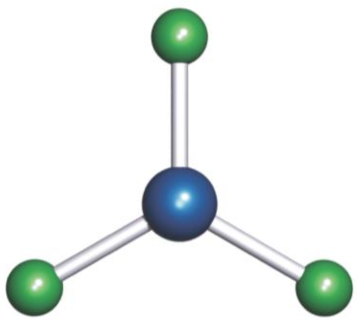
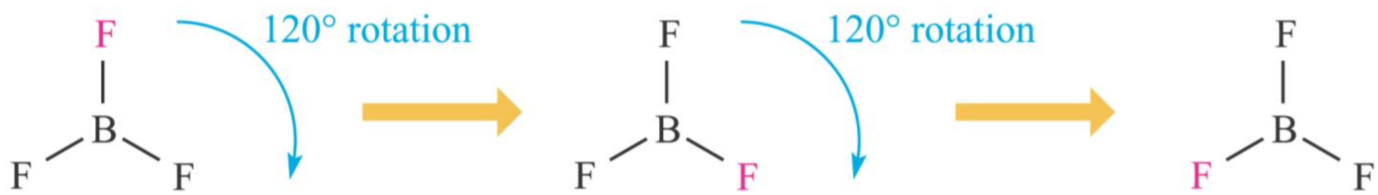
Una molecola ha una ***simmetria*** *se possiede due o più orientazioni nello spazio (o configurazioni) che sono indistinguibili*

Una ***operazione di simmetria*** *muove una molecola (o, in generale, un oggetto) intorno a un elemento di simmetria fino a una configurazione indistinguibile da quella originale*

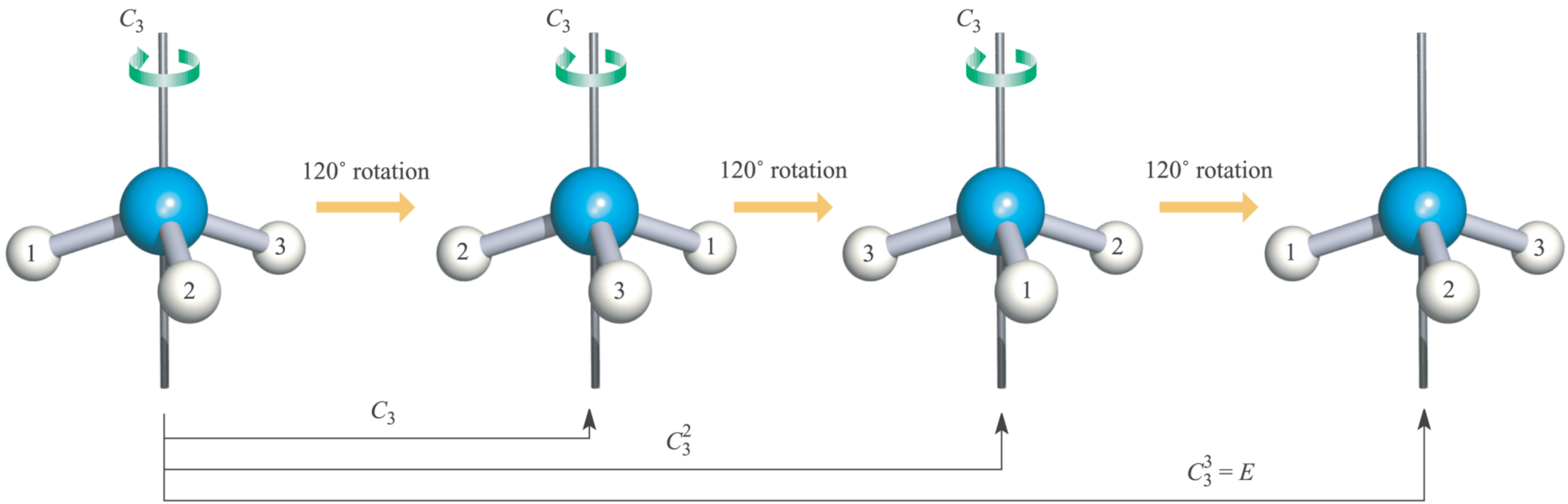
Gli ***elementi di simmetria*** *sono: asse, punto, piano.*

