

❖ Elements of Symmetry

Elements of symmetry may simply be defined as the point, line or plane inside or passing through the molecular geometry about which some operations like rotation, inversion, or reflection generate indistinguishable images. These operations are generally labeled as symmetry operations. A general discussion on different symmetry elements is given below.

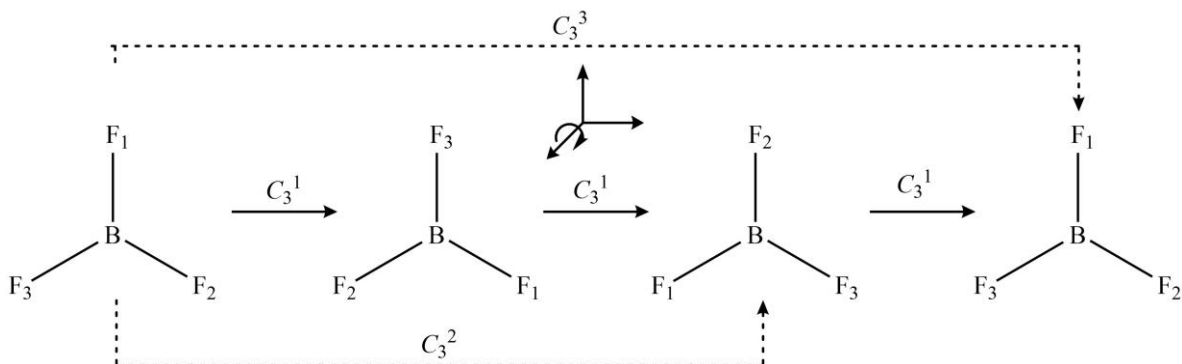
➤ Axis of Rotation (C_n)

The axis of rotation or simply the symmetry axis may simply be defined as the line passing through a molecular geometry about which the rotation through a certain angle generates indistinguishable images.

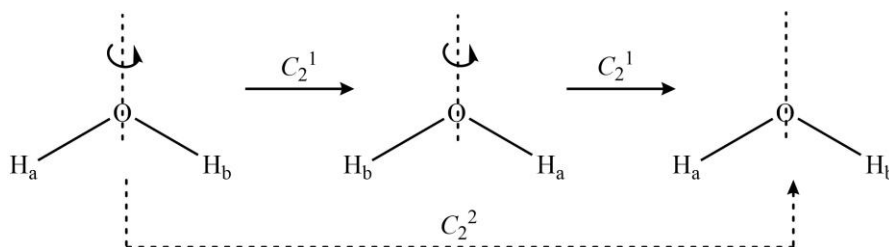
The axis of rotation is generally symbolized by C_n where n can have the value from 1, 2, 3, 4... and so on. The expression for n is

$$n = \frac{360^\circ}{\theta} \quad (5)$$

Where θ is the minimum angle required to generate indistinguishable images. For instance, in the case of a regular trigone or BF_3 molecule, the geometry must be rotated through 120° minimum about the line perpendicular to the molecular plane to get indistinguishable images. Therefore, we can say that it is a C_3 (three-fold) axis of symmetry.



Where C_3^1 , C_3^2 and C_3^3 are the symmetry operations via 120° , 240° , and 360° , respectively. Similarly, for the H_2O molecule, the minimum angle required to generate indistinguishable images is 180° , giving a C_2 axis of symmetry.



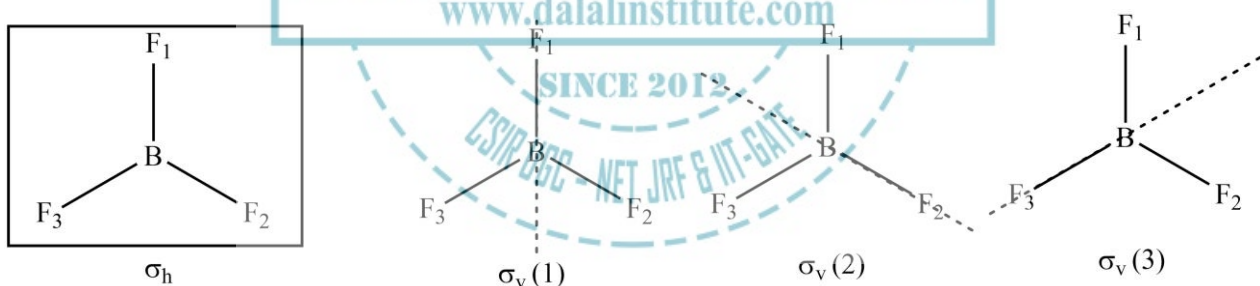
➤ **Plane of Symmetry (σ)**

The plane of symmetry or simply the symmetry plane may be defined as the plane bisecting the molecular geometry in such a way that one half is the mirror image of the other.

