

Determination of Point Group Symmetry

Group theory is a branch of mathematics.

Members of a given group are called elements.

A collection of elements may constitute a group provided certain conditions are met.

These elements of a group are “things”; they could be numbers in a number system ,or symmetry operations or something else.

These elements will constitute a group if they obey certain rules. In fact the definition of a group is a collection of elements which follow a particular set of rules . (The rules need not concern us at the moment.)

The area of group theory in which we have interest is involved with symmetry. It can be shown for a given molecule that the complete collection of symmetry operations associated with the molecule constitutes a mathematical group

In order for symmetry operations to exist there must be symmetry elements present. For example for a reflection to exist there must be a mirror plane.

If a symmetry element is present we can perform a symmetry operation about that element and leave the molecule in an equivalent arrangement. The arrangement may or may not be the same before and after the symmetry operation. The before and after arrangements must however be indistinguishable---so that if we were not watching the symmetry operation we would not know that it occurred.

(see next page for brief examples)

We are interested in point groups.

For molecular point groups, when a symmetry operation is performed while the atoms may be “moved” (rotated for example) to equivalent positions, there is one point, the center of the molecule, which will not be moved. Such symmetry is called point group symmetry. In point group symmetry the molecule will not undergo translation. (There is also space group symmetry, a topic we will not address, which deals with point group symmetry plus symmetry associated with translation of molecules.)

So point group symmetry is associated with molecules that do not move in position

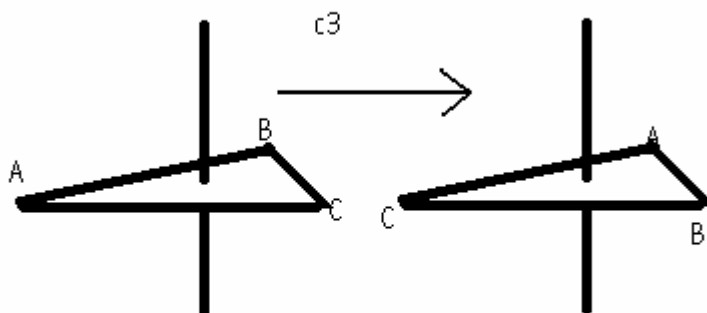
(Space group symmetry involves translation)

Point groups possess some or all of the symmetry operations and elements noted below are:

<u>OPERATION</u>	<u>ELEMENT</u>
Reflection	Mirror plane
Inversion	Center of inversion
Rotation	Axis of rotation
Improper Axis of Rotation	Rotation followed by reflection at right angles to reflection axis
No operation	Identity

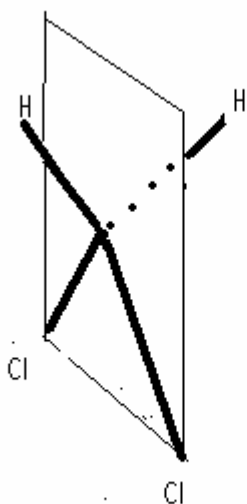
By noting the symmetry elements present in a molecule in a systematic way we can determine the point group to which the molecule belongs. Knowledge of point group symmetry enables one to obtain important molecular information

Example of rotation axis A,B,C are the same atoms



Symbol C_n

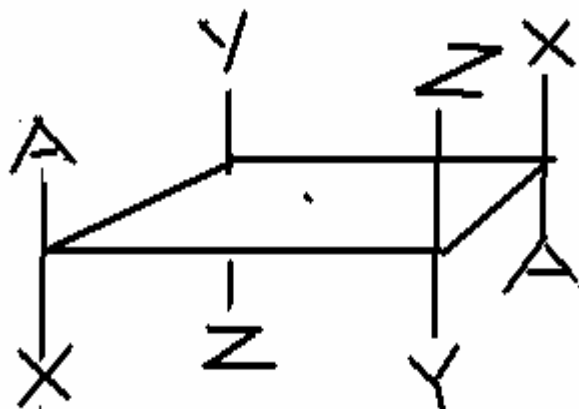
Plane of Symmetry



symbol σ (sigma)

Center of inversion (symbol i)

For a center of inversion to exist every point on the molecule at positions x,y,z must have a corresponding "twin" at $-x,-y,-z$ The center is in center of the molecule



IMPROPER AXIS OF ROTATION

An improper axis of rotation involves a rotation axis and a reflection plane at right angles to the rotation axis. While the two may not actually exist independently, the combined operations should give rise to equivalent molecular arrangements if the axis is present.

The symbol for the Improper Axis of Rotation is S_n

The conformation of ethane illustrated below represents a molecule with an S_6 axis

