SYMMETRY AND GROUP THEORY

Paper: CHNN 404

Unit 1 : Symmetry and Group Theory

Unit 2 : Group theory and its application.

Marks : 35

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GROUP THEORY

Paper: CHNN 404 Unit 1 & 2

Unit 1 : Symmetry and Group Theory

Unit 2 : Group theory and its application.

The symmetry relationship in the molecular structure understand by the basis for mathematical theory is called **Group Theory.** = Algebra of Geometry

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Course: CHNN – 404 (Core compulsory)

Symmetry, Group Theory & Spectroscopy

UNIT-01 Symmetry & Group Theory 16 Hrs

- Outline of symmetry elements and symmetry operation
- Schonflies method for determining the point group of the molecules.
- Multiplication of symmetry operation and multiplication table for C_2v, C_3v, C_{2h}.
- Equivalent symmetry elements, similarity transformation and conjugacy of symmetry operation within the point group
- Matrics: Characteristics, types of matrices(common & special), and Algebra of matrices(Particularly Multiplication)

  Use of Matrix and matrix representation of symmetry Elements and Their point groups(using various Vectors: position vector, translation vector, base vector)
- Γ_{3N} Representation :For H_2O,NH_3,BF_3,$PtCl_4$,PCl_5,SF_6,$POCl_3$,CCl_4,Cis &Trans N_2F_4, $XeOF_4$
- Reducible and Irreducible Representation& charactor Table
- Characteristics of Irreducible Representation: The great orthogonality theorem
- Construction of Character Table For C_3v using properties of irreducible Representation
- Direct product and its utility.

UNIT 02 : Group theory and its applications **16 Hrs**

- Character table and their presentation
- Reduction formula for reducible representation of any matrix presentation of particular point groups
- Application of symmetry to hybrid orbital, molecular orbital
- Hybridisation schemes for sigma-orbitals (for AB_3 : planar triangle, trigonal pyramidal e.g. BF_3 & NH_3 , AB_4 : tetrahedral and square planar molecules e.g. CH_4 & $[PtCl_4]^{-2}$, AB_5 : trigonal bipyramidal & square pyramidal e.g. PCl_5 & IF_5 and AB_6 : octahedral e.g. SF_6 and pi-orbital for AB_3 (e.g. BF_3) AB_6 (e.g. SF_6)
- Application of symmetry to molecular vibrations, interpretation of IR & Raman activity. (spectral data)

God geometrized everything in nature & Nature loves

Syn-metron

SYMMETRY…

To measure together

- ✓ One of the fundamental property of nature
- ✓ Kind of balancing act
- ✓ Beauty and harmony

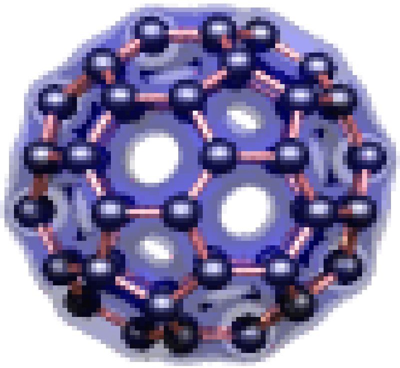
- ➢ Science basic concept
- ➢ Begins as the first property of geometrical figures
- ➢ One of the physical property of molecules
- ➢ It is an essential and important theme for defining molecular structure.

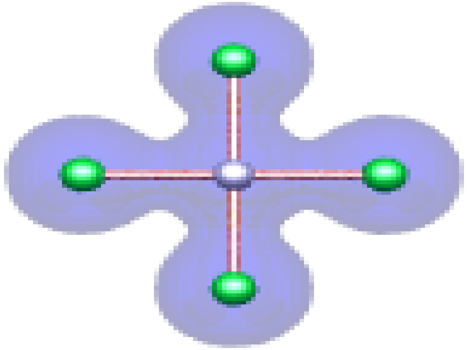
The symmetry relationship in the molecular structure understand by the basis for mathematical theory is called Group Theory.

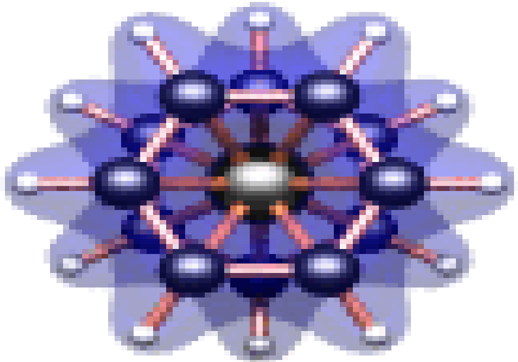
= Algebra of Geometry

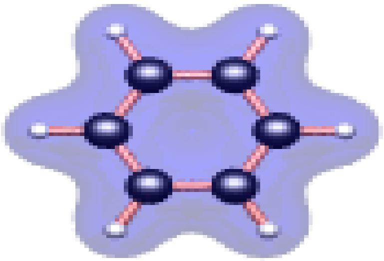
The symmetry arises because…..

- An atom or a group of atoms is repeated in a regular rhythmatic way to from a pattern.





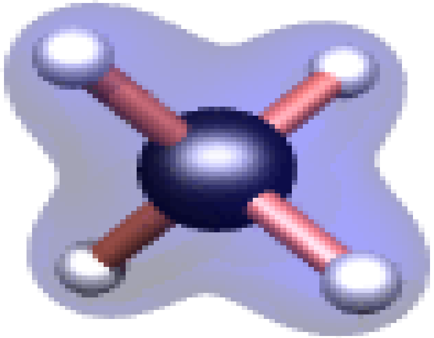


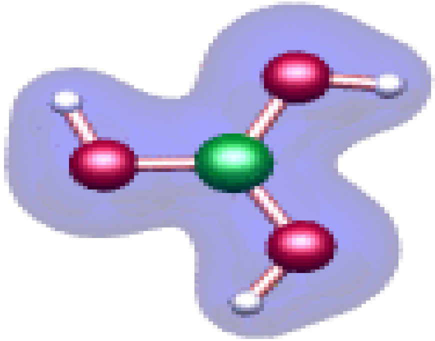


- In order to quantify the extent of this repetitive pattern and the amount of symmetry contained in the molecule,

We need to describe certain ……

"SYMMETRY OPERATIONS"





SYMMETRY OPERATIONS….

is not just any operation.

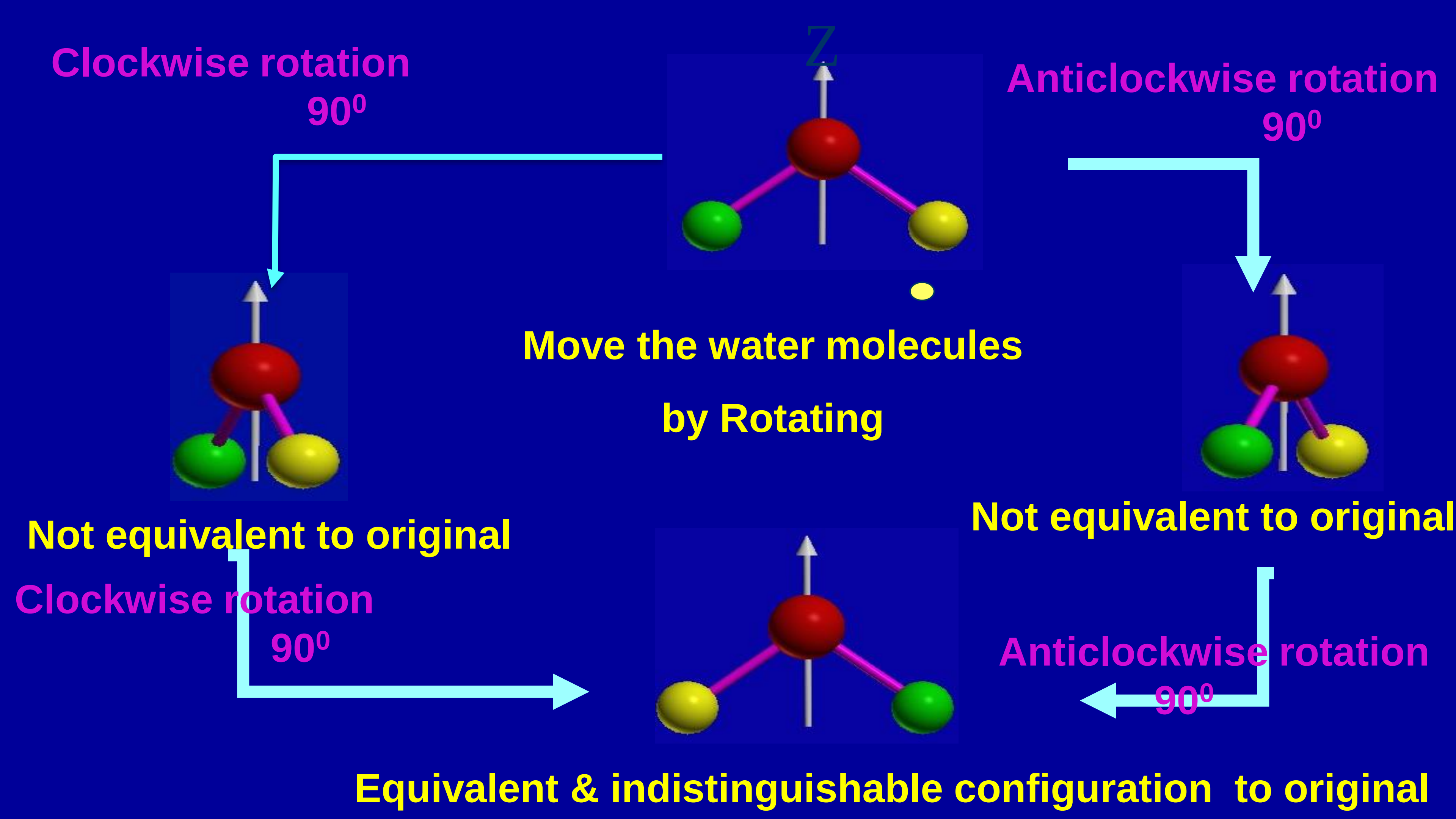
But, it is an operation with a

restriction

or

a specific condition..

A symmetry operation is a movement of the molecules such that the resulting configuration of the molecules is equivalent or indistinguishable or conjugated configuration from of the original configuration (ideal).


Z
Clockwise rotation
90^0
Anticlockwise rotation
90^0
Move the water molecules
by Rotating
Not equivalent to original
Not equivalent to original
Clockwise rotation
90^0
Anticlockwise rotation
90^0
Equivalent & indistinguishable configuration to original

We can move any molecules by..

- Rotating
- Reflecting
- Inversing

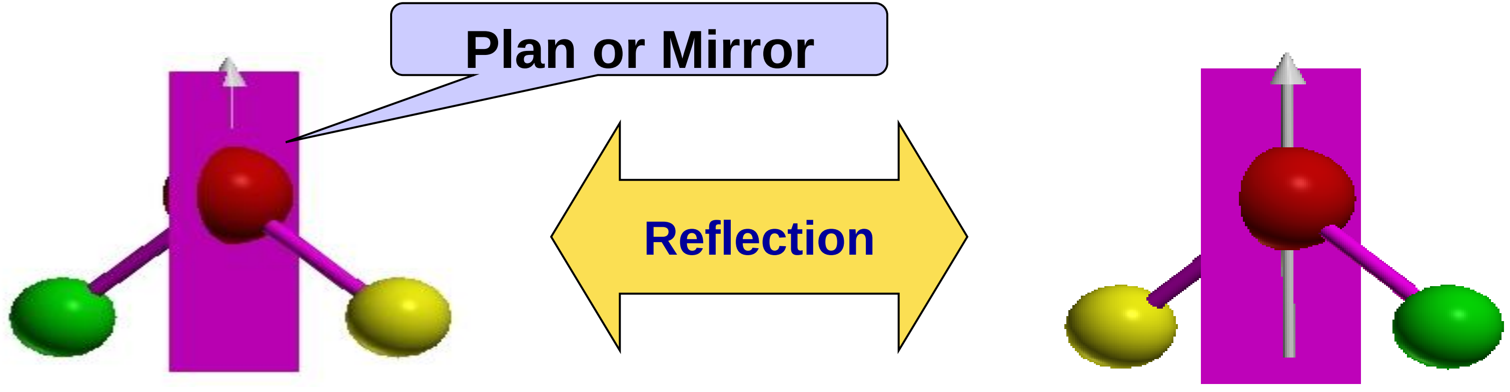
Operation….

Rotation – **Rotate the Molecules on any point [axis] to get an equivalent configuration.**

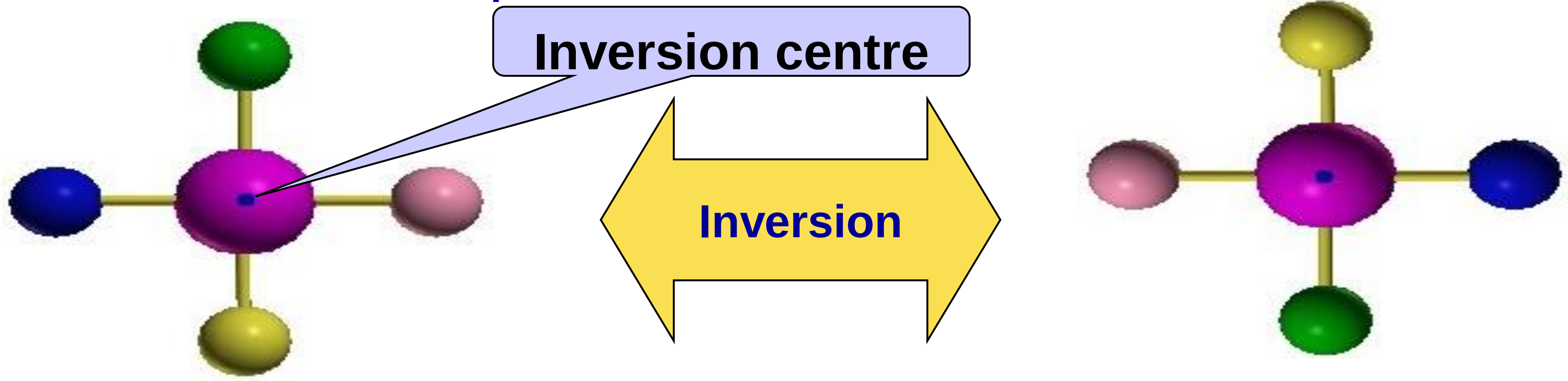
Reflection – **Reflect form any plane which is devising to molecules in same atoms or element..**

Inversion – **Inverted the group or atoms through the center of molecule.**
[transfer from one to one oppositely]

Reflection in water molecule.



