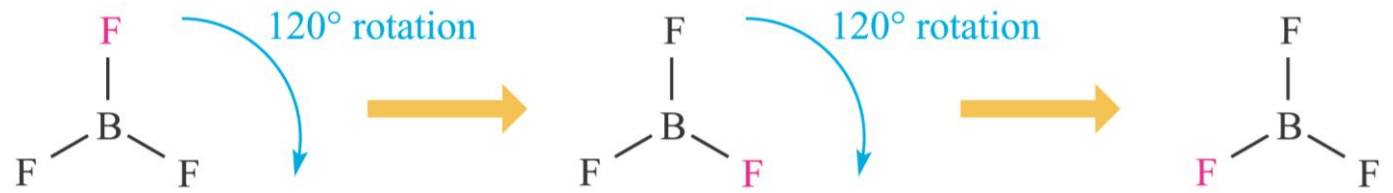
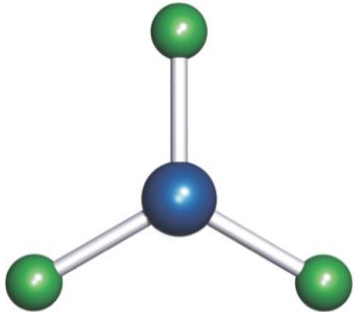


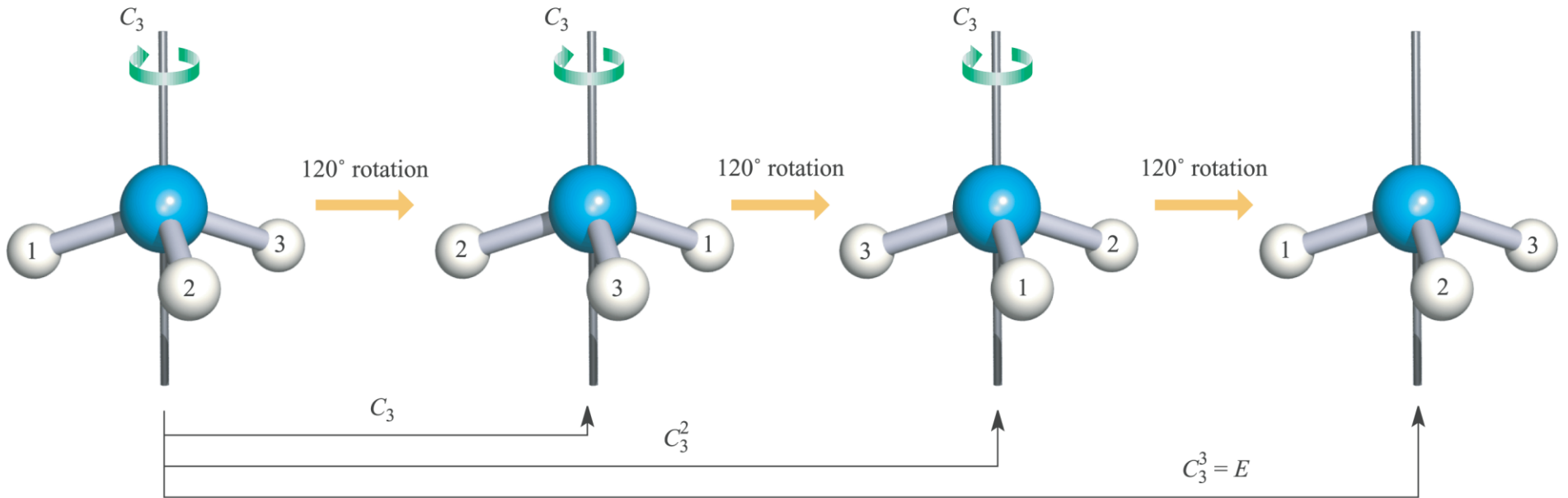
*Una molecola ha una **simmetria** se possiede due o più orientazioni nello spazio (o configurazioni) che sono indistinguibili*

*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*

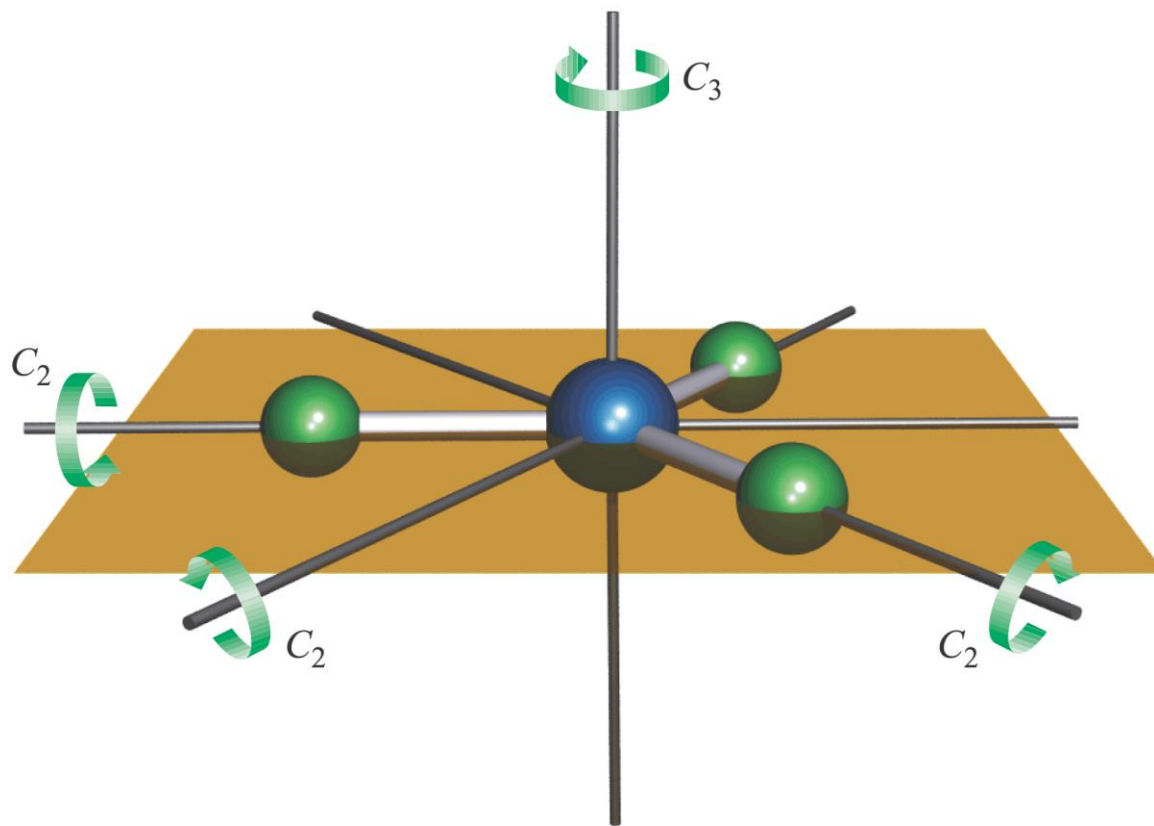
Asse $C_n = \text{rotazione di } 360^\circ/n$



