

In una molecola EX_n contenente legami singoli $E-X$ ogni coppia elettronica del guscio di valenza di E , sia di legame σ che solitaria, è stereochimicamente attiva

Table 2.6 The basic arrangement of regions of electron density according to the VSEPR model

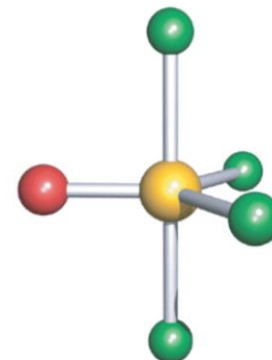
Number of electron regions	Arrangement
2	Linear
3	Trigonal planar
4	Tetrahedral
5	Trigonal bipyramidal
6	Octahedral

Repulsione fra le coppie

coppia solitaria – coppia solitaria > coppia solitaria – coppia di legame > coppia di legame – coppia di legame

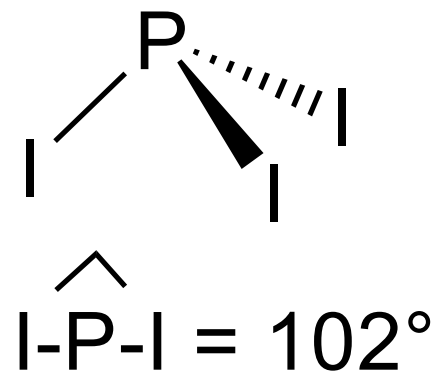
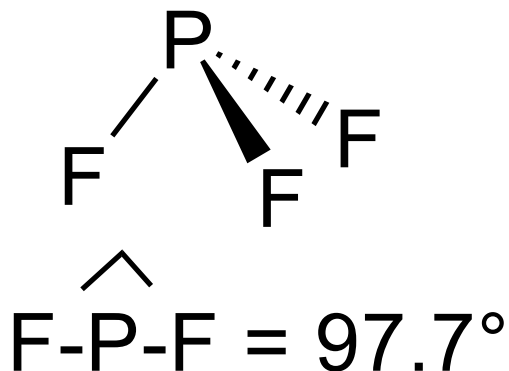
CH_4 (109.5°), NH_3 (107°), H_2O (104.5°)

legame triplo – legame singolo > legame doppio – legame singolo > legame singolo – legame singolo



coppie di legame verso atomi (o gruppi) elettronegativi occupano meno spazio di quelle verso atomi più elettropositivi

OSF_4

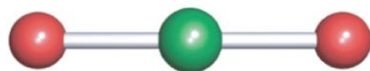


numero sterico = numero di coppie di legame e di non legame intorno all'atomo centrale. Se non ci sono legami E-H:

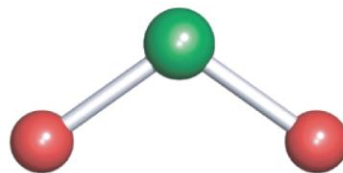
$$\text{n.s.} = \underbrace{\text{elettroni di valenza } (\pm \text{ carica})/8}_{\text{Legami}} + \underbrace{\text{resto}/2}_{\text{Coppie solitarie}}$$

*Il numero sterico determina la **geometria delle coppie**, che non necessariamente coincide con la **geometria molecolare***

