

Fundamentals Of Group Theory



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Introduction

- It is extremely important aspect in the study of chemical bonding, spectroscopy etc.
- Group Theory** is the systematic discussion of symmetry incorporating mathematical principles
- An object is said to possess **Symmetry** if it can take up two or more spatial orientations that are indistinguishable from each other i.e, if it can take up two or more equivalent orientations.



Symmetry operation and symmetry element

- A **symmetry operation** is an action which when performed on a molecule yields a new orientation of it that is indistinguishable from the original though not necessarily identical with it
- A **symmetry element** is a geometrical entity such as a line, a plane or a point with respect to which a symmetry operation may be performed.
- The existence of a symmetry element is dependent on the existence of a symmetry operation and vice versa.



Elements of symmetry and the associated symmetry operations



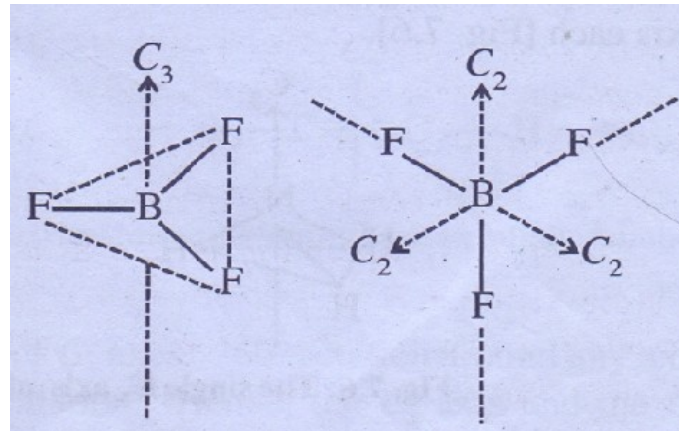
Identity operation- identity element

- ❖ identity operation is one that leaves the **system unchanged**
- ❖
- ❖ The symmetry element associated with the identity operation is called the identity element and is given the symbol **E**
- ❖ The identity operation is trivial and all molecules possess the identity element, the concept is very important while considering sequential symmetry operations and mathematically very useful in the application of group theory



Proper rotation operation- proper rotation axis

- A proper rotation axis or an axis of symmetry is a line about which rotation through a certain angle brings an object into an orientation that is indistinguishable and superimposable on the original.
- The axis of symmetry is a symmetry element – C_n
- The highest fold proper rotation axis is considered as the **principal axis**



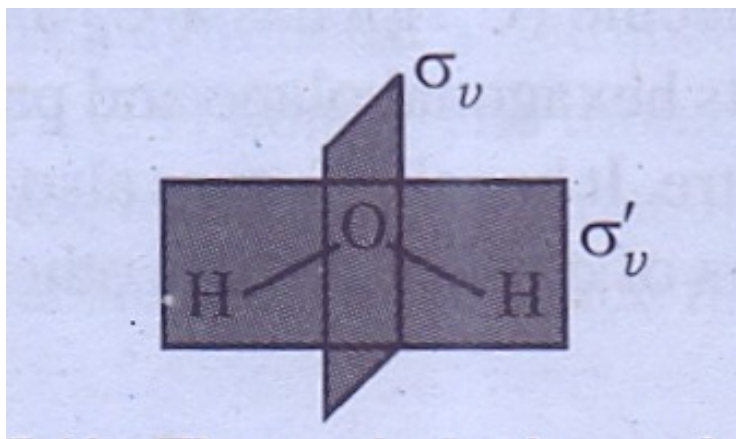


The reflection operation- plane of symmetry or mirror plane

- ❖ If reflection of all the atoms of molecule through a plane bisecting the molecule gives a configuration equivalent to the original one, the molecule is said to have a plane of symmetry - σ
- ❖ A symmetry plane that contains the principal axis of the molecule is called a vertical plane of symmetry - σ_v
- ❖ A symmetry plane perpendicular to the direction of the principal axis of the molecule is called horizontal plane of symmetry - σ_h



- ❖ A symmetry plane that contains the principal axis and at the same time bisects the angle between two similar C_2 axes adjacent to it in the molecule is called a dihedral plane of symmetry – σ_d

