Point Groups

Molecules are classified and grouped based on their symmetry. Molecules with similar symmetry are into the same *point group*. A point group contains all the molecular symmetries that leave a point invariant, and also any distance to that point.

Symmetry Elements

Symmetry elements are mirror planes, axis of rotation, centers of inversion, etc.

A molecule has a given symmetry element if the operation leaves the molecule <u>appearing</u> as if nothing has changed (even though atoms and bonds may have been moved.)

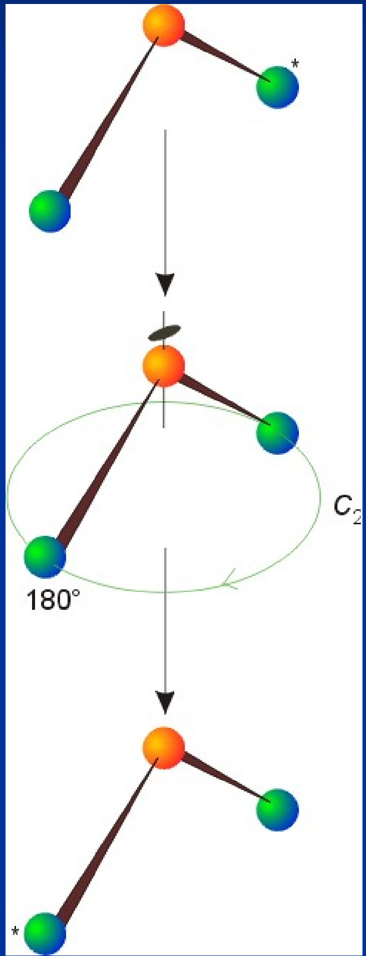
Symmetry Elements

Element	Symmetry Operation	Symbol
	Identity	E
n-fold axis	Rotation by $2\pi/n$	C_n
Mirror plane	Reflection	σ
Center of inversion	Inversion	I
n-fold axis of improper rotation	Rotation by $2\pi/n$ followed by reflection perpendicular to the axis of rotation	S_n

Identity, E

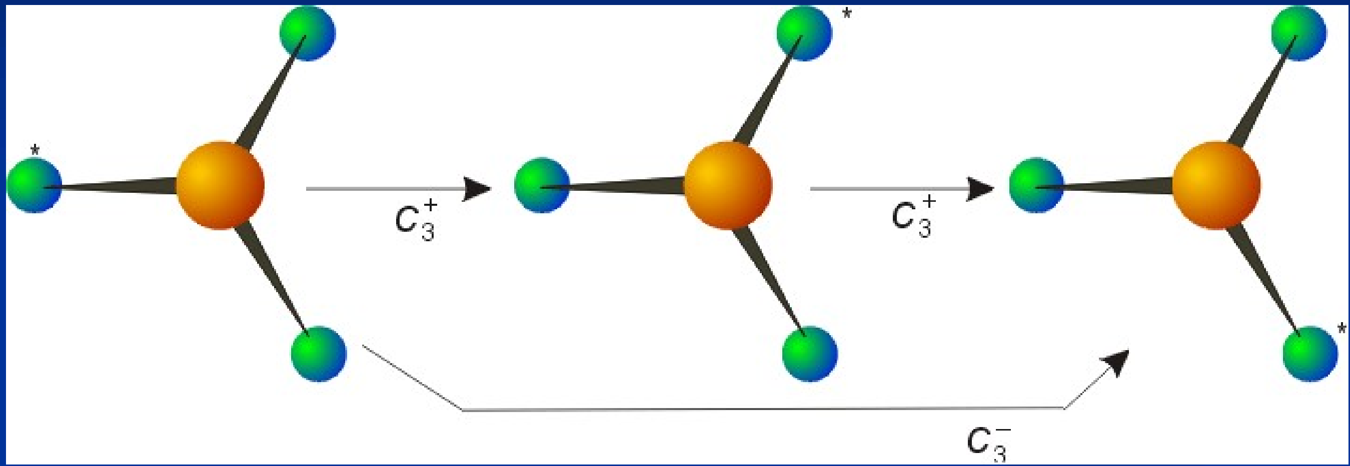
All molecules have Identity. This operation leaves the entire molecule unchanged. A highly asymmetric molecule such as a tetrahedral carbon with 4 different groups attached has only identity, and no other symmetry elements.

n-fold Rotation



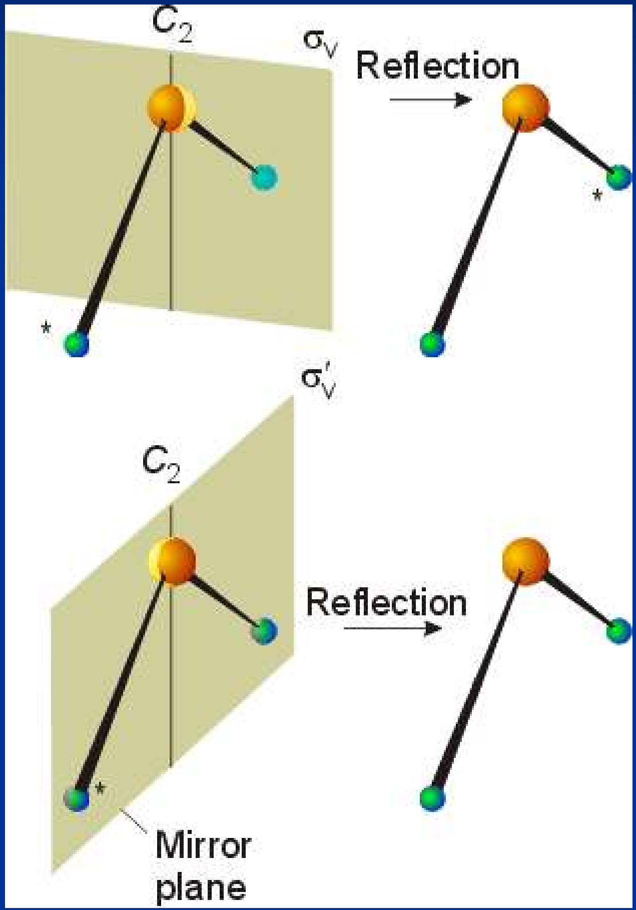
Water has a 2-fold axis of rotation. When rotated by 180°, the hydrogen atoms trade places, but the molecule will look exactly the same.

n-fold Axis of Rotation



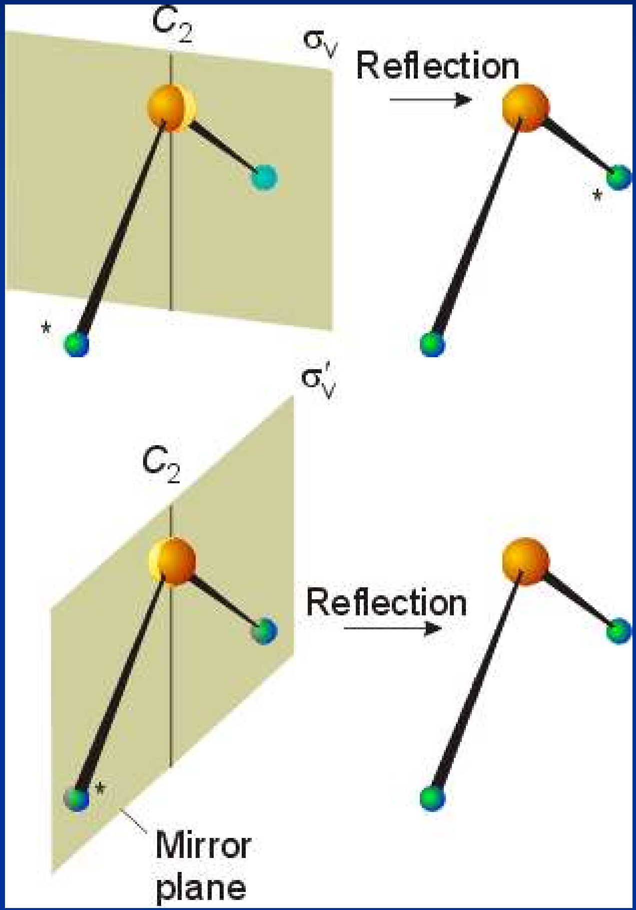
Ammonia has a C_3 axis. Note that there are <u>two</u> operations associated with the C_3 axis. Rotation by 120^o in a clockwise or a counterclockwise direction.