Inversion in $PtCl_4$ molecule.



Symmetry operation is some physical movement on the molecules in order to get an equivalent configuration……...

which in turn generate the corresponding…

" Symmetry Element "

- **it is intricately related with the Symmetry Operation.**
- it is geometrical entity i.e. a point, a line, a plane.

In all,…

There are five type of symmetry elements..

1. **Rotational axis of symmetry. [C_n]**
2. **Plane of symmetry. [σ]**
3. **Inversion centre of symmetry. [i]**
4. **Improper rotational axis of symmetry. [S_n]**
5. **Identity of molecule..[E]**

All S.E. pass through a single point, and the operation generation all S.E. leave just one point unmoved.

it Is nothing but the **‘Centre of Gravity’**.

1. Rotational axis of symmetry. [C_n]

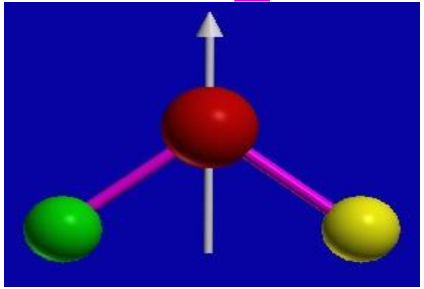
Rotate the molecule ones OR several times by minimum angle θ on any axis to obtain an equivalent configuration

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

Where n = 360/ θ

= order of the axis

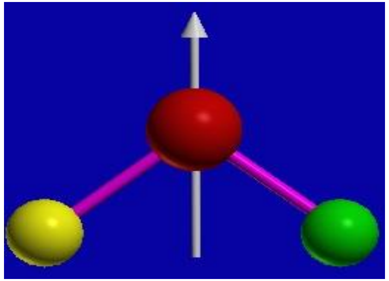
Z



Original configuration

θ = 180 rotation

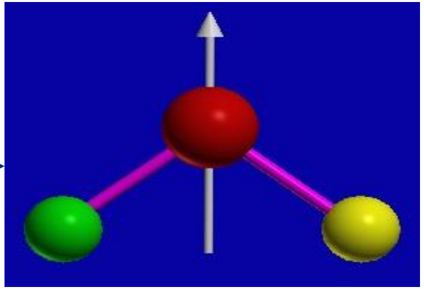
C^1_2



Equivalent configuration to original

θ = 180 rotation

C^2_2

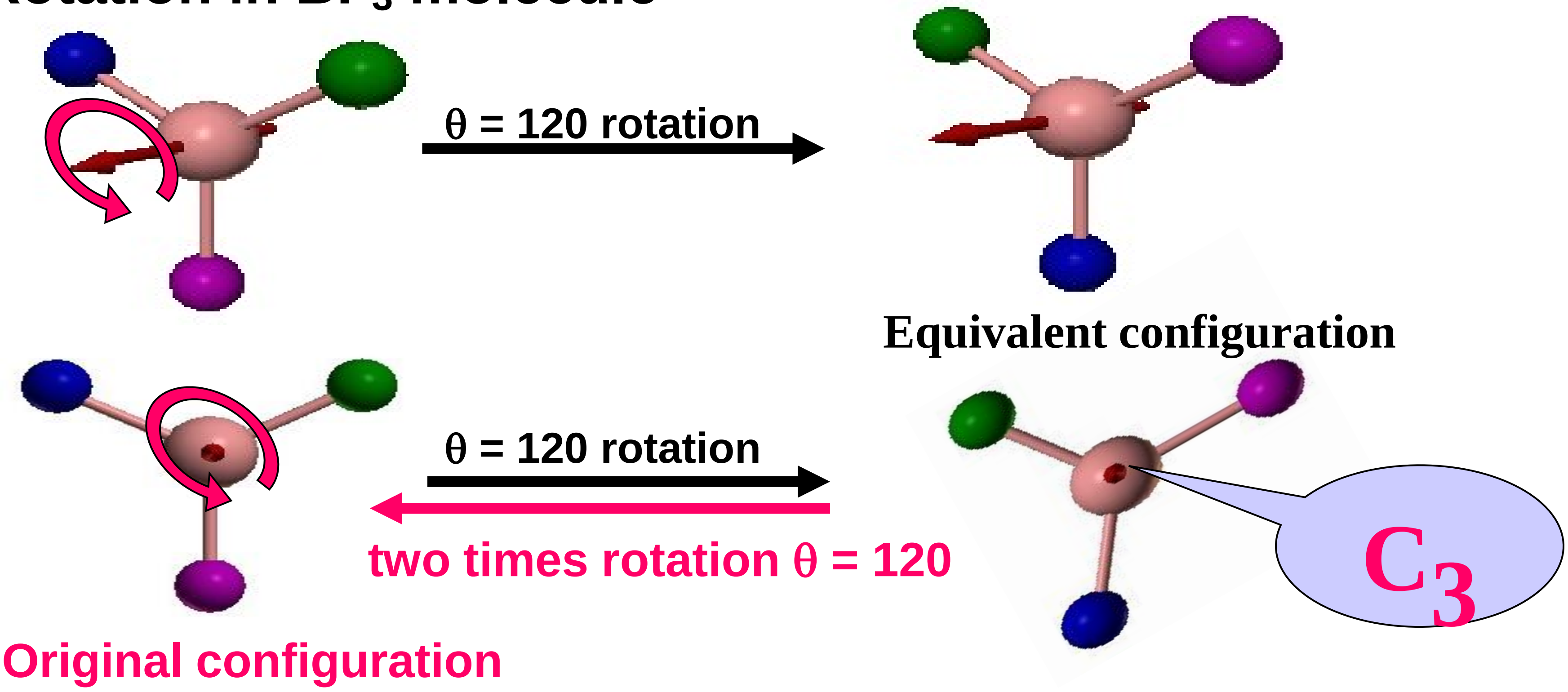


Ideal configuration

In water molecule, $n = 2$

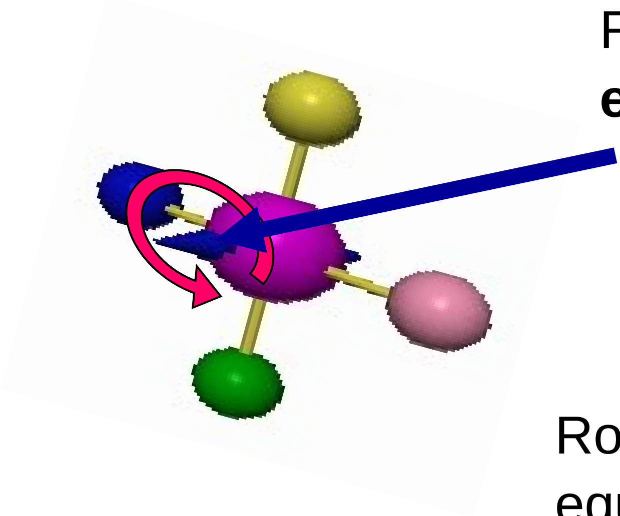
i.e.C_2 rotational axis is present in water molecule.

Rotation in BF_3 molecule



n=360/120= C_3 rotational axis is present in BF_3

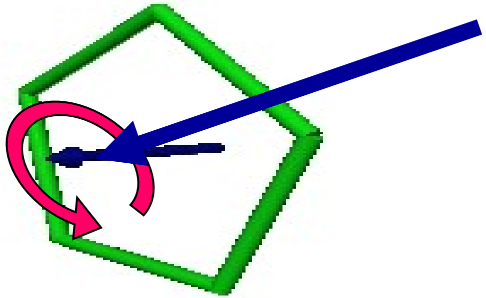
C_4 & C_5 rotational axis



Rotate the $PtCl_4$ molecule to $\boldsymbol{\theta = 90}$ to get **equivalent configuration.**

C_4 rotational axis

When rotate the $PtCl_4$ to **four** times, we get **ideal configuration**

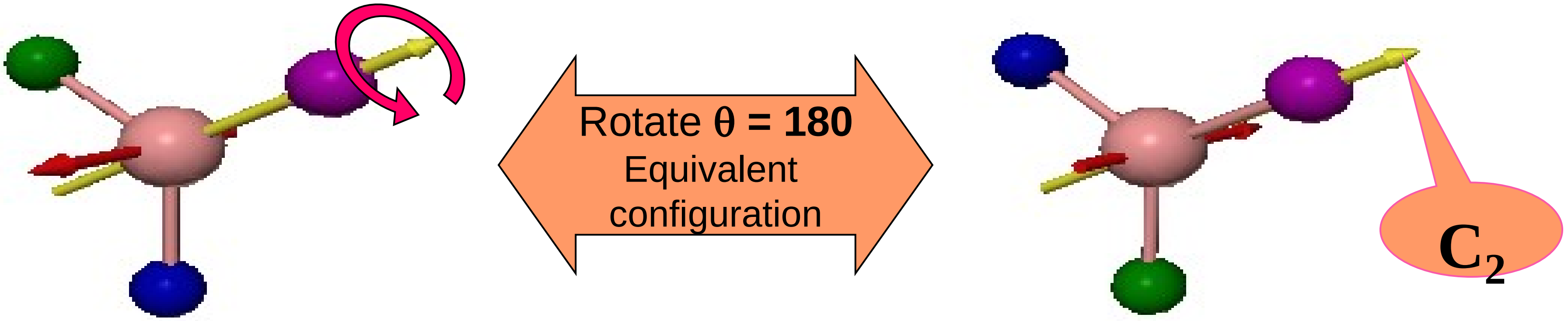


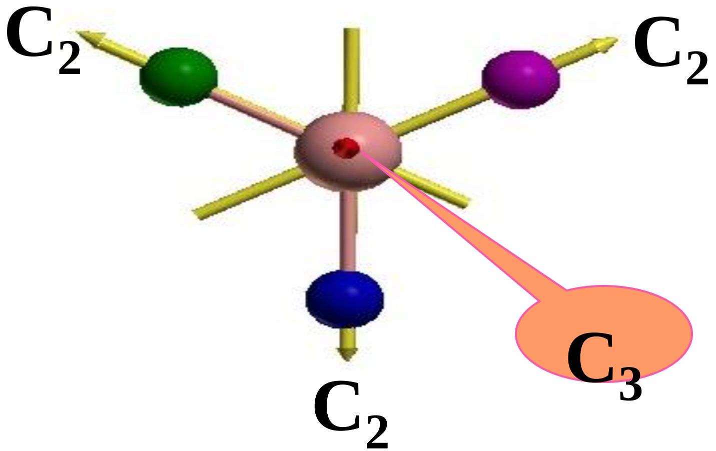
Rotate the C_5H_5 molecule to $\boldsymbol{\theta = 72}$ to get equivalent configuration.

C_5 rotational axis

When rotate the $\mathbf{C_5H_5}$ to **five** times, we get **ideal configuration**

Other Rotational axis in BF3 molecule…..





Total No of Rotational axis in BF_3

One C_3

Three C_2

(which is perpendicular to C_3 **)**

There are in general two types of R. A.

1. Principal R.A. [Cn] Where n is highest.

   e.g. highest fold R.A.

2. Simple OR Secondary R.A.

   these may be often C_2 axis

   it is perpendicular to P.R.A.

   No of S.R.A. = the order of P.R.A.(n)

Rotational axis in BF_3

One C_3 is called P.R.A.

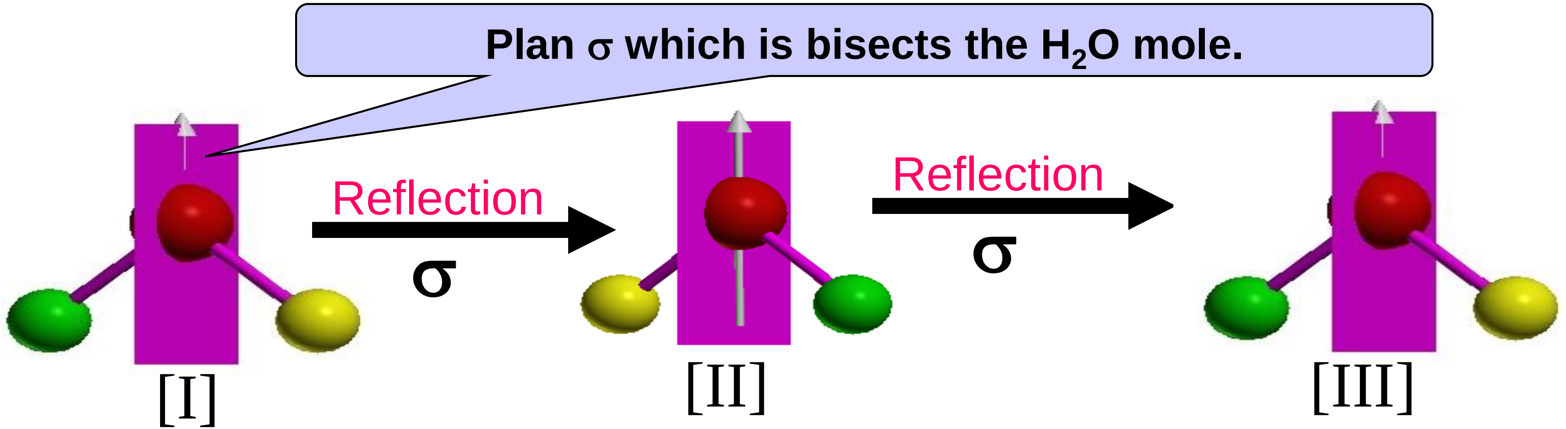
Three C_2 is called S.R.A.(which is perpendicular to C_3)

In R.A. values of $n = 2,3,4,\ldots\ldots\infty$

When $\theta = 0$, then $n = \infty$

2. Plane of symmetry. [σ]

It can be simply obtained by the reflection operation from any plane of molecules



σ^1 (once reflection)= [II]= Equivalent configuration

σ^2 (twice reflection)= [III]= identical configuration=[I]