Asse C_n = rotazione di 360°/n



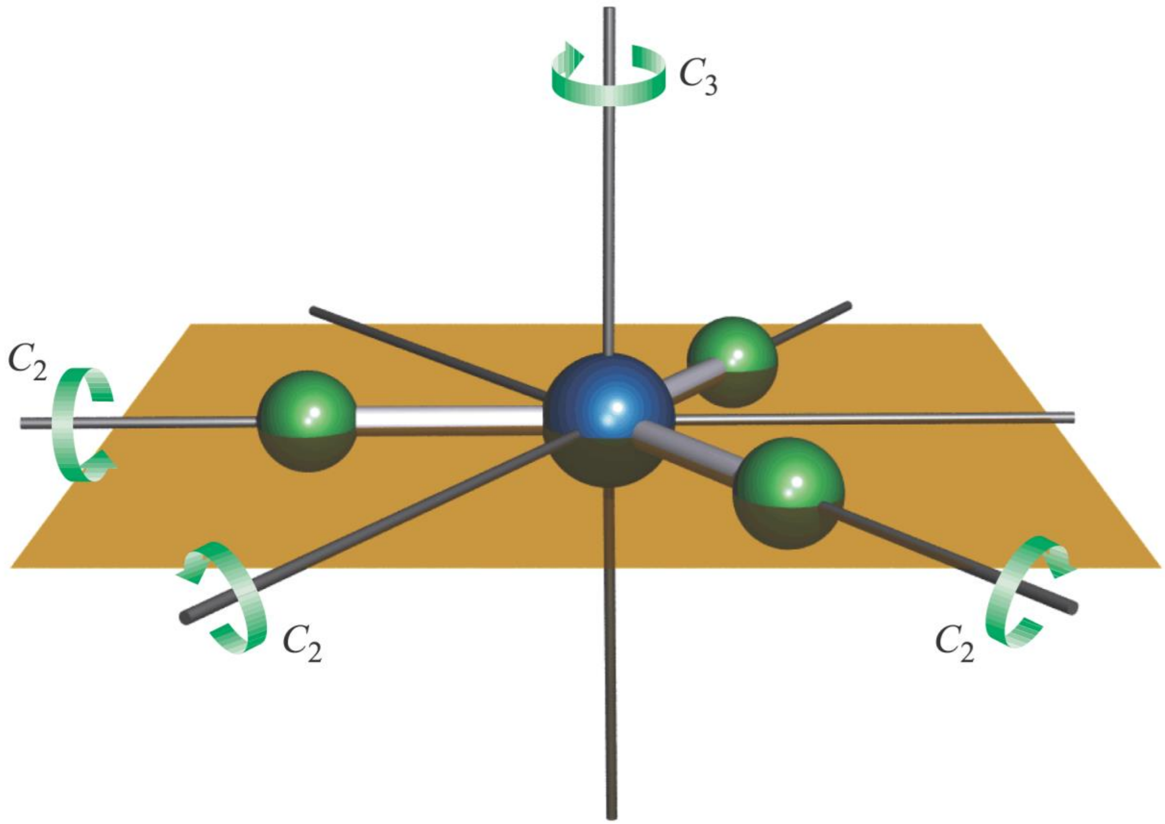


$$C_n^{\,n} = E$$

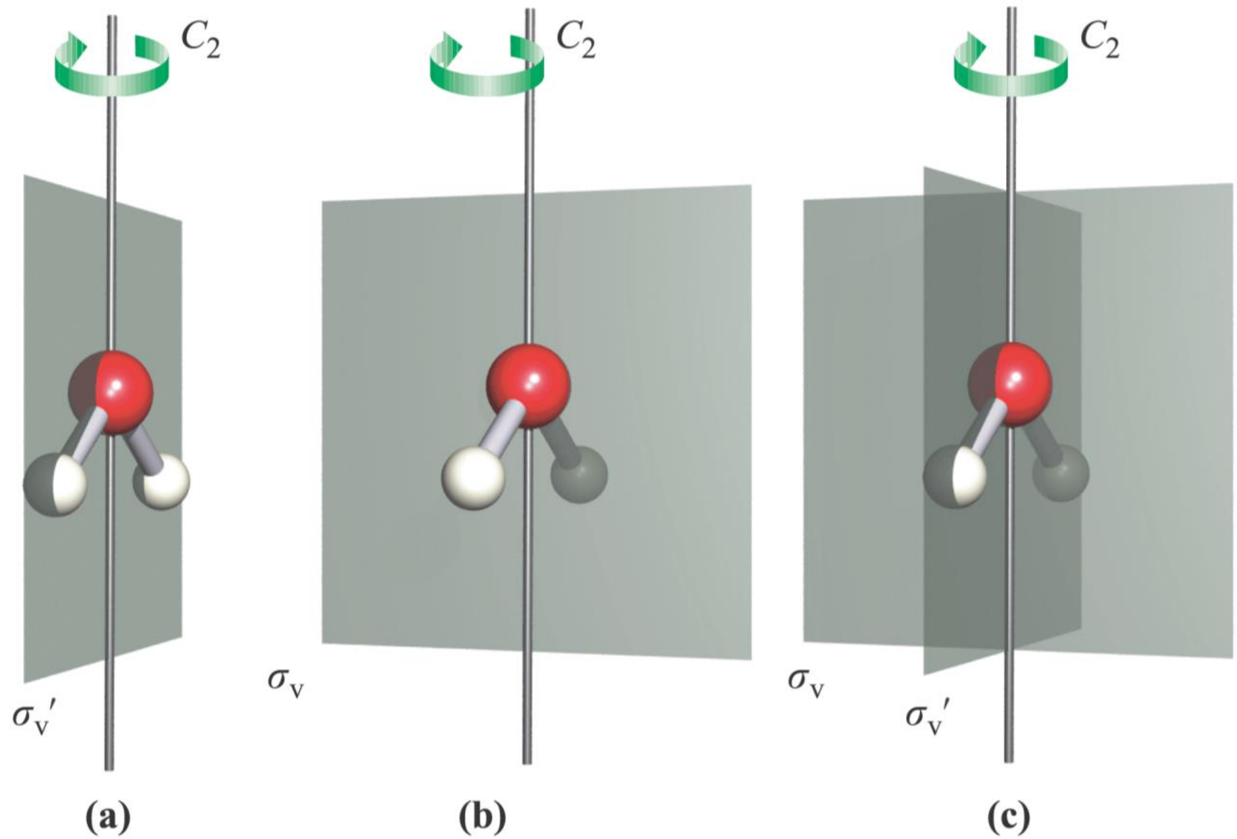


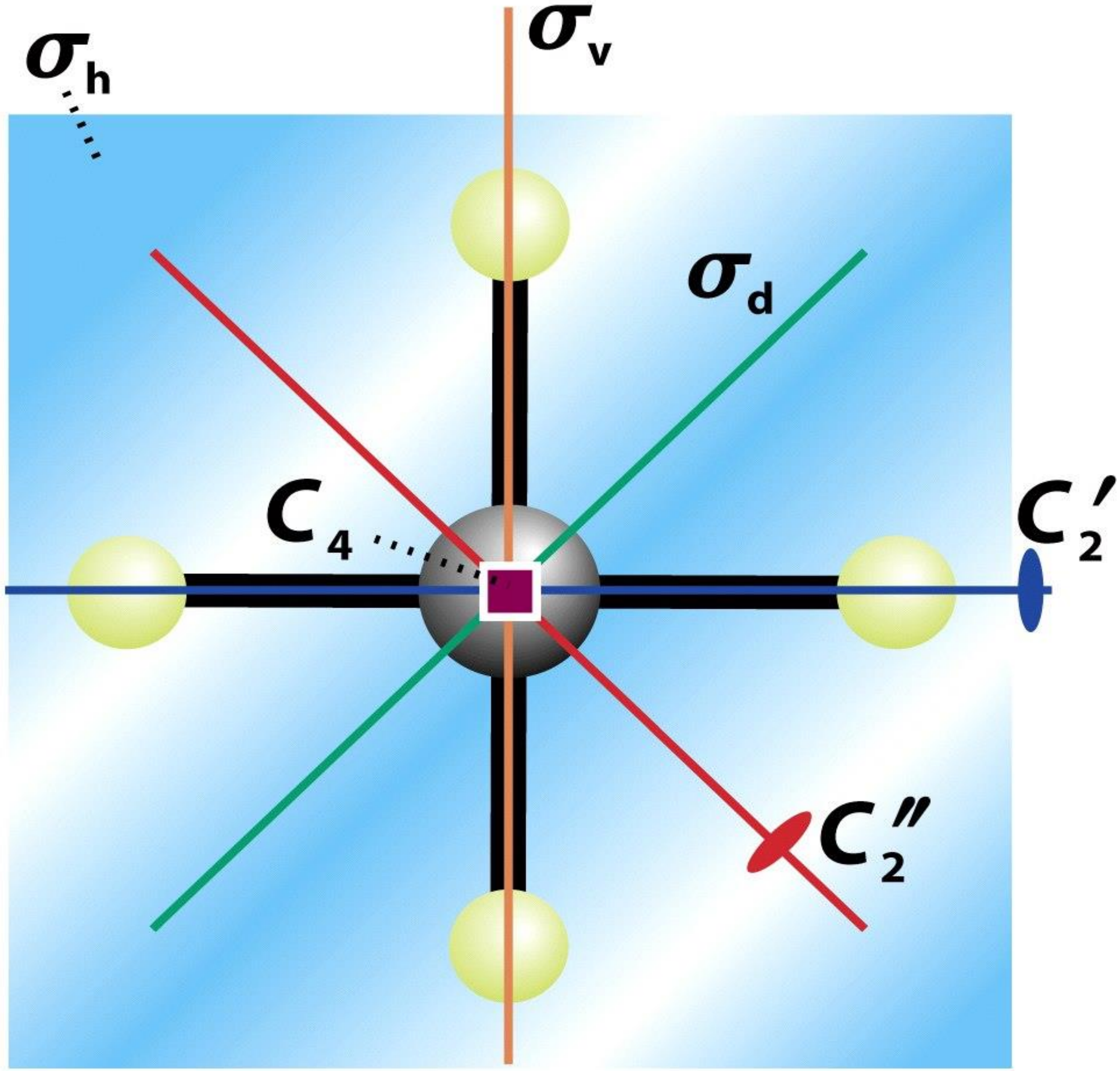
C_3
120° rotation
C_3
120° rotation
C_3
120° rotation
1
2
3
2
3
1
3
1
2
1
2
3
C_3
C_3^2
$C_3^3 = E$

Asse principale

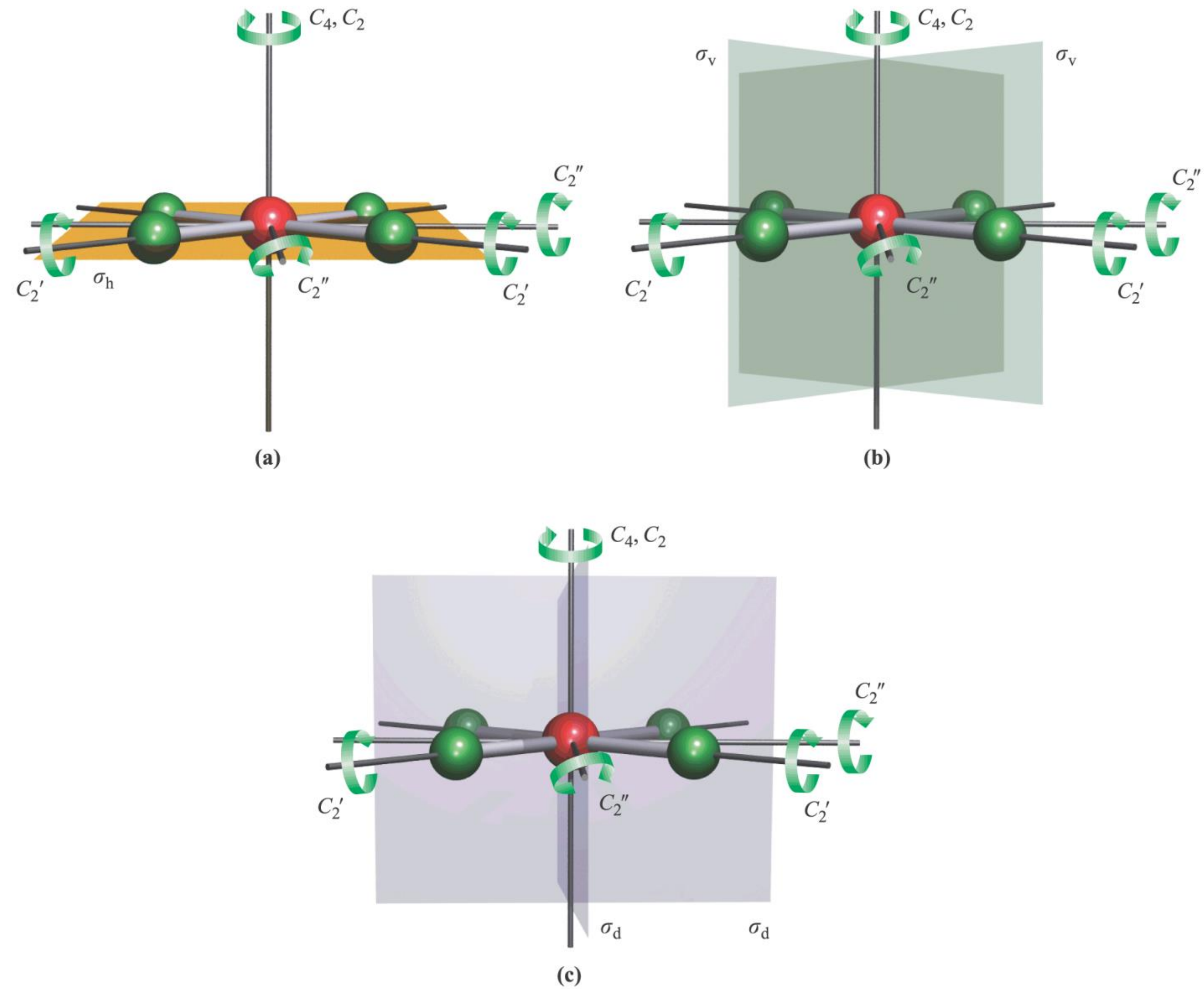


Piani di simmetria: σ_v, σ_h, σ_d



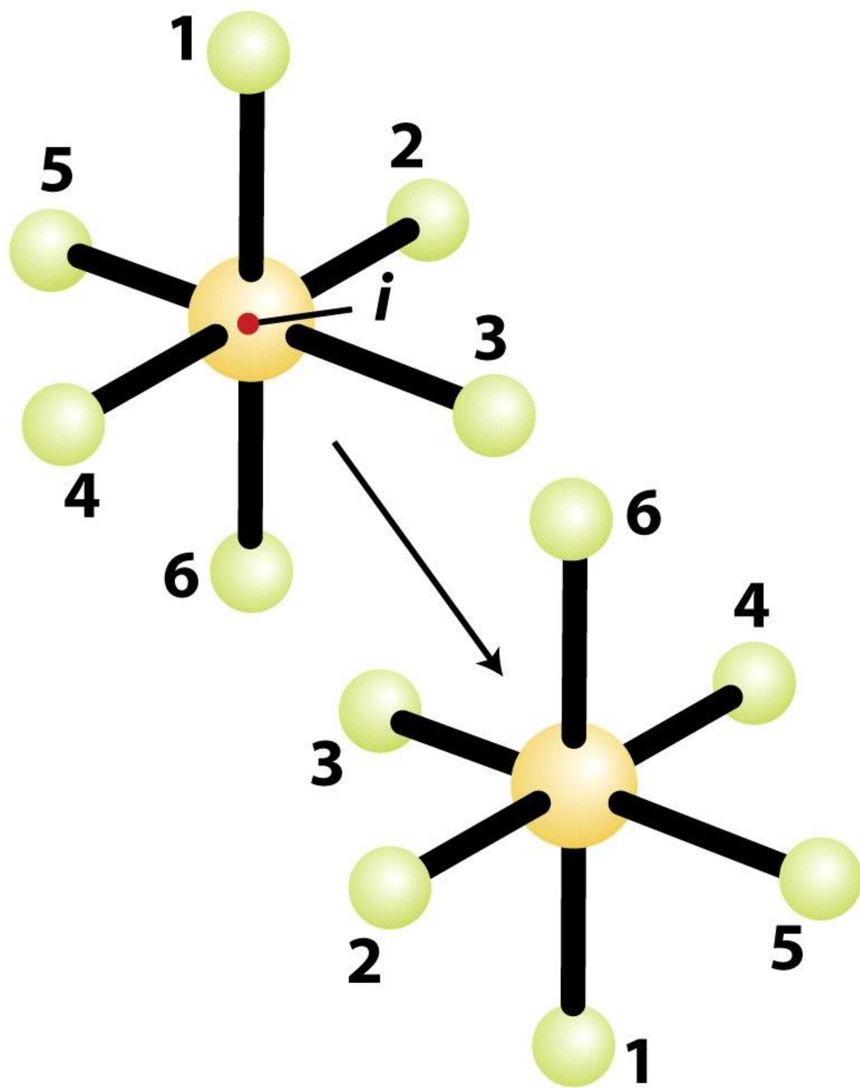


σ_h
σ_v
σ_d
C_4
C_2'
C_2''