2-Coordinate

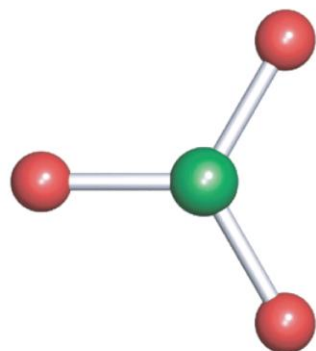


Linear

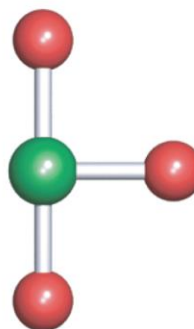


Bent

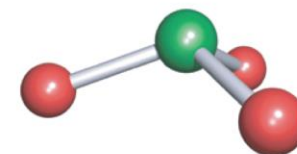
3-Coordinate



Trigonal planar



T-shaped

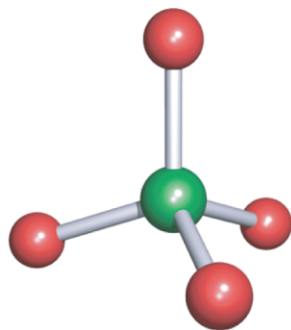


Trigonal pyramidal

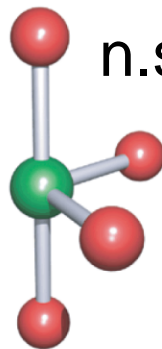


$n.s. = 5$

4-Coordinate

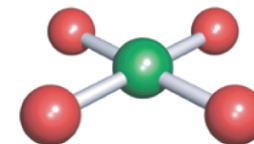


Tetrahedral



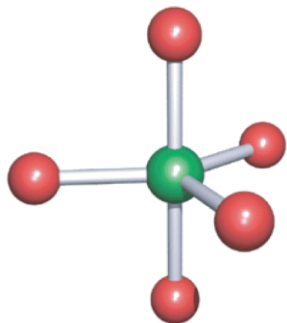
n.s. = 5

Disphenoidal

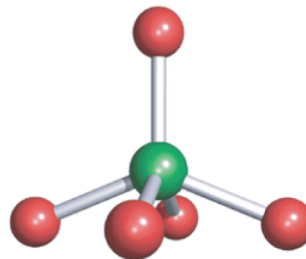


Square planar

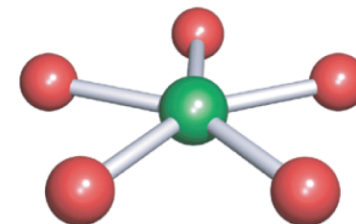
5-Coordinate



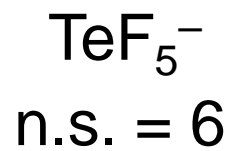
Trigonal bipyramidal



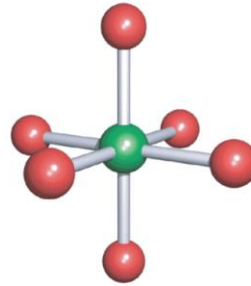
Square-based pyramidal



Pentagonal planar

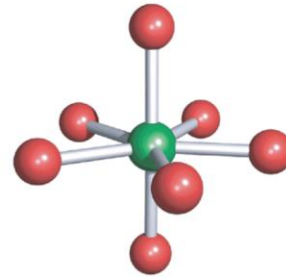


6-Coordinate



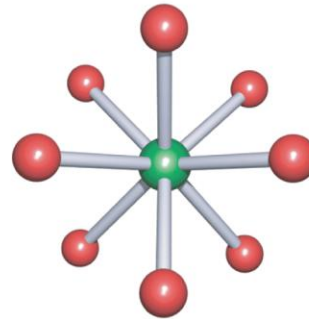
Octahedral

7-Coordinate



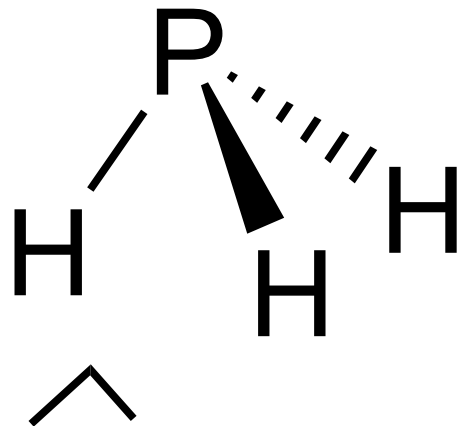
Pentagonal bipyramidal

8-Coordinate



Square antiprismatic

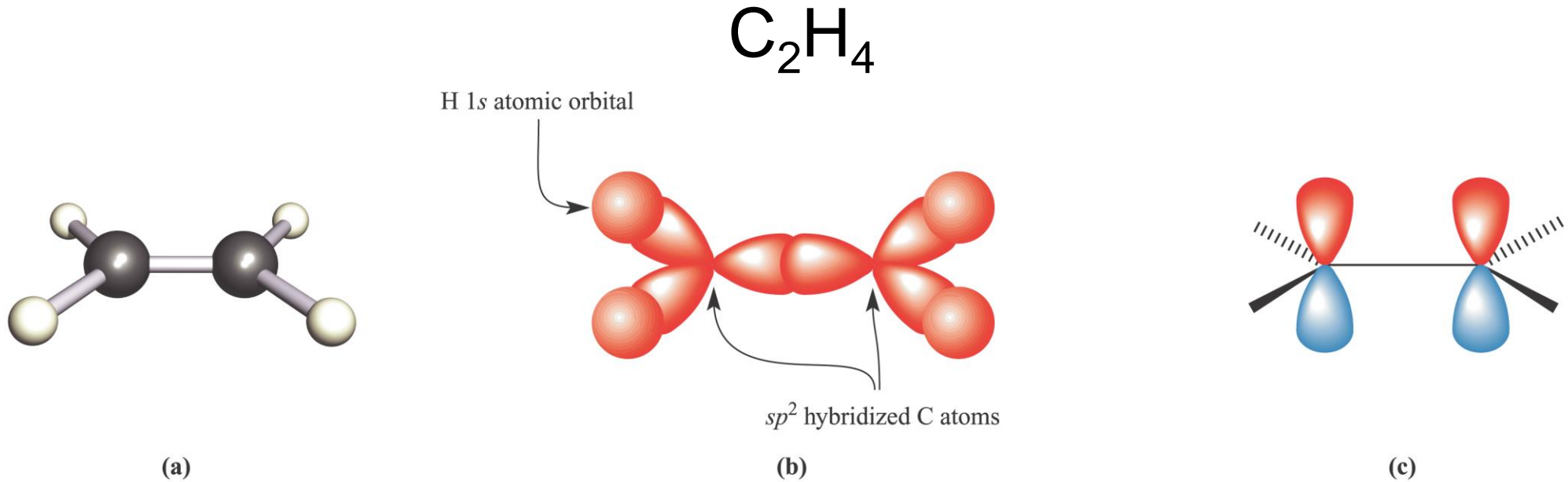
Coppie solitarie stereochimicamente inattive