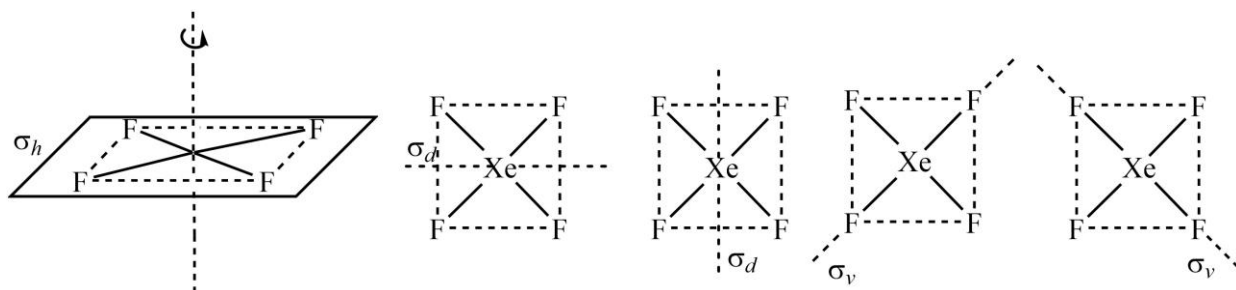
The axis of rotation is generally symbolized by σ_h or σ_v , where the subscript h or v is to denote whether the plane is parallel or perpendicular to the principal axis (symmetry axis of the highest order). There is also a third kind of plane of symmetry called the dihedral plane (σ_d): In other words, we can say that a dihedral plane bisects two σ_v planes. On a final note, a plane of symmetry can also be designated by the Cartesian orientation encompassing it, e.g., (yz -plane) or (xz -plane). For instance, there are two σ_v planes in water molecules as shown below.



Similarly, there are a total of three vertical (σ_v) planes and one horizontal (σ_h) plane in the case of BF_3 molecules as shown below.



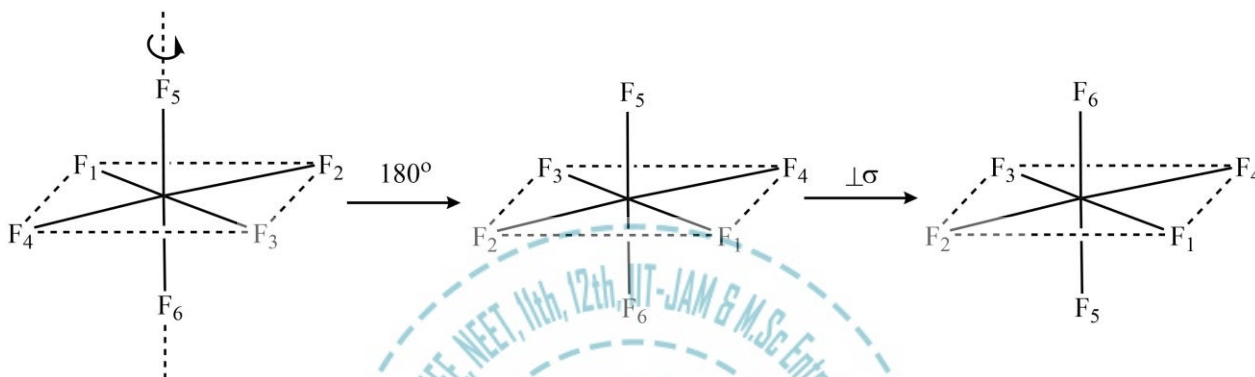
Similarly, there are a total of two vertical (σ_v) planes and one horizontal (σ_h) and two dihedral planes in the case of XeF_4 molecules as shown below.