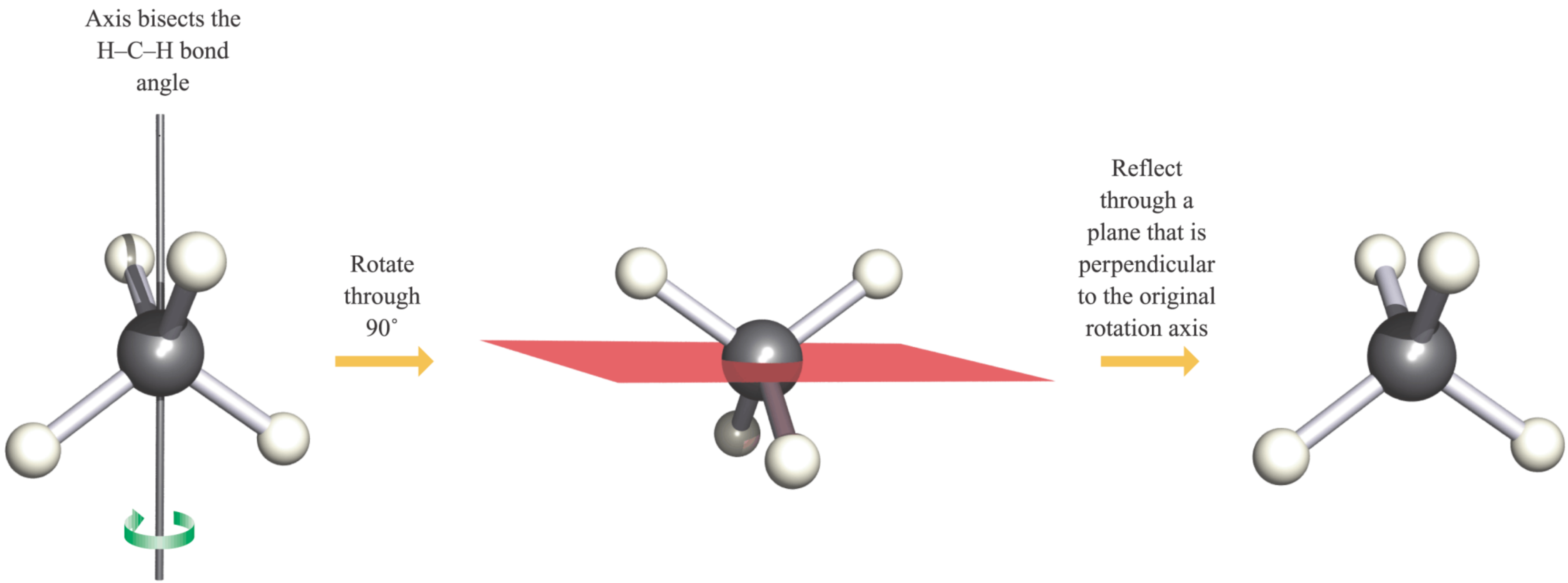


C_4, C_2
C_2''
C_2'
σ_h
C_2''
C_2'
(a)
C_4, C_2
σ_v
σ_v
C_2''
C_2'
C_2''
C_2'
(b)
C_4, C_2
C_2''
C_2'
C_2''
C_2'
σ_d
σ_d
(c)

Centro di simmetria (centro di inversione), *i*



Rotazione impropria o roto-riflessione
Assi S_n



$$S_1 = \sigma \text{ e } S_2 = i$$

Esempi

cis-$C_2H_2Cl_2$ (σ_v, σ_h, C_2)
trans-$C_2H_2Cl_2$ (σ_h, C_2)

Etano:
conformazione eclissata (C_3, $3C_2$, σ_h, $3\sigma_v$, S_3)
conformazione sfalsata (C_3, $3C_2$, $3\sigma_d$, i, S_6)

BCl_3 *vs* PCl_3 ($C_3 + 3C_2 + 3\sigma_v + \sigma_h$ vs $C_3 + 3\sigma_v$)

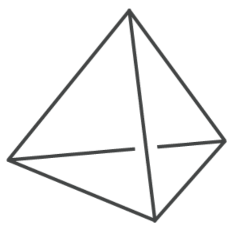
Gruppi puntuali

L’insieme degli elementi di simmetria di una molecola forma un gruppo di simmetria o **gruppo puntuale**.
Ogni gruppo puntuale è identificato con un simbolo, detto **Simbolo di Schoenflies**.

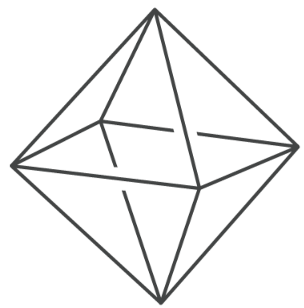
Gruppi puntuali

Simboli di Schoenflies

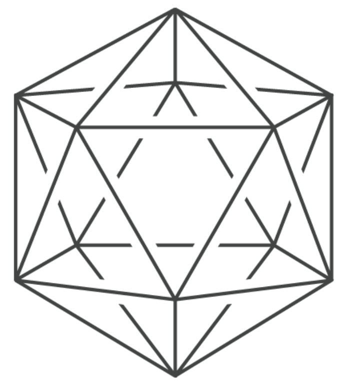
Point group	Characteristic symmetry elements	Comments
C_s	E, one σ plane	
C_i	E, inversion centre	
C_n	E, one (principal) n-fold axis	
C_{nv}	E, one (principal) n-fold axis, n σ_v planes	
C_{nh}	E, one (principal) n-fold axis, one σ_h plane, one S_n-fold axis which is coincident with the C_n axis	The S_n axis necessarily follows from the C_n axis and σ_h plane For $n = 2$, 4 or 6, there is also an inversion centre
D_{nh}	E, one (principal) n-fold axis, n C_2 axes, one σ_h plane, n σ_v planes, one S_n-fold axis	The S_n axis necessarily follows from the C_n axis and σ_h plane For $n = 2$, 4 or 6, there is also an inversion centre
D_{nd}	E, one (principal) n-fold axis, n C_2 axes, n σ_v planes, one S_{2n}-fold axis	For $n = 3$ or 5, there is also an inversion centre
T_d		Tetrahedral
O_h		Octahedral
I_h		Icosahedral



Tetrahedron

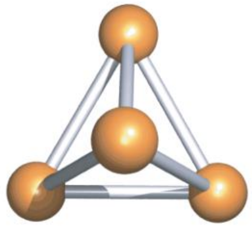


Octahedron

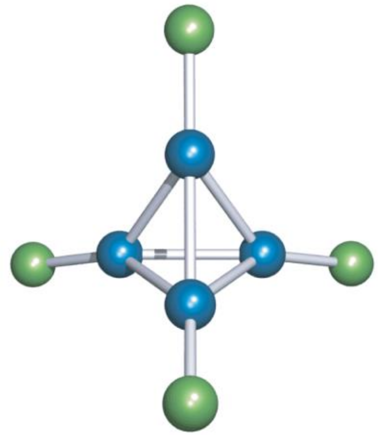


Icosahedron

P_4



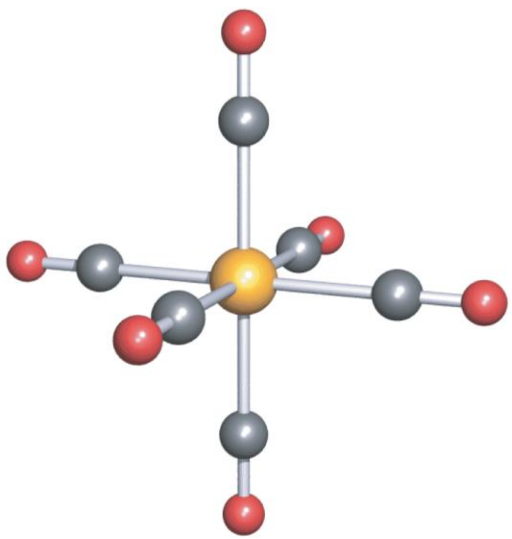
(a)



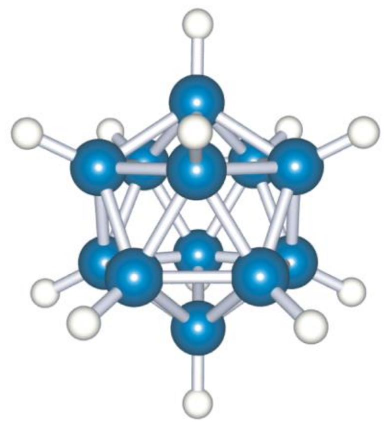
B_4Cl_4

(b)

$W(CO)_6$

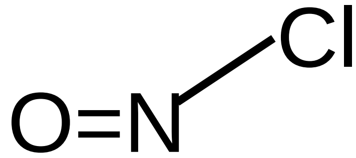


(c)



$[B_{12}H_{12}]^{2-}$

(d)



Point group	Characteristic symmetry elements	Comments
C_s	E, one σ plane	
C_i	E, inversion centre	
C_n	E, one (principal) n-fold axis	
C_{nv}	E, one (principal) n-fold axis, n σ_v planes	
C_{nh}	E, one (principal) n-fold axis, one σ_h plane, one S_n-fold axis which is coincident with the C_n axis	The S_n axis necessarily follows from the C_n axis and σ_h plane For $n = 2$, 4 or 6, there is also an inversion centre
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O_h		Octahedral
I_h		Icosahedral