Mirror Planes



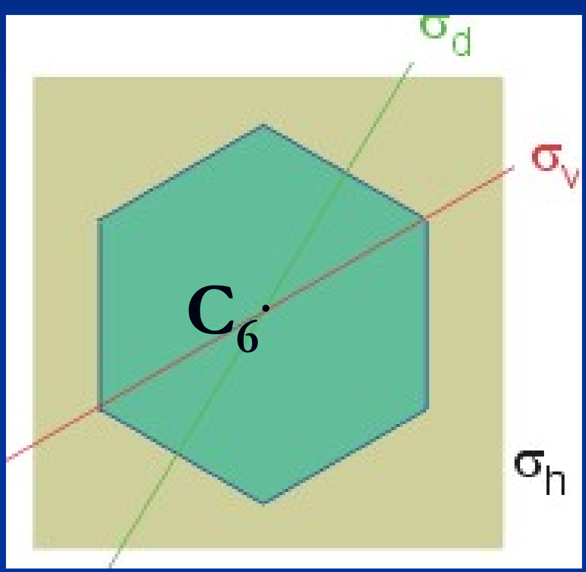
The reflection of the water molecule in either of its two mirror planes results in a molecule that looks unchanged.

Mirror Planes



The subscript "v" in σ_v, indicates a vertical plane of symmetry. This indicates that the mirror plane includes the principal axis of rotation (C_2).

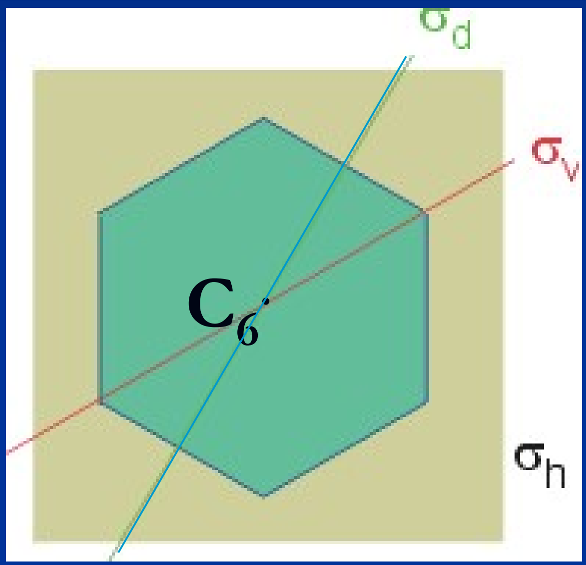
Mirror Planes



The benzene ring has a C_6 axis as its principal axis of rotation.

The molecular plane is perpendicular to the C_6 axis, and is designated as a horizontal plane, σ_h.

Mirror Planes

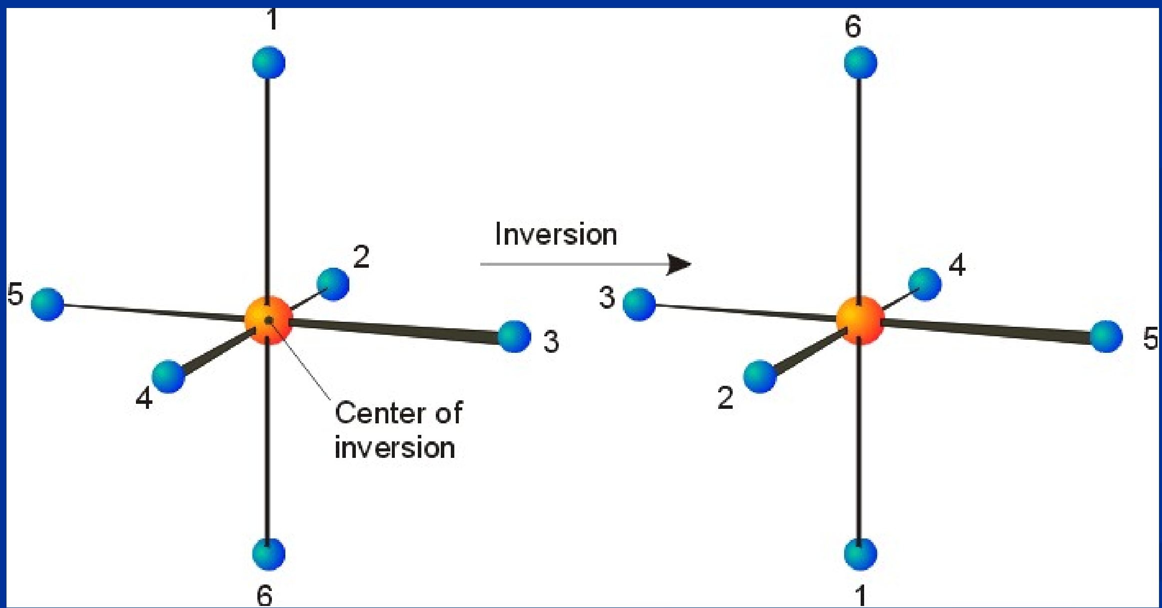


The vertical planes, σ_v, go through the carbon atoms, and include the C_6 axis.

The planes that bisect the bonds are called *dihedral* planes, σ_d.

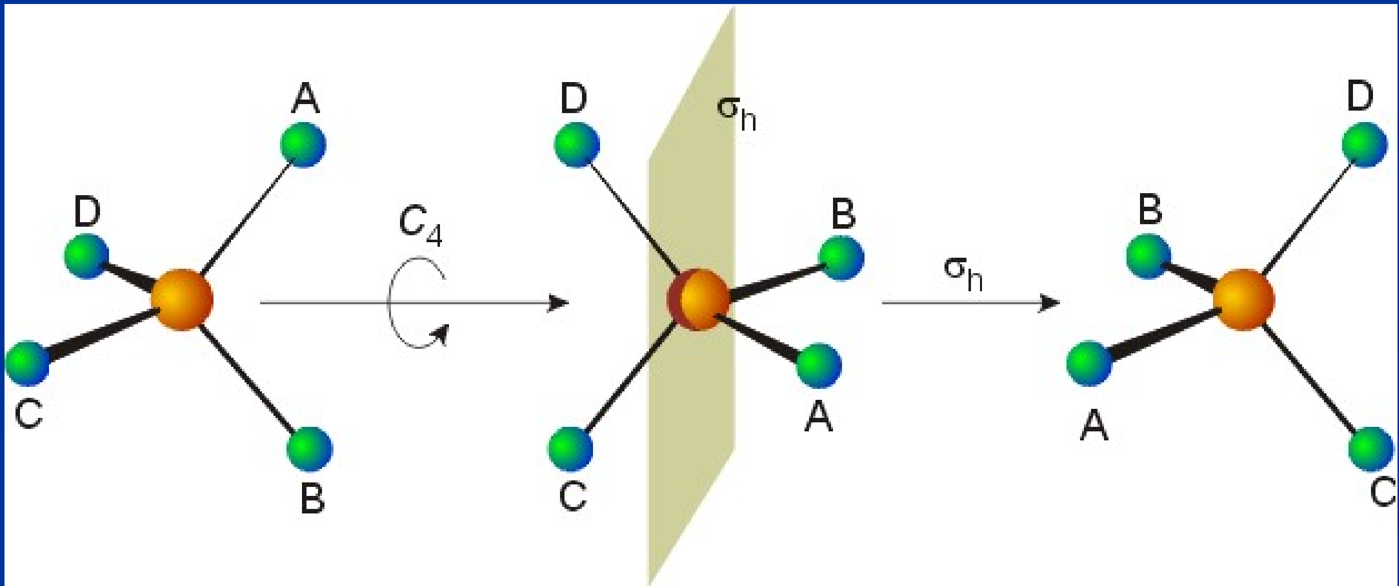
Inversion I

The inversion operation projects each atom through the center of inversion, and across to the other side of the molecule.