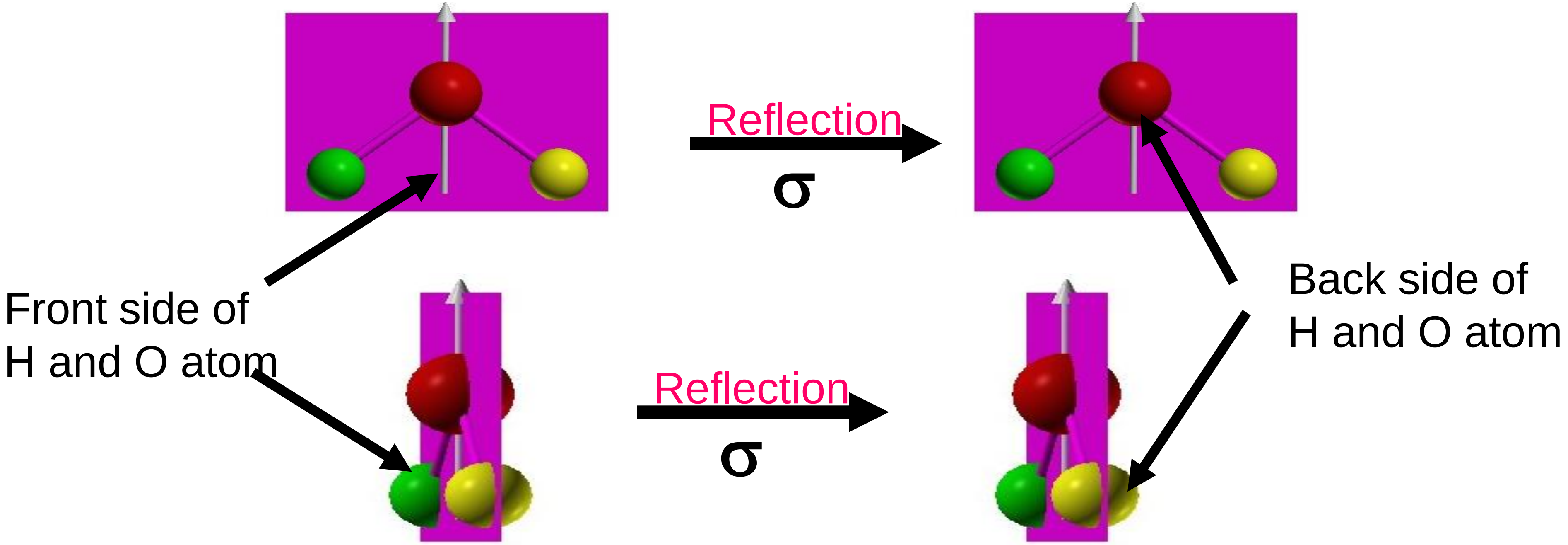
σ^3 (thrice reflection)= [II]= Equivalent configuration

σ^n (n=odd)= [II]= Equivalent configuration

(n=even)= [I]= identical configuration

The plane in fact bisects the **H_2O** molecule into two halves so that one half of the molecule is reflected into the other.

There is another plane in **H_2O mole. (Molecular plane)**



There are two plane in H2O Molecule.

As regularity in structure of mol. Increases,
it possible to discover more and new sets of planes,
All of which can be classified into…

[i] Vertical planes (σ_v)

[ii] Dihedral planes (σ_d)

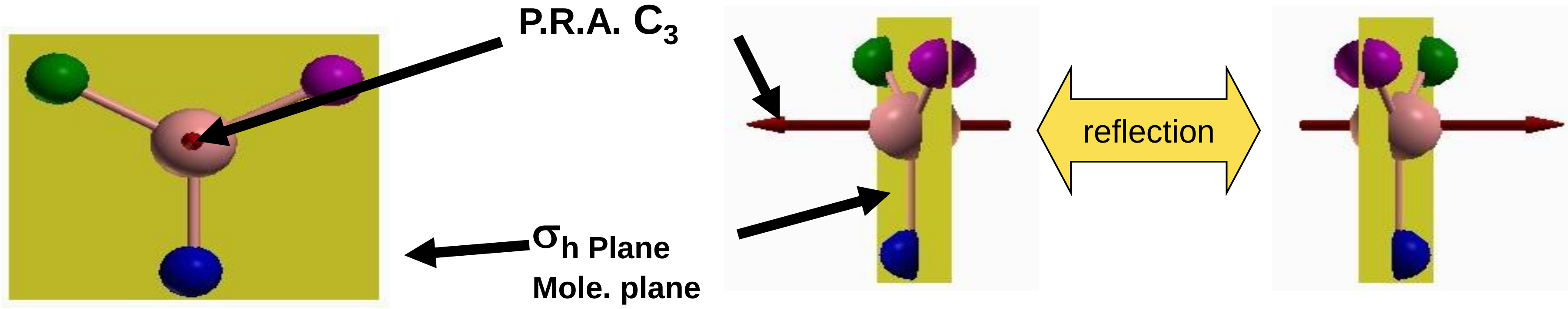
[iii] Horizontal planes (σ_h)

The planes are classified depending on their relationship with either the P.R.A. or S.R.A.

[iii] Horizontal planes (σ_h)

It is perpendicular to the P.R.A.
This is a special and unique plane which is present in many molecules.

In BF_3 (Trigonal planer) mole. Containing σ_h plane which is perpendicular to the P.R.A. C_3



Horizontal planes (σh) in BF_3 contain 3 B-F bonds and bisect all 3F and B atoms.

[i] Vertical planes (σ_v)

It is contains the P.R.A.

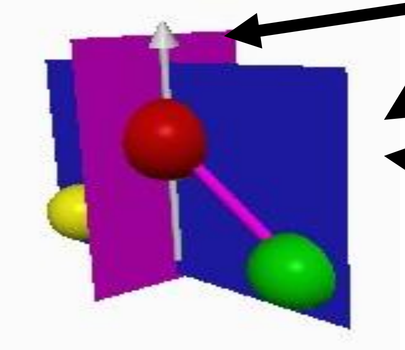
In H_2O molecule two σv planes,

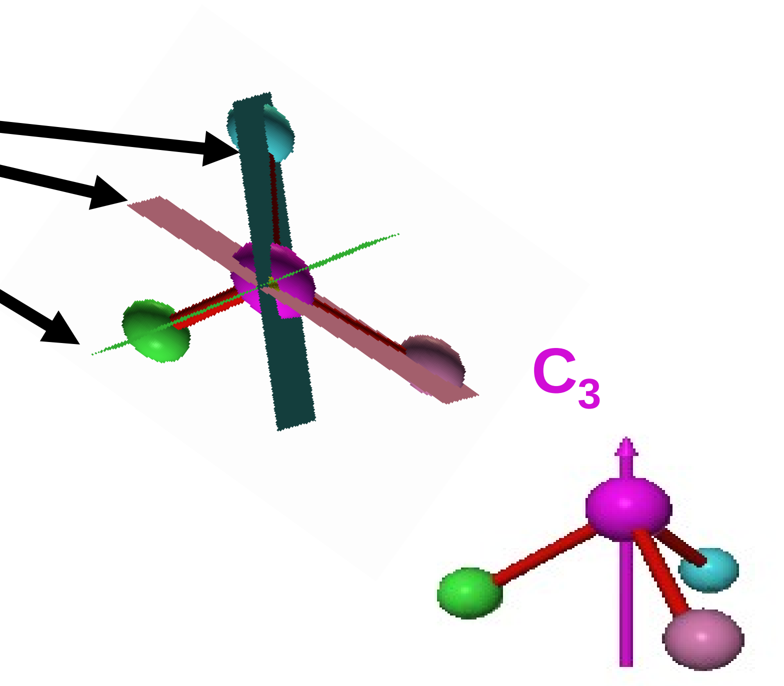
One of the σv plane contains the whole molecule = Molecular plane

Other σv plane bisect the molecule

all plane contains the P.R.A.

σ_v





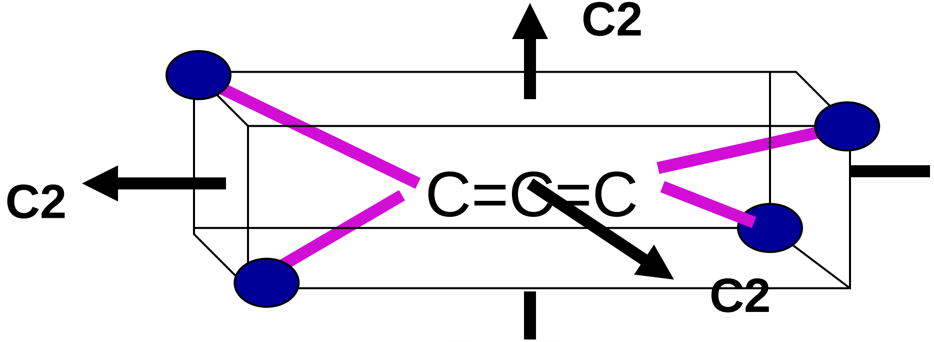
In NH_3 molecule three σv planes

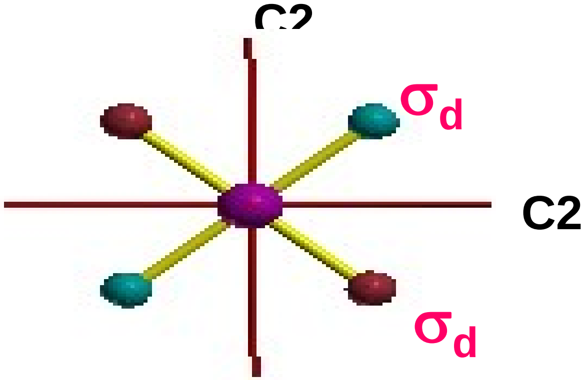
There is no molecular plane in NH_3

[ii] Dihedral planes (σ_d)

A dihedral planes is one which bisects the angle subtended between two similar consecutive C_2 axes. (S.R.A.)

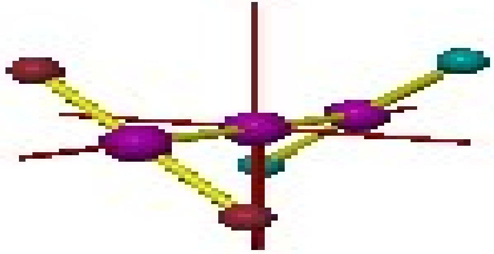
Allene, Methane and staggered ethane are contain only this type of planes



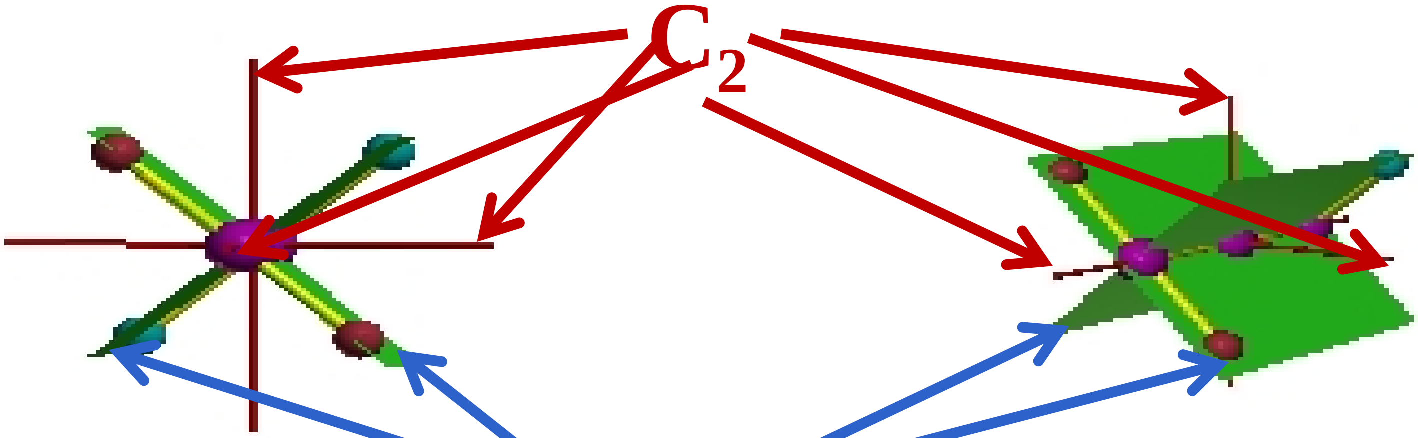


Newman projection

Aline

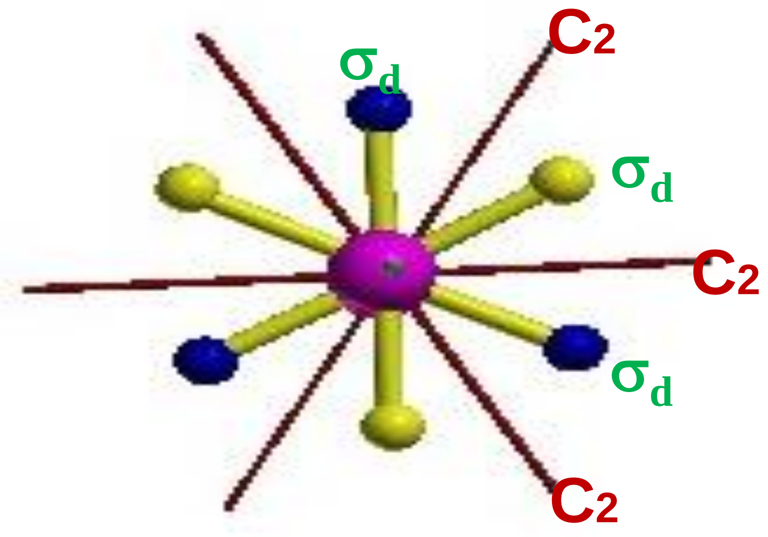


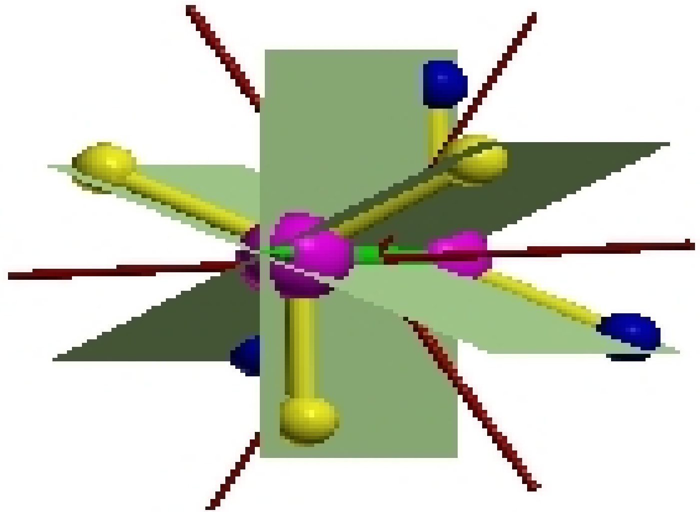
Horse projection



There are $3C_2$ and $2\sigma_d$ (which is bisect the $2C_2$ In the aline.