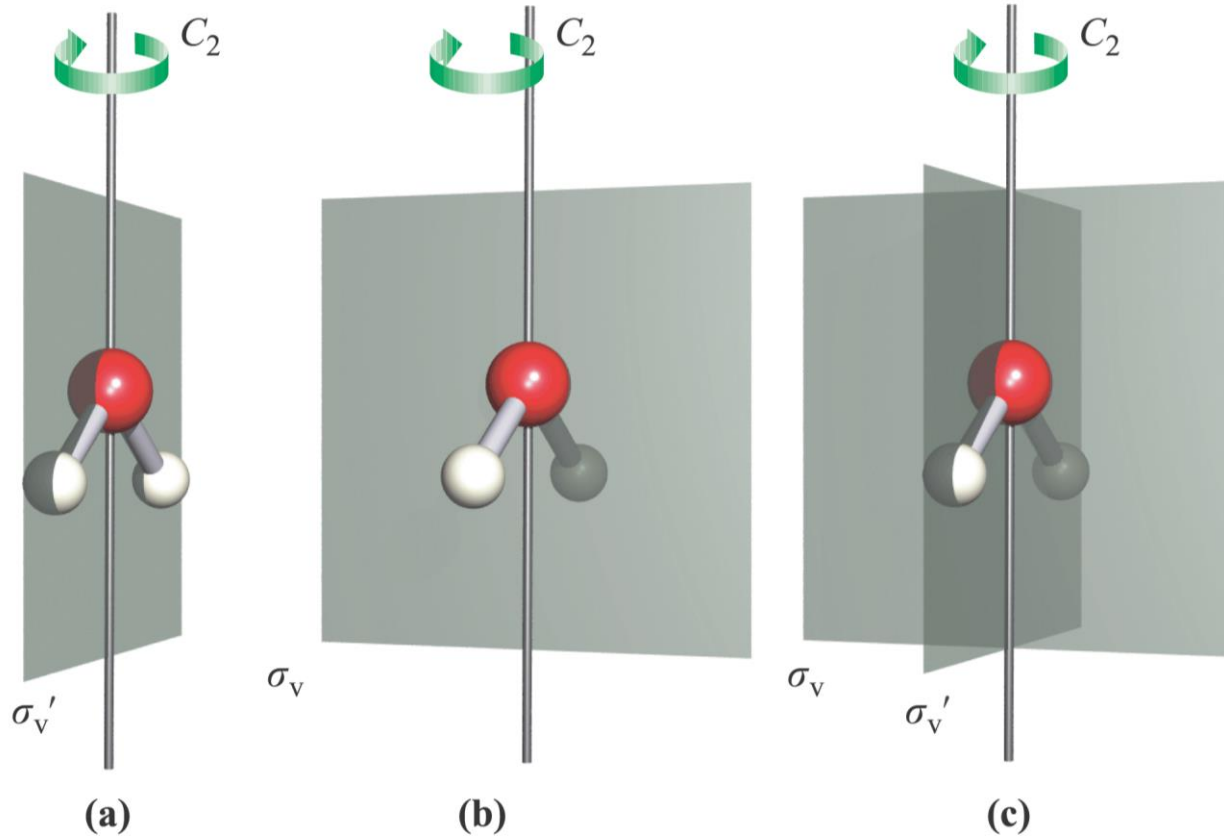
$$C_n^n = E$$

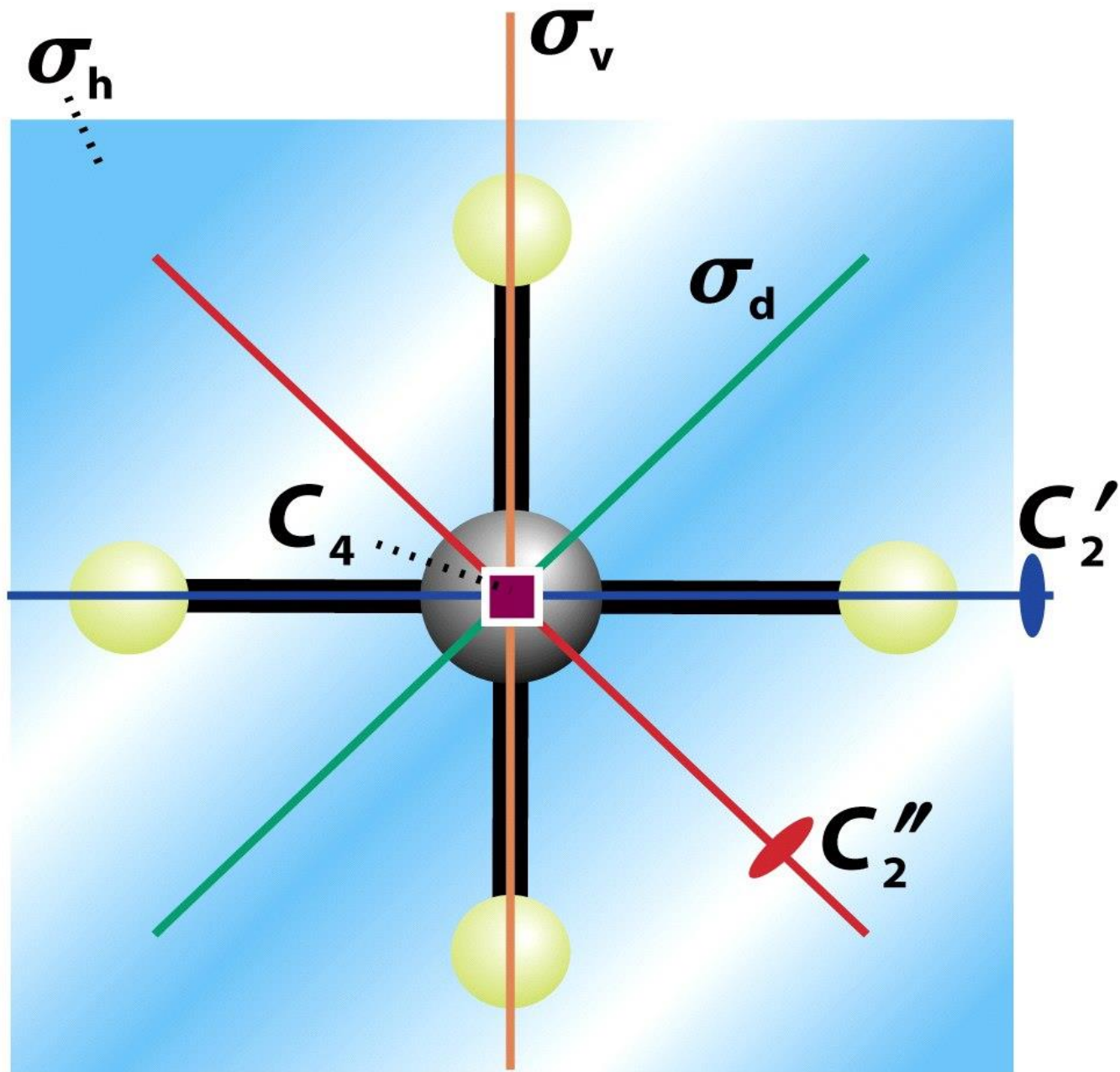


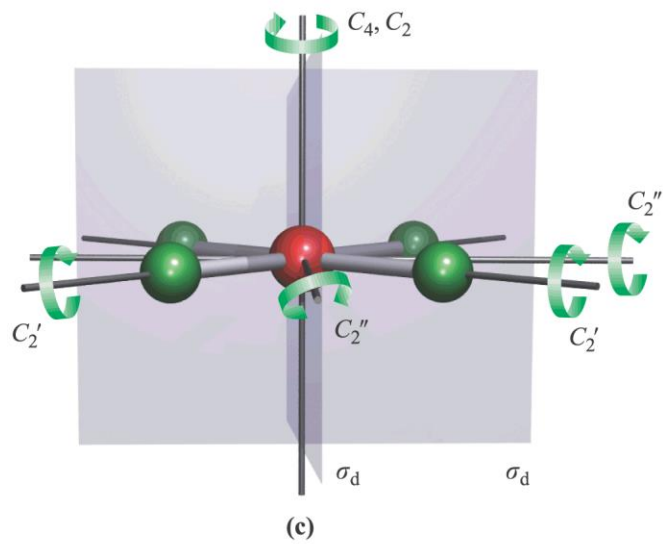
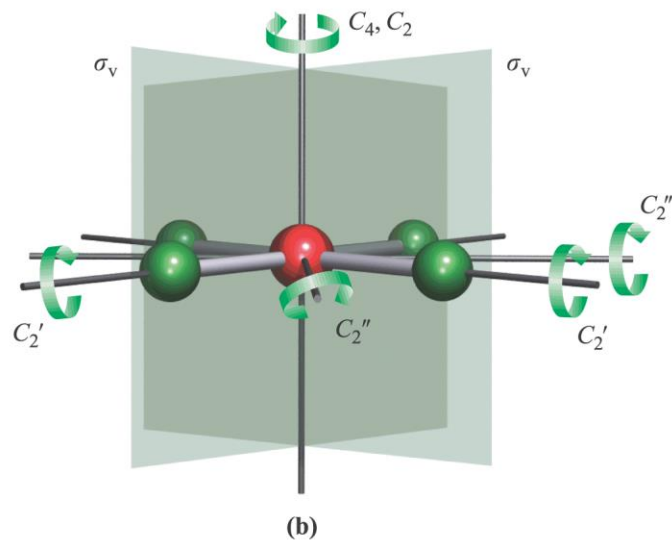
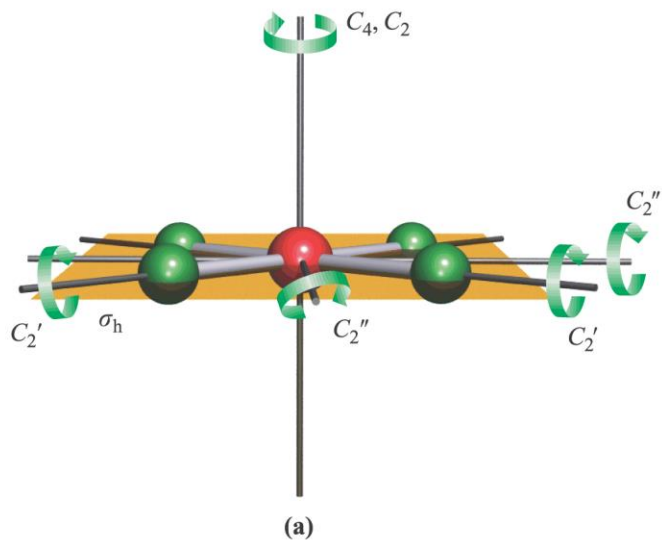
Asse principale