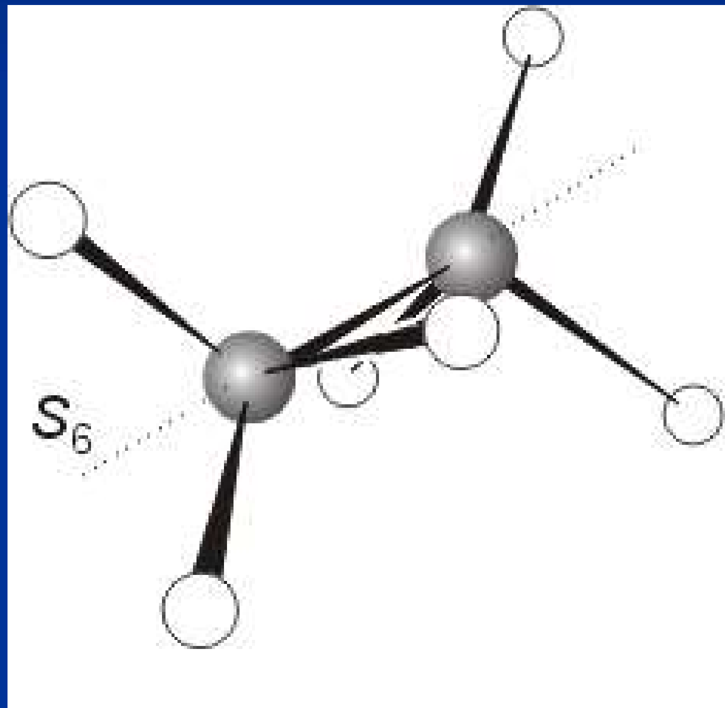
Improper Rotation

An improper rotation is rotation, followed by reflection in the plane perpendicular to the axis of rotation.



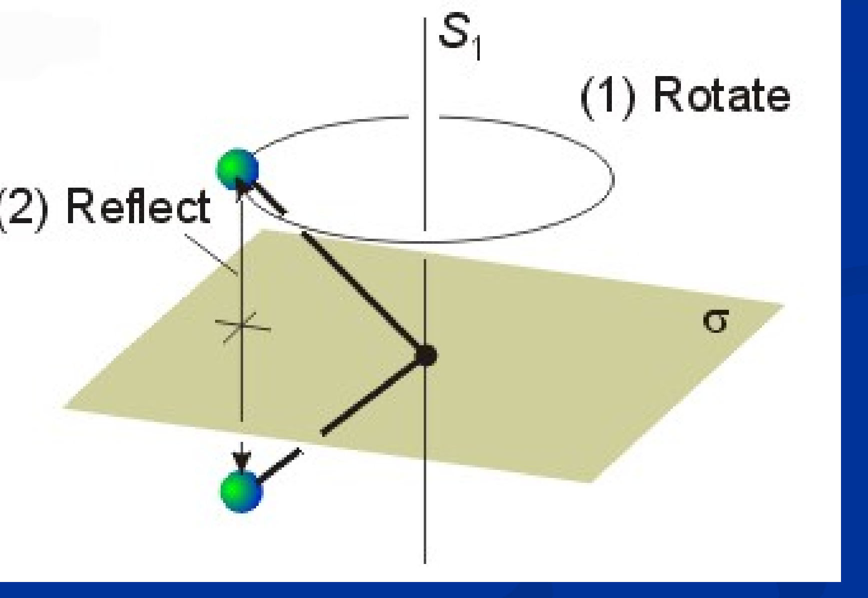
Improper Rotation

The staggered conformation of ethane has an S_6 axis that goes through both carbon atoms.



Improper Rotation

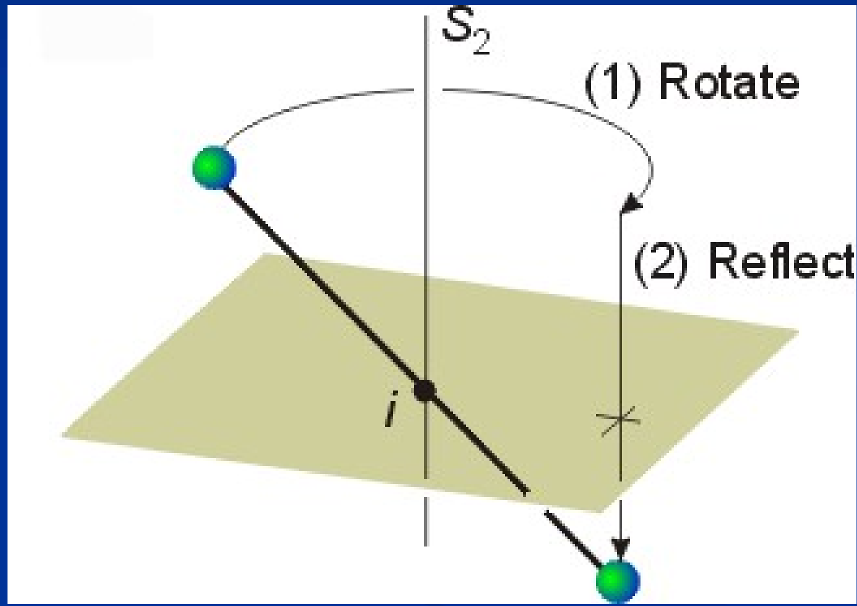
Note that an S_1 axis doesn't exist; it is same as a mirror plane.



Improper Rotation

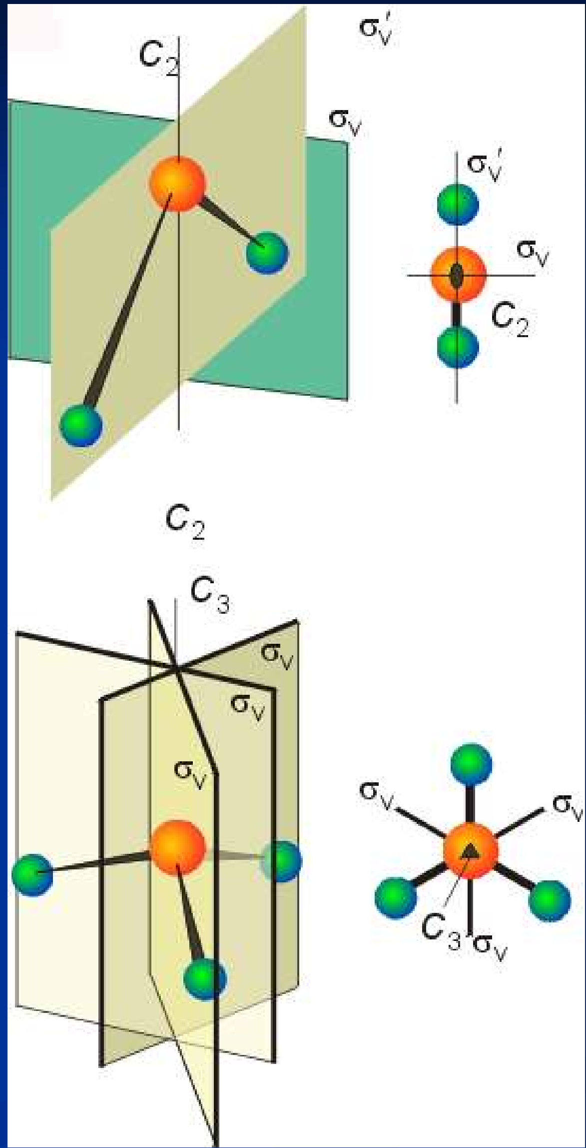
Likewise, an S_2 axis is a center of inversion.

$$S_2 \equiv I$$



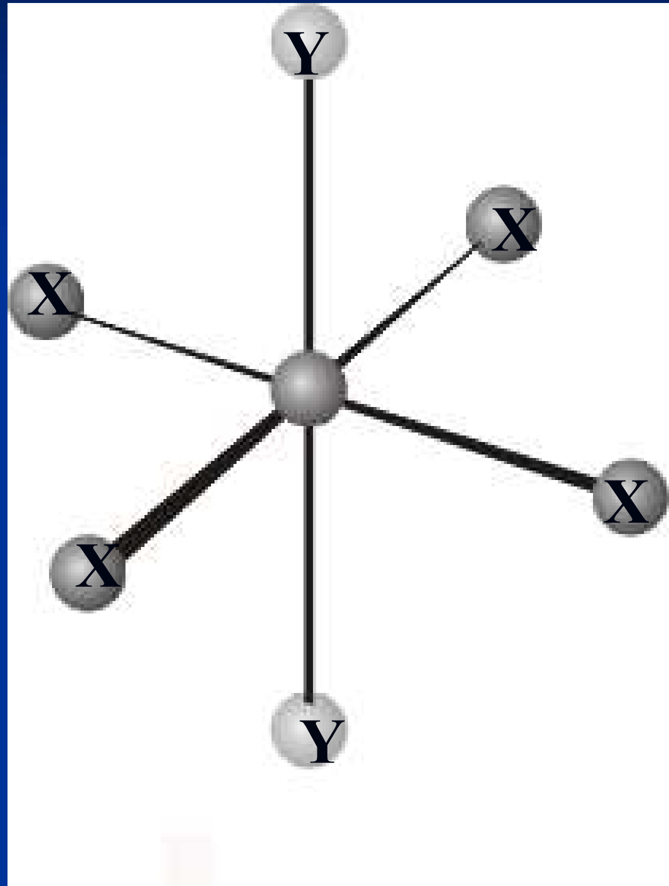
Point Groups

Water and ammonia both belong to the C_{nv} class of molecules. These have vertical planes of reflection, but no horizontal planes.