H-P-H ca. 90°



Molecole poliatomiche secondo la teoria VB

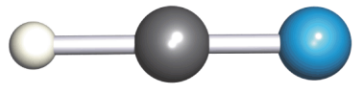


598 kJ mol^{-1} vs $2 \times 346 \text{ kJ mol}^{-1}$

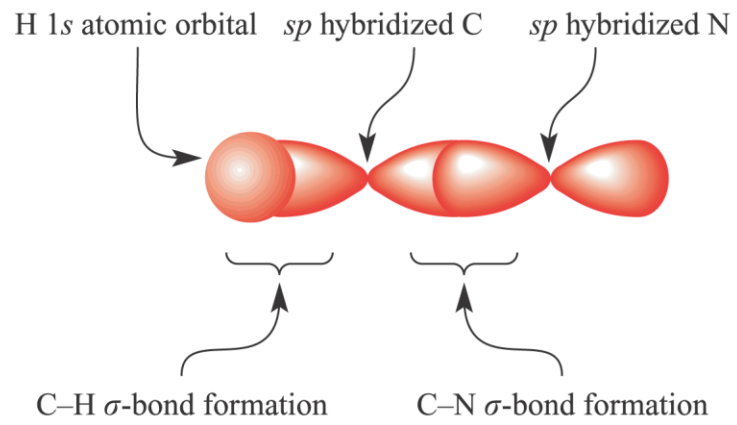
$\sigma + \pi$

2σ

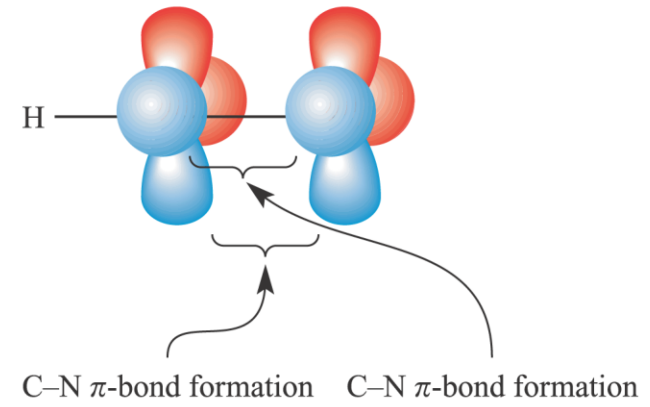
HCN



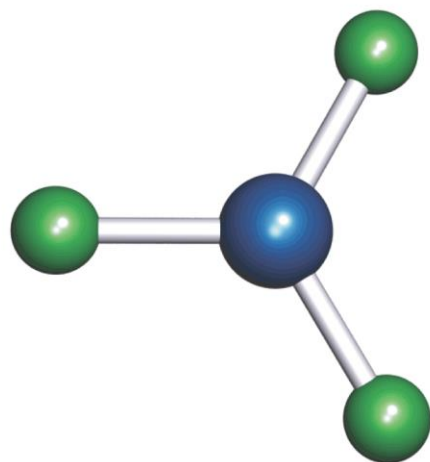
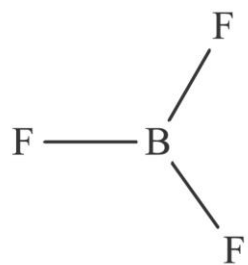
(a)



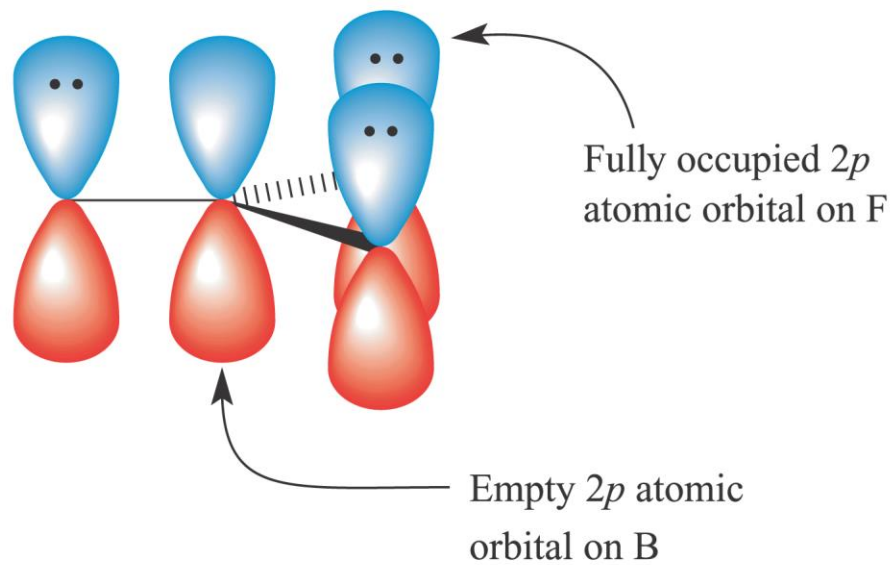
(b)



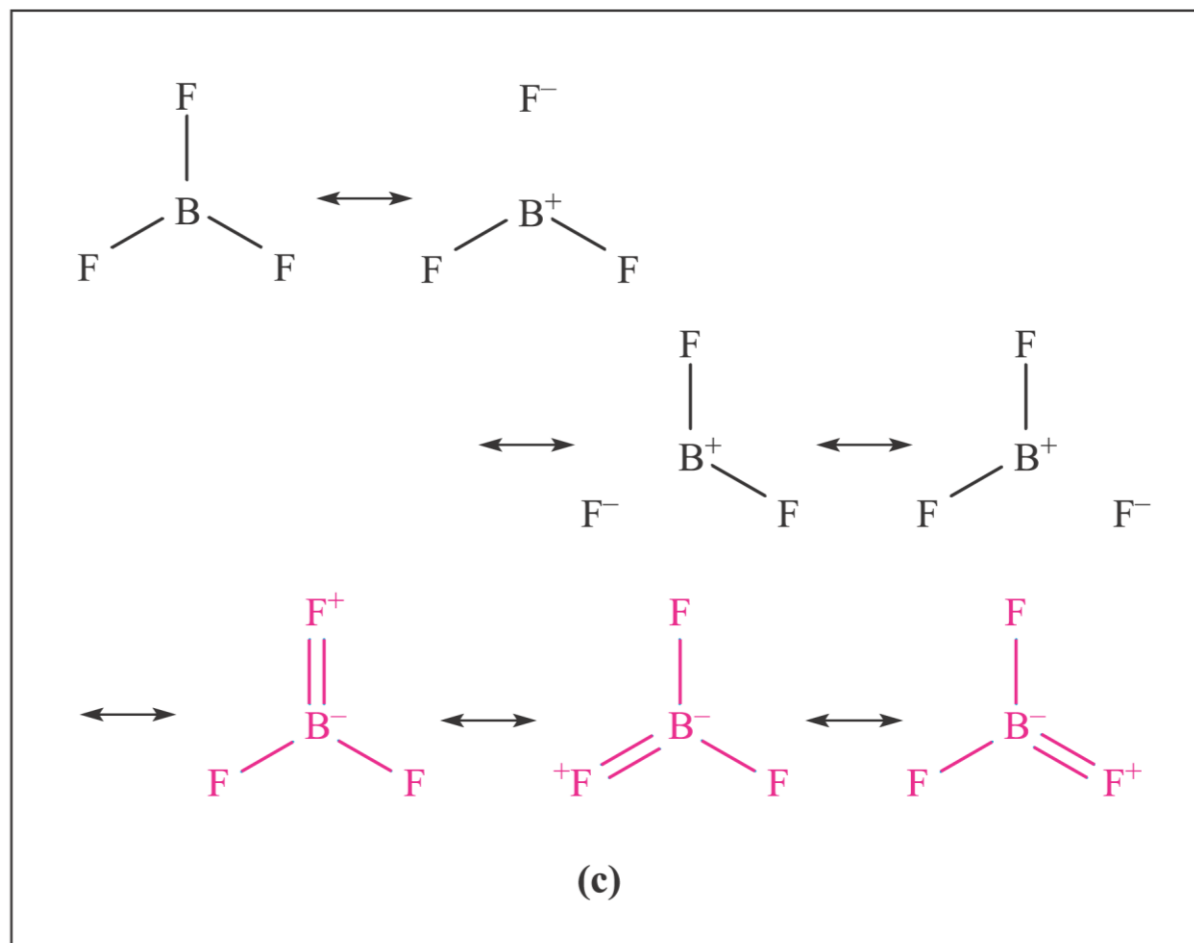
(c)