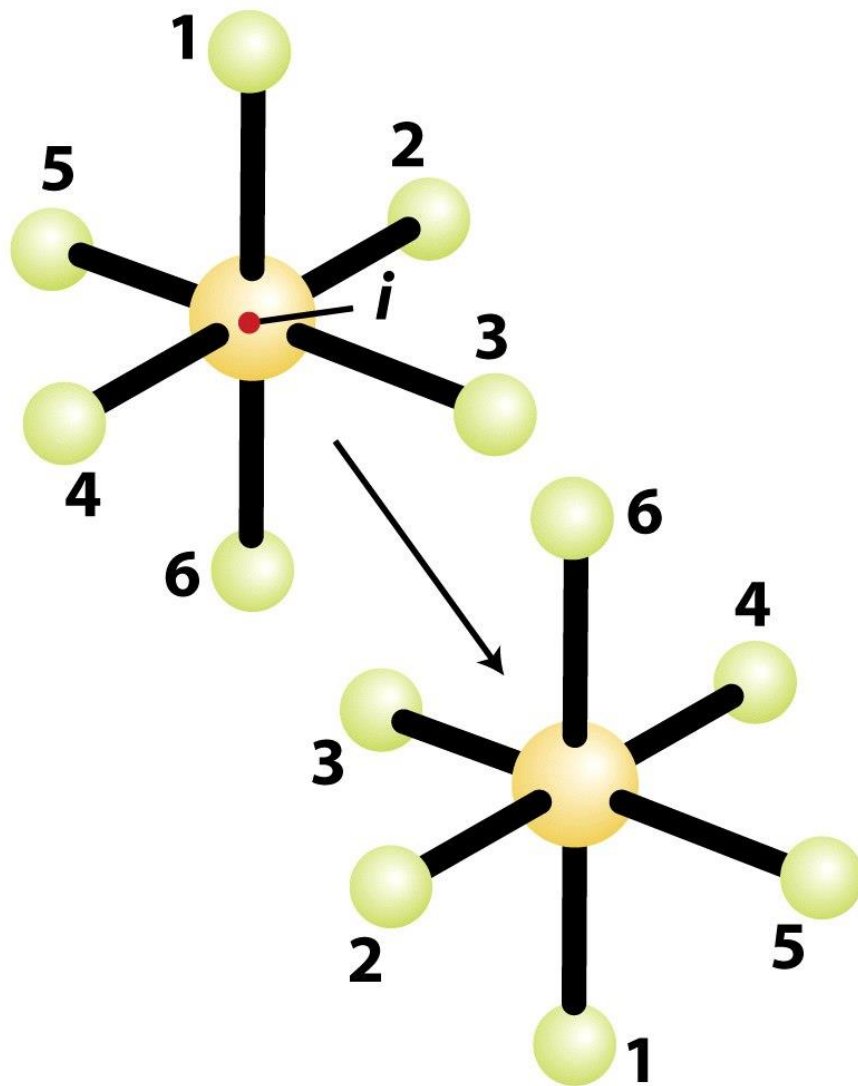
Piani di simmetria: σ_v , σ_h , σ_d





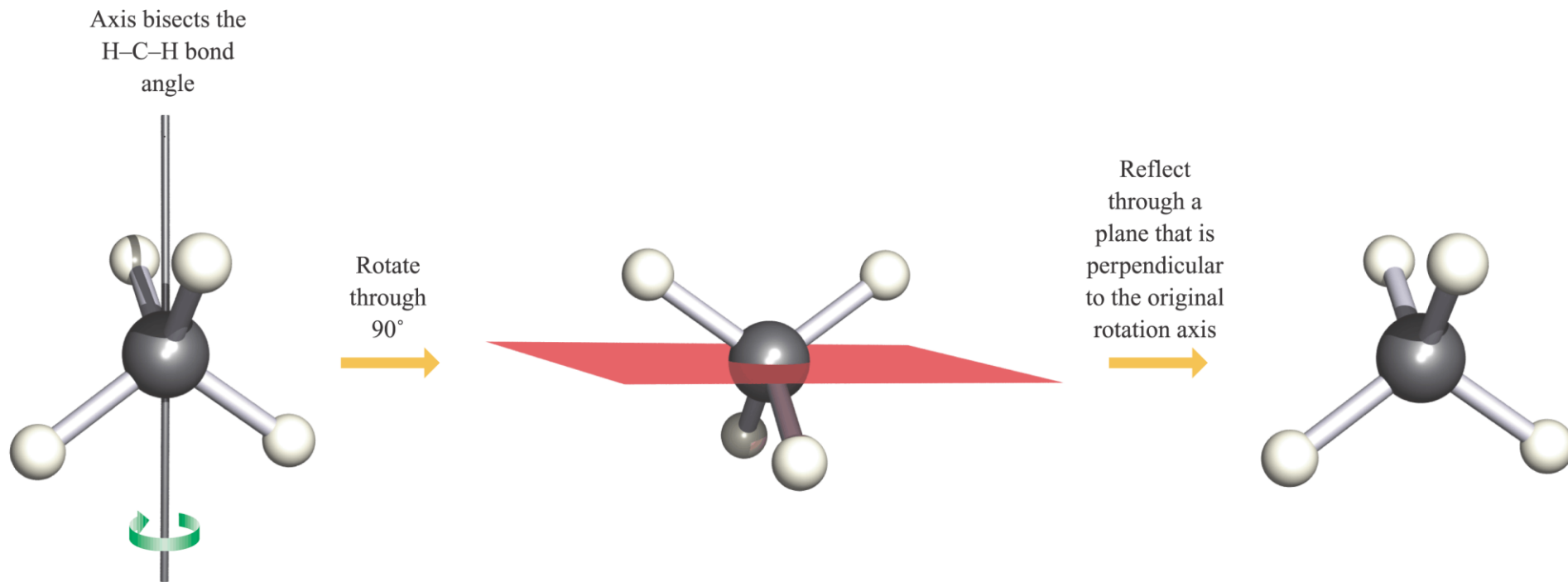


Centro di simmetria (centro di inversione), i



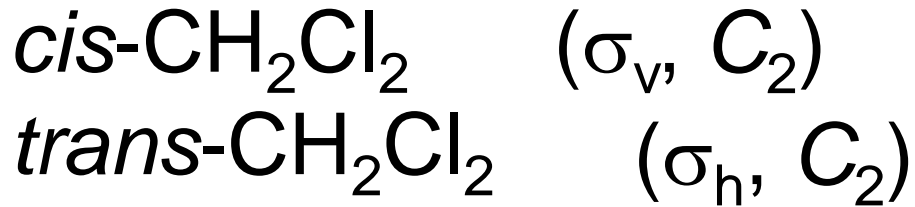
Rotazione impropria o roto-riflessione

Assi S_n

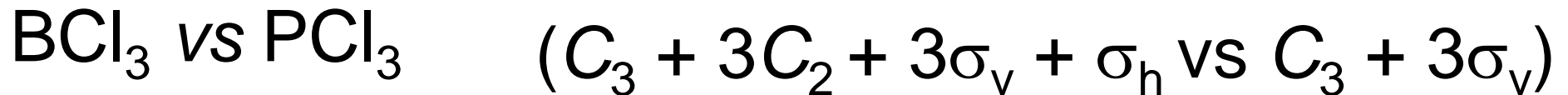


$$S_1 = \sigma \quad e \quad S_2 = i$$

Esempi



Etano:



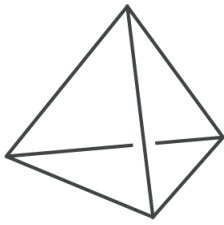
Gruppi puntuali

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**.

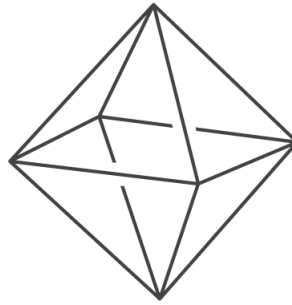
Gruppi puntuali

Simboli di Schoenflies

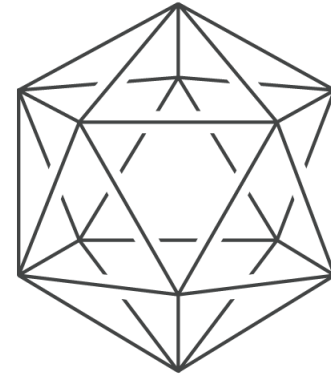
Point group	Characteristic symmetry elements	Comments
