Symmetry in Chemistry

Symmetry:- Symmetry is a geometrical properties in which the structure is proportion and well balanced.

Symmetry Operations:-

A symmetry operation is a movement of a body such that after the movement has been carried out, every point of the body is coinciden with an equivalent point (or the same point) of the body in its original orientation.

Ultimately we can define the symmetry operation as the geometrical operation such as reflection, rotation, inversion etc. which leads to a configuration indistinguishable from the original.

It means the two configurations are not exactly identical, but they look like in all respects.

Symmetry Elements:-

A symmetry element is a geometrical entity such as a line, a plane, or a point with respect to which one or more symmetry operations may be carried out.

Or

A line, A plain or a point with respect to which one or more symmetry operations can be carried out is called symmetry element.

Role of Symmetry elements and Symmetry Operations

Symmetry elements and symmetry operations are so closely interrelated because the operation can be defined only with respect to the element, and the same time the existence of a symmetry element can be demonstrated only by showing that the appropriate symmetry operation exist. Thus, since the existance of the element is contingent on the existence of the operation or operations and viceversa. The related types of elements and operations are tables as follows.

Symmetry Elements		Symmetry Operation
1. Centre of symmetry or Inversion Centre	→	Inversion of all atoms through the Centre
2. Plane of symmetry	→	Reflection in the plane.
3. Proper axis	→	One or more rotation about the axis.
4. Improper axis	→	One or more repetitions of the sequence: rotation followed by reflection in a plane perpendicular to the rotation axis.

Symmetry Operations

1. Identity (E): -

It is an "operation of doing nothing."
When we do not do anything and leave the system unchanged and identical to the original system in all respects, the operation is called Identity.
and it is denoted by 'E'.
identity is represented as symbol E.

2. Centre of Symmetry

or

Inversion Centre: -

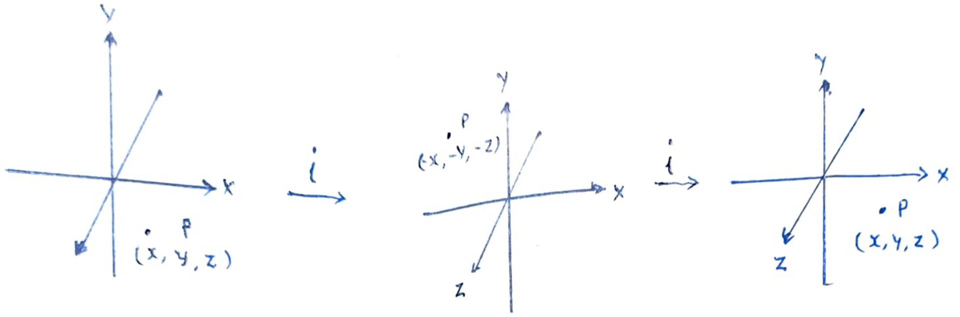
If a molecule can be brought into an equivalent configuration by changing the co-ordinates (x, y, z) of every atom,
where the co-ordinates origin point lies within at a point in atom,
or
where the origin of co-ordinates lies at a point within the molecule, into (-x, -y, -z), then the point at which origin lies is said to be a centre of symmetry or centre of inversion.

In other words, this is an imaginary point in the centre of the molecule, though which the reflection of each atom can be carried out, to result in its co-incidence with an equivalent atom.

The symbol for the inversion centre or for the operation of inversion is represented or denoted by '*i*' (italic *i*)

All atoms in the molecule are inverted during an inversion operation, except the atom at the Centre of Symmetry. The unpaired atom (if any) has to be at the Centre of Symmetry. Thus, a molecule with more than one unpaired atom will not have Centre of Symmetry.

Inversion operation can be shown as follows.



On the basis of above structure it is obvious that repeat of inversion operation (i^2) gives initial representation.

Hence $i^n = E$ (where E is identity)
If n is even

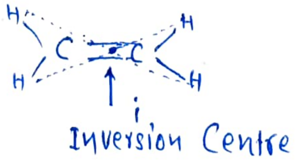
and

$i^n = i$

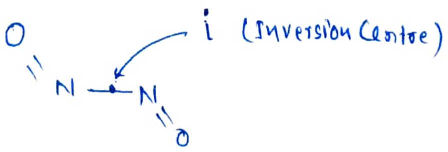
If n is odd.

Examples: Molecules have Centre of Symmetry.