σ_d Plane and C_2 axis in St. Ethane





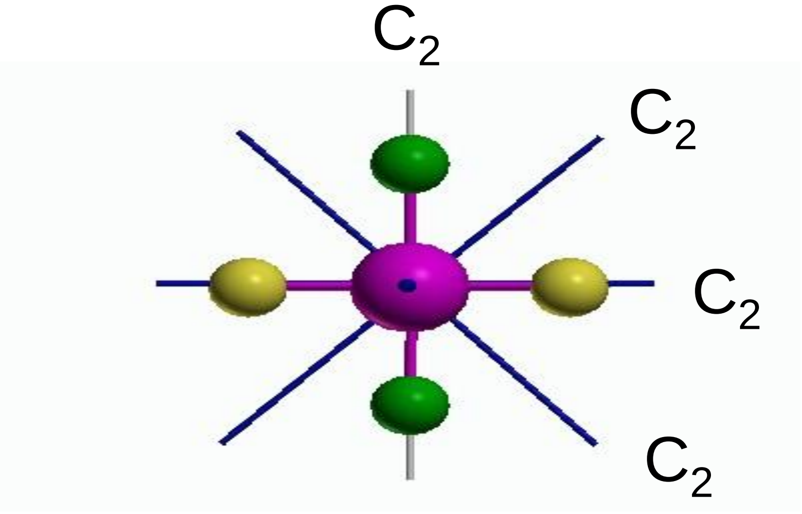
In this molecules,

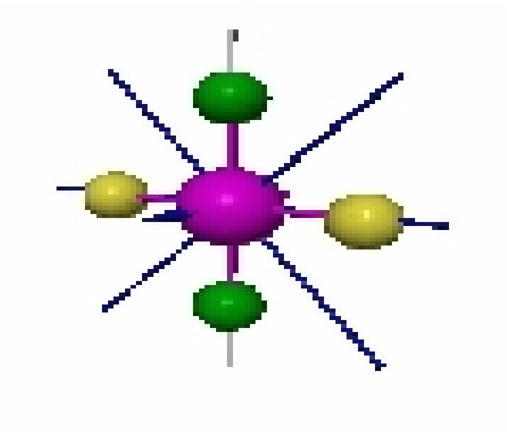
there are 3C_2, which is passed only C-C bone, angle between the two C_2 axis is 120.

There are 3σ_d Plane, which is passed 2C and 2Hwhich are lies in opposite position

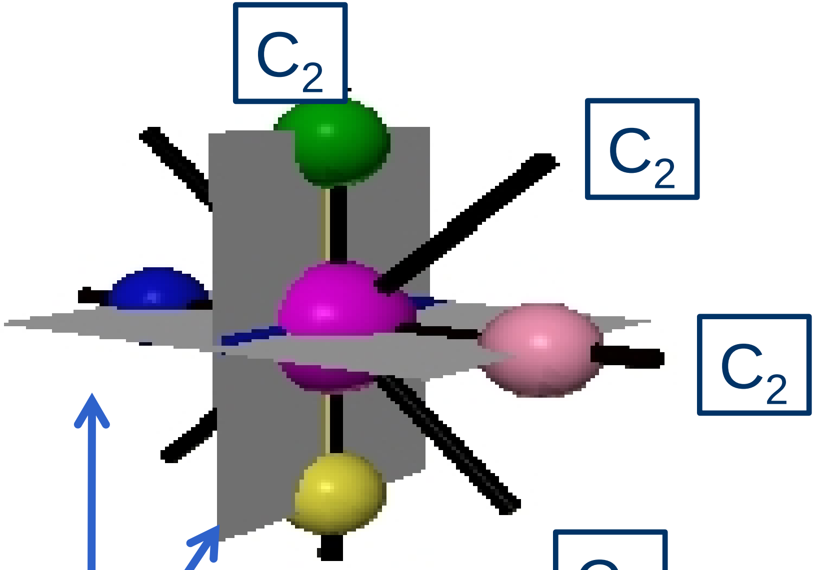
The dihedral planes is difficult to distinguished from σ_v

There are four C_2 In $PtCl_4$

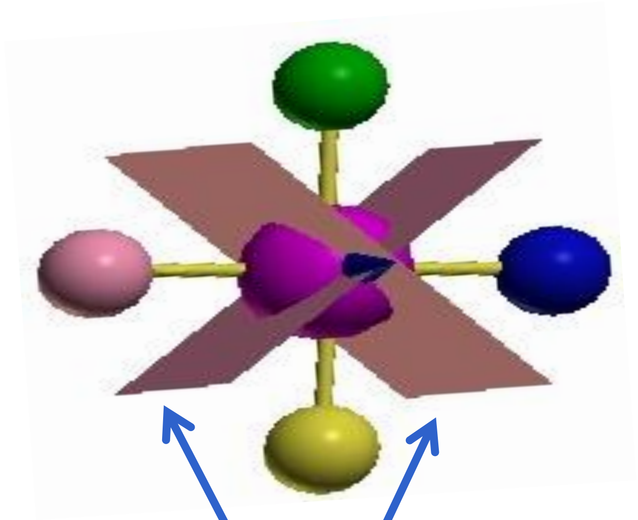




All Plane contain C_2 axis, as well as all the four plane bisects the angle between the two C_2 axis.

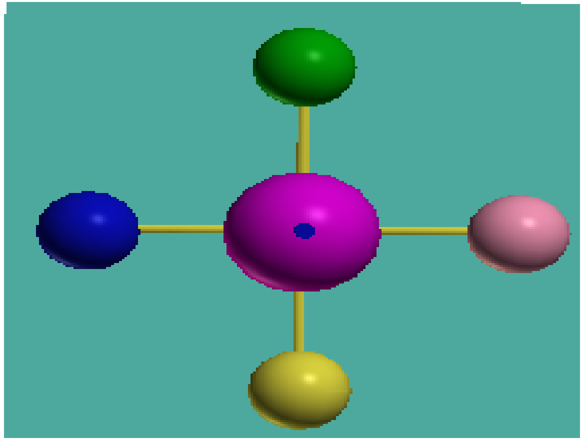


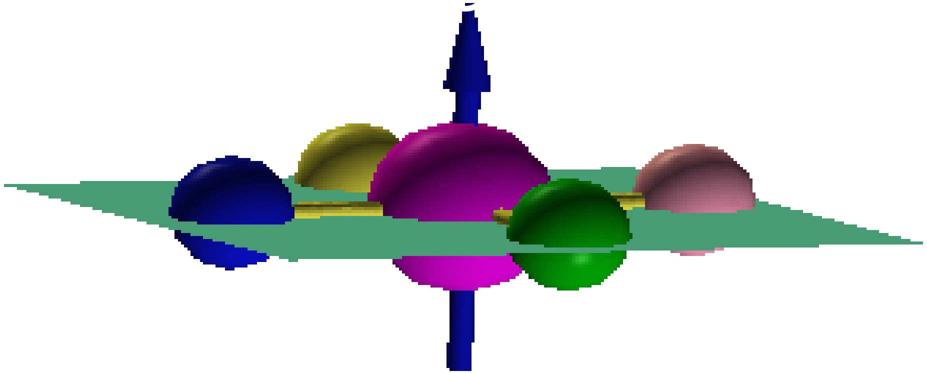
σ_v plan passes through the largest number of atoms group or molecules



σ_d plan passes through the least number of atoms group or molecules

Horizontal planes (σ_h) in $PtCl_4$





There are five planes in $PtCl_4$

Two Dihedral planes (σ_d)

Two Vertical planes (σ_v)

One Horizontal planes (σ_h)

Improper rotational axis of symmetry. [S_n]

Combination axis = Rotation – Reflection axis.

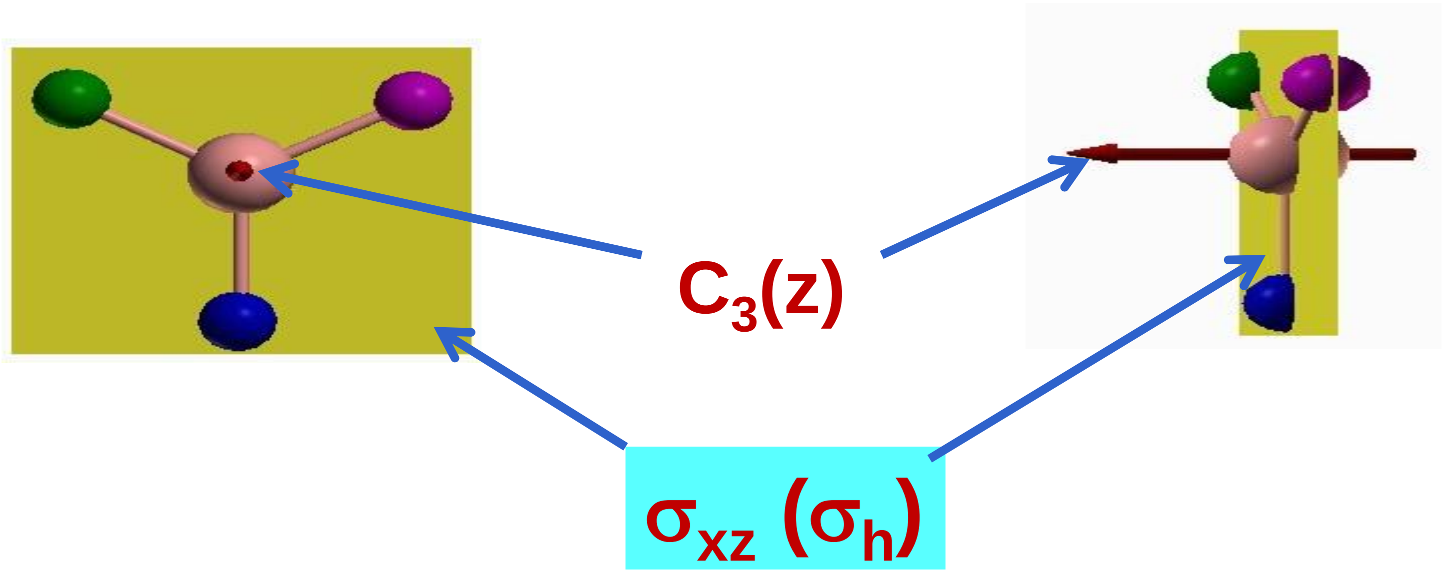
This element is generated by rotating the mole. by an angle and then taking reflection in plane perpendicular to the rotational axis

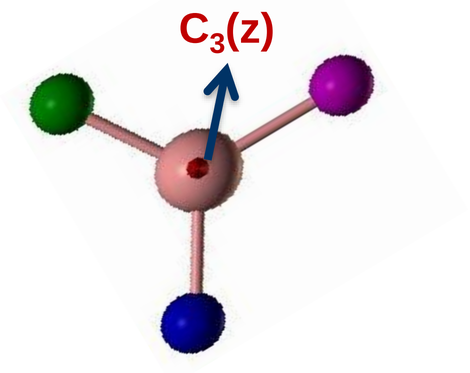
If there is C_n axis along Z-axis and σ_{xz} is a plane perpendicular to axis than,

$$C_n(z) . \sigma_{xz} = S_n$$

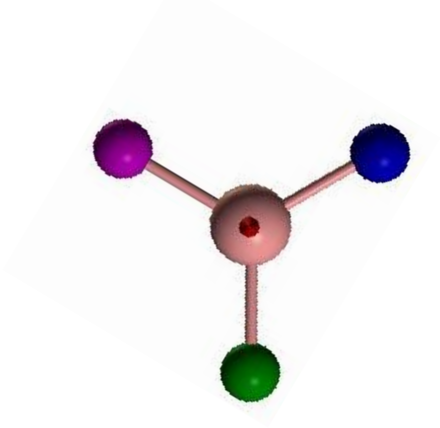
In the BF_3 molecules

There is $C_3(z)$ axis and σ_{xz} (σ_h) plane which is perpendicular to the $C_3(z)$ axis exist separately, then S_3 (z) axis is present in BF_3





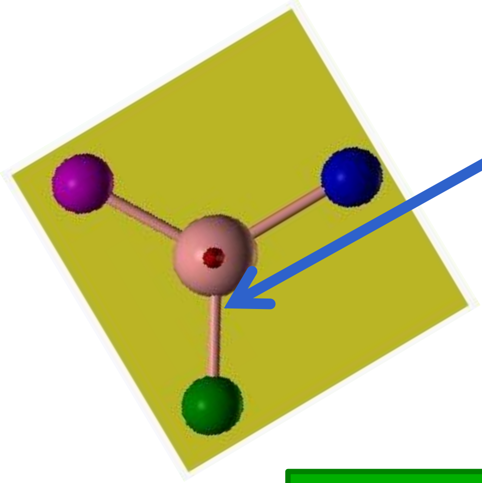
Rotation C_3^1 (120)
Anticlockwise



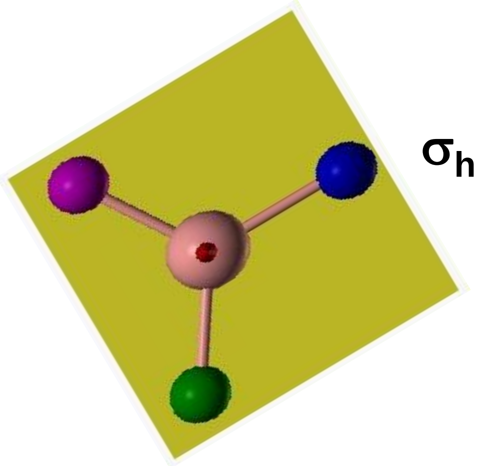
Front side of all B and 3F atoms.