Point group	Characteristic symmetry elements	Comments
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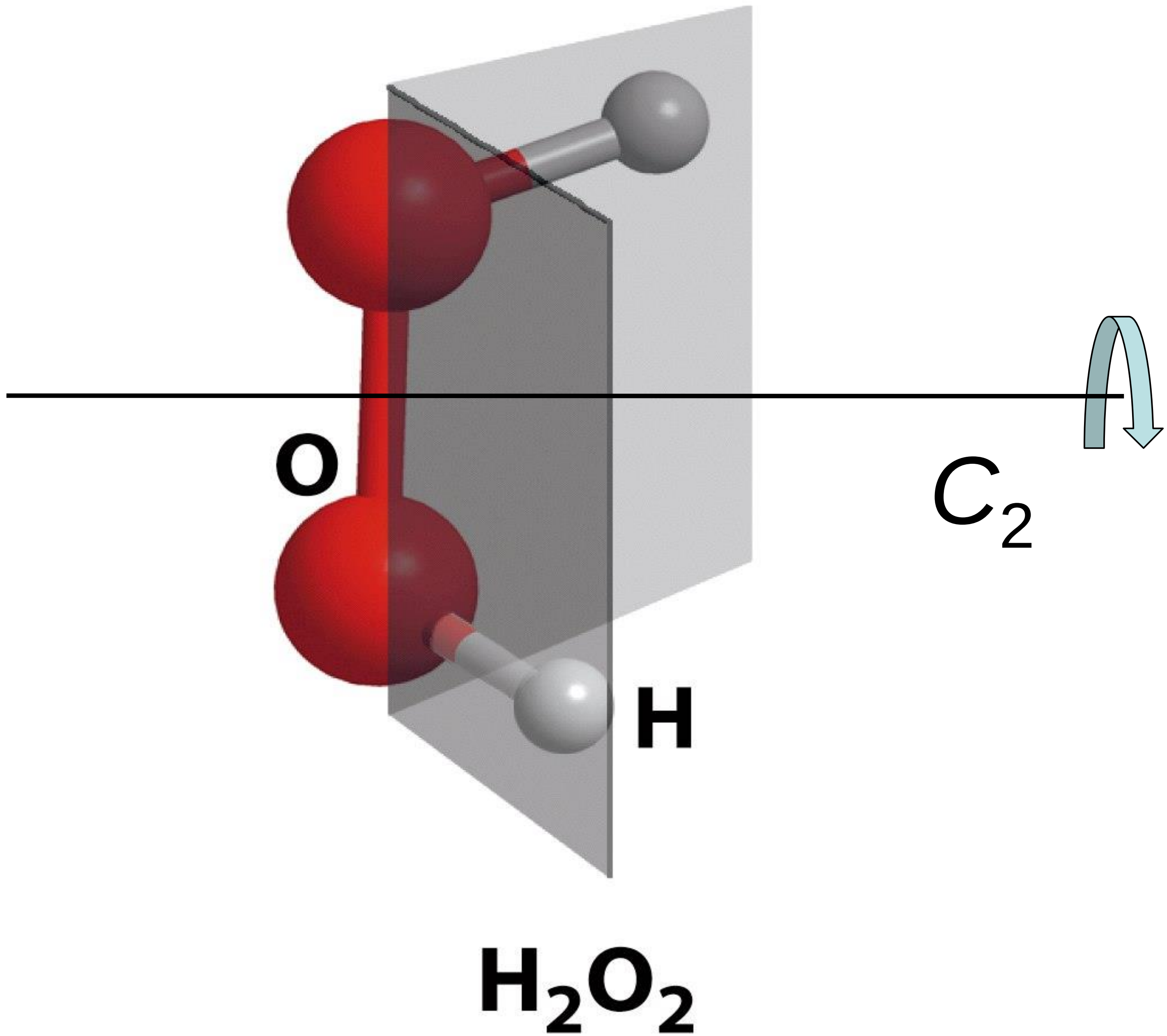

O
H
C_2
H_2O_2

Point group	Characteristic symmetry elements	Comments
C_s	E, one σ plane	
C_i	E, inversion centre	
C_n	E, one (principal) n-fold axis	
C_{nv}	E, one (principal) n-fold axis, n σ_v planes	
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T_d		Tetrahedral
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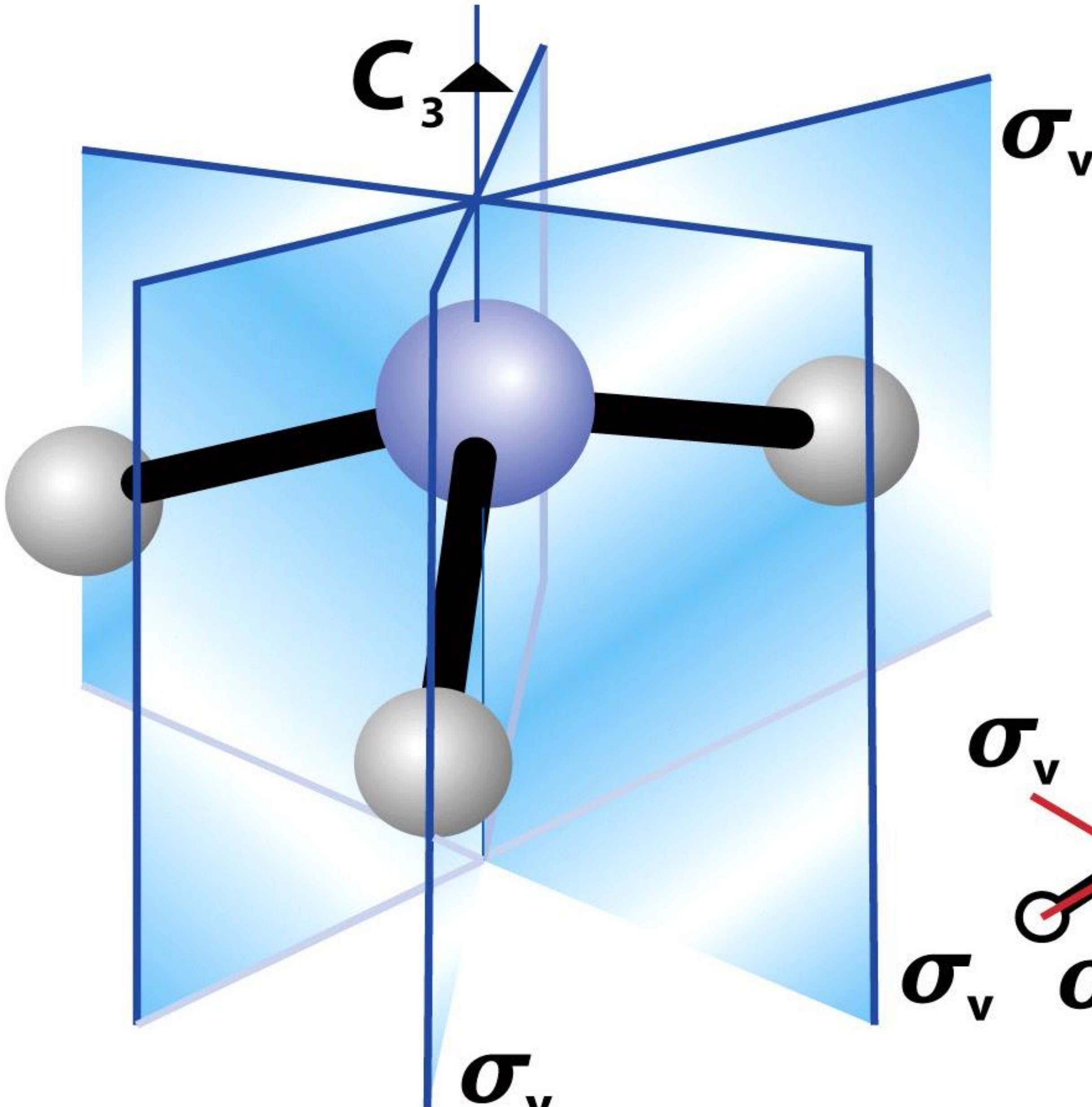
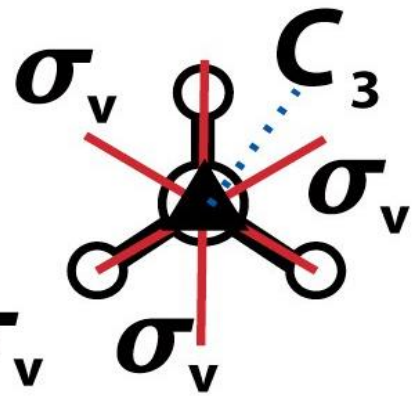
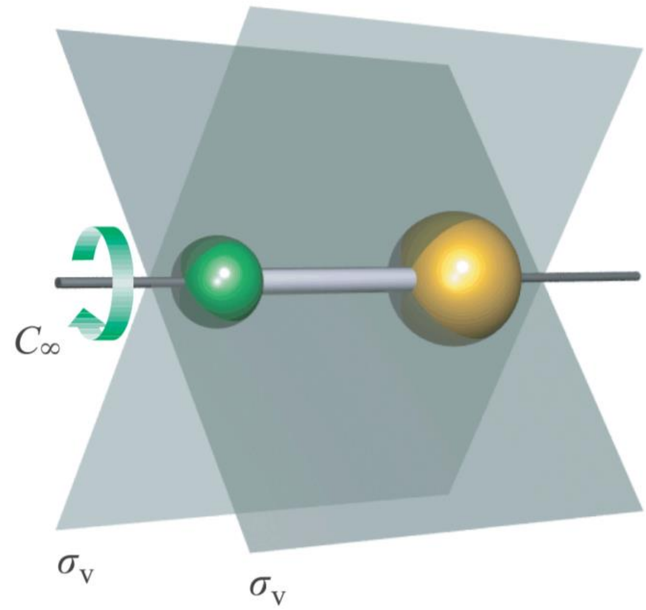
I_h		Icosahedral