Point Groups

The D_{nh} groups have a horizontal plane in addition to vertical planes. Many inorganic complexes belong to these symmetry groups.



$[MX_4Y_2]$, D_{4h}

OPERAÇÕES DOS GRUPOS DE PONTO CRISTALINOS

ROTOREFLEXÕES

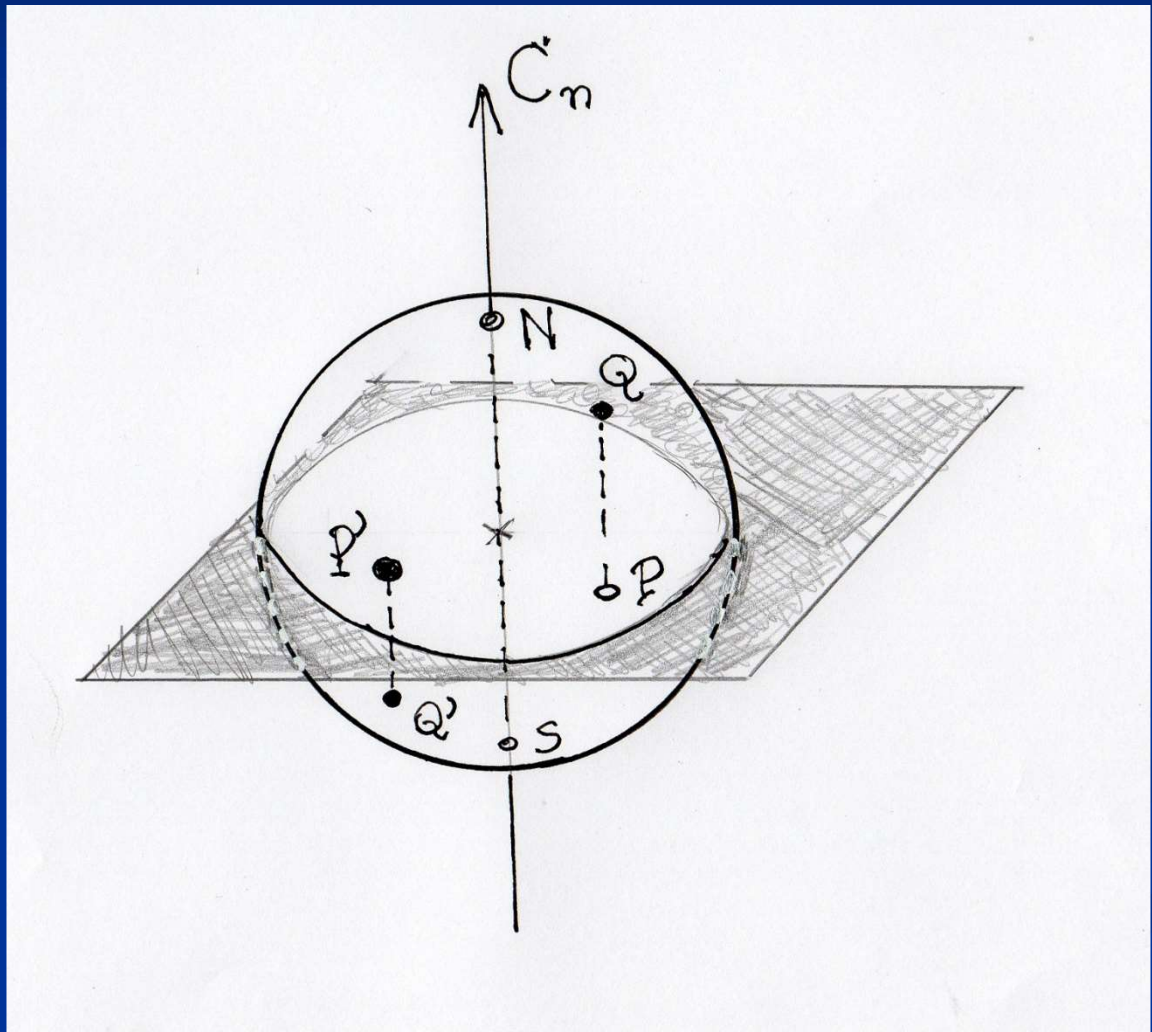
ROTAÇÕES

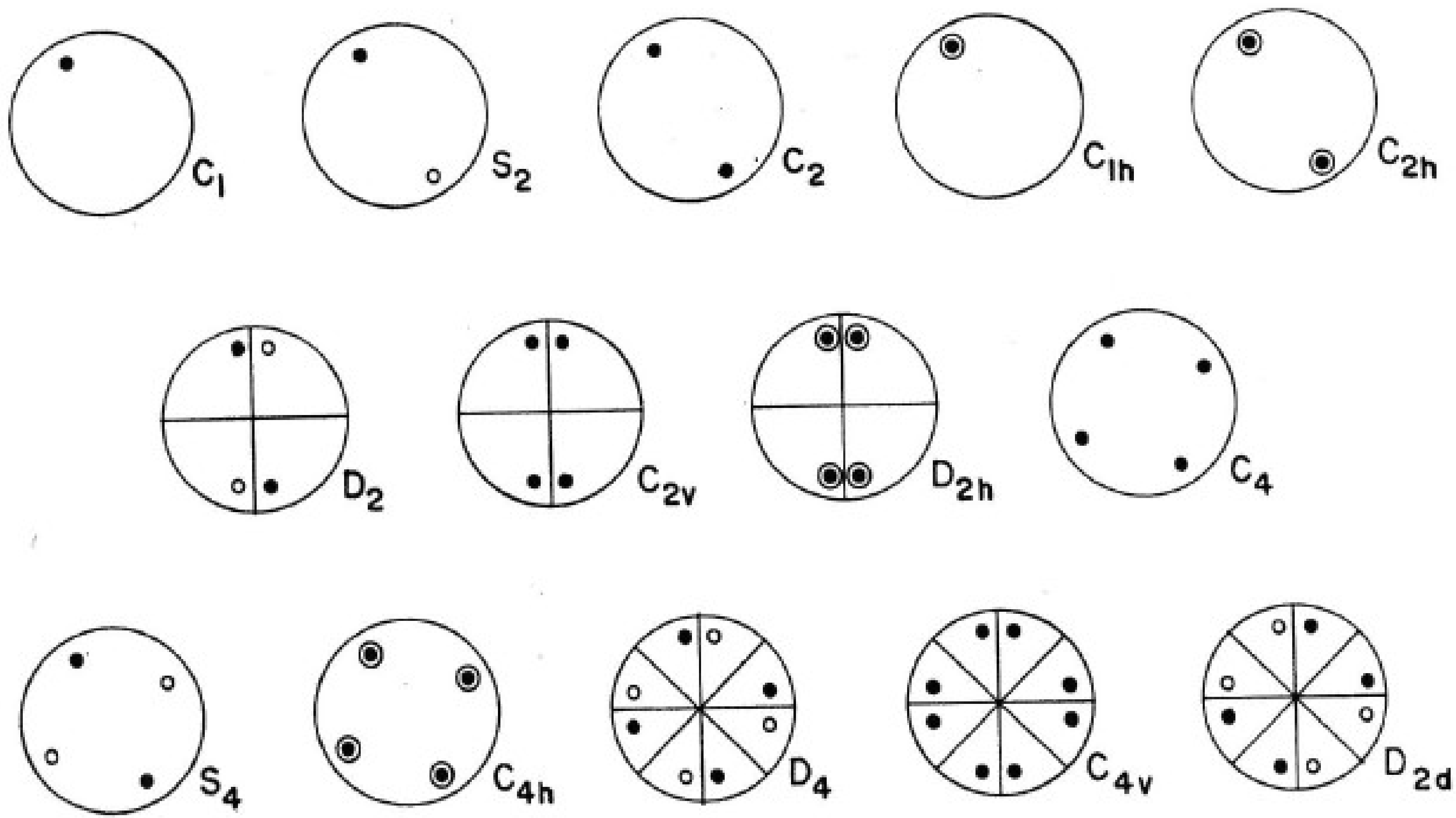
Internacional	Schönflies
1	C_1
2	C_2
3	C_3
3_2	C_3^{-1}
4	C_4
4_3	C_4^{-1}
6	C_6
6_5	C_6^{-1}