Two structure are not identical but equivalent s

S_3^1

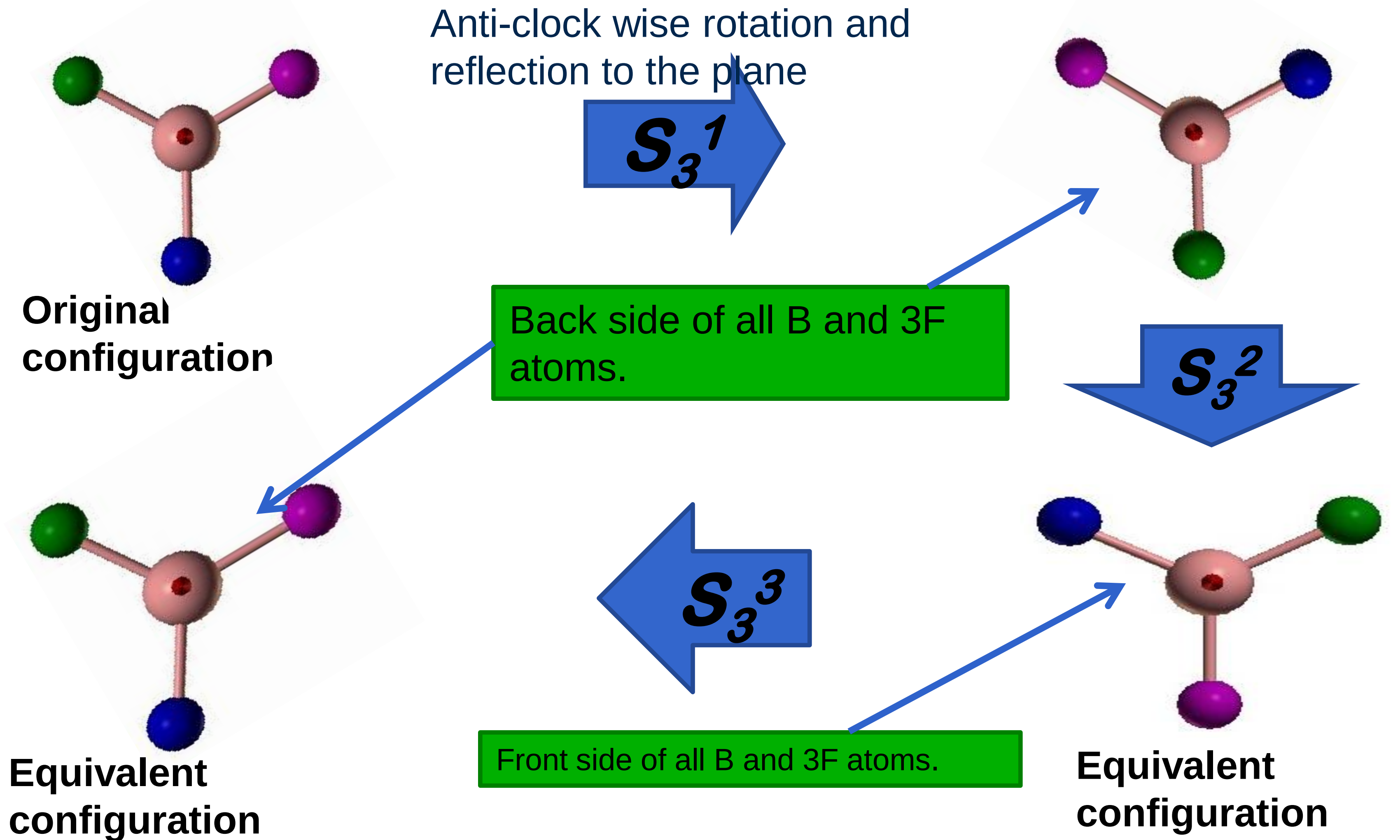


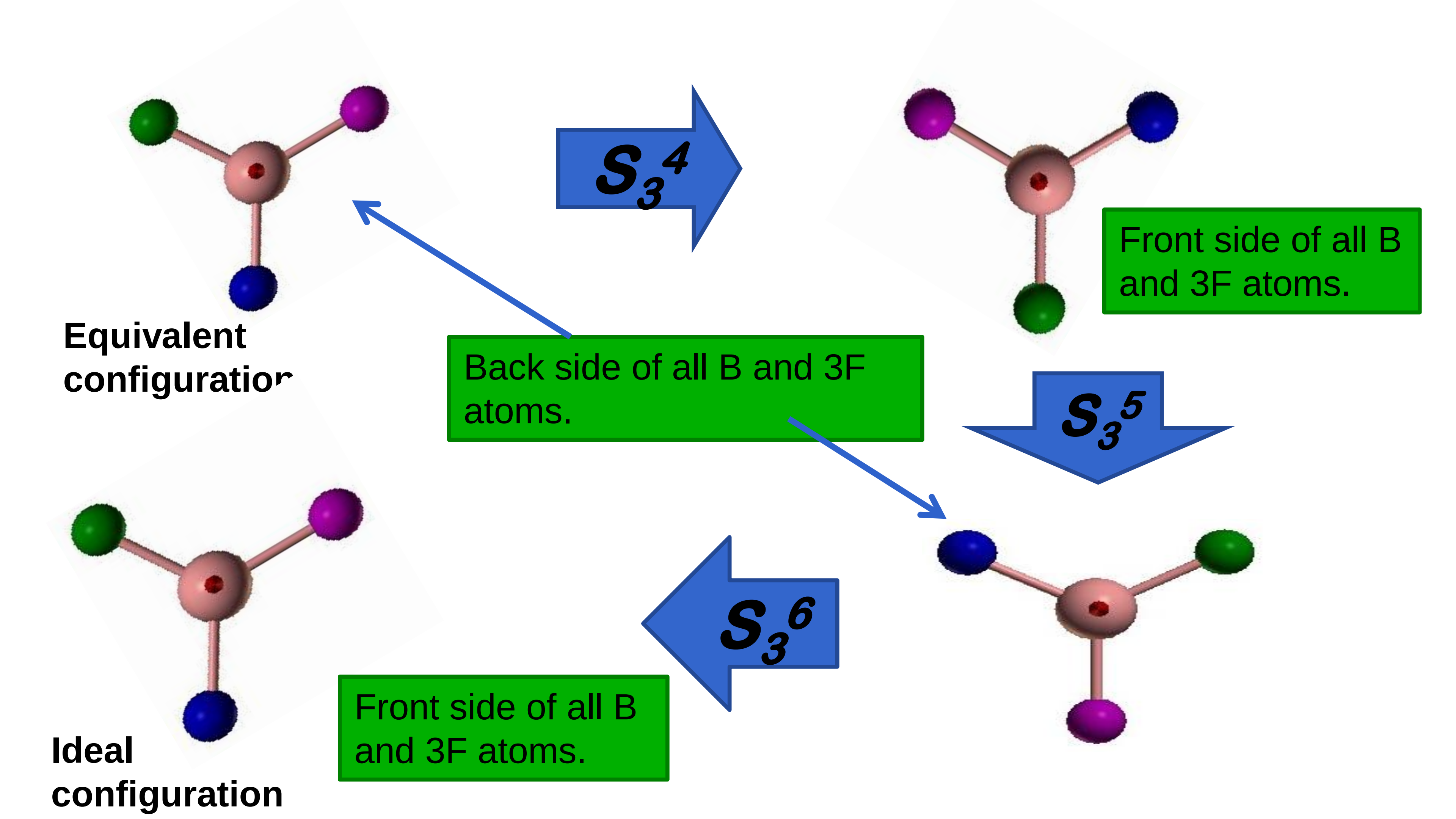
Reflection
σ_{xz} (σ_h)



σ_h

Back side of all B and 3F atoms.


Anti-clock wise rotation and reflection to the plane
S_3^1
Original configuration
Back side of all B and 3F atoms.
S_3^2
S_3^3
Equivalent configuration
Front side of all B and 3F atoms.
Equivalent configuration


S_3^4
Front side of all B and 3F atoms.
Equivalent configuratio
Back side of all B and 3F atoms.
S_3^5
S_3^6
Ideal configuration
Front side of all B and 3F atoms.

Relationship of Improper rotational axis with E(identity)

$$S_n^n = S_n^1 \cdot S_n^2 . S_n^3 . S_n^4 ....S_n^n = E[where..n = even]$$

EXEMPLE :
PtCl4(S4); Eclipesed dibenzene cromium(S6), SF6(Oh)(S4)

$$S_n^{2n} = S_n^1 \cdot S_n^2 . S_n^3 . S_n^4 ....S_n^{2n} = E[where..n = odd]$$

EXEMPLES:
Eclipesed ehane(S3); BF3(S3); Eclipesed ferrocene (S5)

From the discussed, it is conclude that,

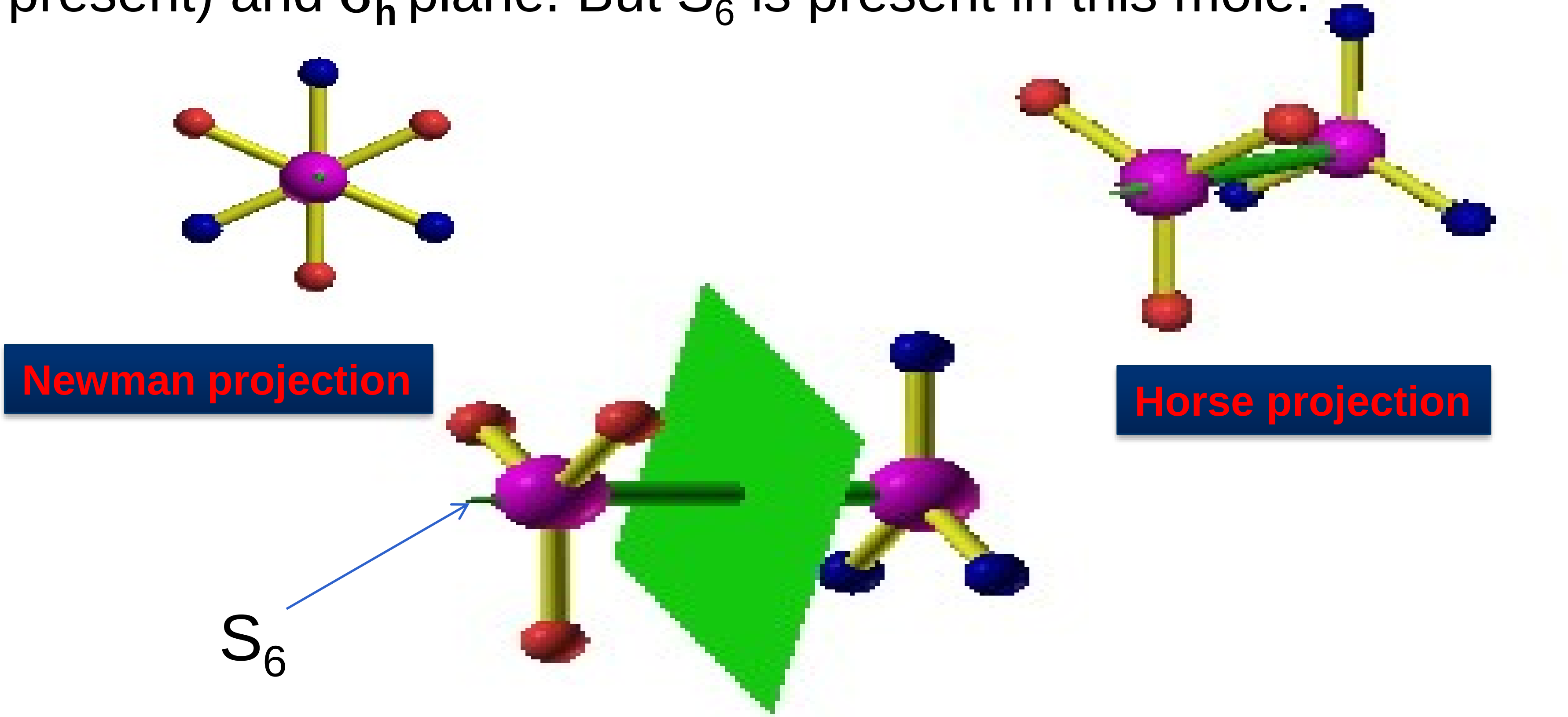
If a C_n and a σ plane perpendicular to it exist separately, then S_n is necessarily present in molecules.

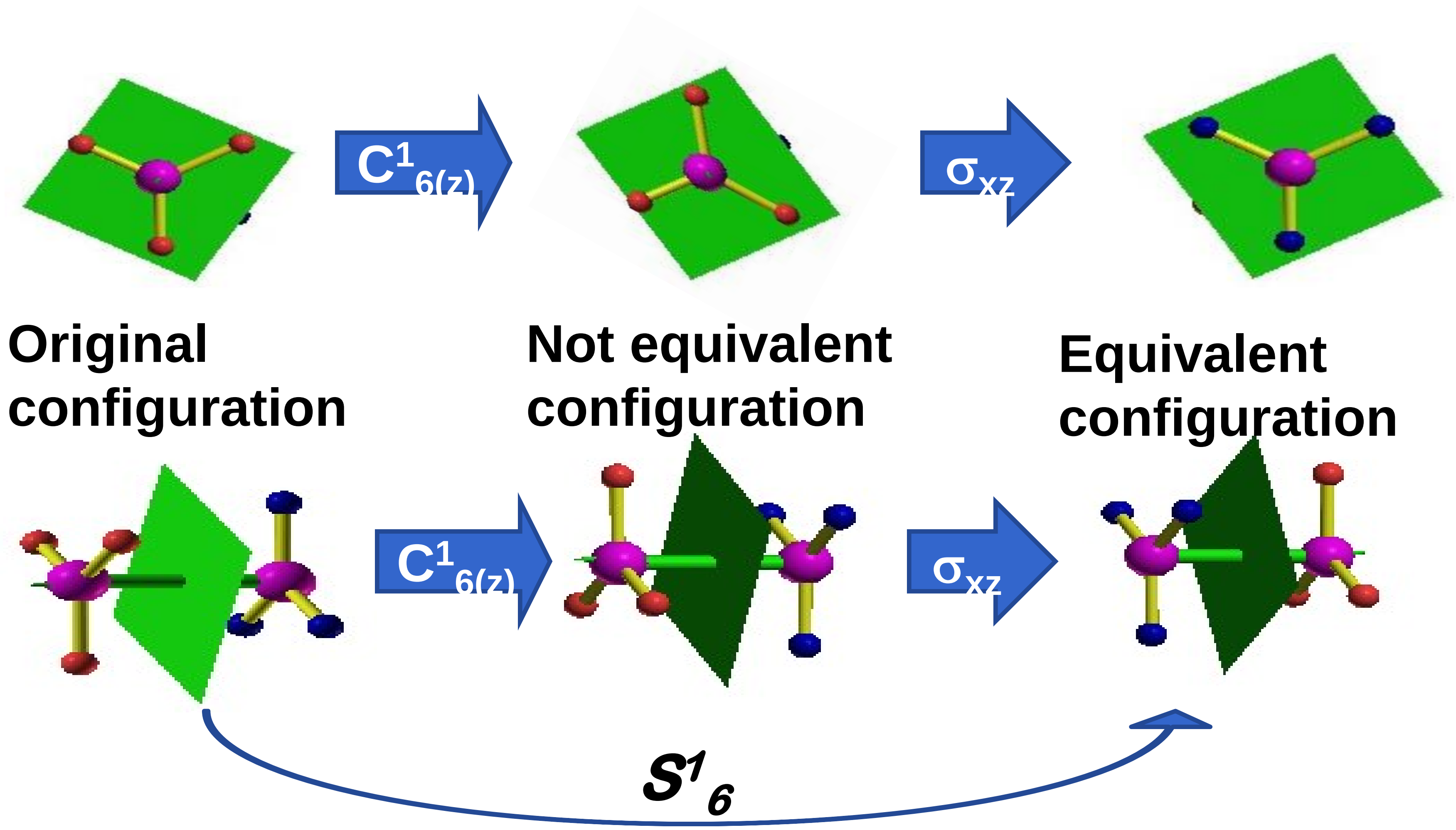
Examples: Eclipesed ehane(S3); BF3(S3); eclipesed ferrocene(S5); PtCl4(S4); Eclipesed dibenzene cromium(S6).