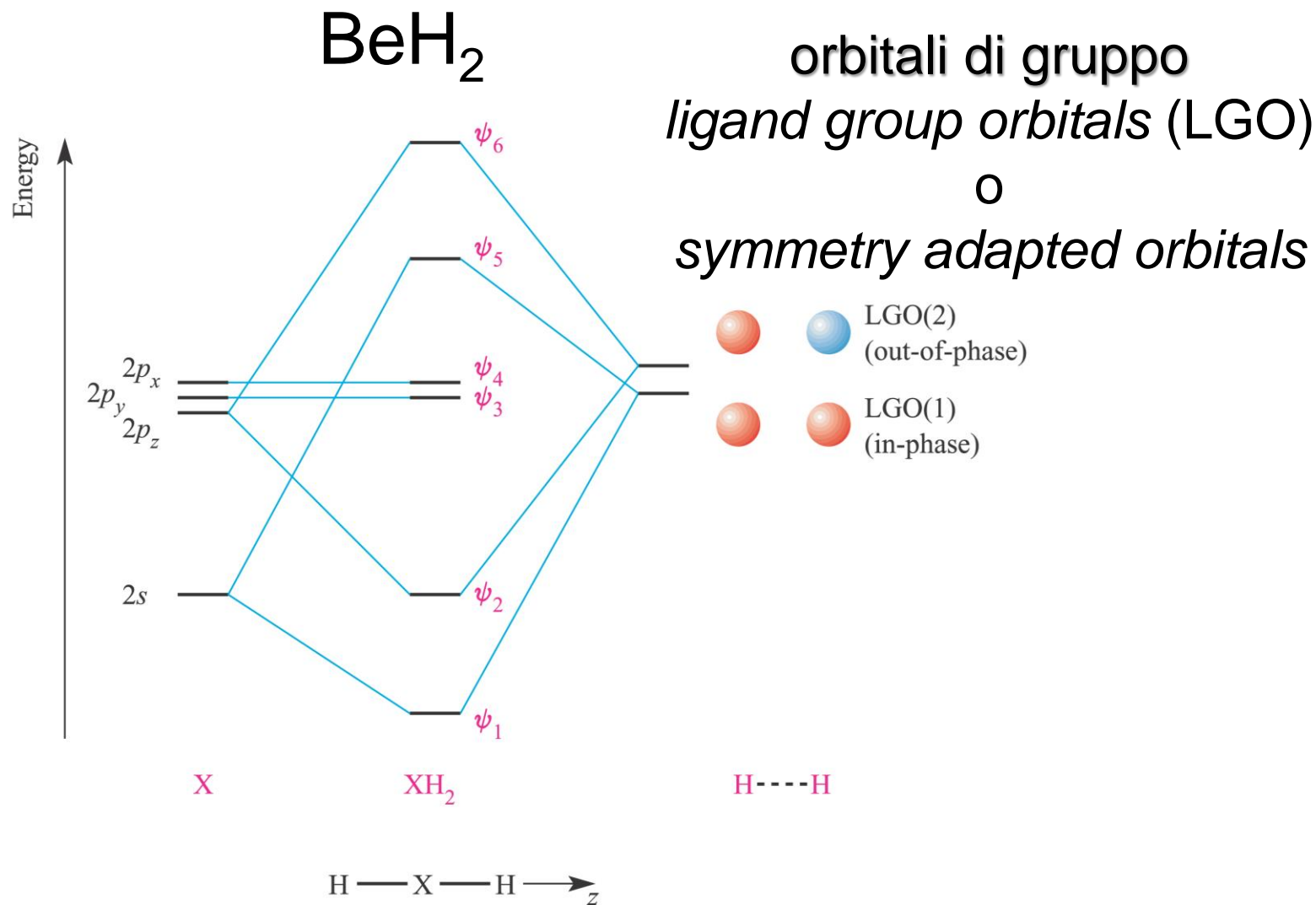
(a)