C_{3v}



$C_{\infty v}$



Point group	Characteristic symmetry elements	Comments
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C_i	E, inversion centre	
C_n	E, one (principal) n-fold axis	
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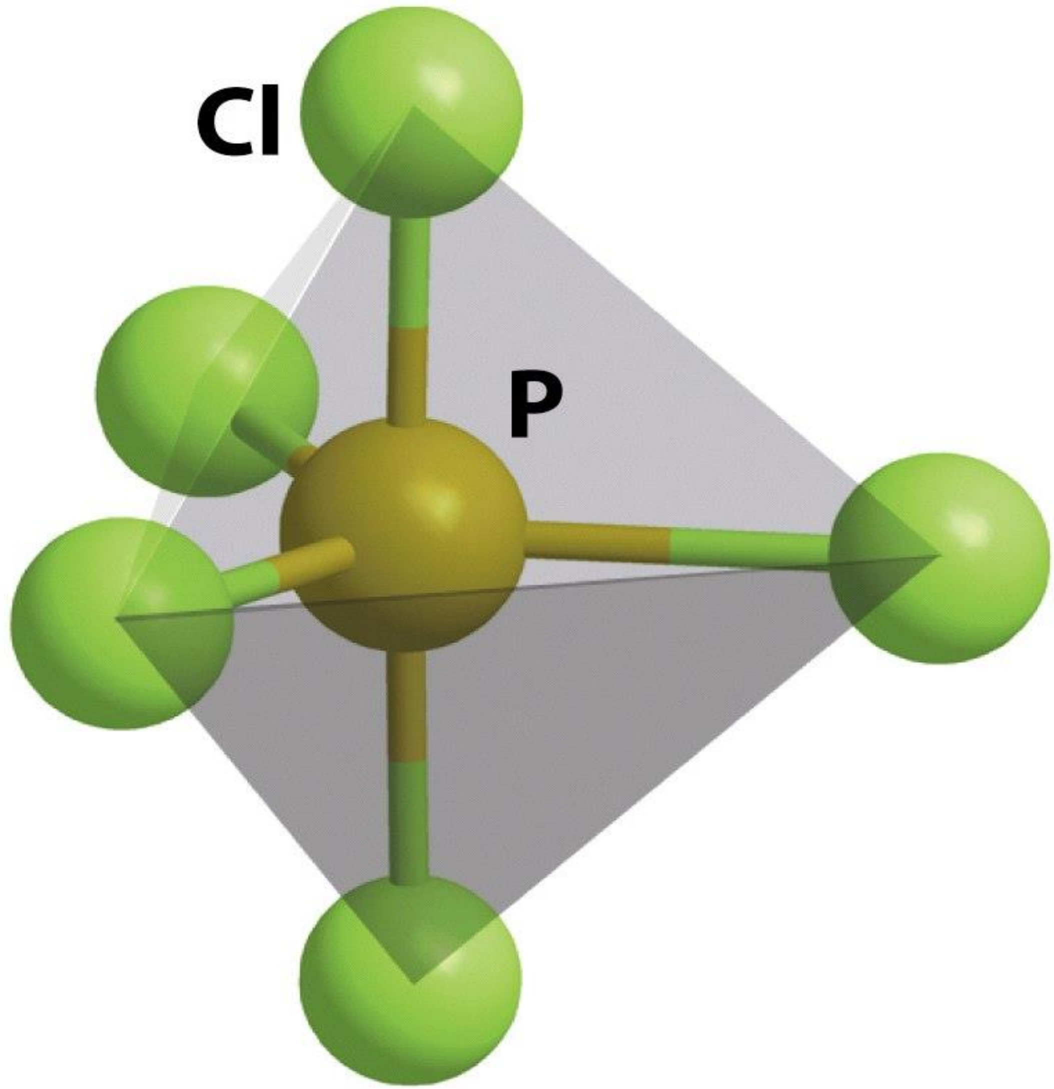
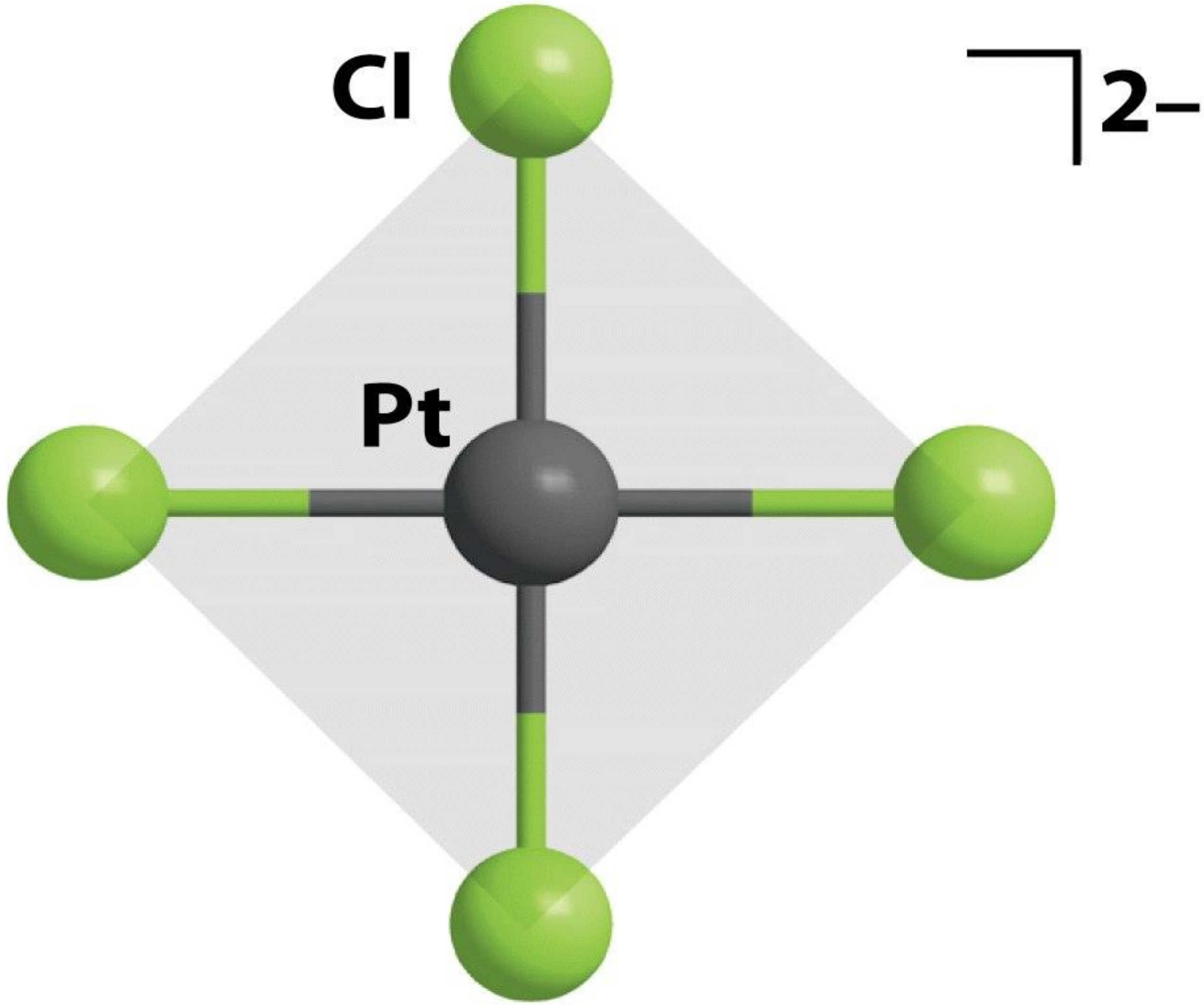
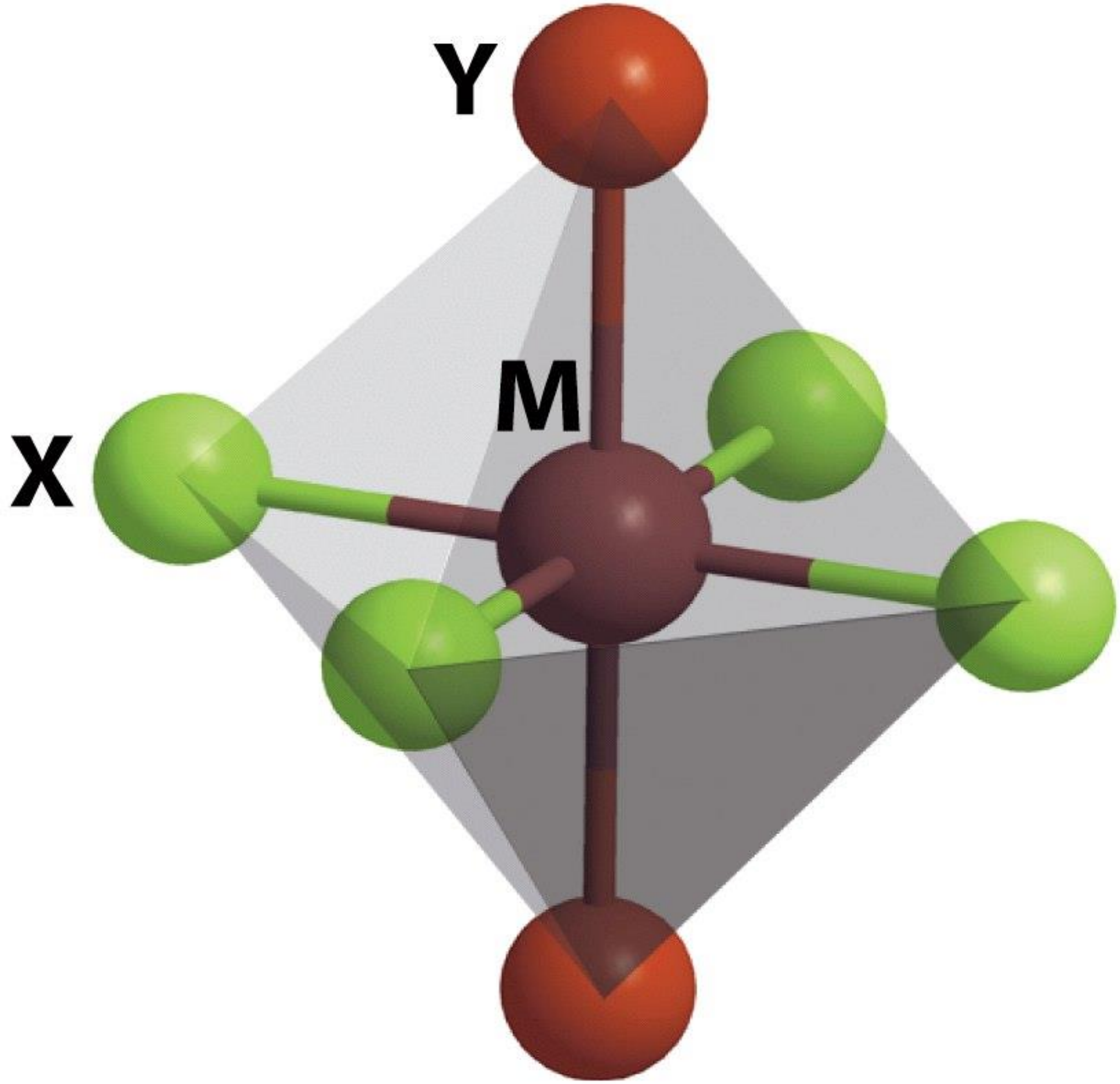
T_d		Tetrahedral
O_h		Octahedral
I_h		Icosahedral