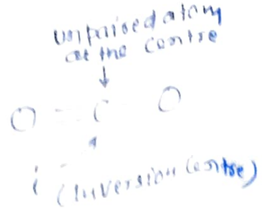
(1) C_2H_4



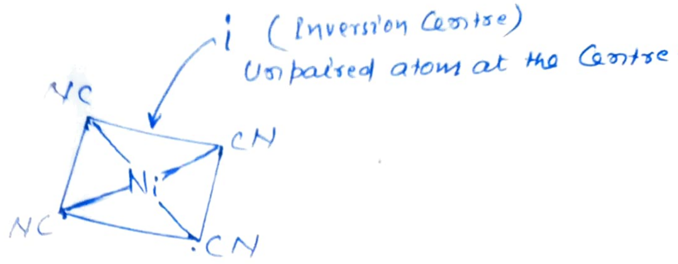
(2) N_2O_2



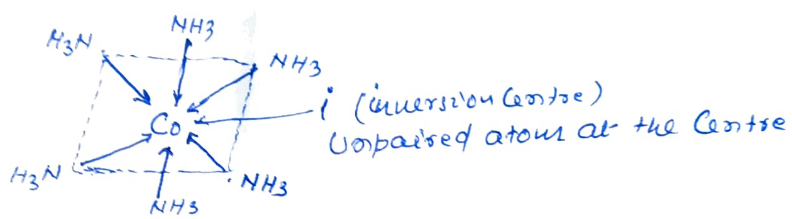
(3) CO_2



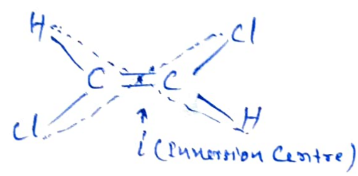
(4) $[Ni(CN)_4]^{2-}$



(5) $[Co(NH_3)_6]$



(6) trans - $C_2H_2Cl_2$



(7) Benzene :- C_6H_6

(8) P- disubstituted Benzene

However, there are some molecules which do not have a Centre of Symmetry.

Examples are (i) CH_4 (ii) Cis $C_2H_2Cl_2$

(iii) O- disubstituted Benzen

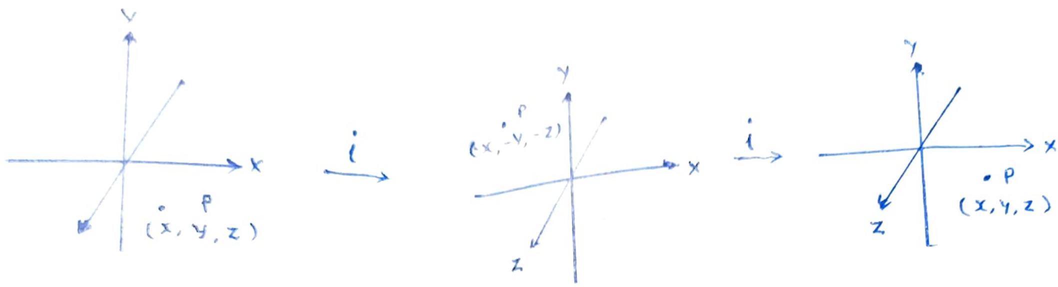
(iv) m - disubstituted Benzene

etc.

Its Structure may be represented as follows.

All atoms in the molecule except the atom at the Centre of Symmetry are inverted during an inversion operation. The unpaired atom (if any) has to be at the Centre of Symmetry. Thus, a molecule with more than one unpaired atom will not have Centre of Symmetry.

Inversion operation can be shown as follows.



On the basis of above structure it is obvious that repeat of inversion operation (i^2) gives initial representation.

Hence $i^n = E$ (where E is identity) if n is even

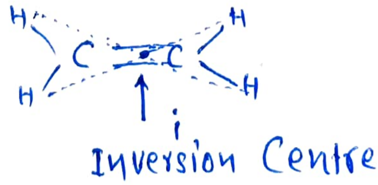
and

$i^n = i$

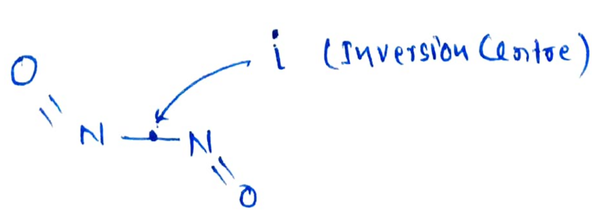
if n is odd.

Examples: Molecules have Centre of Symmetry.

(1) C_2H_4



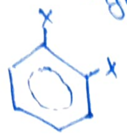
(2) N_2O_2



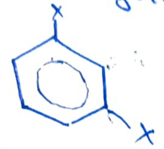
CH_4

Cis - $C_2H_2Cl_2$

O - distributed Benzene



m - distributed Benzene



Axis of Symmetry

or

(Rotation about an axis) C_n -

Axis of Symmetry is an imaginary axis passing through the molecule, around which the molecule can be rotated clockwise to take the nuclear frame work from one position to another indistinguishable position.

i.e the rotation around the axis takes the molecules from one orientation to another equivalent orientation.

This is represented by C_n

where n being the order of the axis.

Hence, if θ is the smallest angle by which we rotate the object with respect to an axis and get an indistinguishable configuration, the rotation is referred to as a symmetry operation, C_n. Where

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

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 consider 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 consider as principal axis or z axis. So an axis passing through a large number of bonds is consider as z axis or Principal axis.

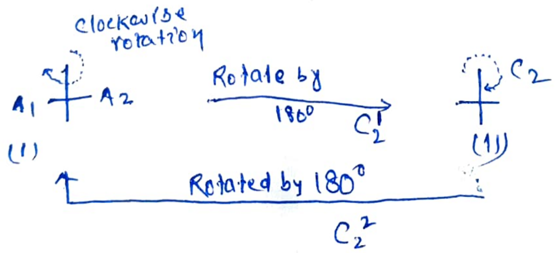
(3) In a planar molecule the rotational axis perpendicular to the plane of the molecule is taken as Z-axis.

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 $\theta = 180°$

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.