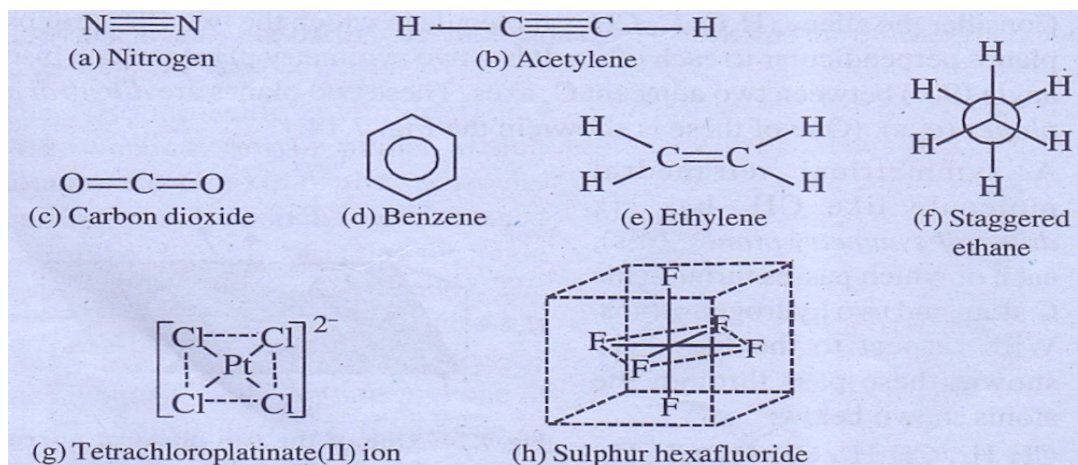


- ❖ The water molecule has two symmetry planes perpendicular to each other. Both contain the C_2 axis and are thus vertical symmetry planes, represented as σ_v and σ'_v



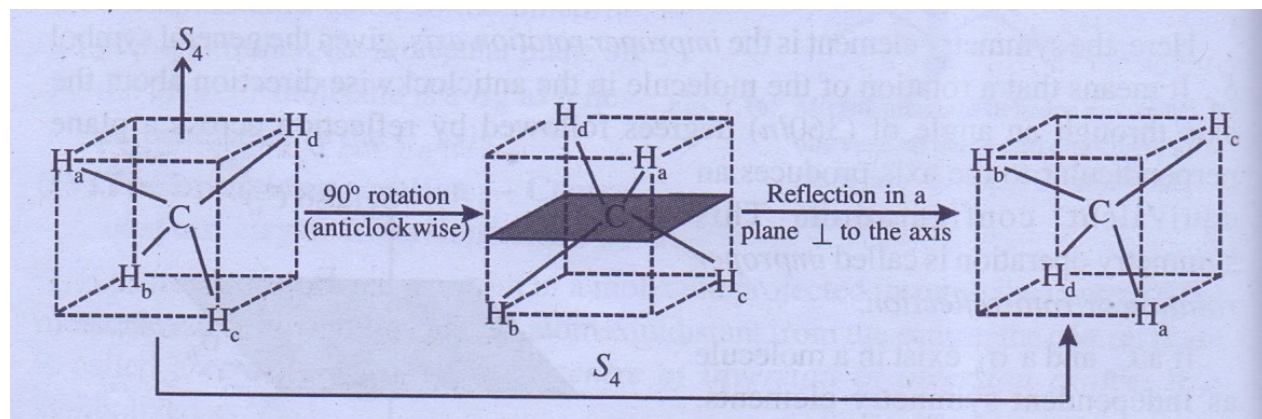
The inversion operation- Centre of symmetry

- ❖ If a straight line from any atom in a molecule projected through the Centre of the molecule encounters an equivalent atom equidistant from the Centre, the central point is called a Centre of symmetry or Centre of inversion - **i**



Improper rotation operation – improper rotation axis

- ❖ If rotation of a molecule about an axis through a certain angle followed by reflection in a plane perpendicular to the axis yields an equivalent configuration the axis is called an improper rotation axis or roto-reflection axis- S_n