PCl_5, D_{3h}



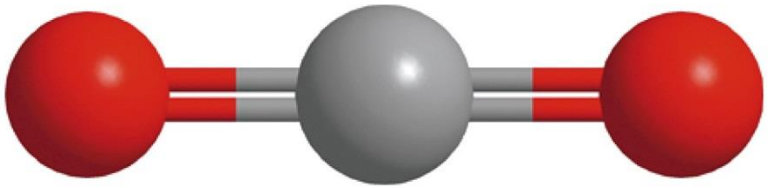
$[PtCl_4]^{2-}$, D_{4h}



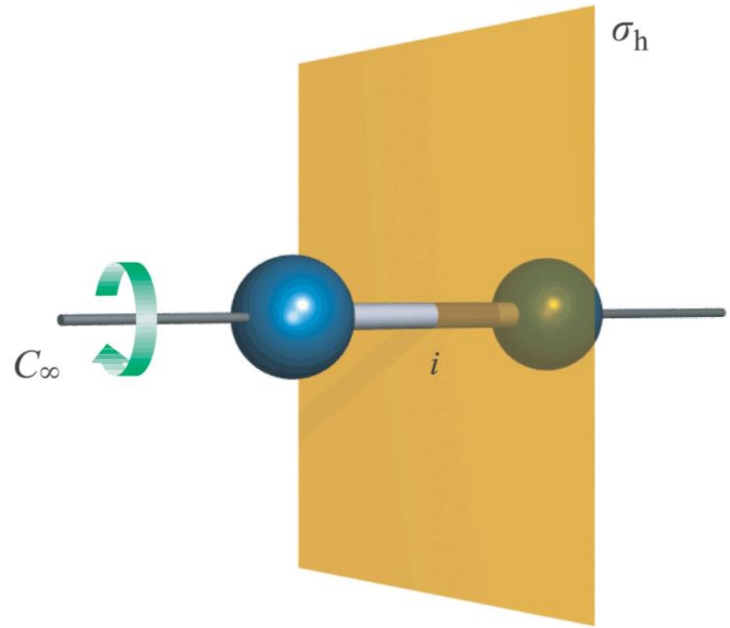
$[MX_4Y_2]$, D_{4h}

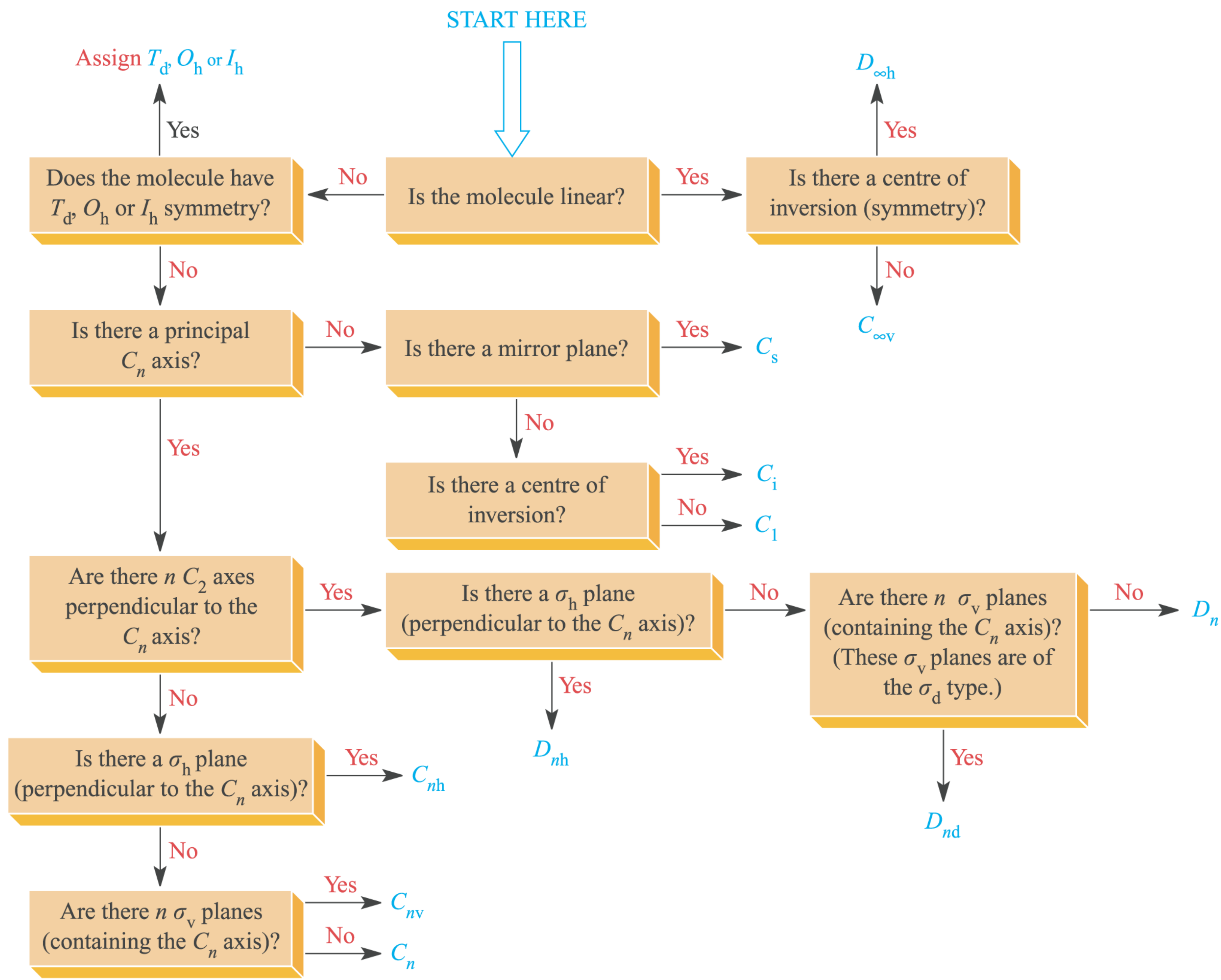
Geometria ottaedrica, simmetria inferiore