C_s	E , one σ plane	
C_i	E , inversion centre	
C_n	E , one (principal) n -fold axis	
C_{nv}	E , one (principal) n -fold axis, n σ_v planes	
C_{nh}	E , one (principal) n -fold axis, one σ_h plane, one S_n -fold axis which is coincident with the C_n 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

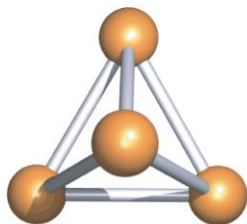


Octahedron

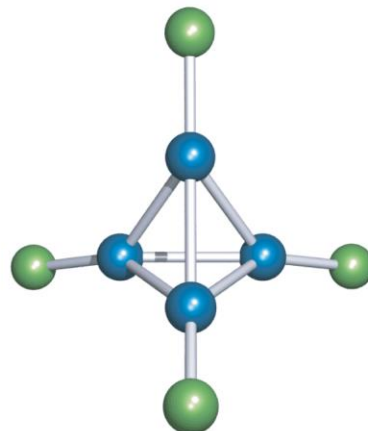


Icosahedron

P_4



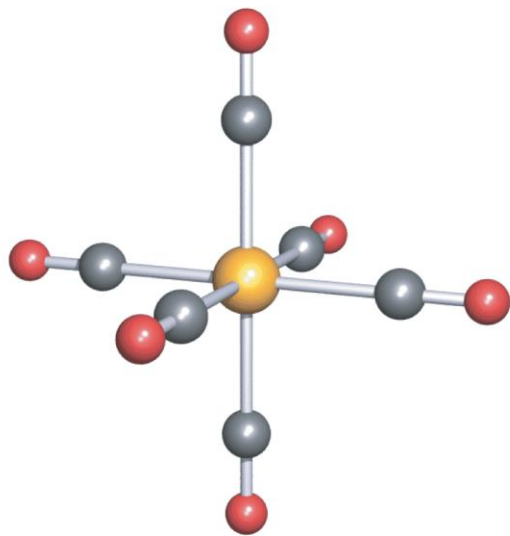
(a)



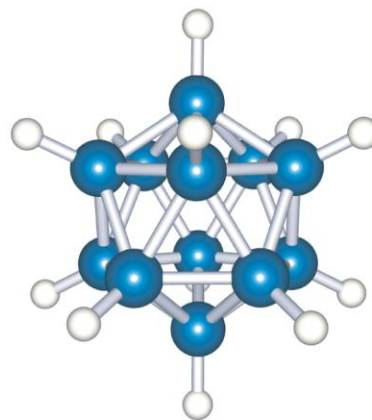
(b)

B_4Cl_4

$W(CO)_6$

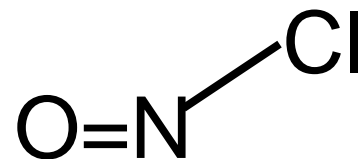


(c)



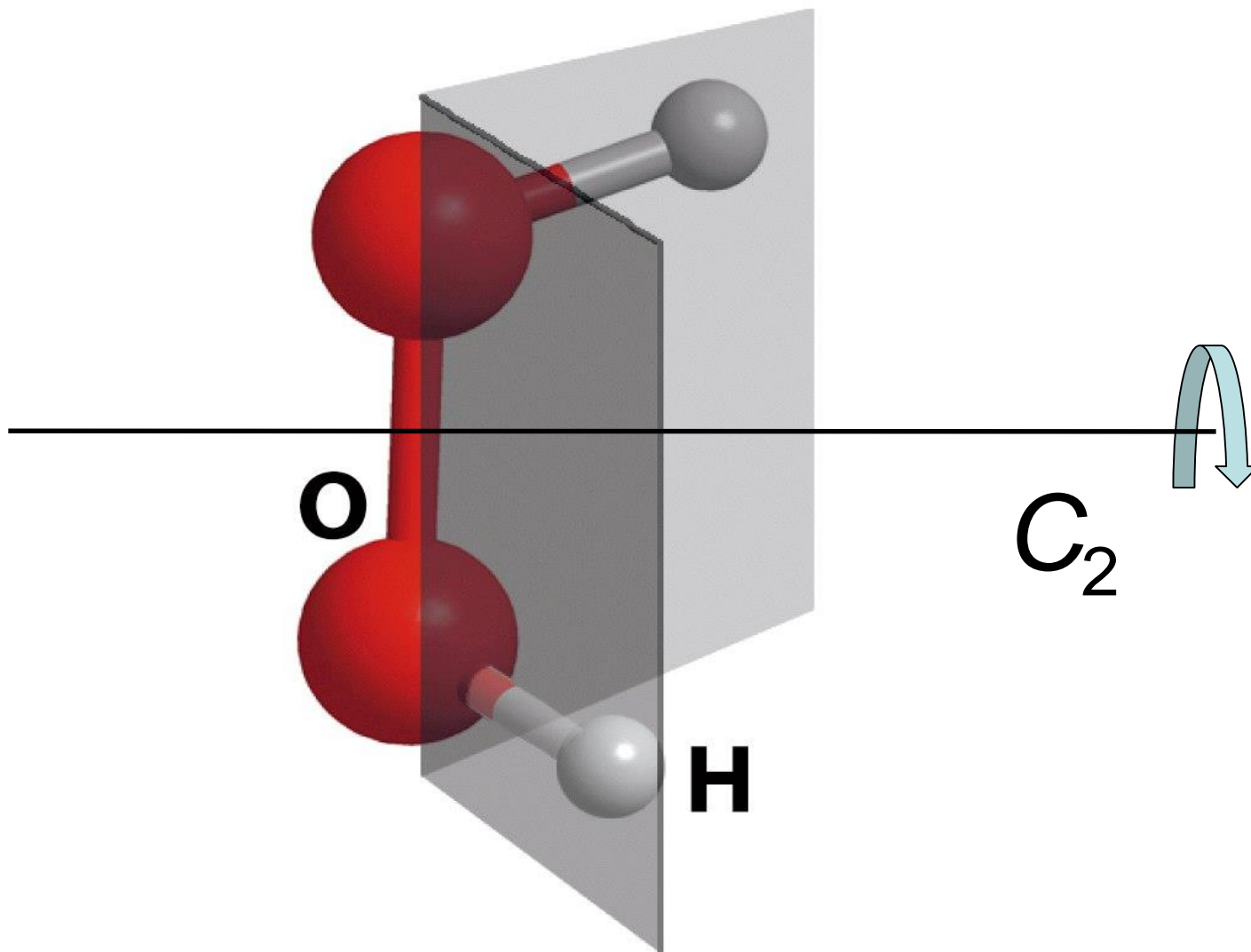
(d)