Introduction to group theory

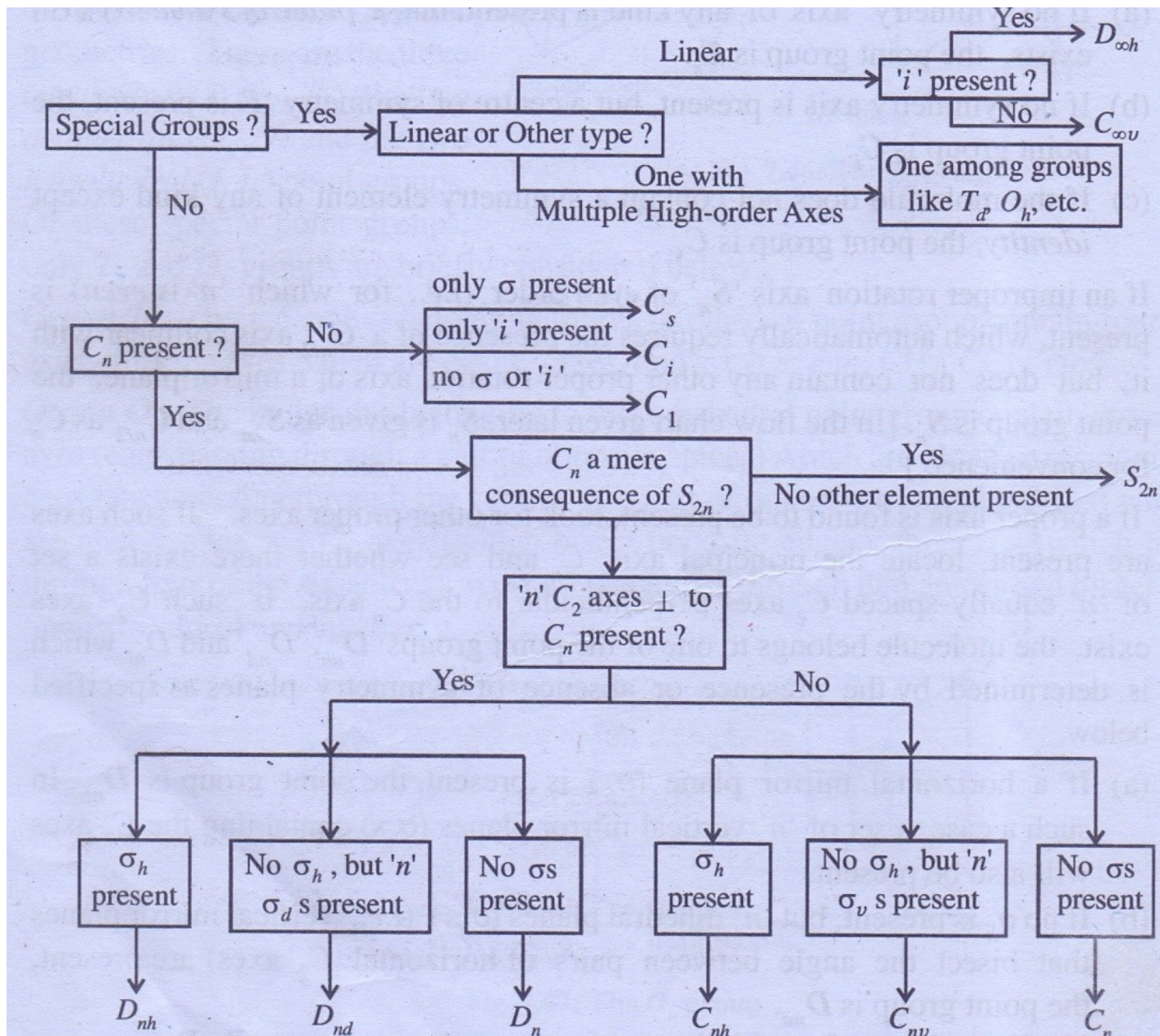


Mathematical groups and point group

- ❖ A group is a collection of mathematical objects known as elements or members which are related to each other according to certain rules called closure rule, identity rule, associative rule and inverse rule
- ❖ A point group is set of all the symmetry operation, the action which leaves at least one point of the molecule unmoved or invariant.