REFLEXÕES

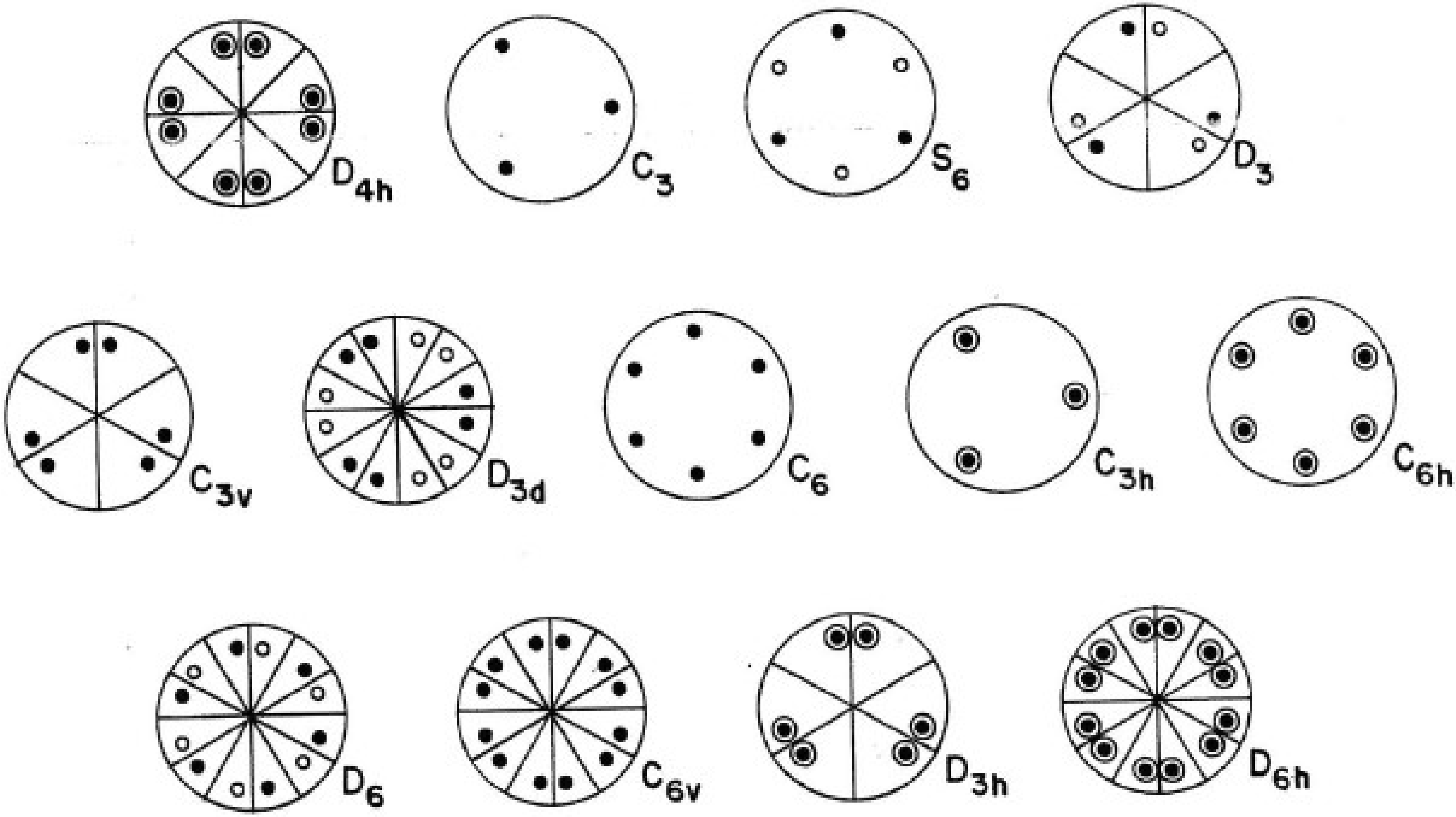
Internacional	Schönflies
$\bar{1}$	$I \equiv S_2$
$\bar{2} \equiv m$	$\sigma \equiv S_1$
$\bar{3}$	S_6^{-1}
$\bar{3}_2$	S_6
$\bar{4}$	S_4^{-1}
$\bar{4}_3$	S_4
$\bar{6}$	S_3^{-1}
$\bar{6}_5$	S_3

Stereographic Projection





C_1
S_2
C_2
C_{1h}
C_{2h}
D_2
C_{2v}
D_{2h}
C_4
S_4
C_{4h}
D_4
C_{4v}
D_{2d}



D4h
C3
S6
D3
C3v
D3d
C6
C3h
C6h
D6
C6v
D3h
D6h

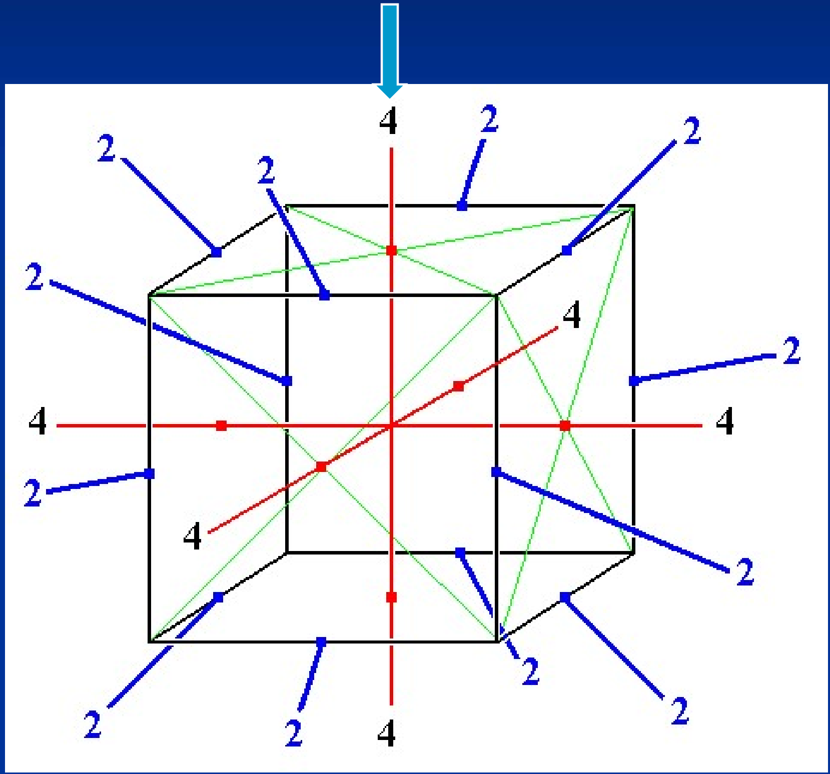
AXIAL GROUPS	GENERATORS
C_n	C_n
C_{nv}	$C_n \, , \sigma_v$
C_{nh}	$C_n \, , \sigma_h$
S_n	$S_n = C_n \sigma_h$
D_n	$C_n \, , U_2 = C'_2$
D_{nh}	$C_n \, , U_2 \, , \sigma_h$
D_{nd}	$C_n \, , U_2 \, , \sigma_d$

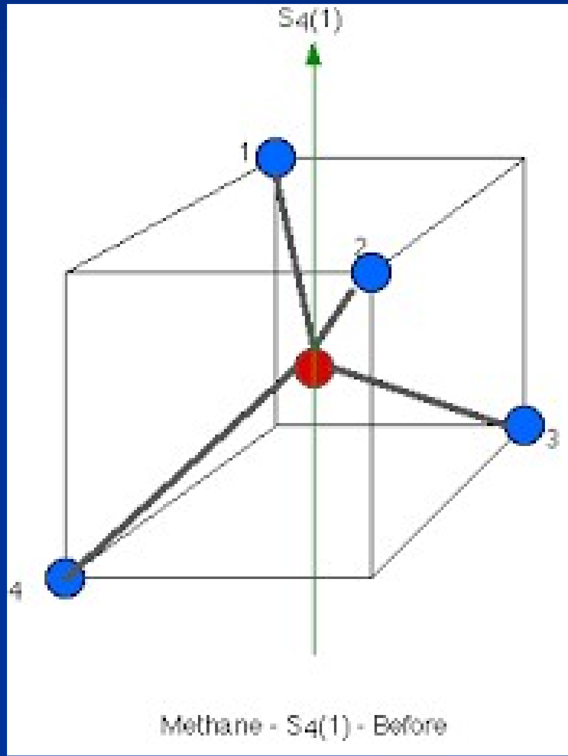
Cubic Groups

Highly symmetrical molecules, such as identically substituted tetrahedrons or octahedrons belong to their own point groups (T_d or O_h respectively).