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

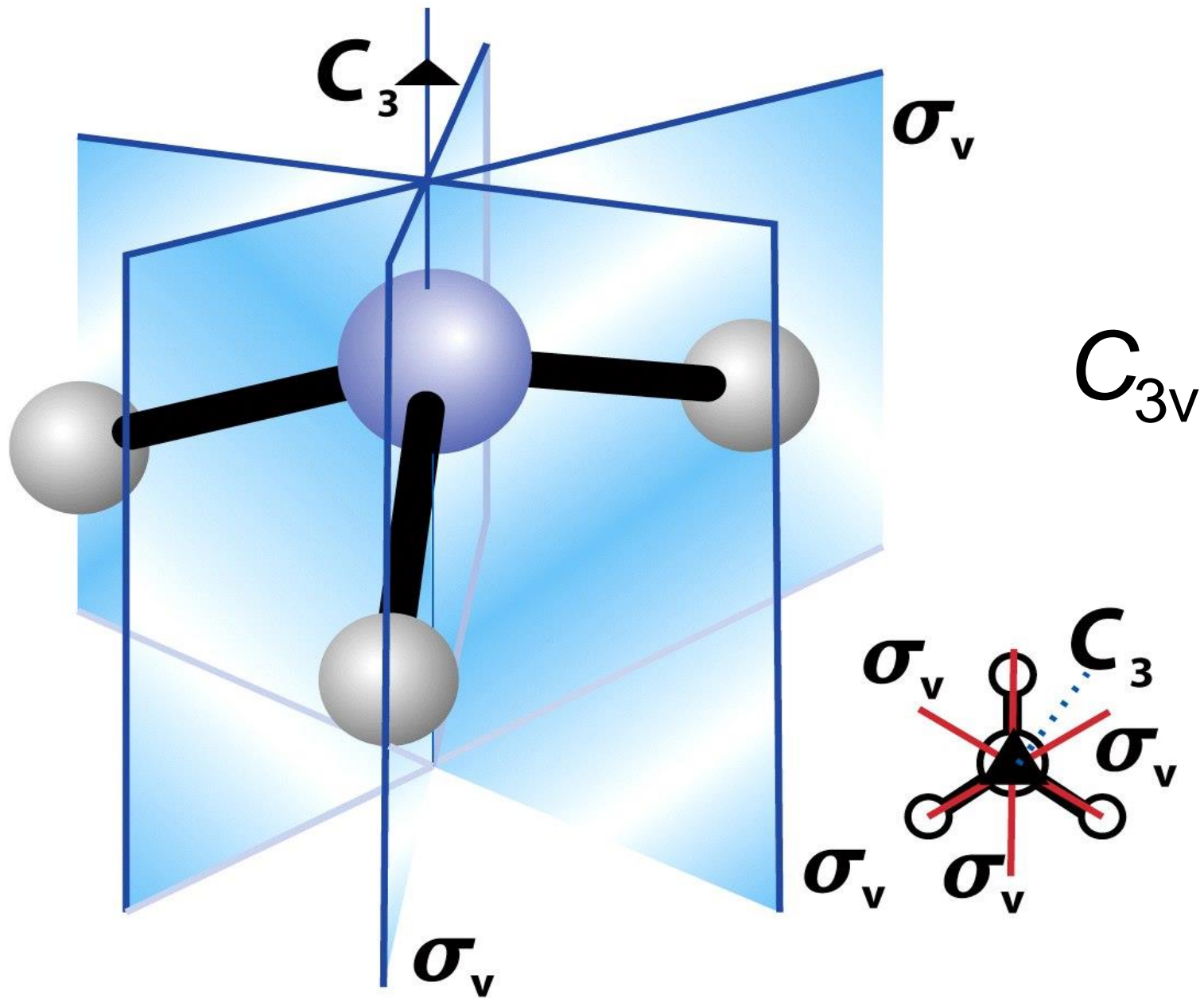


Point group	Characteristic symmetry elements	Comments
C_s	E , one σ plane	
C_i	E , inversion centre	
C_n	E , one (principal) n -fold axis	
C_{nv}	E , one (principal) n -fold axis, n σ_v planes	
C_{nh}	E , one (principal) n -fold axis, one σ_h plane, one S_n -fold axis which is coincident with the C_n 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