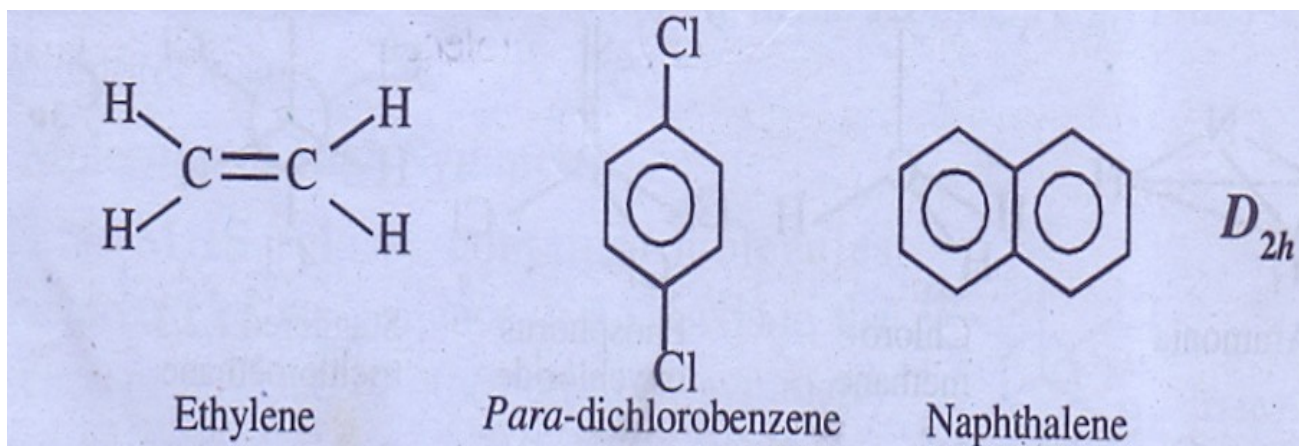
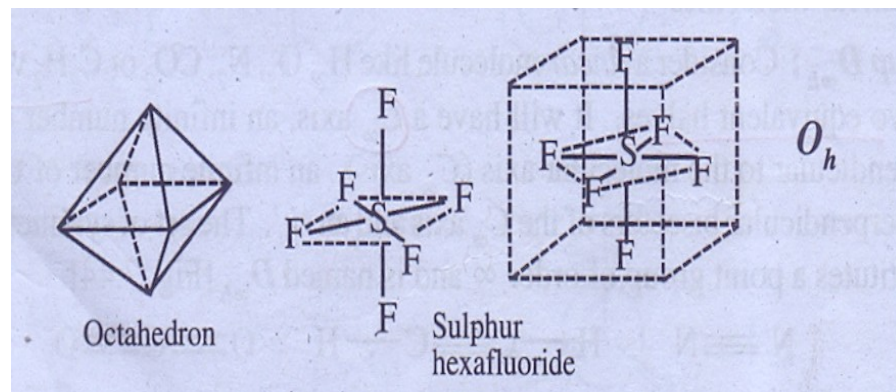
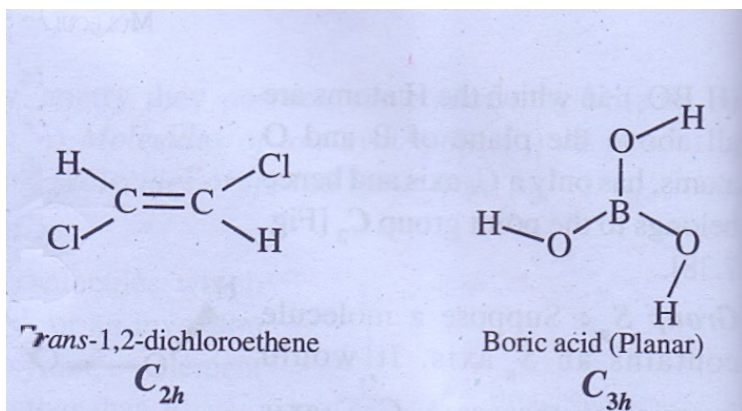
A systematic procedure for the identification of point groups