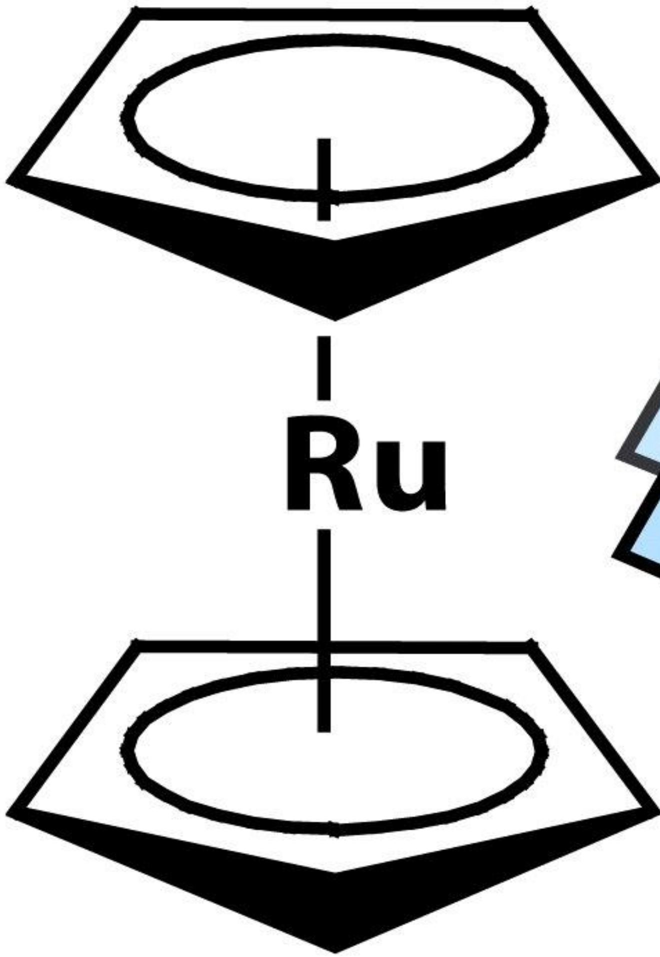
$D_{\infty h}$



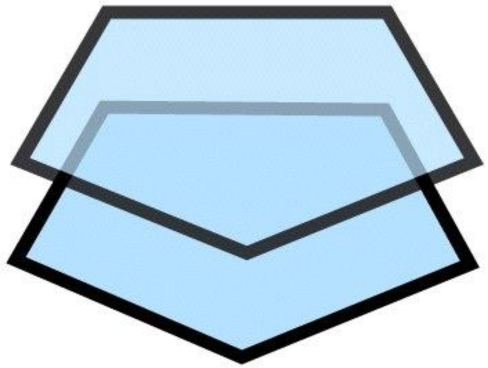
CO_2

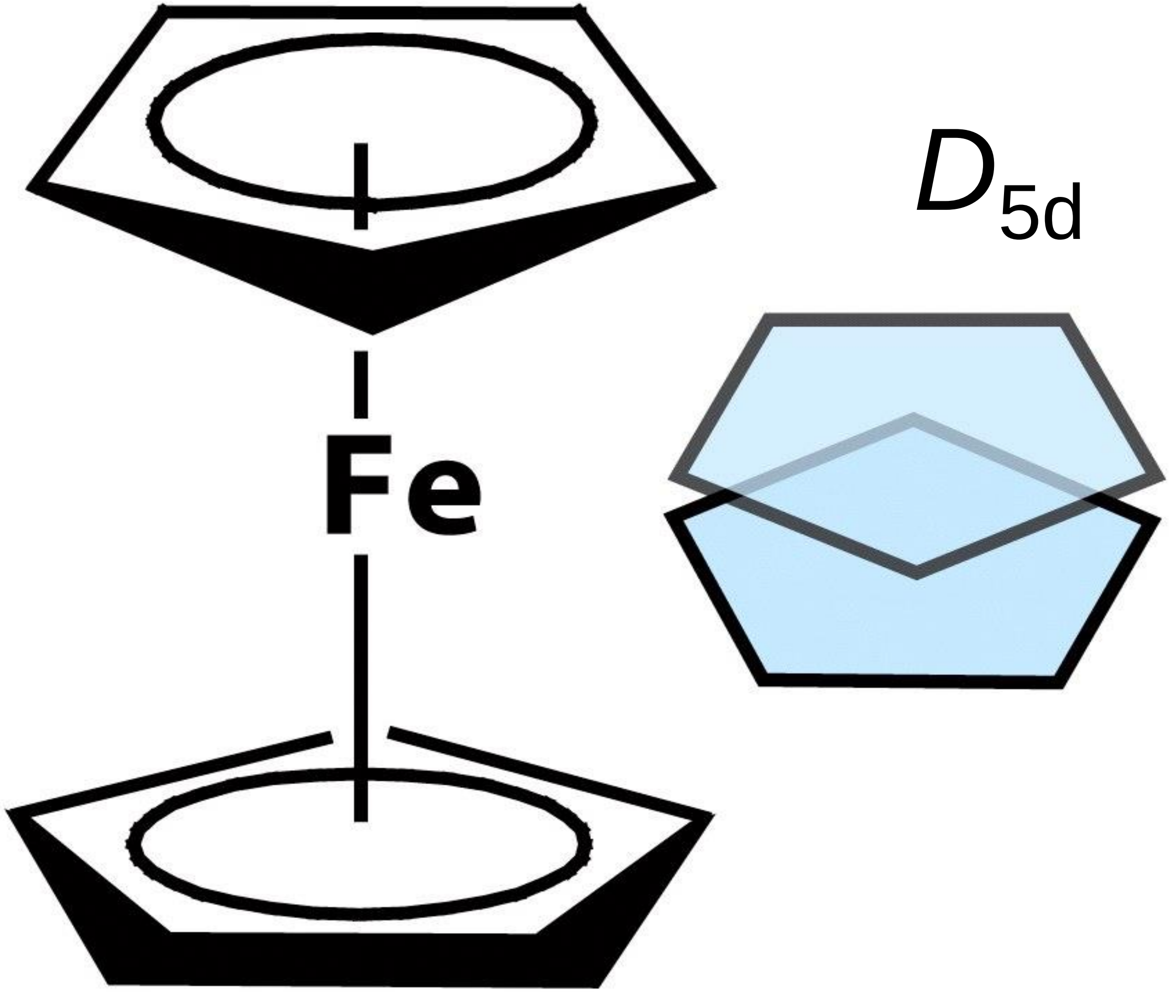


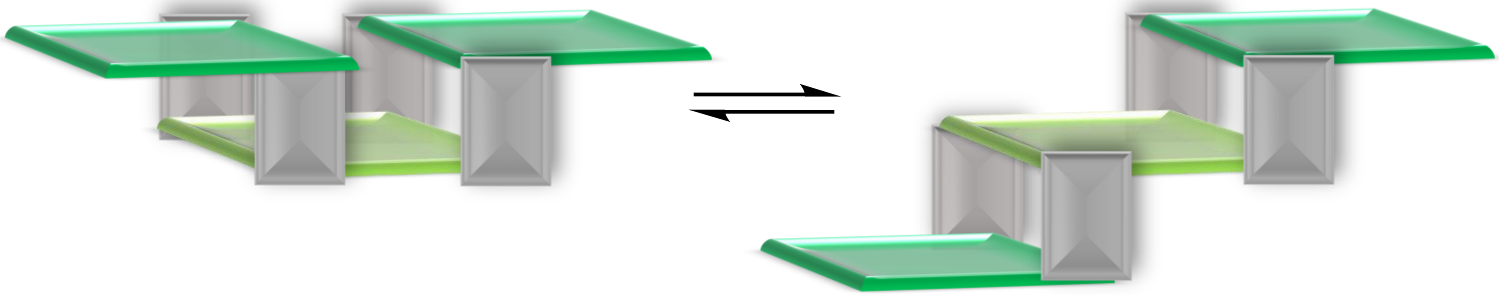

START HERE
Is the molecule linear?
Yes
Is there a centre of inversion (symmetry)?
Yes
$D_{\infty h}$
No
$C_{\infty v}$
No
Does the molecule have T_d, O_h or I_h symmetry?
Yes
Assign T_d, O_h or I_h
No
Is there a principal C_n axis?
No
Is there a mirror plane?
Yes
C_s
No
Is there a centre of inversion?
Yes
C_i
No
C_1
Yes
Are there n C_2 axes perpendicular to the C_n axis?
Yes
Is there a σ_h plane (perpendicular to the C_n axis)?
Yes
D_{nh}
No
Are there n σ_v planes (containing the C_n axis)? (These σ_v planes are of the σ_d type.)
No
D_n
Yes
D_{nd}
No
Is there a σ_h plane (perpendicular to the C_n axis)?
Yes
C_{nh}
No
Are there n σ_v planes (containing the C_n axis)?
Yes
C_{nv}
No
C_n