However, S_n may exist even when C_n and σ_h perpendicular to C_n do not exist independently.

Examples: St.ethane(S6); St.Ferrocine(S10); St.Cr(C6H5)2

Staggered ethane do not contain the C_6 axis (C_3 is present) and σ_h plane. But S_6 is present in this mole.





C16(z)
σxz
Original configuration
Not equivalent configuration
Equivalent configuration
C16(z)
σxz
S16

Original configuration

$C^1_{6(z)}$

Not equivalent configuration

σ_{xz}

Equivalent configuration

S^1_6

S^2_6

Equivalent configuration

S^3_6

Equivalent configuration

S^4_6

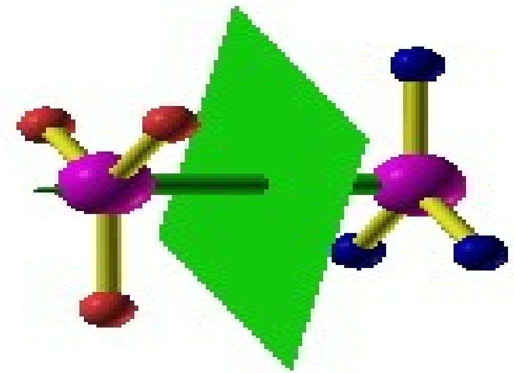
Equivalent configuration

S^5_6

Equivalent configuration

S^6_6

Identical configuration



Inversion centre of symmetry. [*i*]

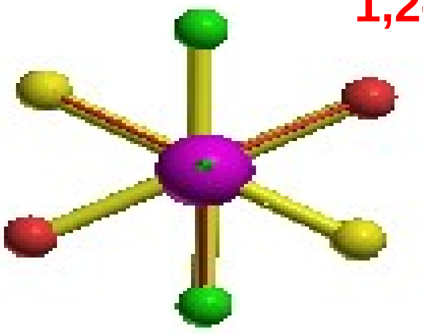
[*i*] *is* Generated when all the atoms or groups are inverted through the center of the molecules.

This operation requires :

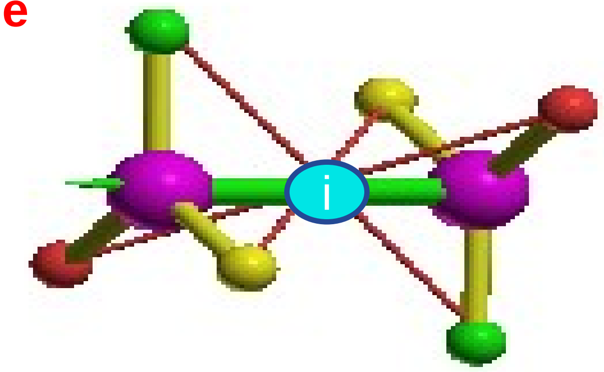
- ✓All the atoms or groups lying out side the center of gravity of the mole.
- ✓All atoms or groups must always occur in identical pairs or twins.
- ✓All the atoms or groups must be diagonally placed with each other.

Examples of molecules having Inversion centre [*i*]

1,2-dichloro 1,2-dibromoethane



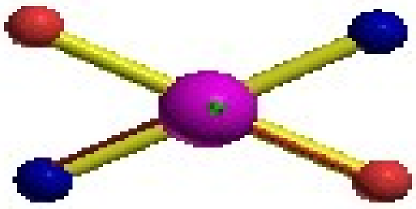
Cl
Br
H
C



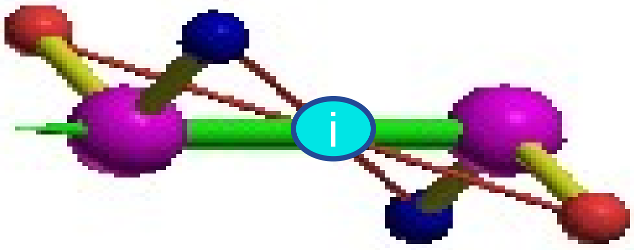
Newman projection

P_2F_4

Horse projection

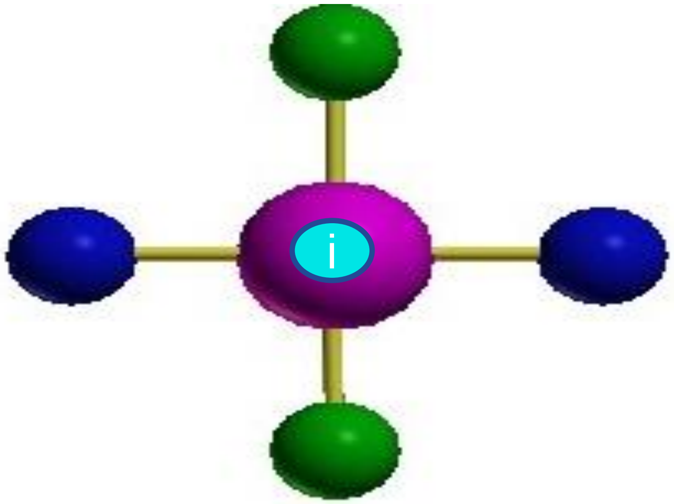


F1
F2
P



An atom may or may not be located at the inversion center.

- In P_2F_4 and ClBrCH-CHBrCl mole. An atom may not located at the Inversion center.
- In $PtCl_4$ mole. Pt atom located at the I.C.

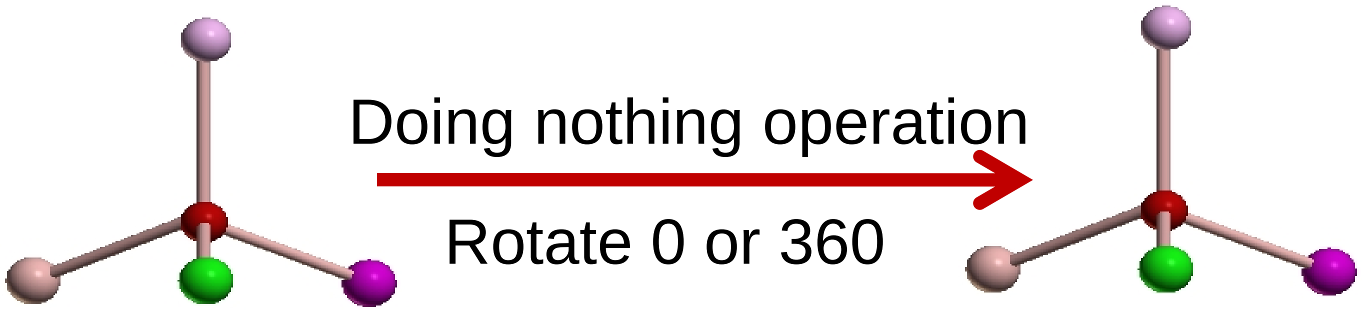


Identity (E)

This element is obtained by an operation ‘ identity operation’ (doing-nothing operation).
Every molecule has this element of symmetry.

After this operation, the molecule remains as such.
This situation can be visualized by two ways.

1. Do not do any thing on molecules.
2. Rotate the molecules by 360.

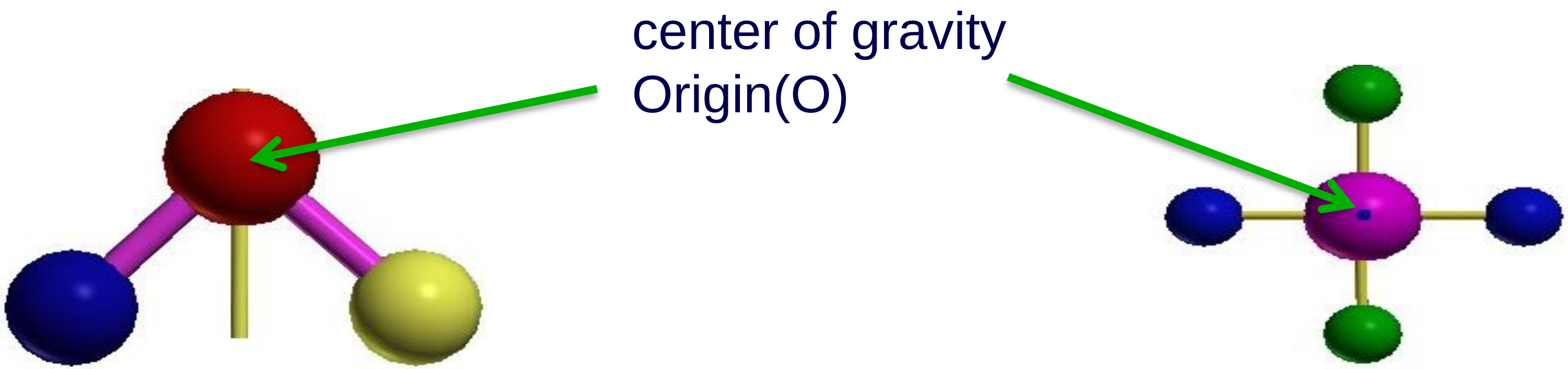


Cartesian coordinate system and symmetry element

It is always convenient to place a molecule in Cartesian coordinates(X,Y,Z) system and define its symmetry element .

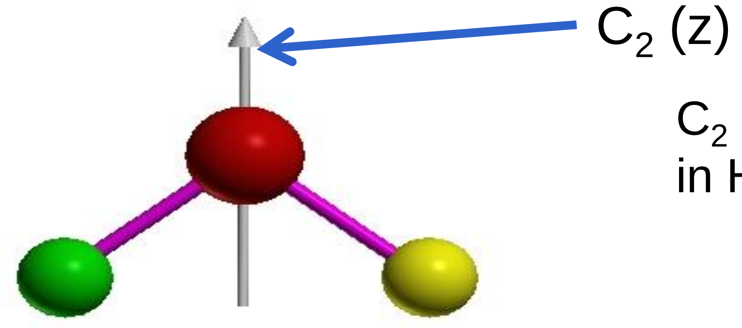
Origin (O):-

Molecules has always the center of gravity and the center of gravity always located at the origin of the coordinate axis system.



Z-Axis:-

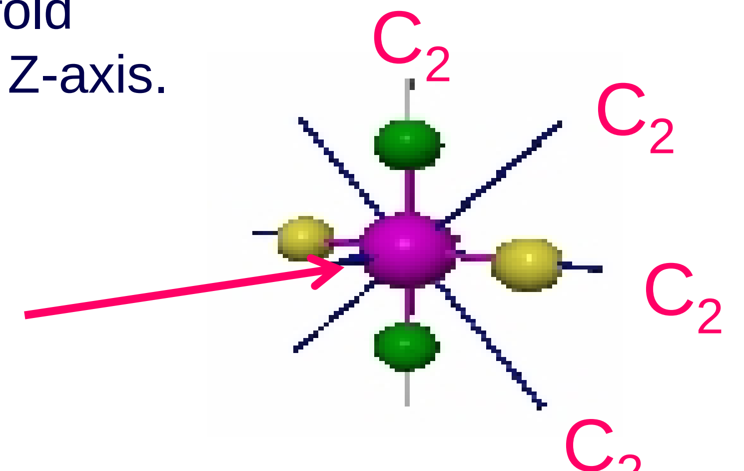
1. if there is only one R.A. of symmetry, it is to be taken as Z-axis.



C_2 (only one R.A.) it is to be selected Z-axis in H_2O.

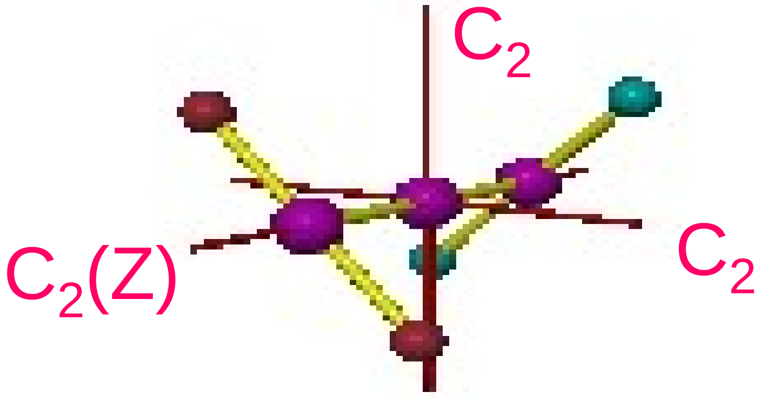
2. if there are more than one R.A. the highest fold rotational axis (P.R.A.) is to be selected as the Z-axis.

C_4 (PRA) is to be selected Z-axis [C_4 (Z)]



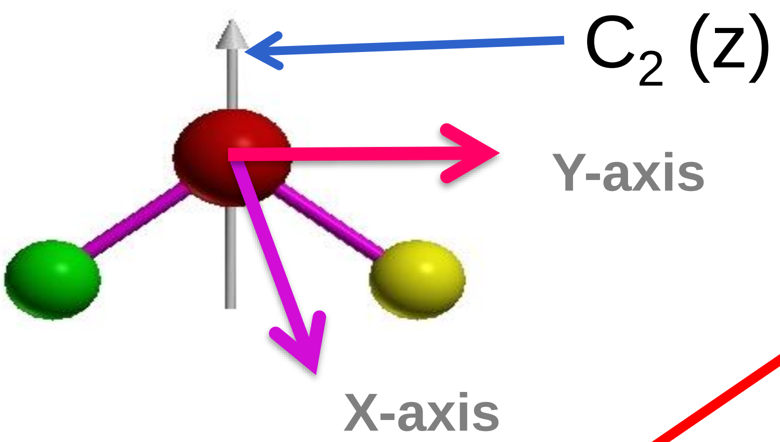
3. if there are more the highest fold rotational axis(P.R.A.), the axis containing more number of atoms should be considered as the z-axis

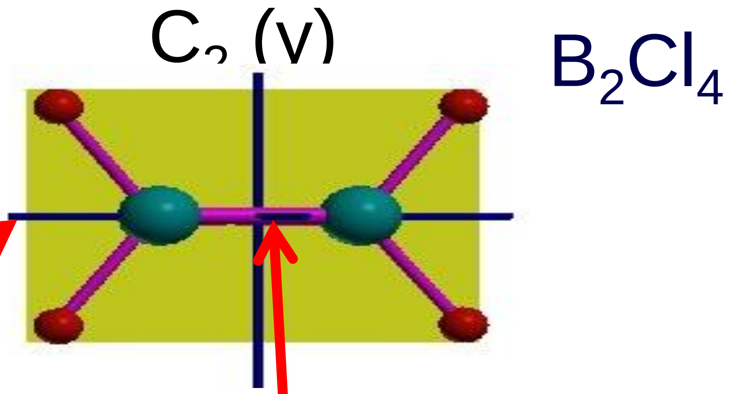
There are three C2 axis in Aline mole, the C2 axis which is containing three C-atoms is to be selected as Z-axis



X & Y-Axis:-

- If the molecules is planer and if Z-axis is lies in this plane then the X-axis is to be chosen as the perpendicular to this plane.
 and Y-Axis then lies perpendicular to the XZ plane.