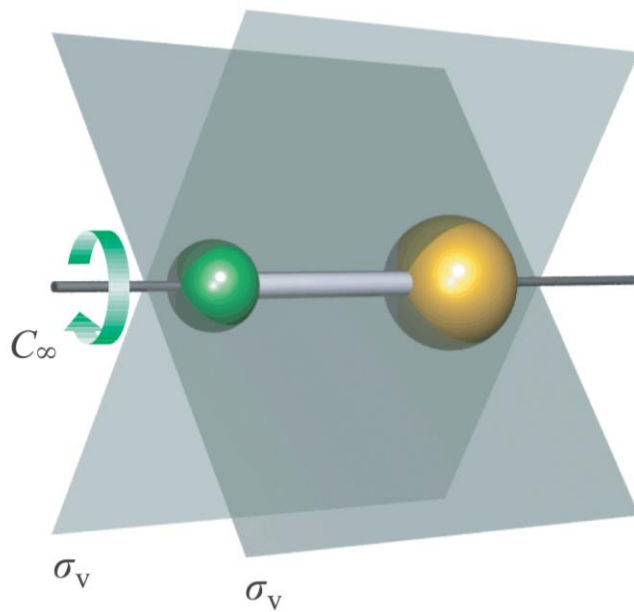
Point group	Characteristic symmetry elements	Comments
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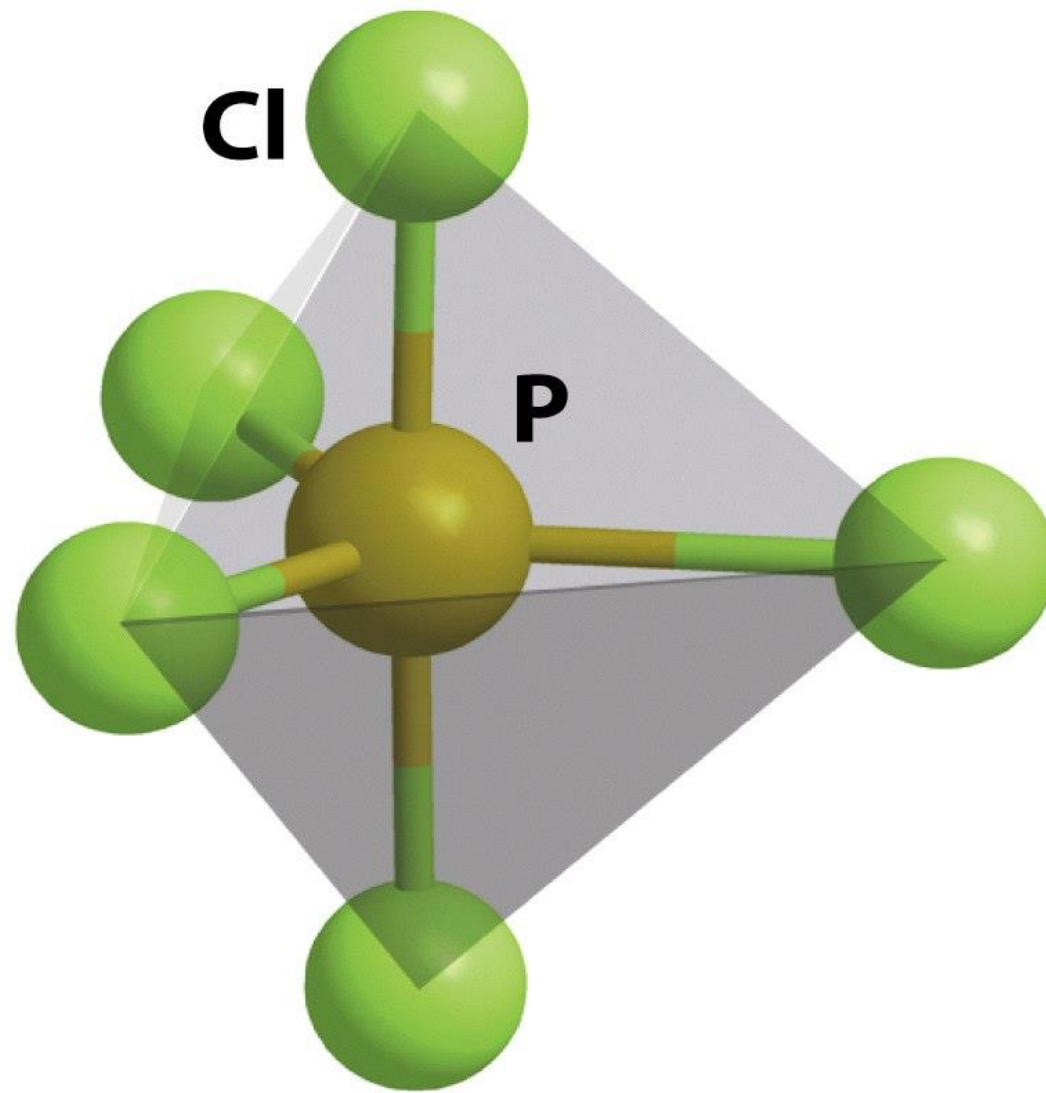
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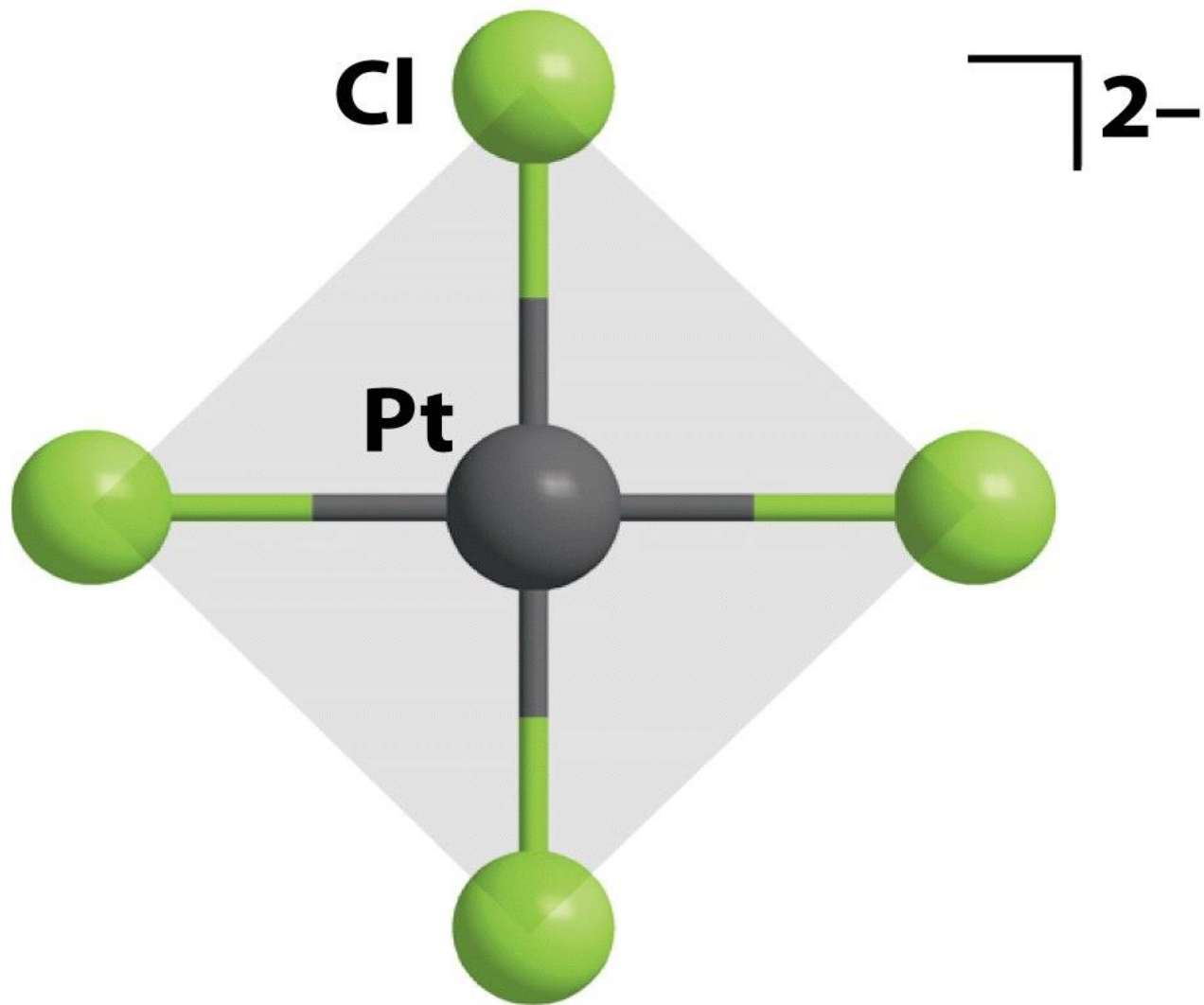
$C_{\infty v}$