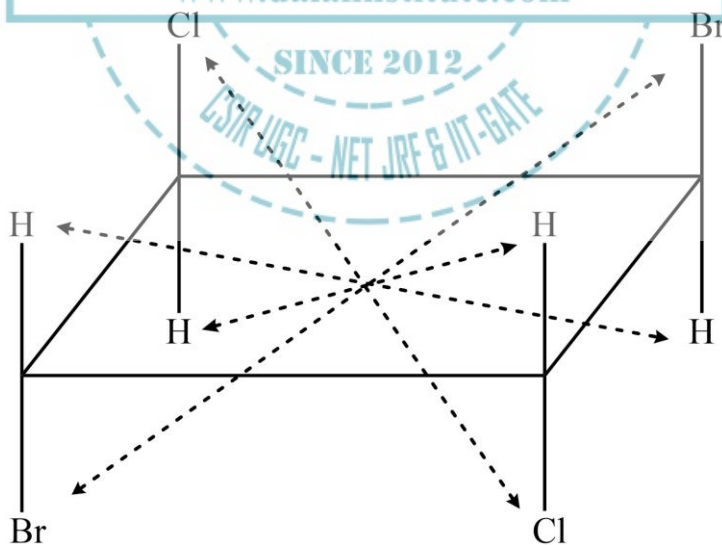
➤ **Center of Symmetry (i)**

The molecular geometry is said to possess the center of symmetry if a rotation through 180° followed by the perpendicular reflection generates an indistinguishable image.

The center of symmetry or simply the 'inversion center' is denoted by the symbol 'i', which is a point inside the geometry at such a position that if an object is inverted about this point, the position vector of any point in an object (say x, y, z) is also inverted ($-x, -y, -z$). For instance, consider the case of the SF_6 molecule.



Similarly, the complete staggered form of CHClBr-CHClBr also possesses the center of symmetry as it produces indistinguishable images after inverting through the center. Furthermore, the center of symmetry in any molecular geometry can also be found by drawing lines of equal length in the opposite direction from the center, provide that similar points are observed.



Similarly, other examples of molecules with the center of symmetry are acetylene, a staggered form of ethane and ethylene.

➤ **Alternating Axis of Symmetry (S_n)**

The alternating axis of symmetry or improper axis of rotation may simply be defined as the line passing through a molecular geometry about which a rotation followed by a perpendicular reflection generates indistinguishable images.

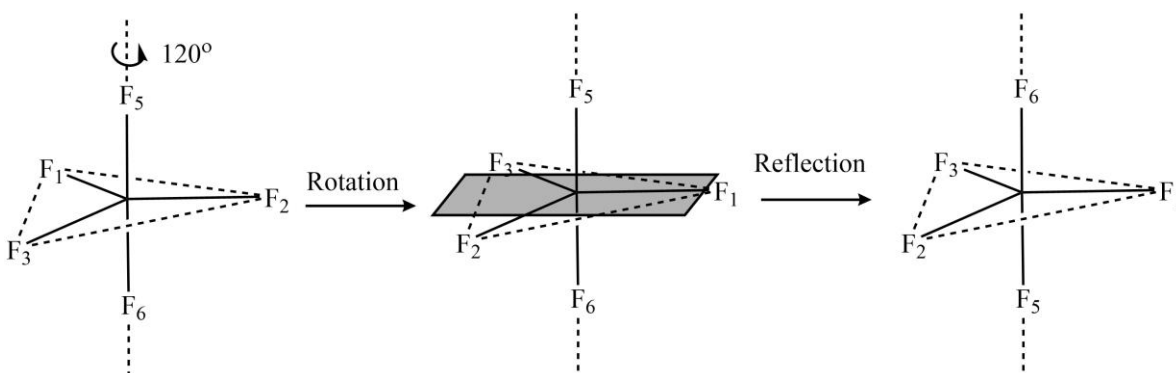
The improper axis of rotation is generally symbolized by S_n where n can have the value from 1, 2, 3, 4... and so on. The expression for n is

$$n = \frac{360^\circ}{\theta} \quad (6)$$

Where θ is the minimum angle required before perpendicular reflection to generate indistinguishable images. For instance, in the case of a regular trigone or CH_4 molecule, the geometry must be rotated through 90° before the reflection in a perpendicular plane is carried out to get indistinguishable images. Therefore, we can say that it is an S_4 (four-fold) alternating axis of symmetry.



Similarly, for the BF_3 molecule, indistinguishable images can also be obtained by rotating the molecule through 120° about a line perpendicular to the molecular plane followed by the reflection. Therefore, we can say that it is an S_3 (three-fold) alternating axis of symmetry.



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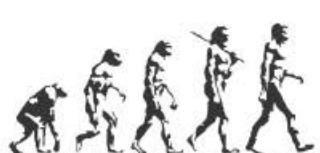
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Volume I

MANDEEP DALAL



First Edition

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