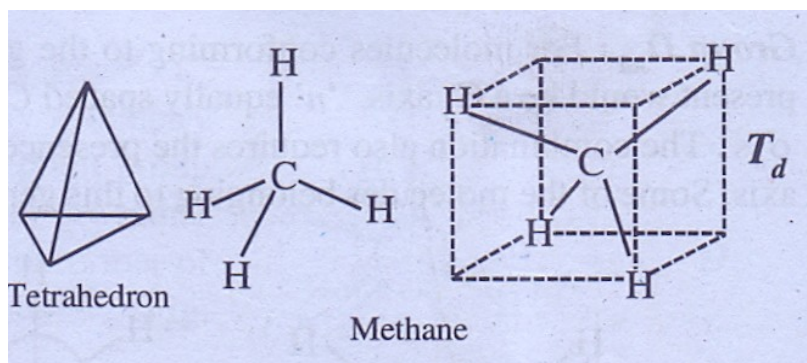
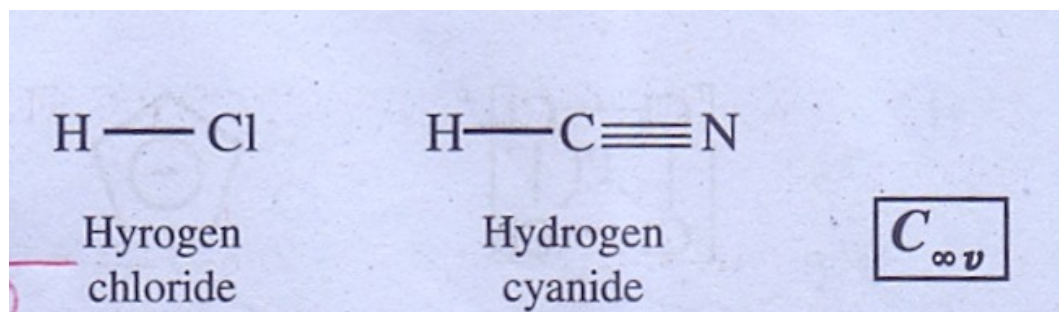
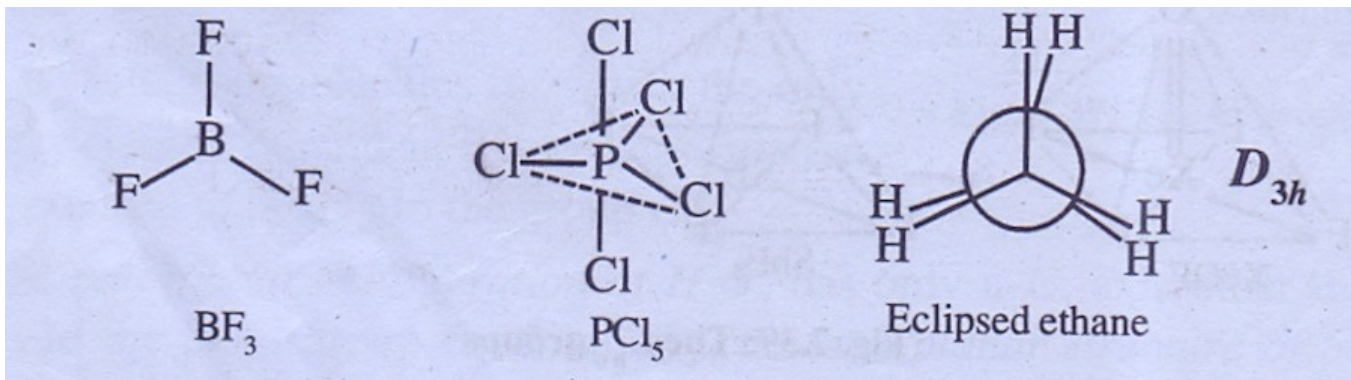




- ❖ Finite groups- there will be limited number of elements. eg: C_{2v} , C_{3v} , C_{2h} etc
- ❖ Infinite group- there will be an unlimited number of elements. Eg: $C_{\infty v}$, $D_{\infty h}$
- ❖ Abelian group – a group in which all elements commute with each other .eg: C_{2v}
- ❖ Non abelian group –a group for which multiplication is not commutative for some pairs of its elements. Eg: C_{3v}

Examples







Reference

- ❖ Principles of physical chemistry-puri sharma pathania
- ❖ Chemical application of group theory-F.A. Cotton-third edition