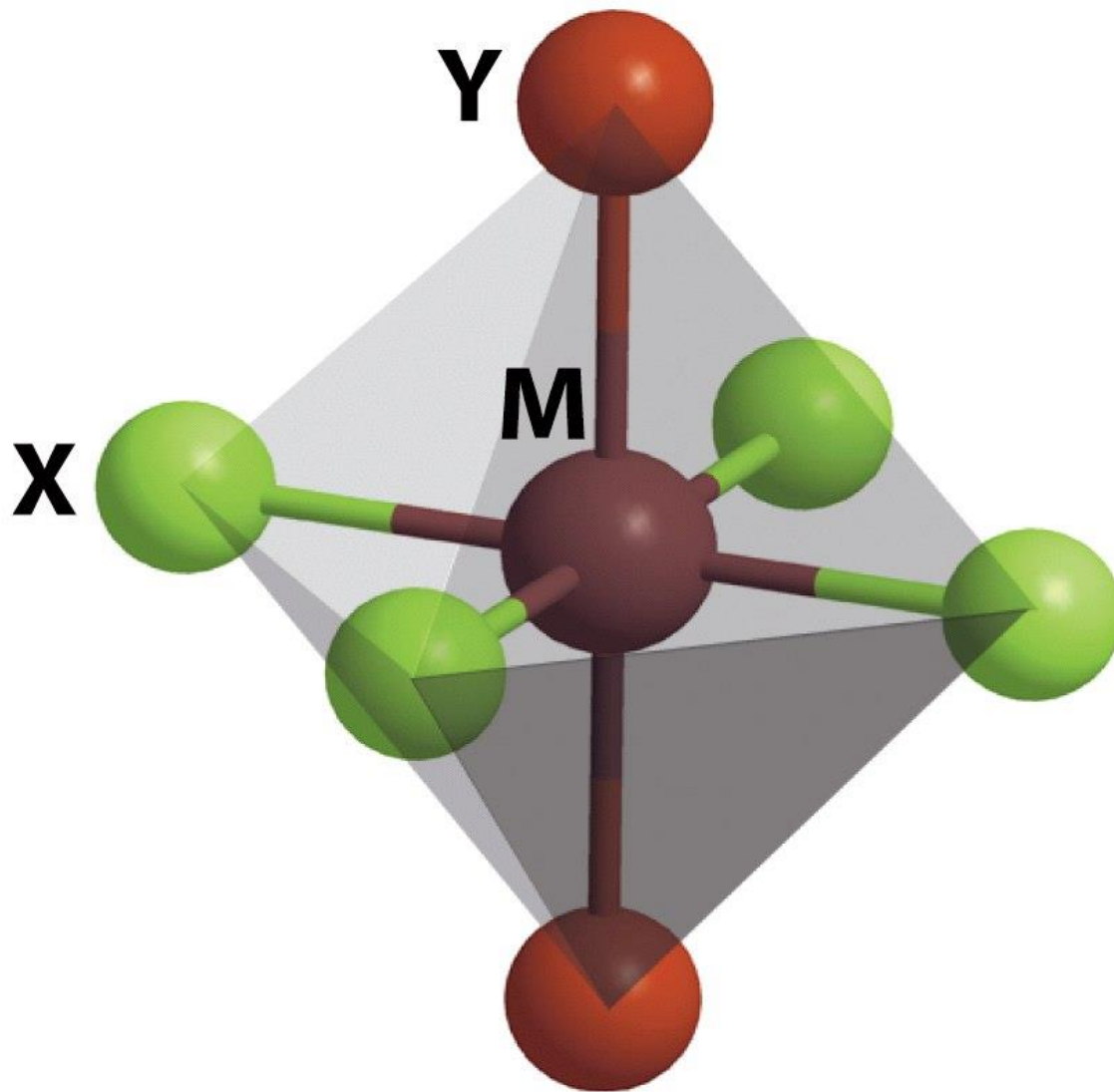


Point group	Characteristic symmetry elements	Comments
C_s	E , one σ plane	
C_i	E , inversion centre	
C_n	E , one (principal) n -fold axis	
C_{nv}	E , one (principal) n -fold axis, n σ_v planes	
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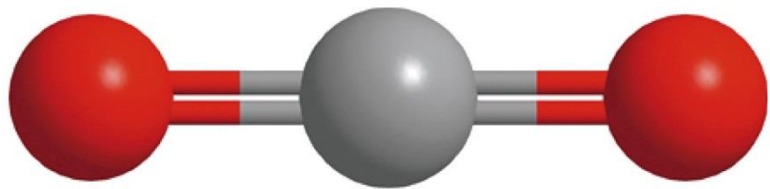
PCl_5, D_{3h}



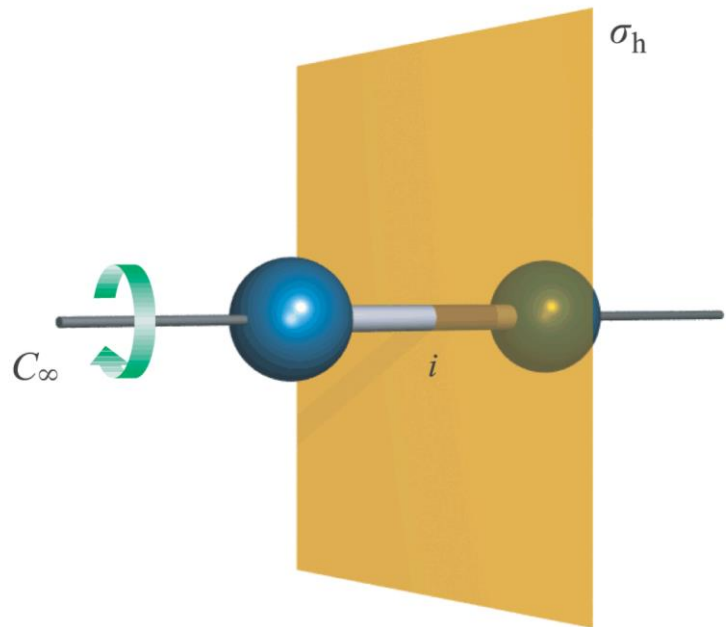


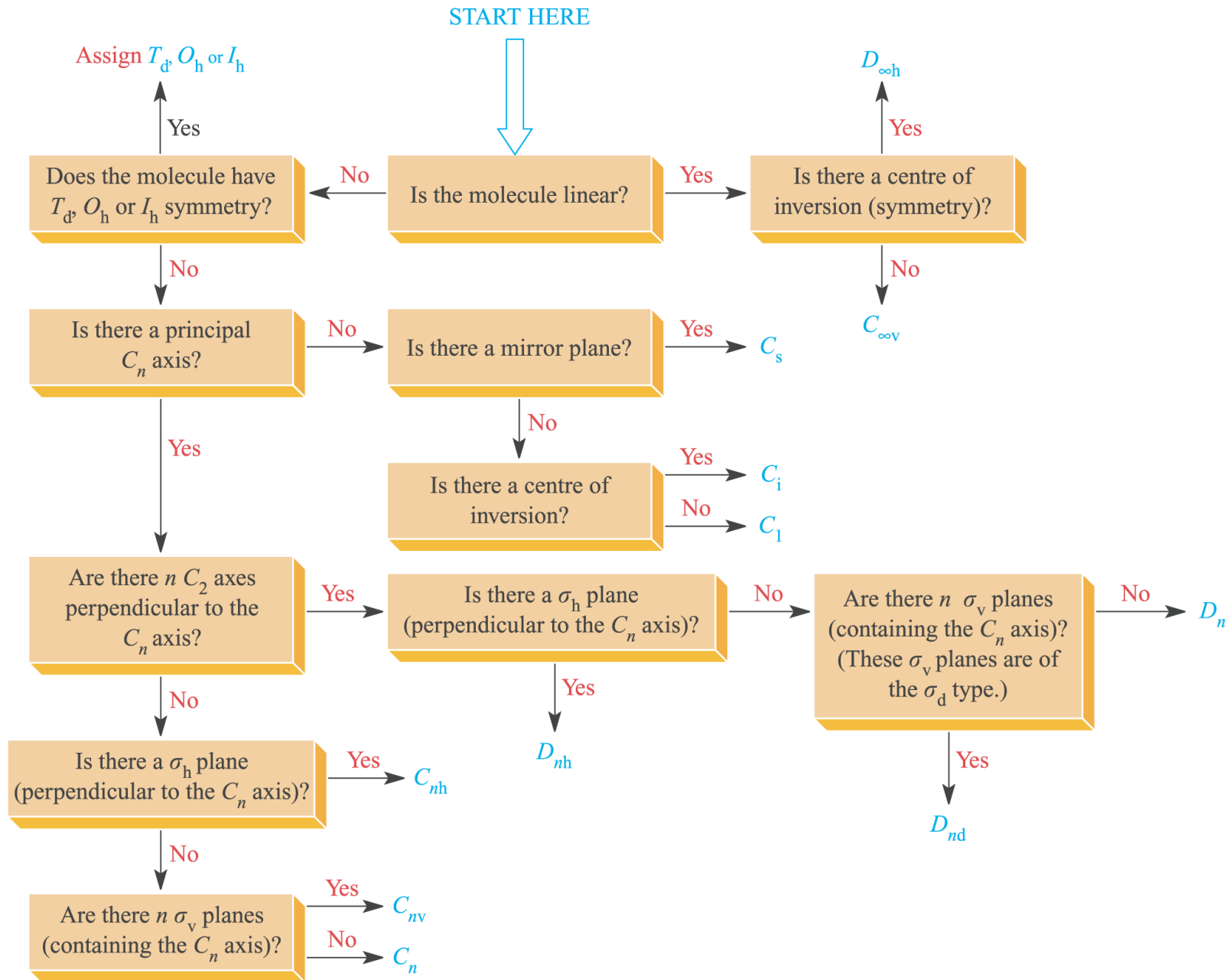
Geometria ottaedrica, simmetria inferiore

