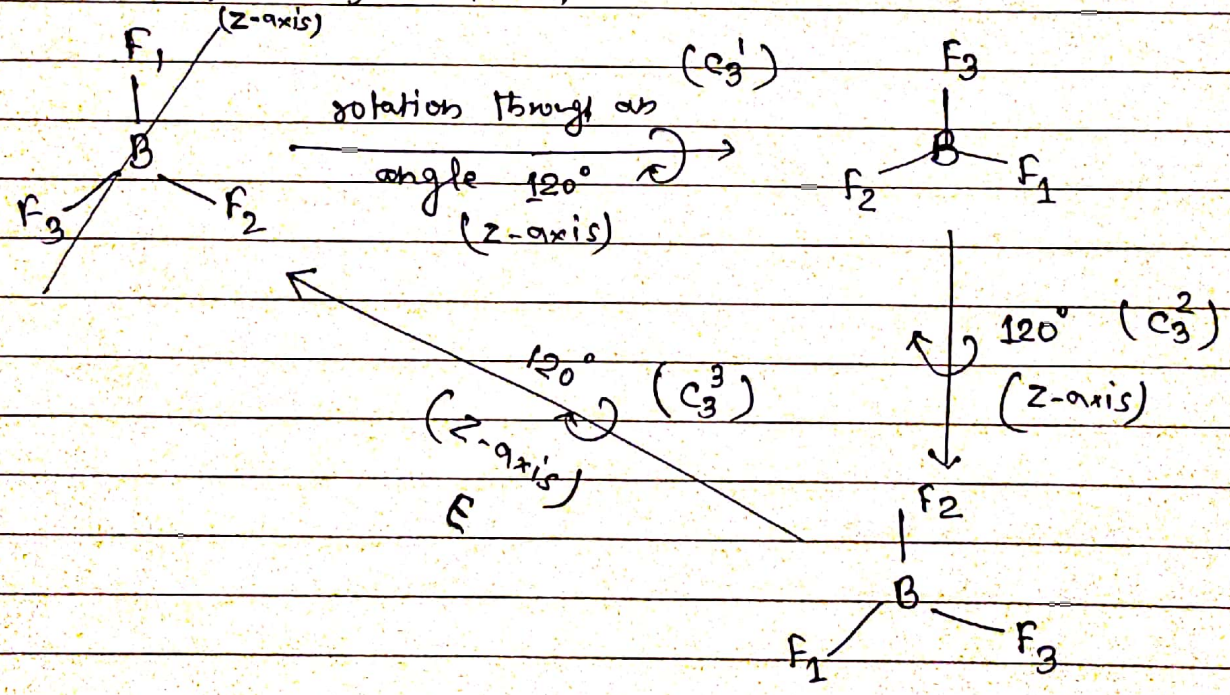
If we perform several operations and we get same configuration then this operation is called Identity.

It means doing nothing.

2). Proper axis of rotation - C_n.

If we perform operations through a line & we get similar configuration then this operation is called proper axis of rotation.

In BF_3 molecule, -



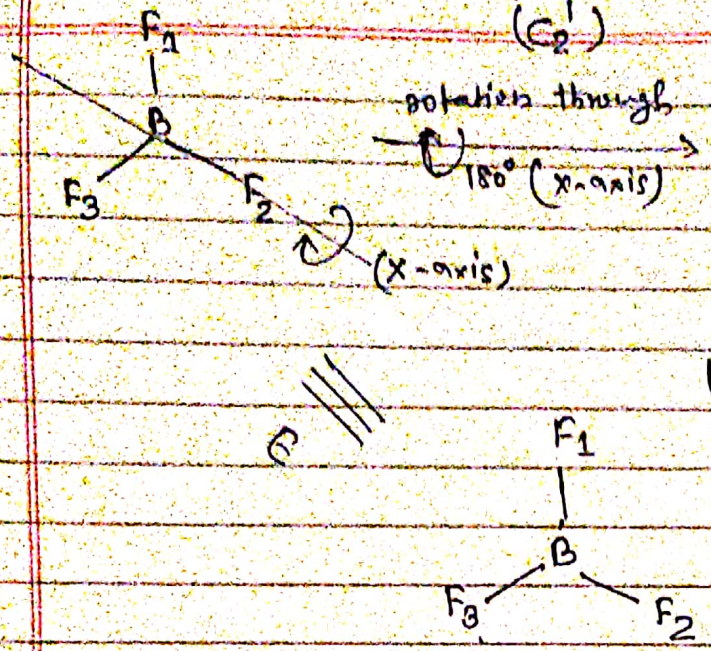
Symmetry Element - C_3

Symmetry operation - C_3^1, C_3^2, $C_3^3 \equiv E$.