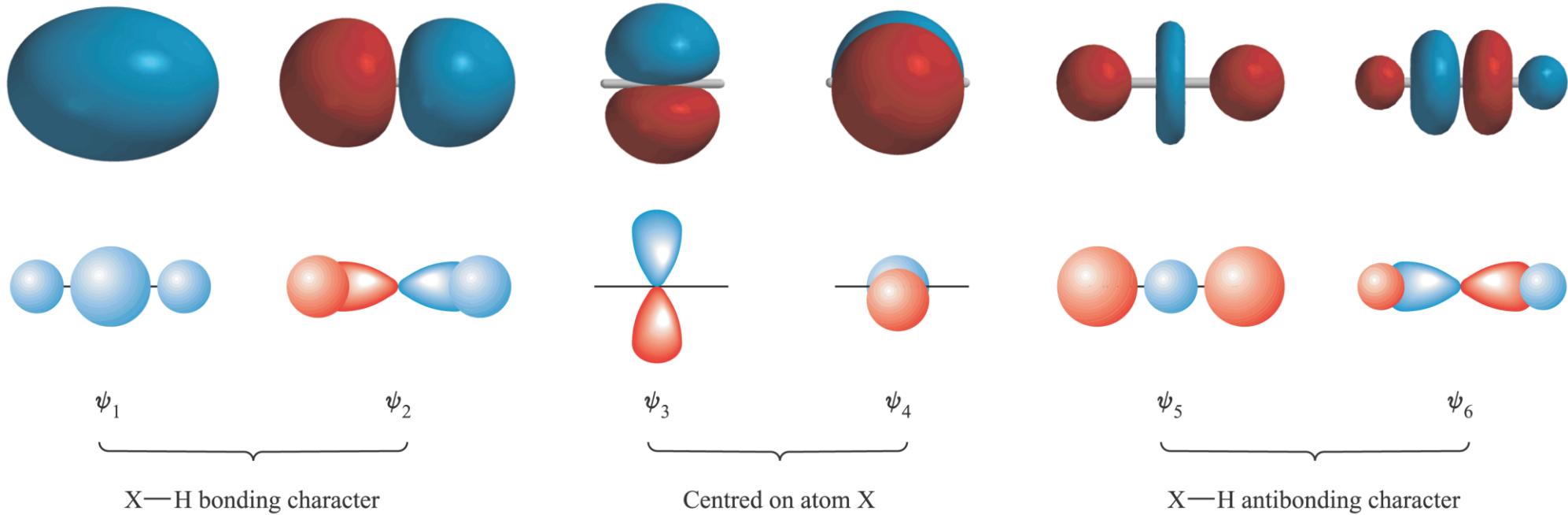
(b)

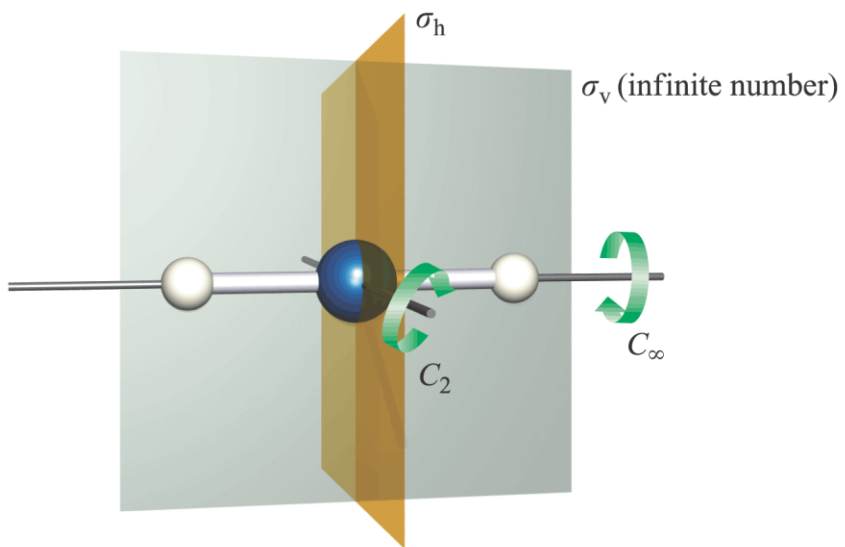


Molecole poliatomiche secondo la teoria MO



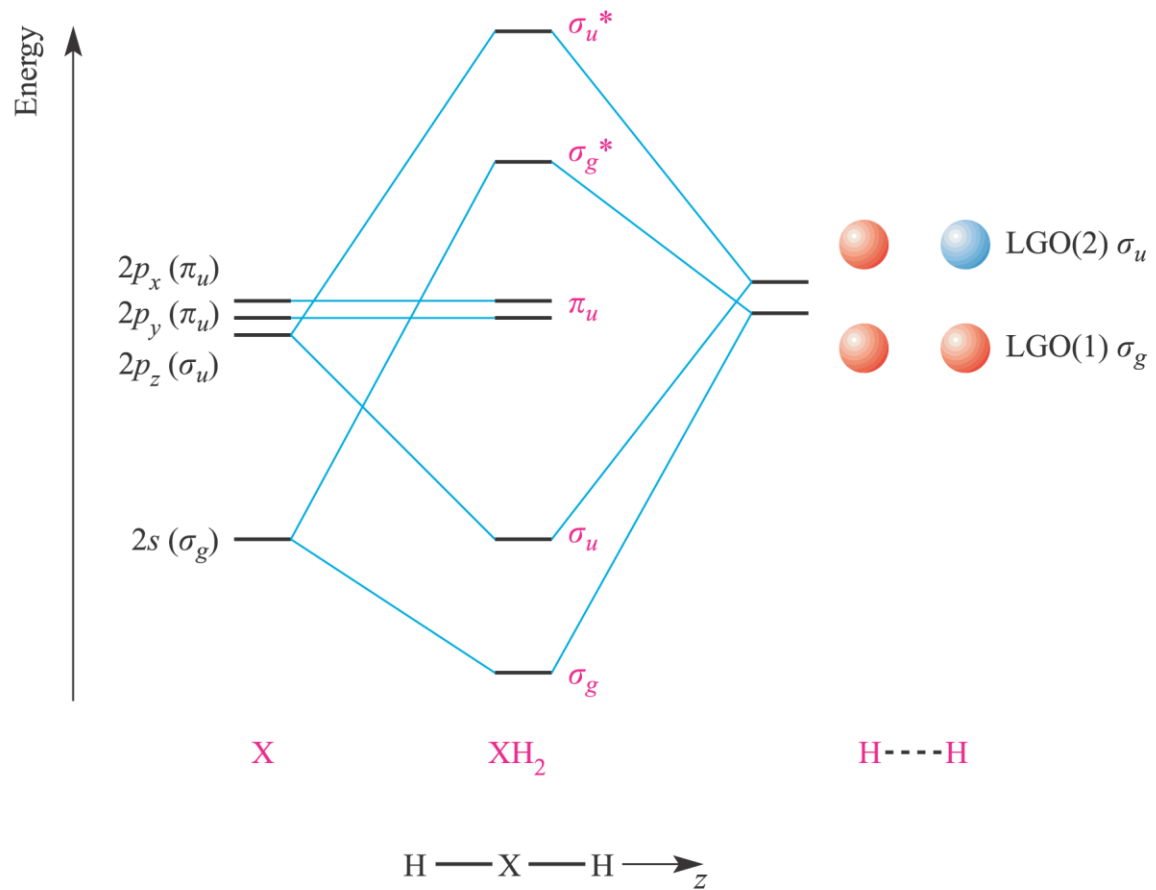
Molecole poliatomiche secondo la teoria MO