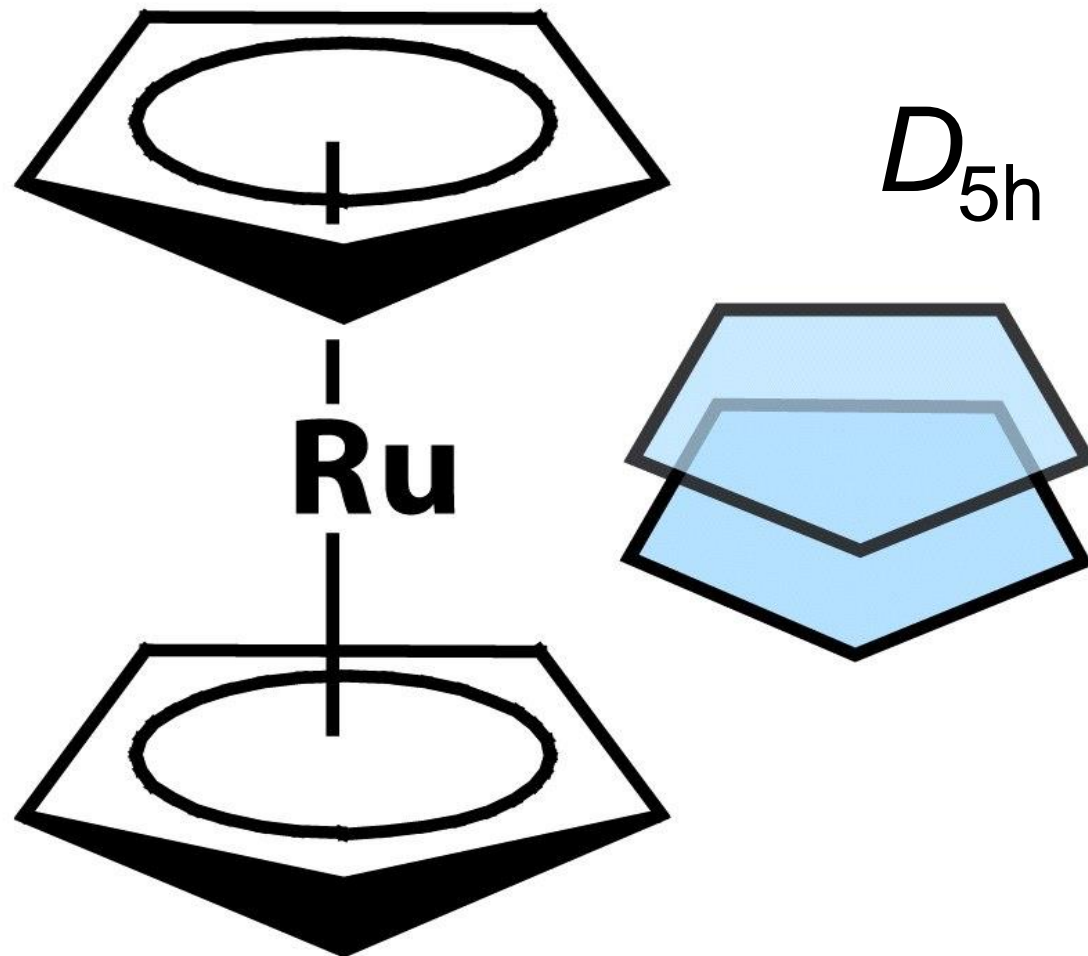
$D_{\infty h}$



CO₂







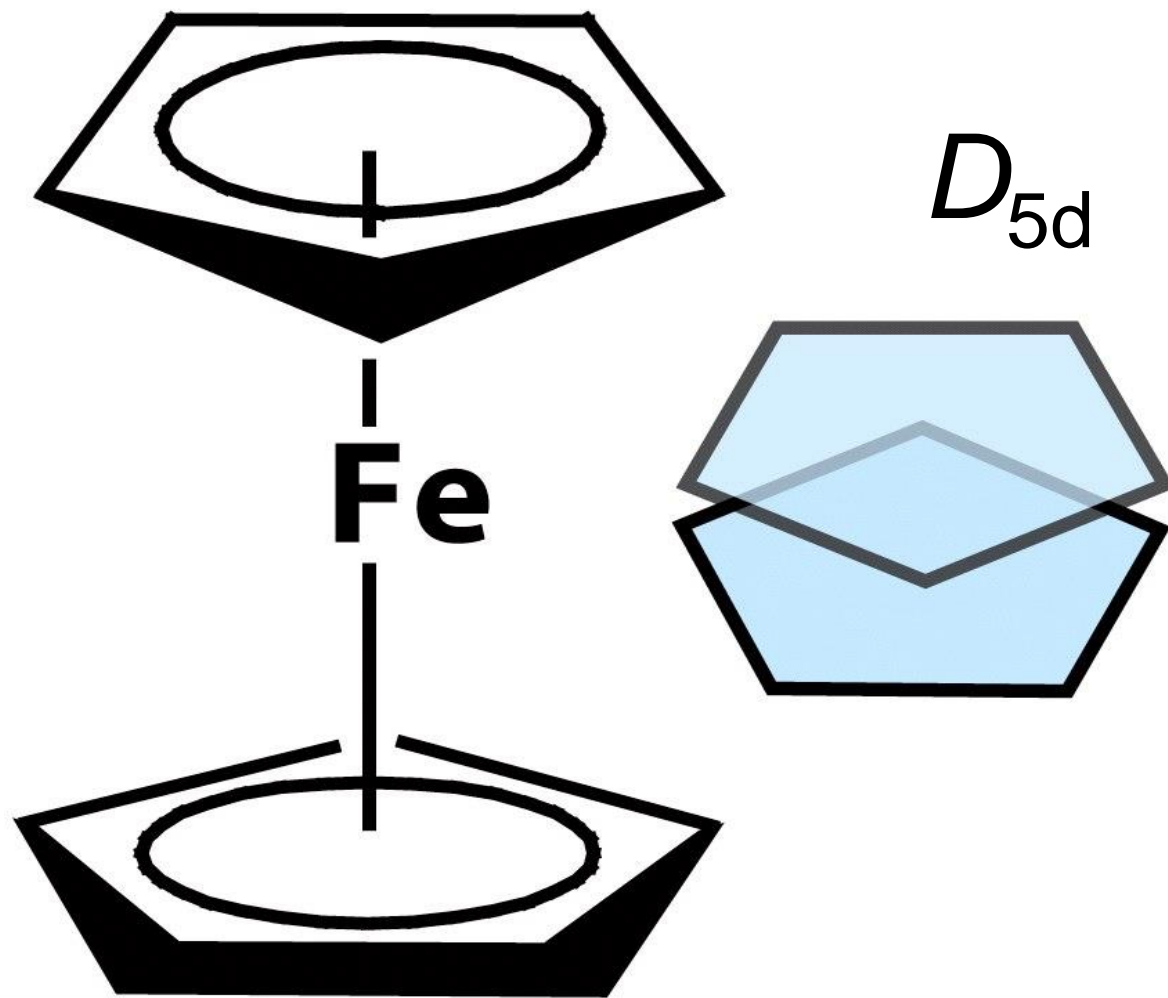


Tabella dei caratteri per il gruppo puntuale C_{2v}

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)	