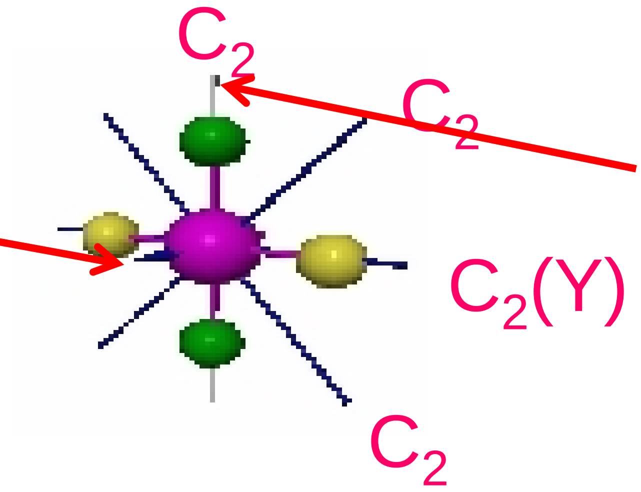
C_2 (z) lies in molecular plane

C_2 (x)perpendicular to the z-axis & plane

X & Y-Axis:-

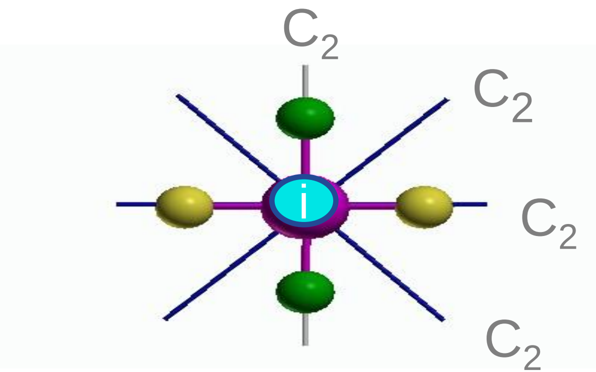
- If the molecules is planer and if Z-axis is perpendicular to this plane then x-axis is chosen as passing through the largest number of atoms or group,
  and Y-Axis is chosen as perpendicular to the XZ plane.

[C_4 (Z)] perpendicular the molecular plan.



[C_2(X)] perpendicular the C_4 (Z). And passing through Pt and 2Cl atoms

How to make the group of total SE for the molecules?



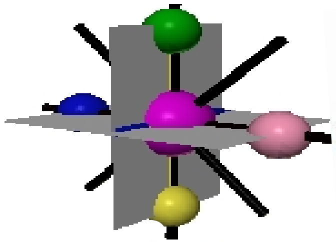
$$Identity = E$$

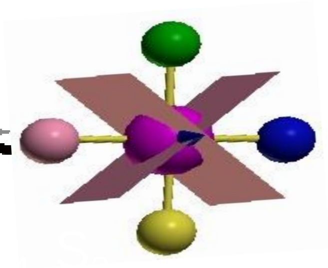
$$P.R.A. = C_4^1, C_4^2, C_4^3, C_4^4, C_4^5, \ldots\ldots C_4^n.$$

$$P.R.A.(2) = C_2^1, C_2^2, C_2^3, C_2^4, C_2^5, \ldots\ldots C_2^n.$$

$$S.R.A. = 4C_2^1, 4C_2^2, 4C_2^3, 4C_2^4, \ldots\ldots 4C_2^n.$$

$$\mathrm{Im}.R.A. = S_4^1, S_4^2, S_4^3, S_4^4, S_4^5, \ldots\ldots S_4^n.$$

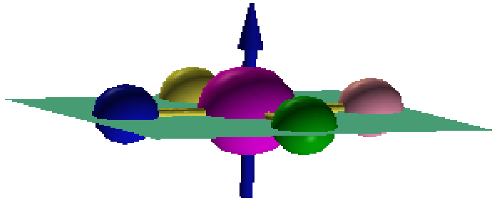




$$\mathrm{Im}.R.A.(2) = S_2^1, S_2^2, S_2^3, S_2^4, \ldots\ldots S_2^n.$$

$$H.Plane = \sigma h^1, \sigma h^2, \sigma h^3, \ldots.\sigma h^n,$$

$$V.Plane = 2\sigma v^1, 2\sigma v^2, 2\sigma v^3, \ldots.2\sigma v^n,$$



$$D.Plane = 2\sigma d^1, 2\sigma d^2, 2\sigma d^3, \ldots.2\sigma d^n,$$

$$I.C. = i^1, i^2, i^3, \ldots.i^n,$$

More about symmetry elements….

- ✓For any given Molecules, it is possible to list the symmetry elements extensively.
- ✓The list of S.E. is called group of molecules.
- ✓And the No of S.E. is called order of group (h)

In one group, S.E. correlated with other S.E.

S.E. implied occurrence other S.E.

- ➢ It is not necessary to indicate such type of S.E.
- ➢ This type of S.E. preclude and than indicate in a group of molecules.

Some important relation of S.E.

S.E.	n	Correlation
C_n^n	n= even or odd	E
σ^n	n= even	E
	n= odd	σ
i^n	n= even	E
	n= odd	i
S_n^n	n= even	E
	n= odd	σ

The implied presence of other S.E. and deducing

The S.E. implied the other S.E. in group , they can be deduced by using the relationship

The presence of Cn axis in a molecule will always imply the presence of a total of *n* distinct S.E.

$$C_n^1 \cdot C_n^2 \cdot C_n^3 \ldots\ldots\ldots\ldots C_n^n . C_n^{n+1} . C_n^{n+2} \ldots\ldots\ldots\ldots$$

$$C_n^{n+1} = C_n^n \cdot C_n^1 = E \cdot C_n^1 = C_n^1$$

Where C_n^{n+1} Is repeated,

When once the repeated element is encountered, the series should be terminated.

Example, when n=even, C_4 axis is present in $PtCl_4$.

P.R.A.	Correlation	
C_4^1		C_4^1
C_4^2	$C_{4/2}^{2/2}$	C_2^1
C_4^3		C_4^3
C_4^4		E
C_4^5	$C_4^{4+1} = C_4^4 \cdot C_4^1 = E \cdot C_4^1 = C_4^1 (repeted)$	

$$C_n^m = C_{n/m}^{m/m} = C_k^1$$

Example, when n=odd, C_3 axis is present in BF_3.

P.R.A.	Correlation	
C_3^1		C_3^1
C_3^2		C_3^2
C_3^3		E
C_3^4	$C_3^{3+1} = C_3^3 \cdot C_3^1 = E \cdot C_3^1 = C_3^1 (repeted)$	

S_n axis are implied other S.E.

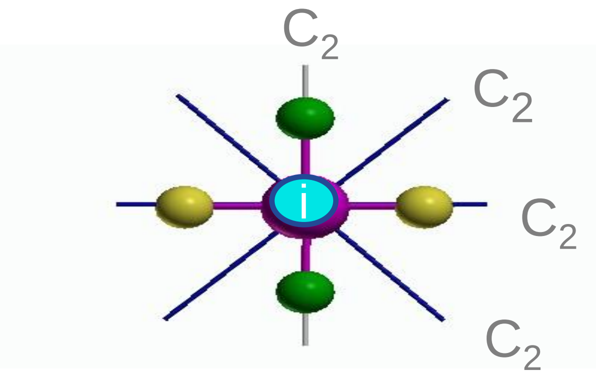
Example, when n=even, S_4 axis is present in $PtCl_4$.

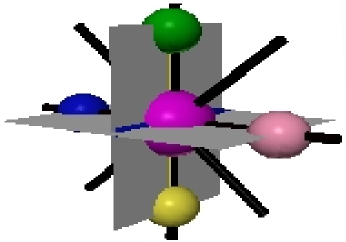
P.R.A.	Correlation	
S_4^1		S_4^1
S_4^2	$S_4^2 = C_4^2 \cdot \sigma^2 = C_2^1 \cdot E = C_2^1$	C_2^1
S_4^3		S_4^3
S_4^4		E
S_4^5	$S_4^{4+1} = S_4^4 \cdot S_4^1 = E \cdot S_4^1 = S_4^1 (repeted)$	

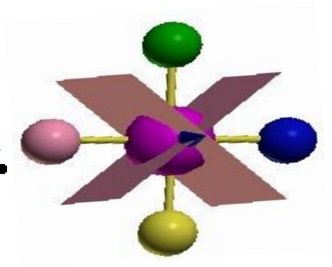
Example, when n=odd, S_3 axis is present in BF_3.

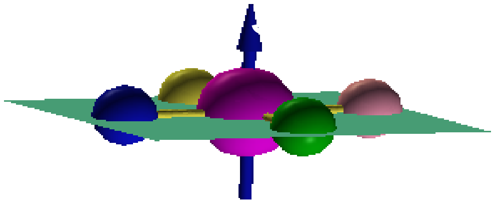
P.R.A.	Correlation	
S_3^1		S_3^1
S_3^2	$S_3^2 = C_3^2 \cdot \sigma^2 = C_3^2 \cdot E = C_3^2$	C_3^2
S_3^3	$S_3^3 = C_3^3 \cdot \sigma^3 = E \cdot \sigma^2 \cdot \sigma = E \cdot E \cdot \sigma = \sigma_h$	σ_h
S_3^4	$S_3^4 = C_3^4 \cdot \sigma^4 = C_3^3 \cdot C_3^1 \cdot E = C_3^1$	C_3^1
S_3^5		S_3^5
S_3^6	$S_3^6 = C_3^6 \cdot \sigma^6 = E$	E
S_3^7	$S_3^{6+1} = S_3^6 \cdot S_3^1 = E \cdot S_3^1 = S_3^1 (repeted)$	

The actual amount of S.E. in $PtCl_4$









$$Identity = E$$

$$P.R.A. = C_4^1, C_4^3,$$

$$P.R.A.(2) = C_2^1,$$

$$S.R.A. = 4C_2^1,$$

$$\mathrm{Im}.R.A. = S_4^1, S_4^3,$$

$$\mathrm{Im}.R.A.(2) = S_2^1, = i$$

$$H.Plane = \sigma h^1$$

$$V.Plane = 2\sigma v^1$$

$$D.Plane = 2\sigma d^1$$

$$I.C. = i^1 \cdot or \cdot S_2^1$$

Total no of S.E.=16

Notation of Point Group

The list of actual amount of S.E. for molecules is called group of S.E. and the group of S.E. is indicated by some symbols, is called P.G. of molecule.

→Every group has a descriptive symbol signifying the presence of some defining combination of S.E.

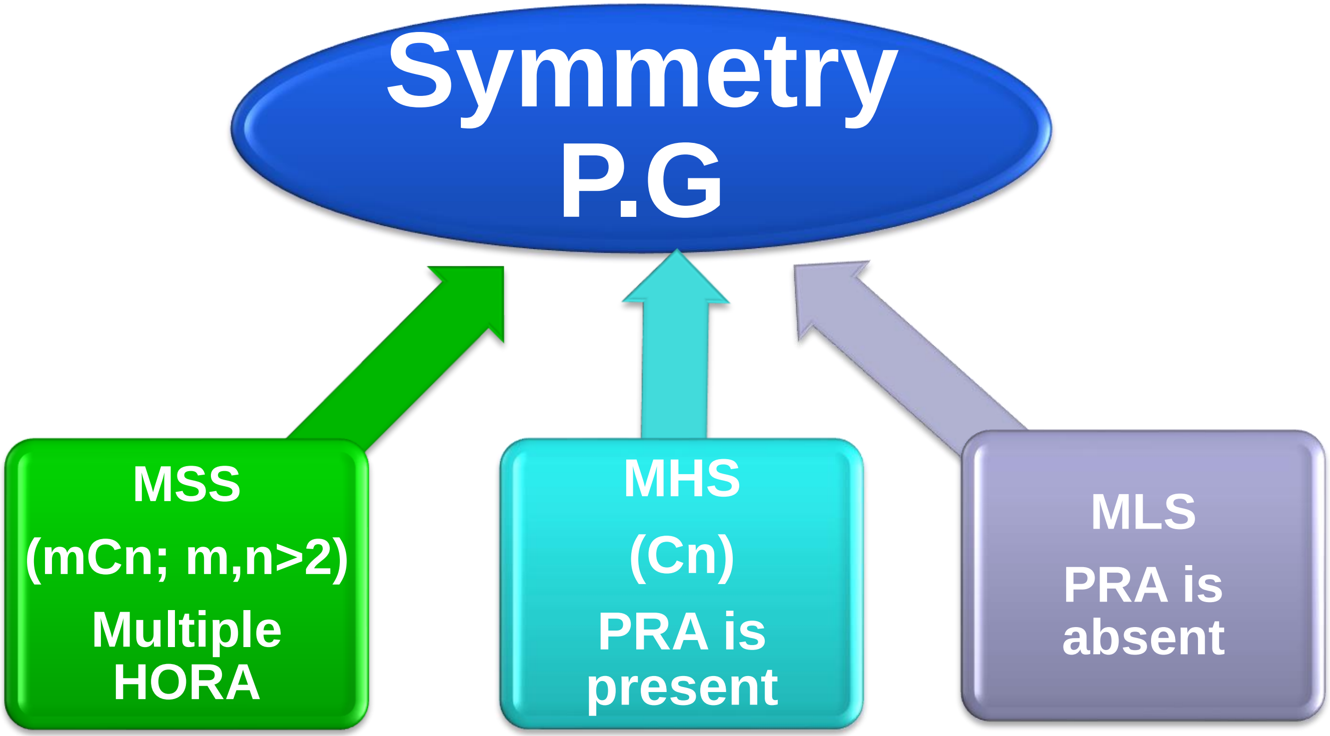
→There are two types of symbolism.