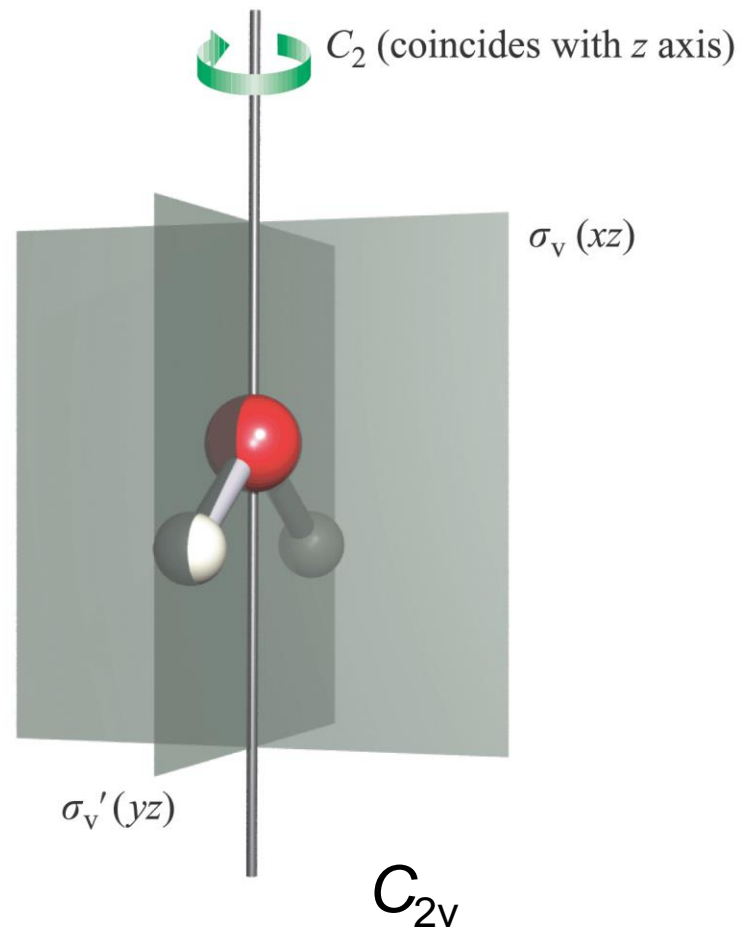


$D_{\infty h}$

(a)



(b)

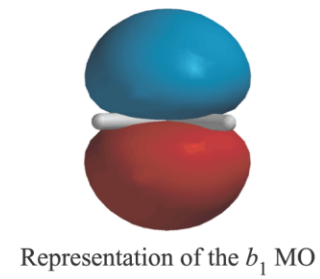
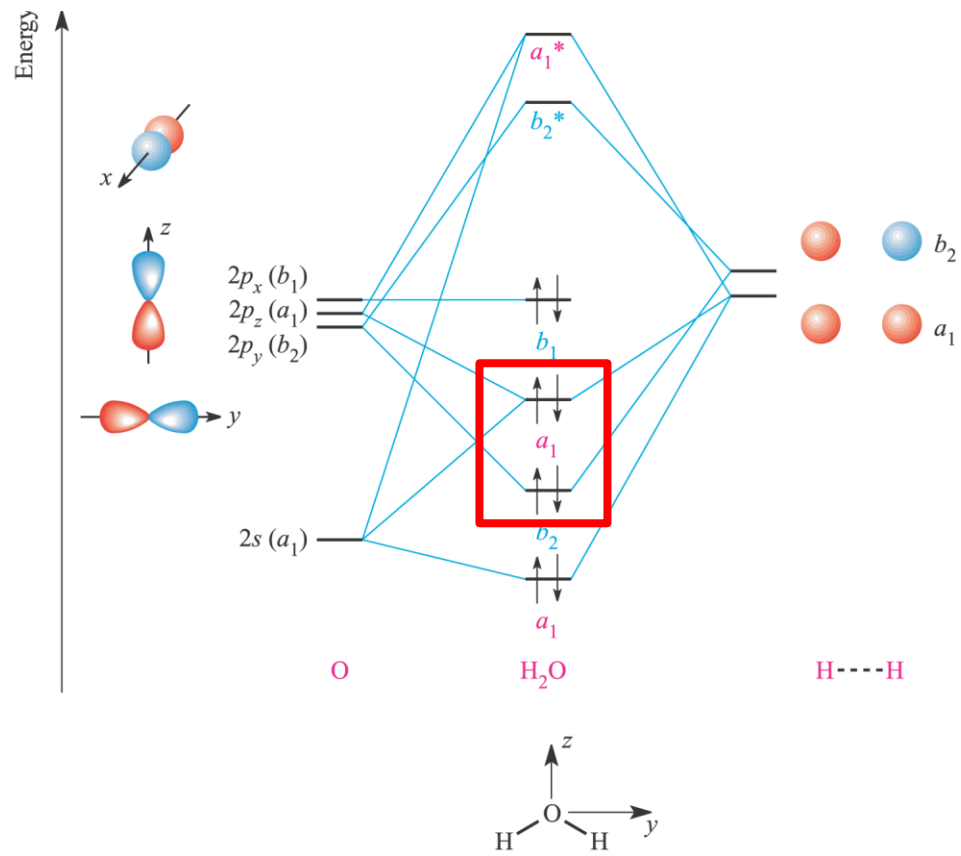