Total $\Rightarrow$ $2C_3$.

Note - C_3 is called principal axis.

other operation (axis of rotation) are -



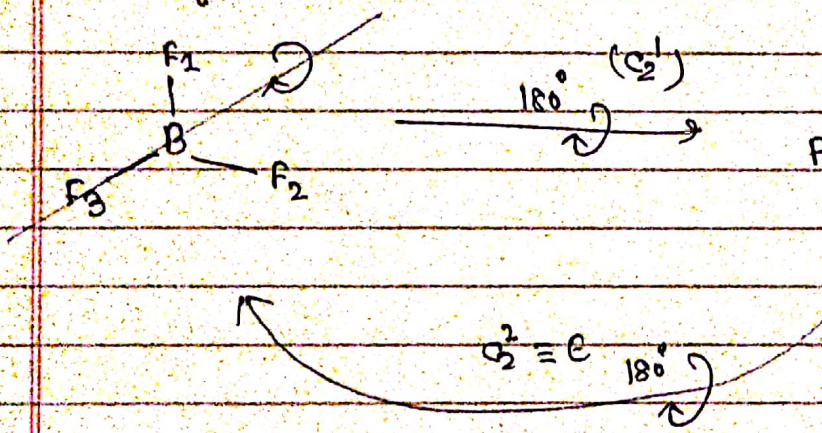
Symmetry element

C_2

Symmetry operation.

C_2', E

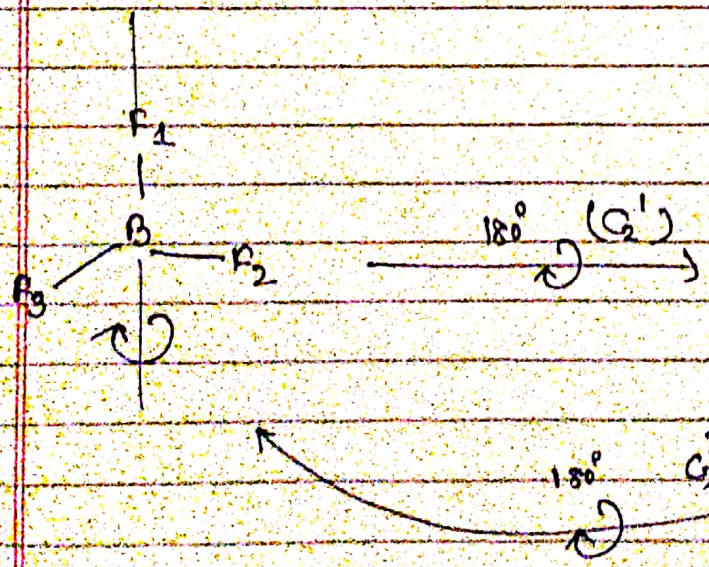
Similarly,



Symmetry element – C_2

Symmetry operation –

C_2', E.



Symmetry element – C_2

Symmetry operation –

C_2', E.

Total symmetry operation - $3C_2$.
(Note - C_2 is called subsidary axis).

(3). Reflection -

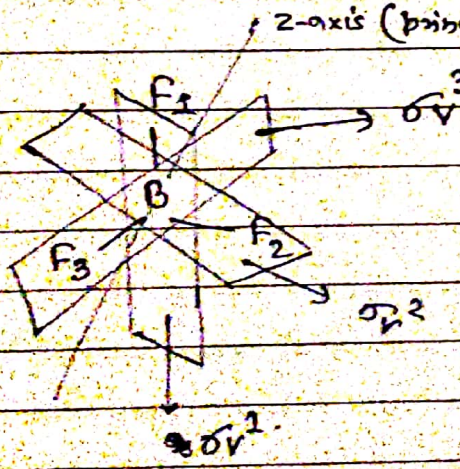
If we perform operation through a plane (xy, yz & xz) and get similar configuration then this operation is called reflection. It is denoted by σ.