CUBIC SYMMETRY

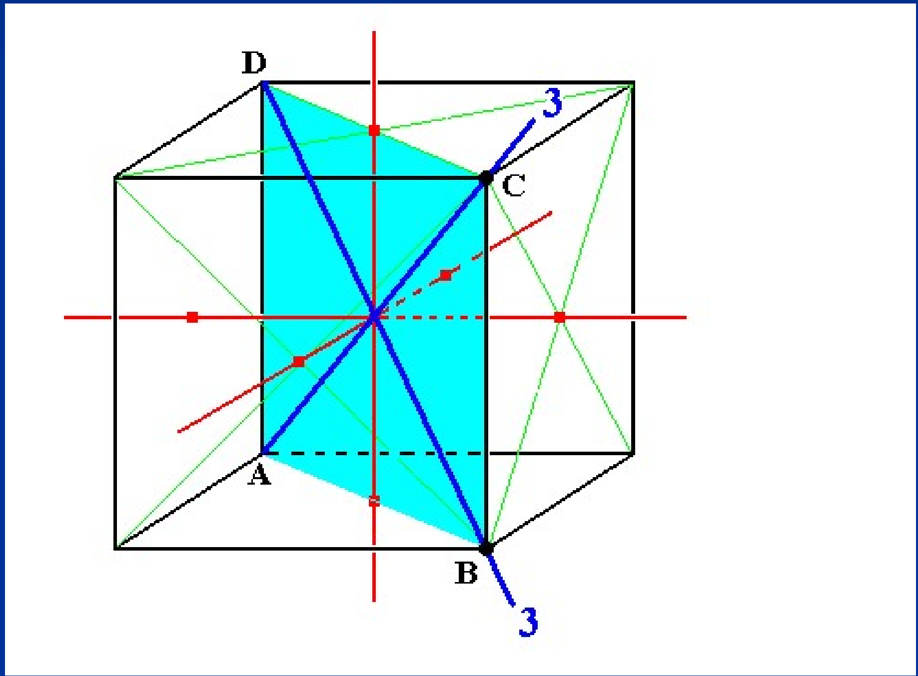
C_4 C_2 S_4

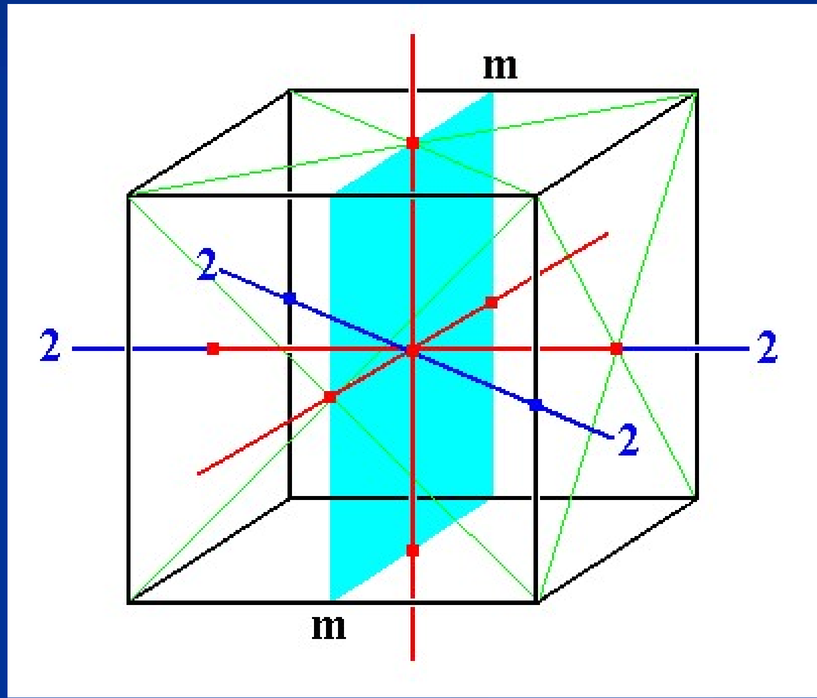




C_3 S_6

MIRROR PLANES

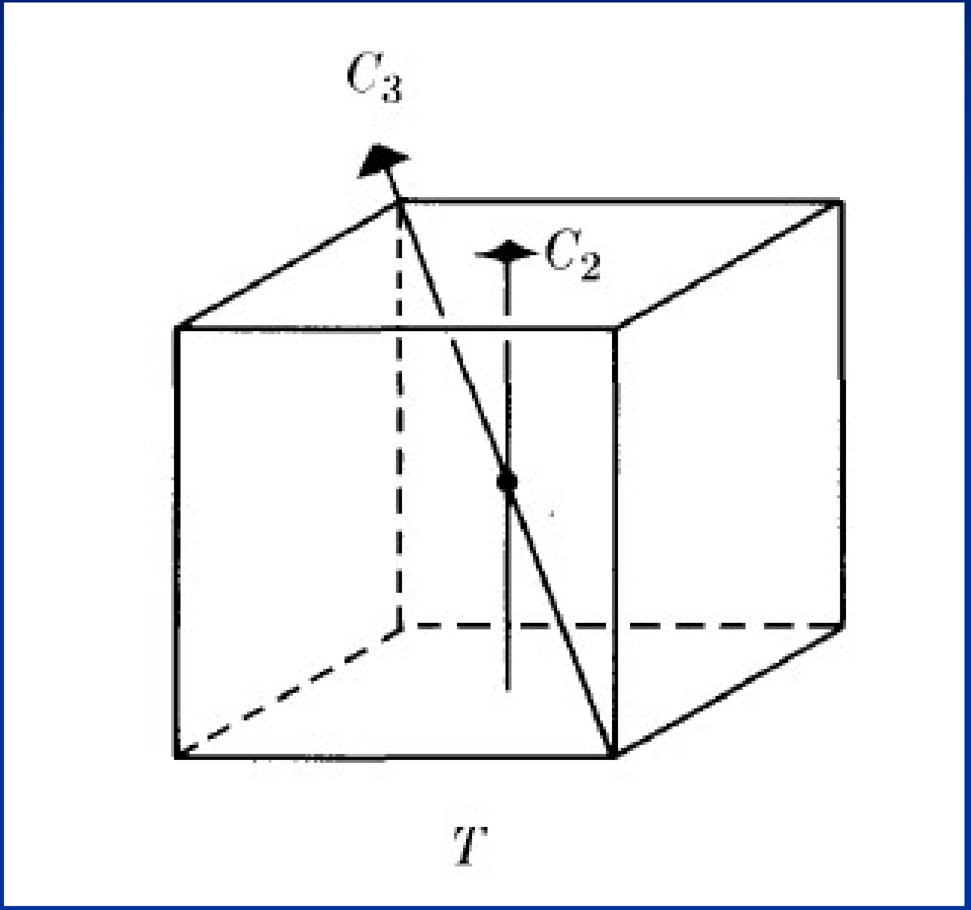




GROUP T (h=12)

Generators (C_3 , C_2)