C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	1	y, R_x	yz

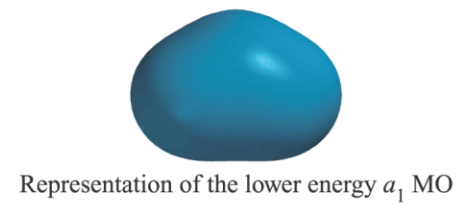
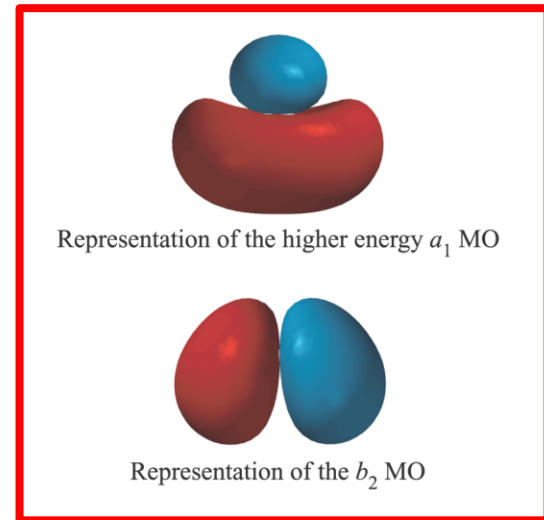
2H