There are three types of reflection -

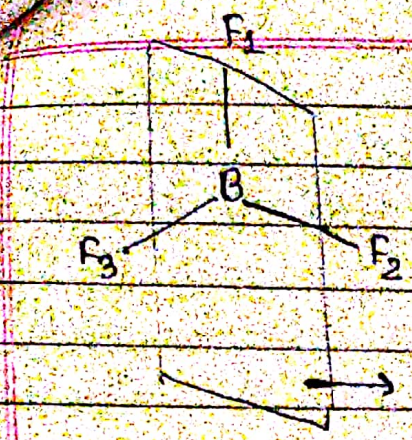
1). Vertical plane of symmetry → σ_v
It contain Principal axis (C_n).

2) Horizontal plane of symmetry → σ_h
It is ⊥ to the Principal axis (C_n).

3) Dihedral plane of symmetry → σ_d.
It contain principal axis (C_n) and bifercate two Sub-sideary axis.



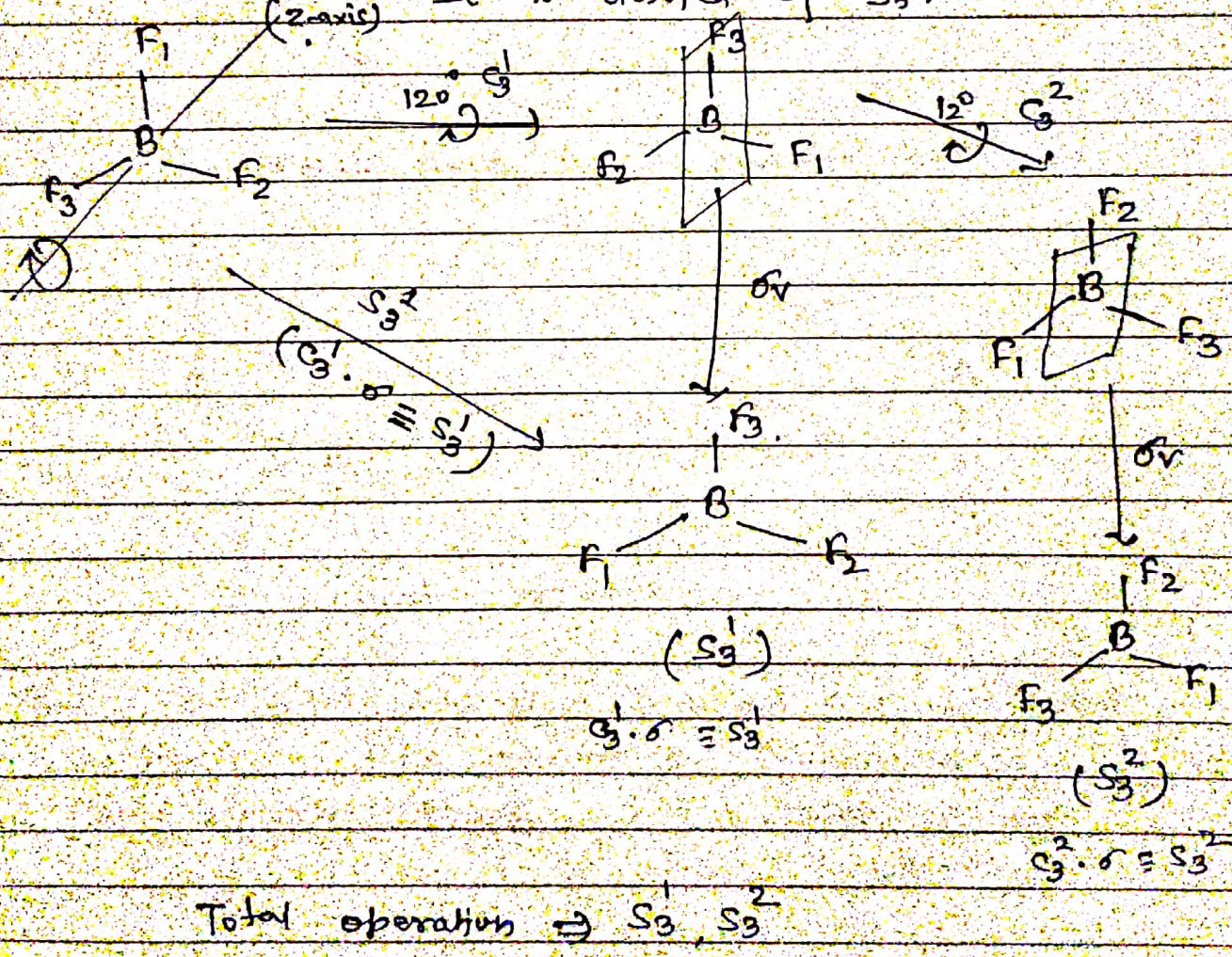
Total operation ⇒ $3\sigma_v$.