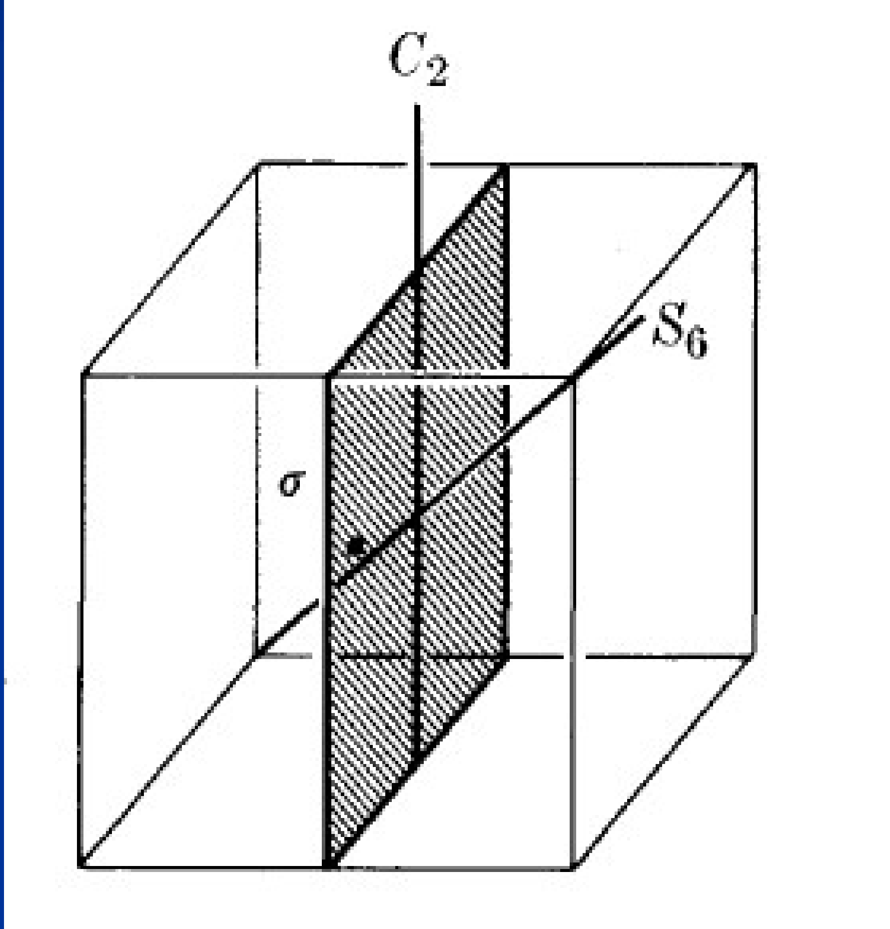
(23)



Classes:

{E}
{$3C_2$}
{$4C_3$}
{$4C_3^2$ }

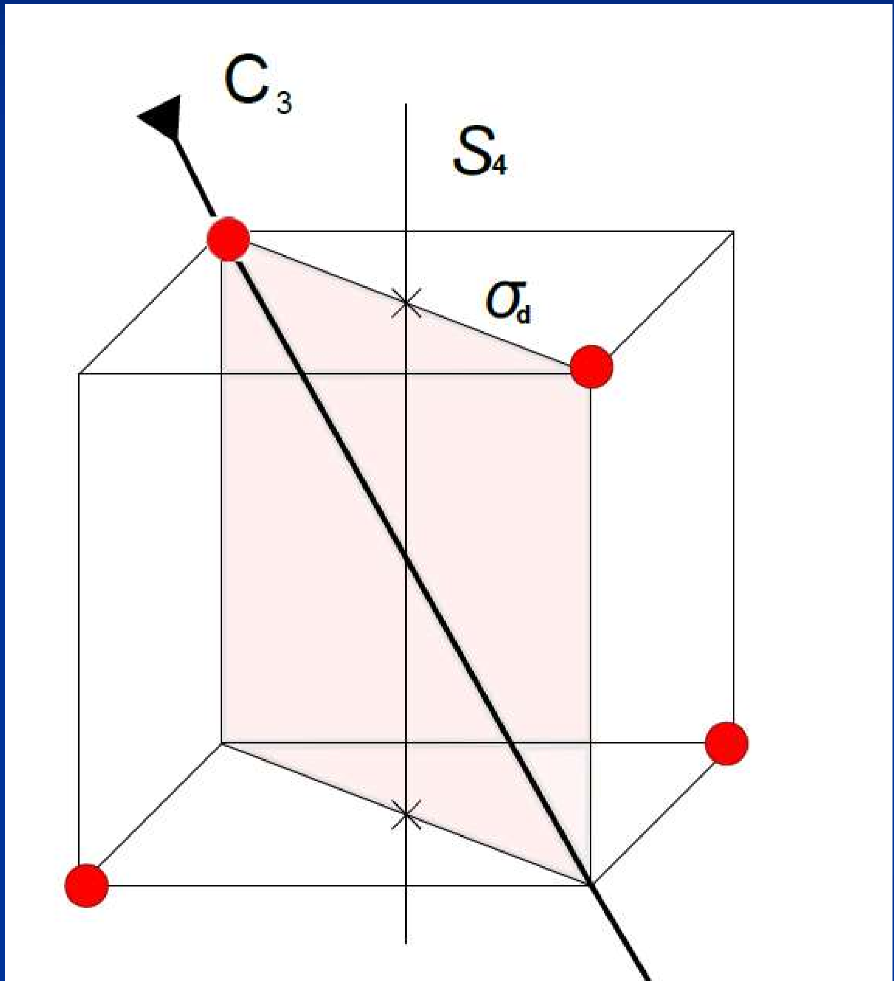
GROUP T_h (h=24) (m3)



Classes:

$\{E\}$, $\{I\}$
$\{3C_2\}$, $\{3\sigma\}$
$\{4C_3\}$, $\{4S_6^5\}$
$\{4C_3^2\}$, $\{4S_6\}$

GROUP T_d (h=24) ($\bar{4}$ 3m)

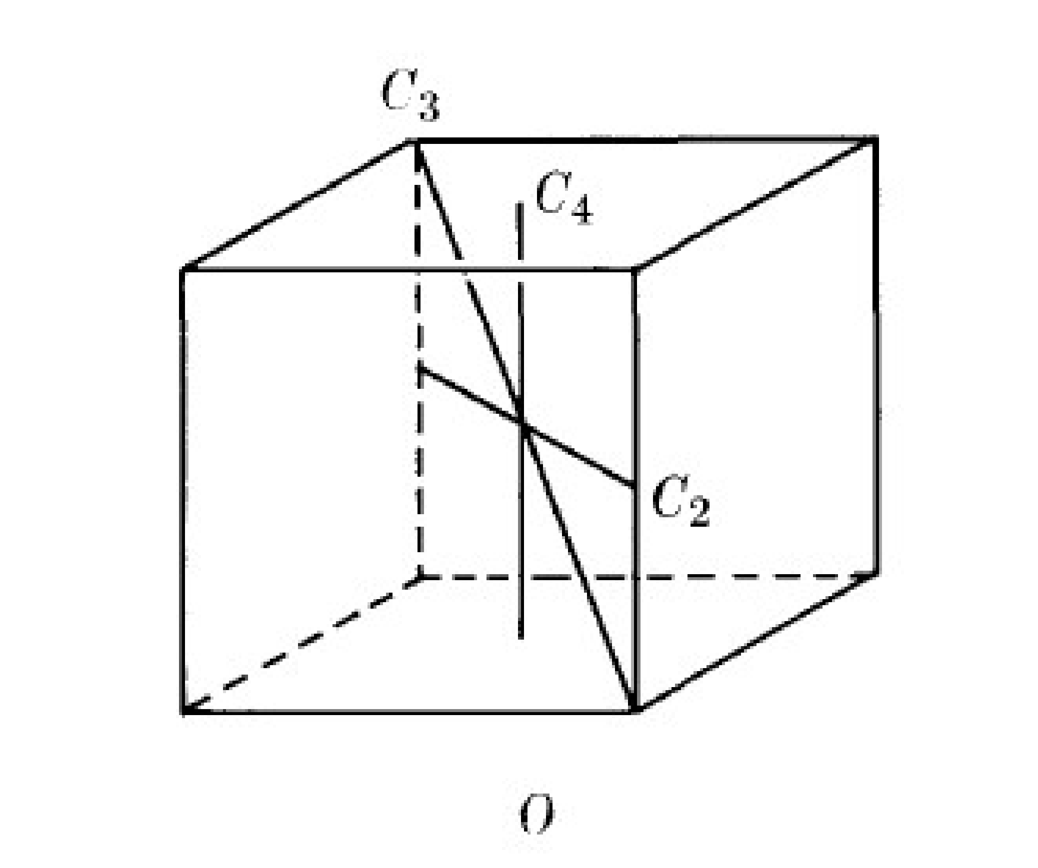


Classes:

$\{E\}$
$\{8C_3\}$
$\{6S_4\}$
$\{3C_2\}$
$\{6\sigma_d\}$

$C_2 = S_4^2$

GROUP O (h=24) (432)