1. Schoenflies Notation
2. Hermann-Mauguin notation

Schoenflies Notation

1. The main symbol (alphabetical) used refers to the axis of highest symmetry in the molecules.
   C- stands for highest-fold proper axis.
   S- stands for highest fold improper axis.
   D- stands for H.F.P.R.A. with nC2 (S.R.A) perpendicular to it.
   T;O;I;- are specially symbols to represent the highly symmetry.
   Tetrahedral; octahedral; icosahedral.
2. The numerical subscripts indicate the order of the H.O.R.A.
   C_1, C_2, C_5,D_2, D_1 D_3,, S_3,
3. Further labeling with alphabetical subscripts indicates the presence of certain type of planes of symmetry.
   v- used for vertical plane. d.-is used for dihedral plane.
   h.-used for horizontal plane.
4. The subscript "*i*" alone is used when the mole. Contains only '*i*' element.(C_i)
5. The subscript "s" alone is used when the mole. Contains only plane of symmetry 'σ' element.(C_s)
6. For the linear mole. Using the symbols Cαh and Dαh depending on the absence or presence of 'I' .

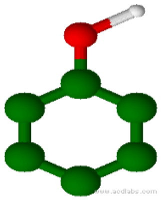
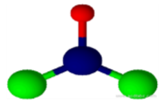
Flow chart of Sy. P.G.



MLS
PRA is absent

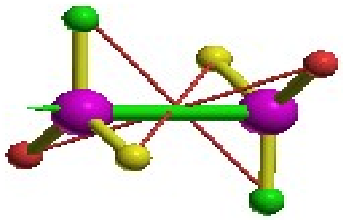
Cs
Only σ

$ClBr-CH_2$
Phenol, HOD,
$SOCL_2$; Aniline

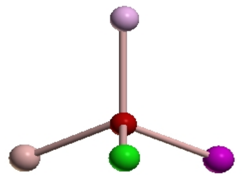
Ci
Only i

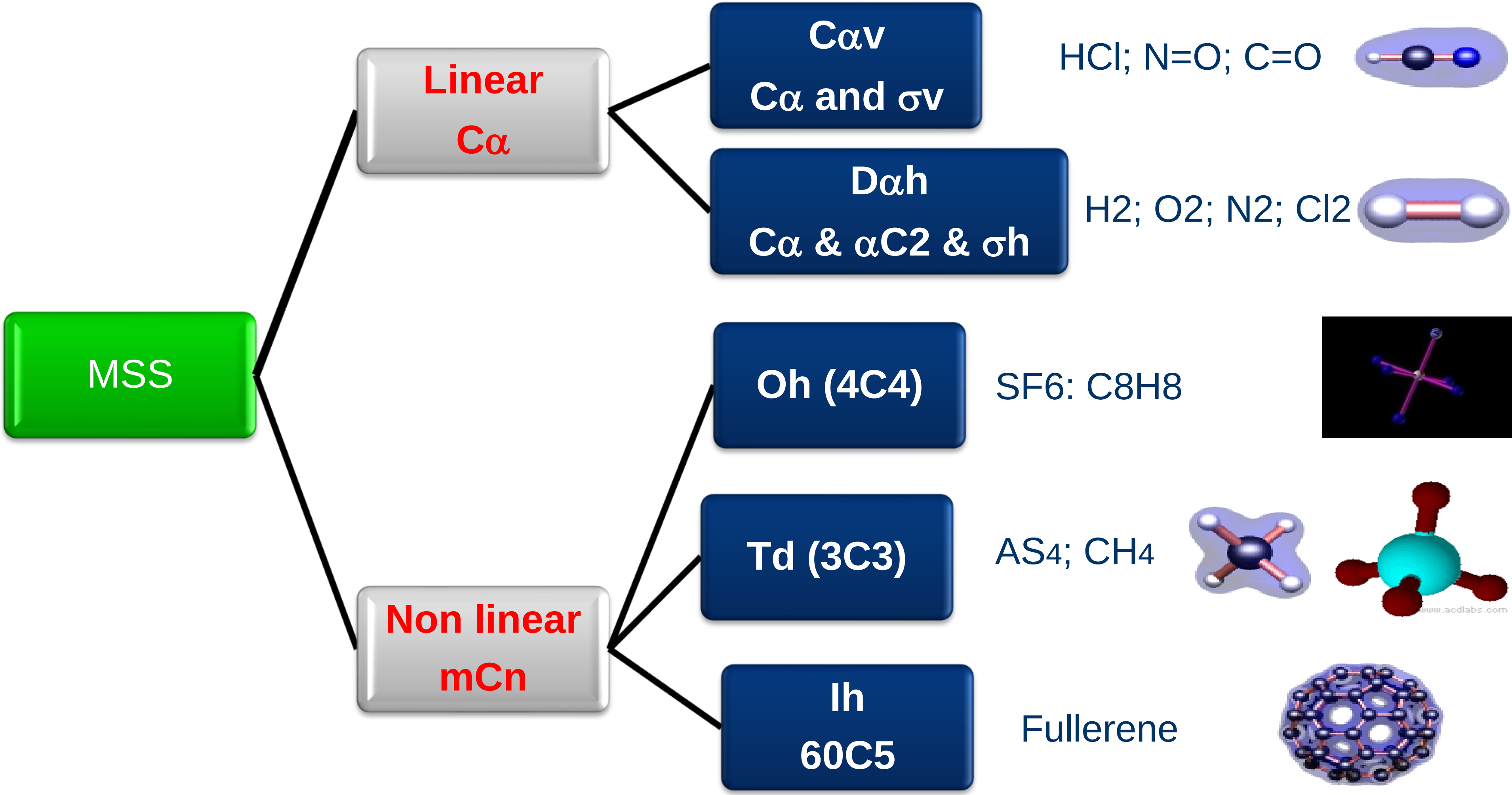
Trans CHFCl-CHFCl



C_1
Only C1

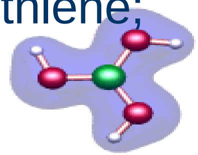
CH-Cl.Br.I



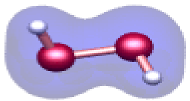

MSS
Linear
Cα
Non linear
mCn
Cαv
Cα and σv
Dαh
Cα & αC2 & σh
Oh (4C4)
Td (3C3)
Ih
60C5
HCl; N=O; C=O
H2; O2; N2; Cl2
SF6: C8H8
AS4; CH4
Fullerene
www.acdlabs.com

MHS

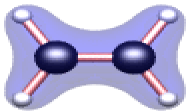
- Only Cn , is present
  - Cnv: Cn and σv — H2O; Pyridene: NH3; Ph3: SO2; SOCl2; PCl3; XeOF4
  - Cnh: Cn & σh — Trans-1.2-dichloroethlene; H3BO3;



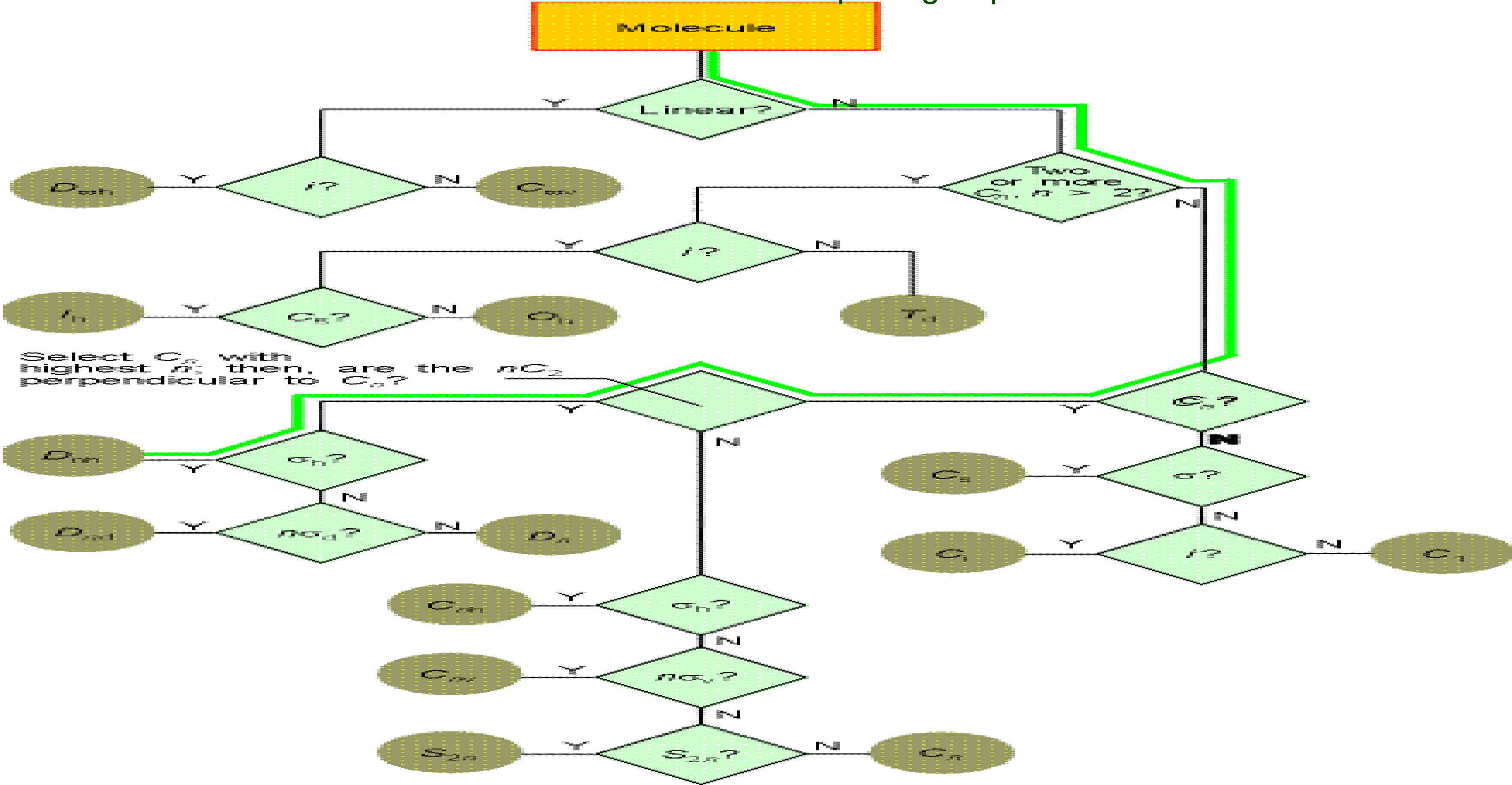
  - Only Cn — Non-planer H2O2; NPh3:PPh3



- Cn ⊥ nC2 present
  - Dn: Only Cn ⊥ nC2 — G-C2H4; G-C2H6
  - D2d: Cn ⊥ nC2 & σd — Allene; S-C2H6; S-Ferrocine; S-Cr(C6H6)2
  - Dnh: Cn ⊥ nC2 & σh — C2H4; B2H6; BF3; PCl5; C6H6; PtCl4; e-C2H6: Borozole(B3N3H6)



Knowing the Symmetry Elements of the molecule we can now use the following flow chart to determine the molecular point group.



Point Group and their detailed list of actual S.E.

Point group	Order of group, h	Type of symmetry elements
C_1	1	$E\ (=C_1)$
C_i	2	$E, I\ (=S_2)$
C_s	2	E, σ
	C_n – groups: (h = n)	
C_2	2	E, C_2
C_3	3	$E\ C_3^1, C_3^2$
C_4	4	$E, C_4^1, C_4^2\ (=C_2), C_4^3$
C_5	5	$E, C_4^1, C_4^2, C_4^3, C_4^4$
	C_{nv} – groups: (h = 2n)	
C_{2v}	4	$E, C_2, 2\sigma$
C_{3v}	6	$E, C_3^1, C_3^2, 3\sigma_v$
C_{4v}	8	$E, C_4^1, C_4^2(=C_2), C_4^3, 2\sigma_v, 2\sigma_v'$
	C_{nh} – groups: (h = 2n)	
C_{2h}	4	$E, C_2, i=(S_2), \sigma_h$
C_{3h}	6	$E, C_3^1, C_3^2, S_3^1, S_3^5, \sigma_h$
C_{4h}	8	$E, C_4^1, C_4^2(=C_2), C_4^3, S_4^1, S_4^3, \sigma_h, i=(S_2)$
	D_n – groups: (h = 2n)	
D_2	4	E, C_2, C_2'
D_3	6	$E, C_3^1, C_3^2, 3C_2$
D_4	8	$E, 2C_4, C_2, 4C_2$

Point Group and their detailed list of actual S.E.

D_{nh} – groups: (h = 4n)		
D_{2h}	8	E, C_2 , $2C_2'$, i=(S_2), σ_h , $2\sigma_v$
D_{3h}	12	E, $2C_3$,$3C_2$, σ_h ,$3\sigma_v$, $2S_3$, (S_3^1, S_3^5)
D_{4h}	16	E, $2C_4$,(C_4^1,C_4^2), C_2=(C_4^2), $2C_2'$,$2C_2''$, σ_h ,$2\sigma_v$,$3\sigma_d$, i , $2S_4$ (S_4^1, S_4^3)
D_{nd}– groups: (h = 4n)		
D_{2d}	8	E, C_2 , $2C_2'$, 2 σ_d, $2S_4$
D_{3d}	12	E, $2C_3$ (C_3^1, C_3^2), $3C_2$,i, $3\sigma_d$, $2S_6$(S_6^1, S_6^3)
D_{4d}	16	E, $2C_4$, (C_4^1, C_4^3), C_2=(C_4^2), $4C_2'$,$4\sigma_d$, $4S_8$(S_8^1, S_8^3 , S_8^5, S_8^7)
S_n (n=even)– groups: (h = n)		
S_4	4	E, S_4^1, S_4^3 , C_2
S_6	6	E, S_6^1, S_4^5, C_3^1, C_3^2, i
S_8	8	E, S_8 ,S_8^1, S_8^3 , S_8^5, S_8^7, C_4^1, C_4^3, C_2=(C_4^2)
Infinite- point group (h=∞)		
$C_{\infty v}$	∞	E, ∞, C_∞, $\infty\sigma_v$
$D_{\infty v}$	∞	E, ∞, C_∞, $\infty\sigma_v$, σ_h, i

How define the Order of Point Group (h) ?

The total no. of symmetry element s is present in point group that is called order of point group.

Method to identify order of Point Group

Allocate Number: 1 for C and S
2 for D
4 for T
6 for O
12 for I

Multiply by principle axis number (n)

Multiply by 2 for any plane (σ), centre of symmetry (i)

C_2v = 1*2*2=h=4

C_i = 1*2=h=2

C_4v = 1*4*2=h=8

Td = 4*3*2=h=24

D_{4h} = 2*4*2=h=16

Oh= 6*4*2=h=48

THANK YOU…THANK YOU….