Molecular plane has also a plane of symmetry called σ_h. ($\perp$ to C_n).

4) Improper axis of rotation :-

Rotation followed by reflection called improper axis of rotation. It is denoted by S_n.



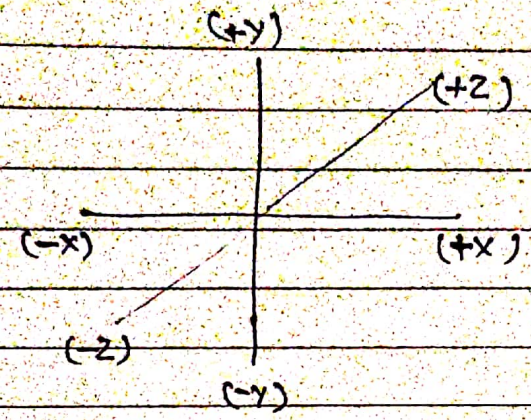
Total operation $\Rightarrow S_3^1, S_3^2$

$\Rightarrow 2S_3$.

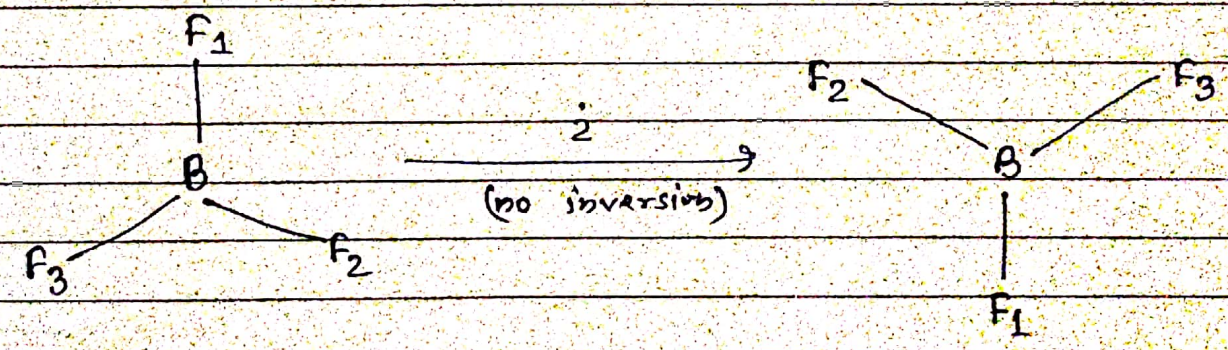
(5) Inversion :-

It represents reflection of all atoms through a point (centre) in the molecule.

Let us consider a point $P(x, y, z)$ lying in first quadrangle. It generates $P'(-x, -y, -z)$ after the process of inversion.



In BF_3 molecule, there is no inversion centre.



No inversion operation.

Thus, the total symmetry elements and symmetry operations in BF_3 molecule is summarised as -

Total symmetry Elements	Total Symmetry operation
E	E
C_3	C_3^1 C_3^2 $(2C_3)$
C_2	B_2^1, C_2^1, C_2^1 $(3C_2)$
σ	$3\sigma_v, \sigma_h$

S_3 S_3^1, S_3^2 $(2S_3)$

Thus, In BF_3 molecule total 12 symmetry operations occurs.

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