CLASSES:

$\{E\}$

$\{6C_2\}$

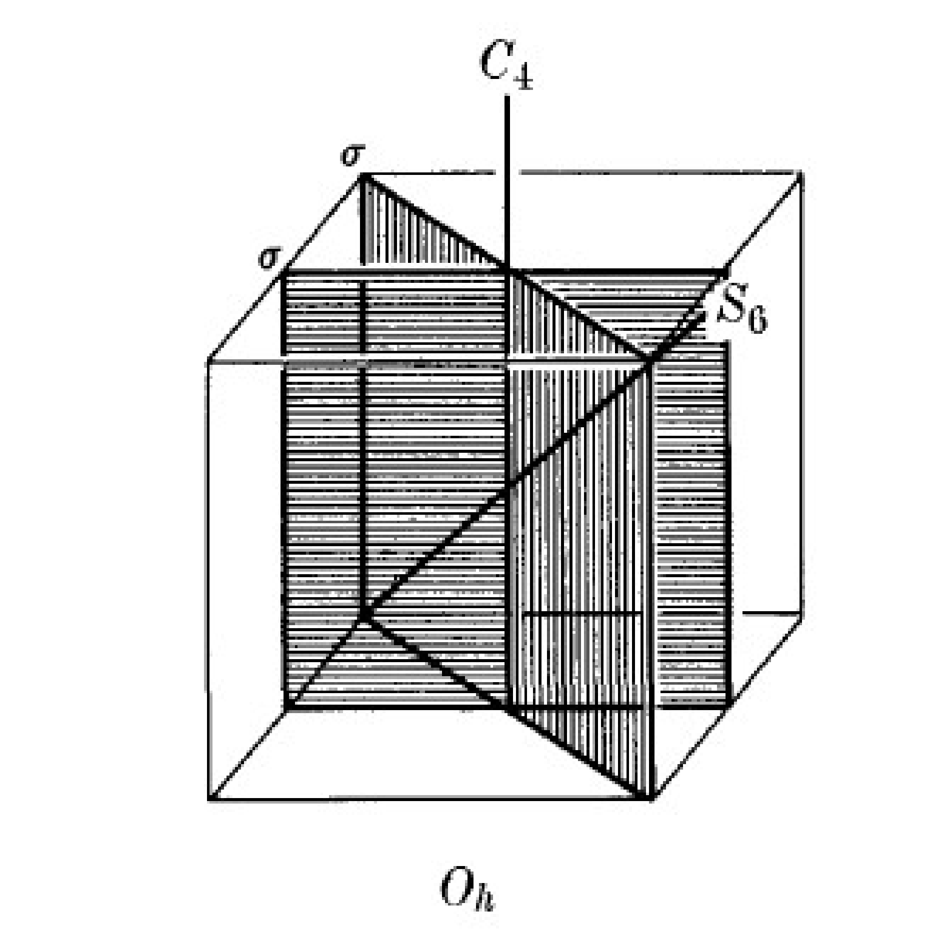
$\{8C_3\}$

$\{6C_4\}$

$\{3C'_2\}$

$C'_2 = C_4^2$

GROUP O_h h=48 (m3m)

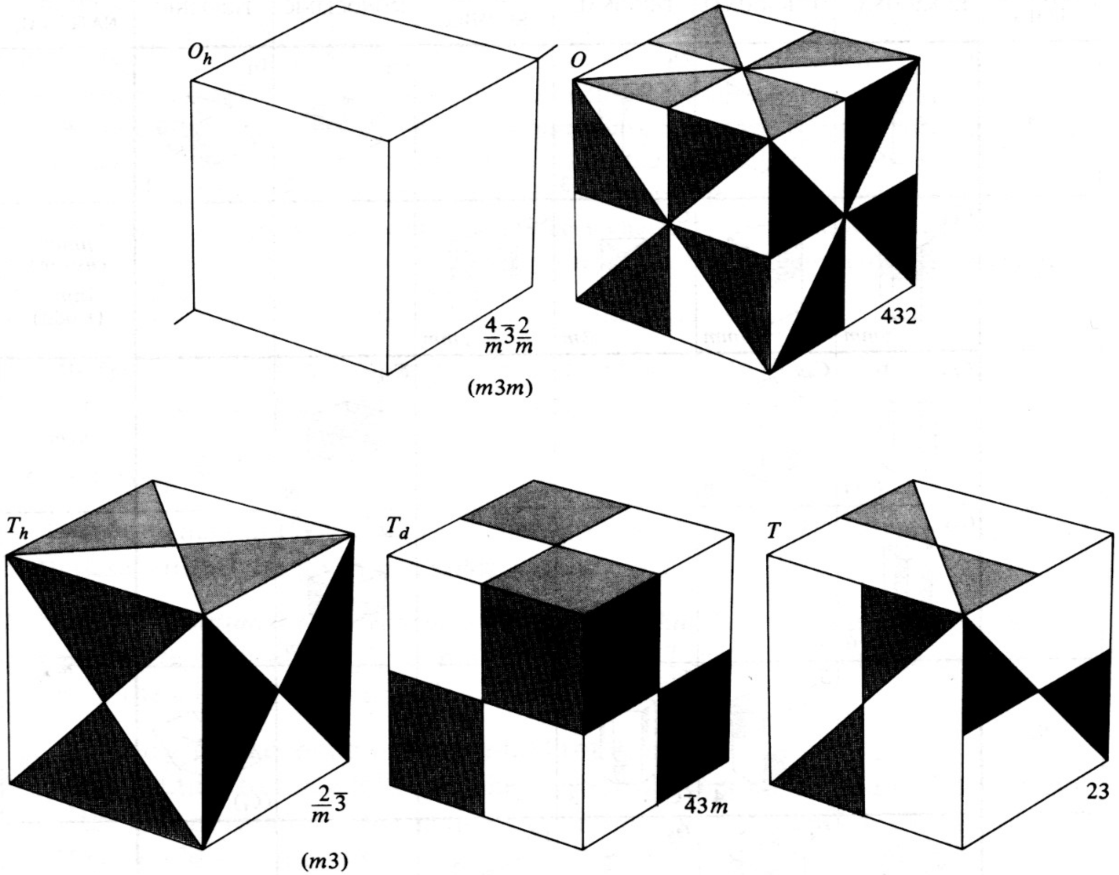


CLASSES:

$\{E\}$, $\{I\}$
$\{6C_2\}$, $\{6\sigma_d\}$
$\{8C_3\}$, $\{8S_6\}$
$\{6C_4\}$, $\{6S_4\}$
$\{3C'_2\}$, $\{3\sigma_h\}$

Table 7.2

OBJECTS WITH THE SYMMETRY OF THE FIVE CUBIC CRYSTALLOGRAPHIC POINT GROUPS[a]



[a] To the left of each object is the Schoenflies name of its symmetry group and to the right is the international name. The unpictured faces may be deduced from the fact that rotation about a body diagonal through 120° is a symmetry operation for all five objects. (Such an axis is shown on the undecorated cube.)

$n = 1, 2, 3, 4, 6.$

$n =$	1	2	3	4	6	TOTAL
C_n (m)	C_1 (1)	C_2 (2)	C_3 (3)	C_4 (4)	C_6 (6)	5
C_{nh} –	C_{1h} (m)	C_{2h} (2/m)	C_{3h} (3/m)	C_{4h} (4/m)	C_{6h} (6/m)	5
C_{nv}	$C_{1v} \equiv C_{1h}$	C_{2v} (2mm)	C_{3v} (3m)	C_{4v} (4mm)	C_{6v} (6mm)	4
S_n	$S_1 \equiv C_{1h}$	S_2 ($\bar{1}$)	$S_3 \equiv C_{3h}$	S_4 ($\bar{4}$)	S_6 ($\bar{3}$)	3
D_n	$D_1 \equiv C_2$	D_2 (222)	D_3 (32)	D_4 (422)	D_6 (622)	4
D_{nh}	$D_{1h} \equiv C_{2v}$	(mmm) D_{2h}	($\bar{6}$m2) D_{3h}	(4/m mm) D_{4h}	(6/mmm) D_{6h}	4
D_{nd}	×	×	×	D_{2d} ($\bar{4}$2m)	D_{3d} ($\bar{3}$m)	2
Grupos cúbicos	T, T_d, T_h, O, O_h					5
						32