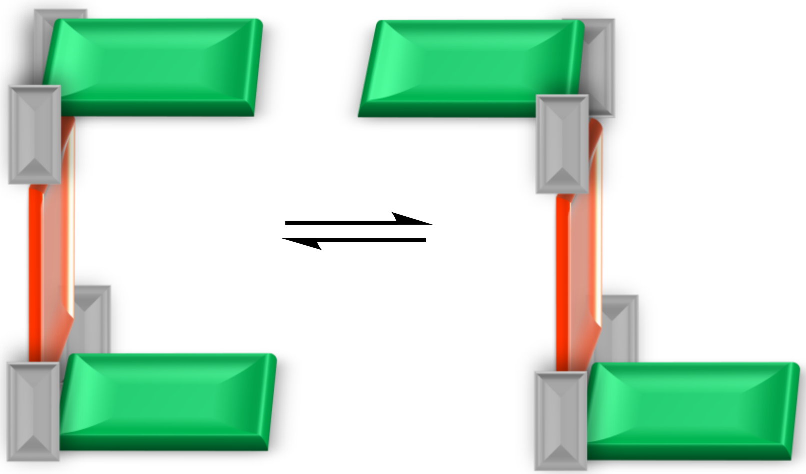


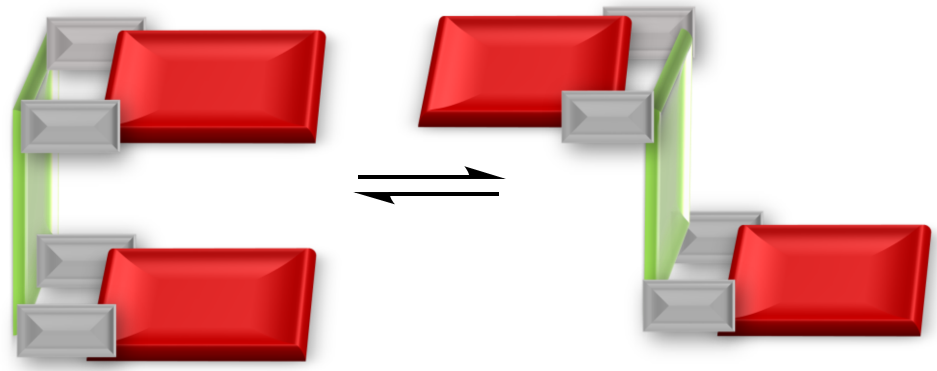
D_{5h}

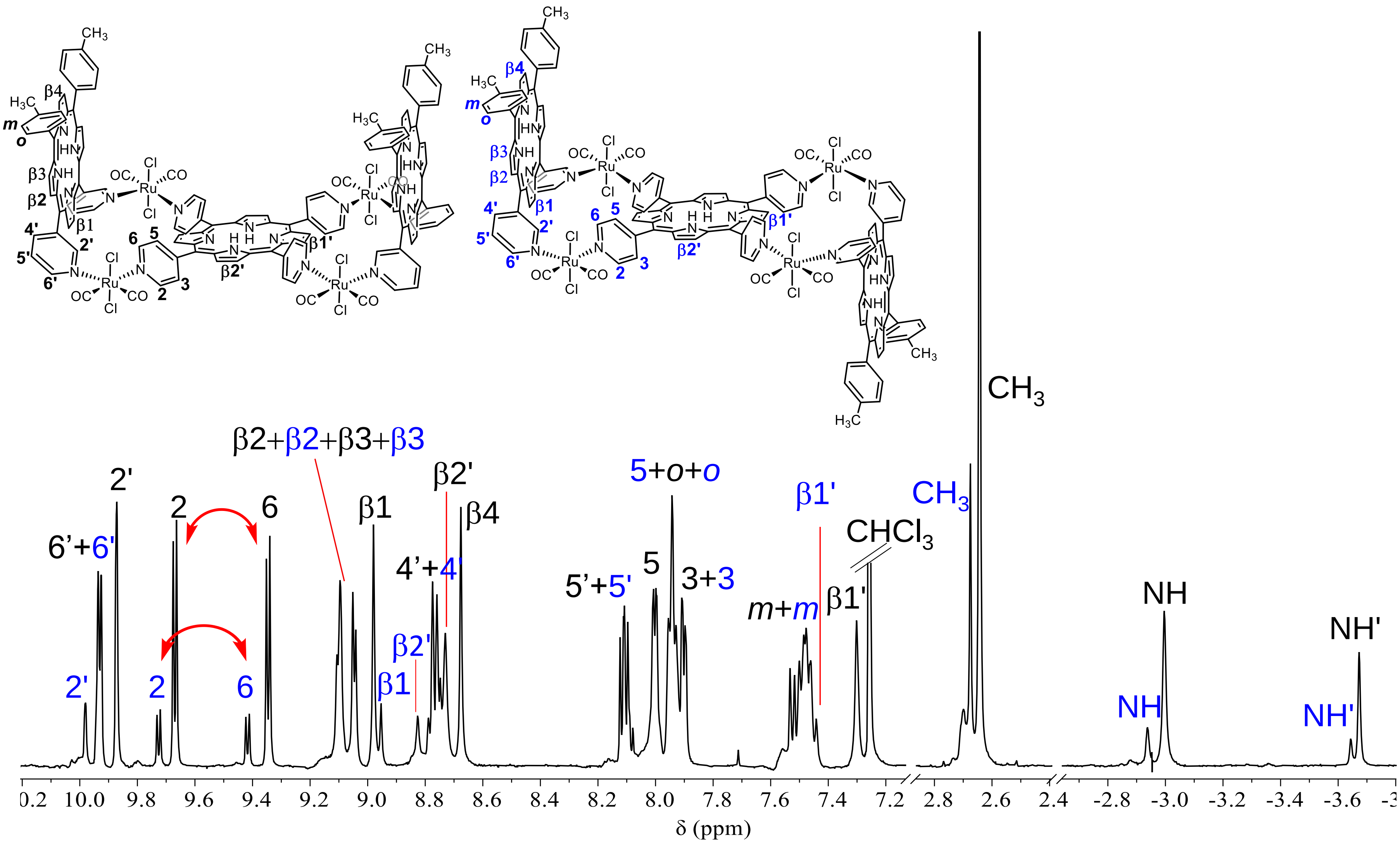



Fe
D5d

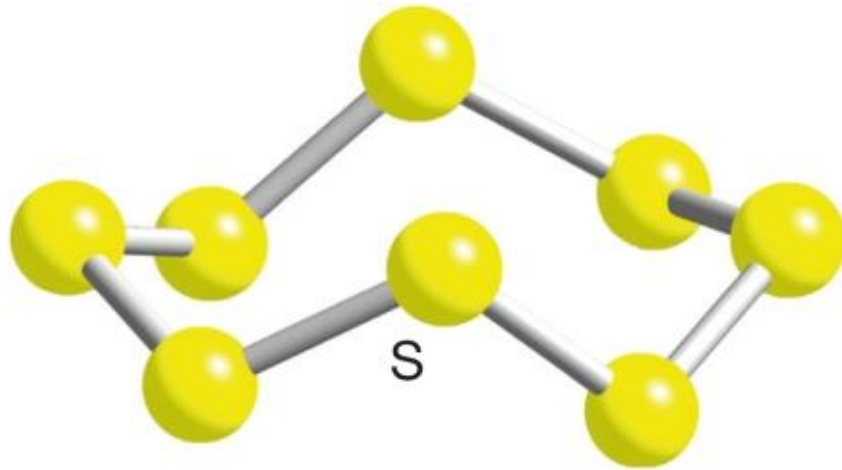








6'+6'
2'
2
6
β2+β2+β3+β3
β1
β2'
β4
4'+4'
5'+5'
5
5+o+o
3+3
β1'
m+m
β1'
CHCl3
CH3
CH3
NH
NH'
NH
NH'
2'
2
6
β1
β2'
δ (ppm)



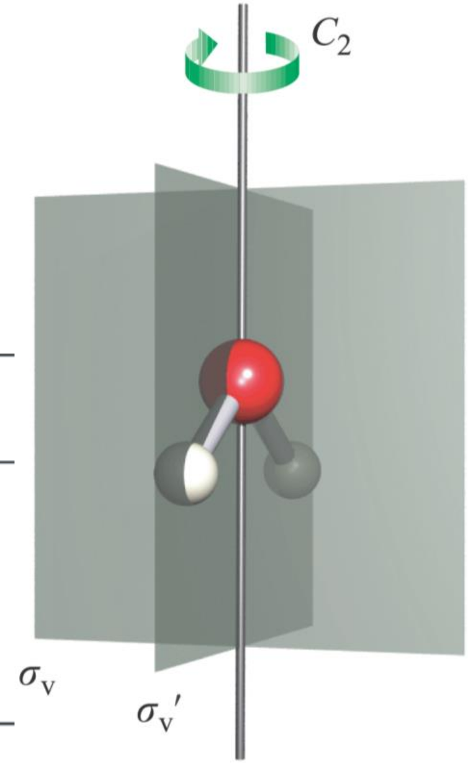
S_8

Tabella dei caratteri per il gruppo puntuale C_{2v}

SIMBOLO DI SCHOENFLIES

OPERAZIONI DI SIMMETRIA

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	−1	−1	R_z	xy
B_1	1	−1	1	−1	x, R_y	xz
B_2	1	−1	−1	1	y, R_x	yz



SIMBOLI DI MULLIKEN
(**Dimensione**)

FUNZIONI DI BASE

PRODOTTI BINARI DI FUNZIONI

RAPPRESENTAZIONI IRRIDUCIBILI

Tabella dei caratteri per il gruppo puntuale C_{3v}

Gruppi puntuali che possiedono assi di rotazione di ordine 3 o superiore possono avere rappresentazioni irriducibili di ***dimensione*** *2 (indicata con E) o 3 (T)*

C_{3v}	E	$2C_3$	$3\sigma_v$		
A_1	1	1	1	z	x^2+y^2, z^2
A_2	1	1	-1	R_z	
E	2	-1	0	$(x, y)\ (R_x, R_y)$	$(x^2-y^2, xy)\ (xz, yz)$

DIMENSIONE 2

COPPIE DI FUNZIONI DI BASE

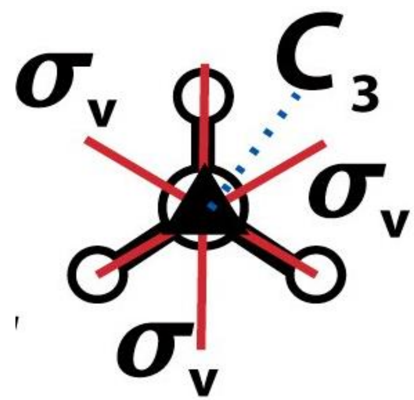
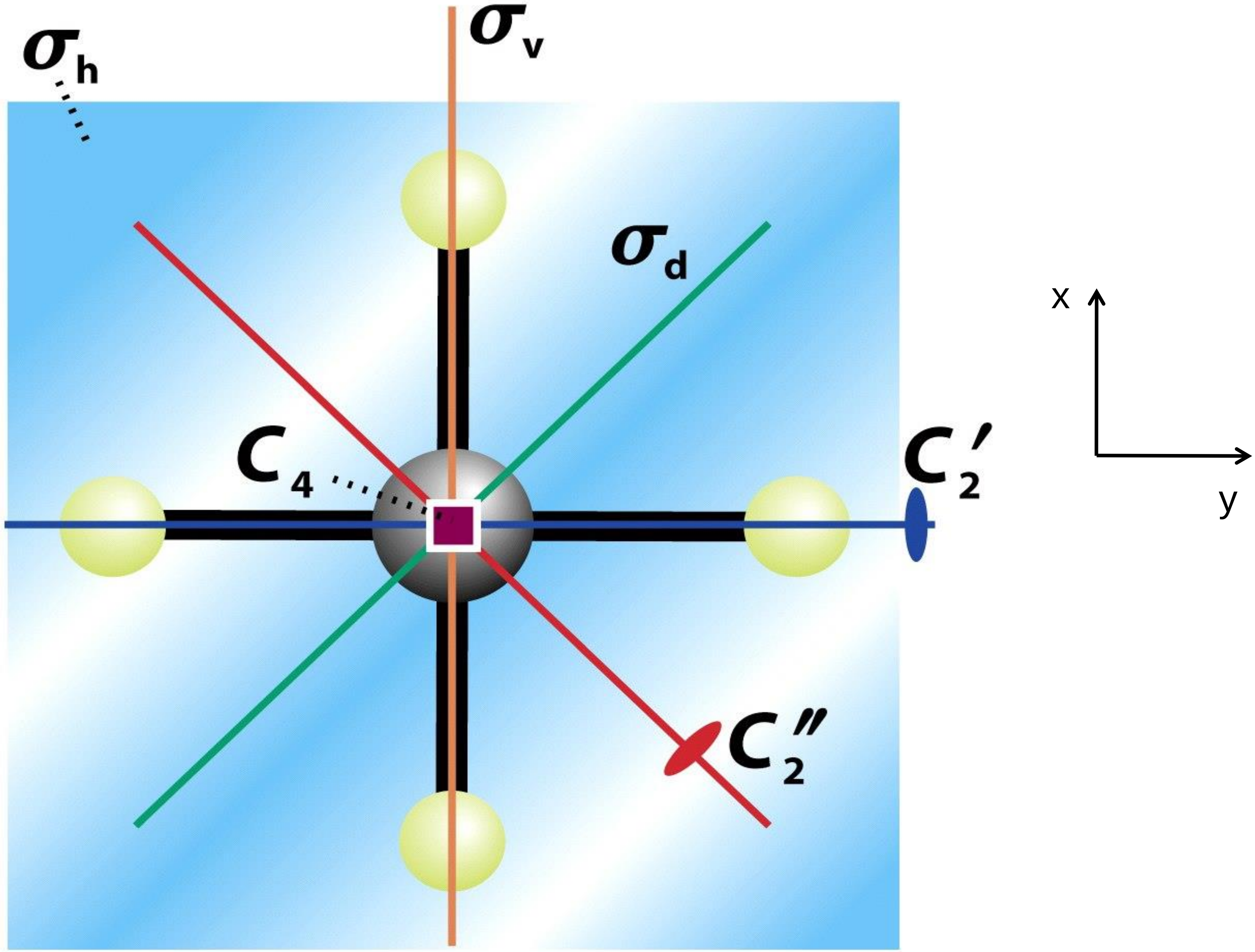


Tabella dei caratteri per il gruppo puntuale D_{4h}

	E	$2C_4$ (z)	C_2	$2C'_2$	$2C''_2$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$	linears, rotations	quadratic
A_{1g}	1	1	1	1	1	1	1	1	1	1		x^2+y^2, z^2
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1	R_z	
B_{1g}	1	-1	1	1	-1	1	-1	1	1	-1		x^2-y^2
B_{2g}	1	-1	1	-1	1	1	-1	1	-1	1		xy
E_g	2	0	-2	0	0	2	0	-2	0	0	(R_x, R_y)	(xz, yz)
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1		
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1	z	
B_{1u}	1	-1	1	1	-1	-1	1	-1	-1	1		
B_{2u}	1	-1	1	-1	1	-1	1	-1	1	-1		
E_u	2	0	-2	0	0	-2	0	2	0	0	(x, y)	



σ_v
σ_h
σ_d
C_4
C_2′
C_2″
x
y