2	0	0	2
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$A_1 + B_2$

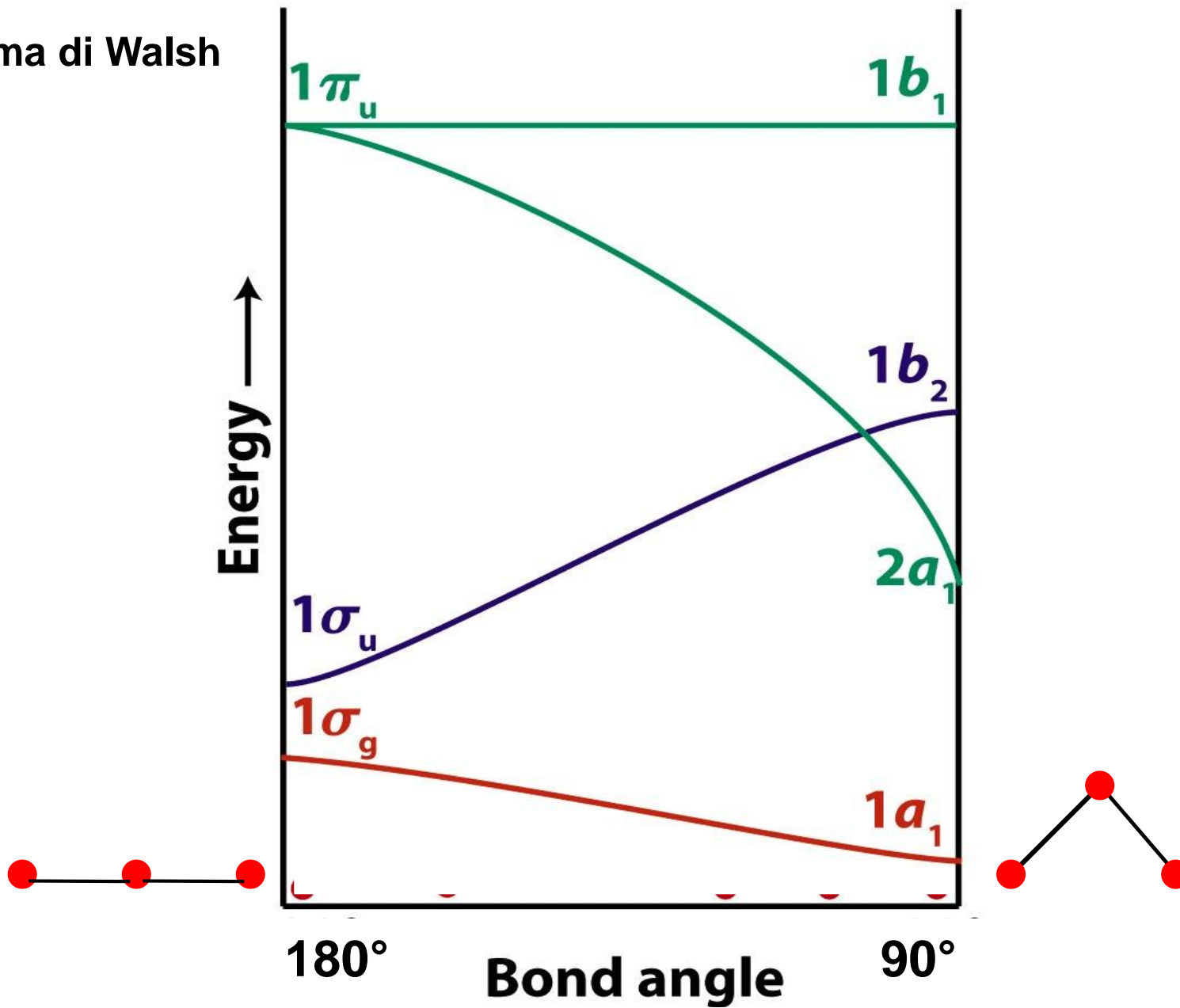


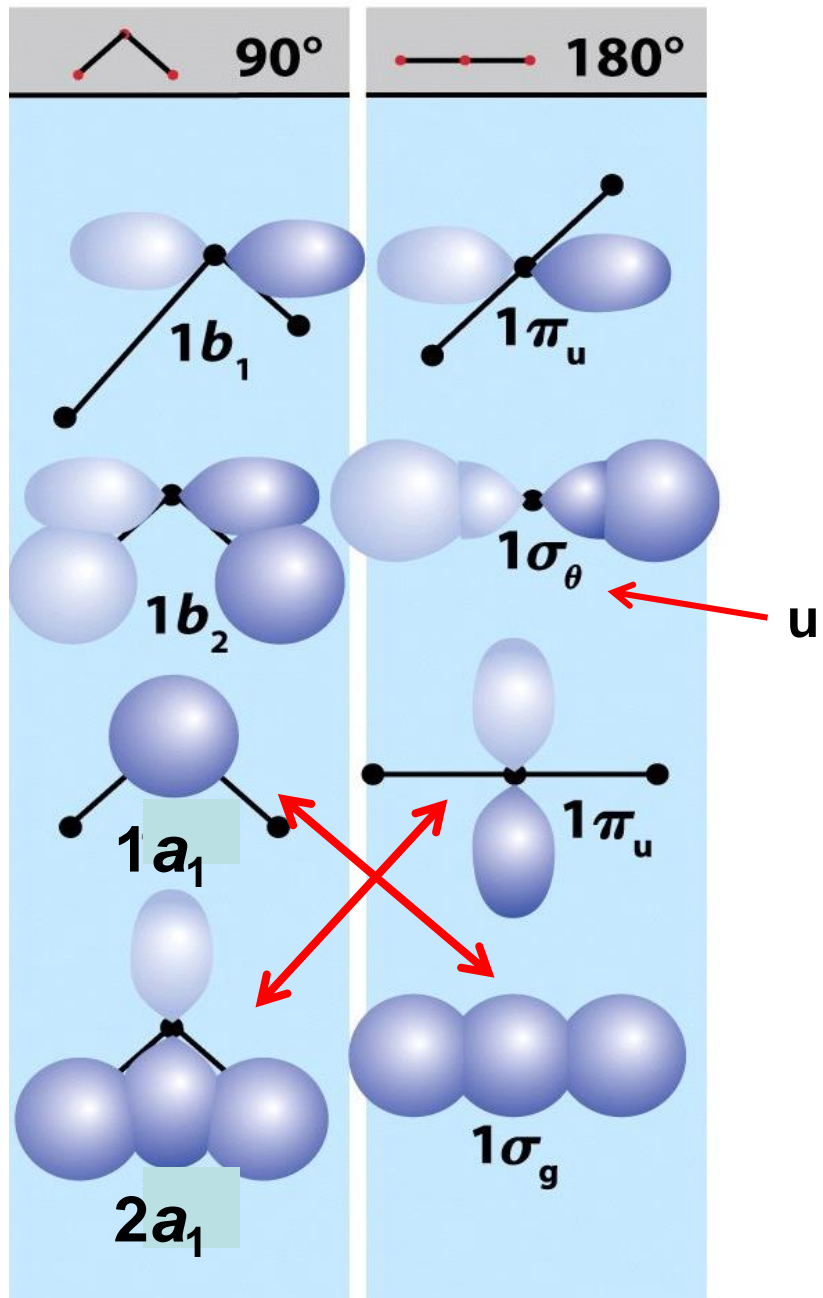
n.l.



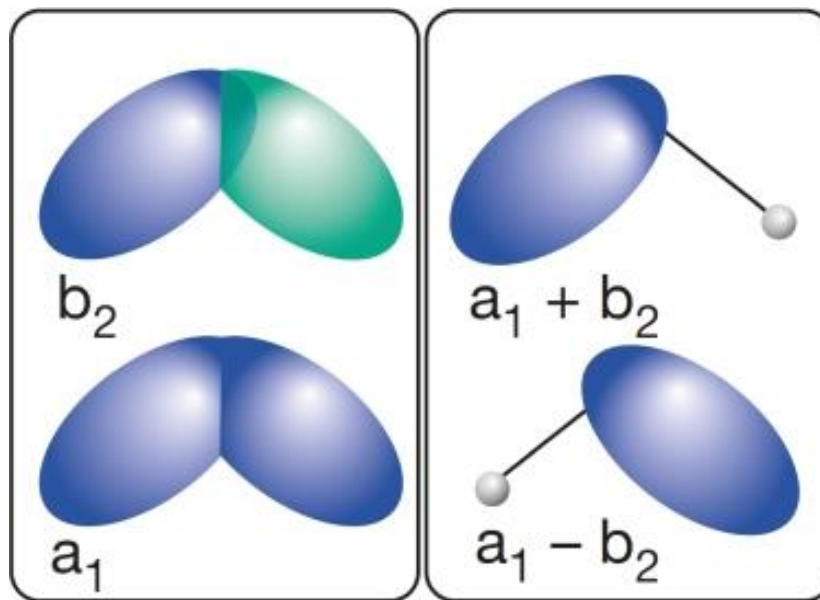
n.l.

Diagramma di Walsh



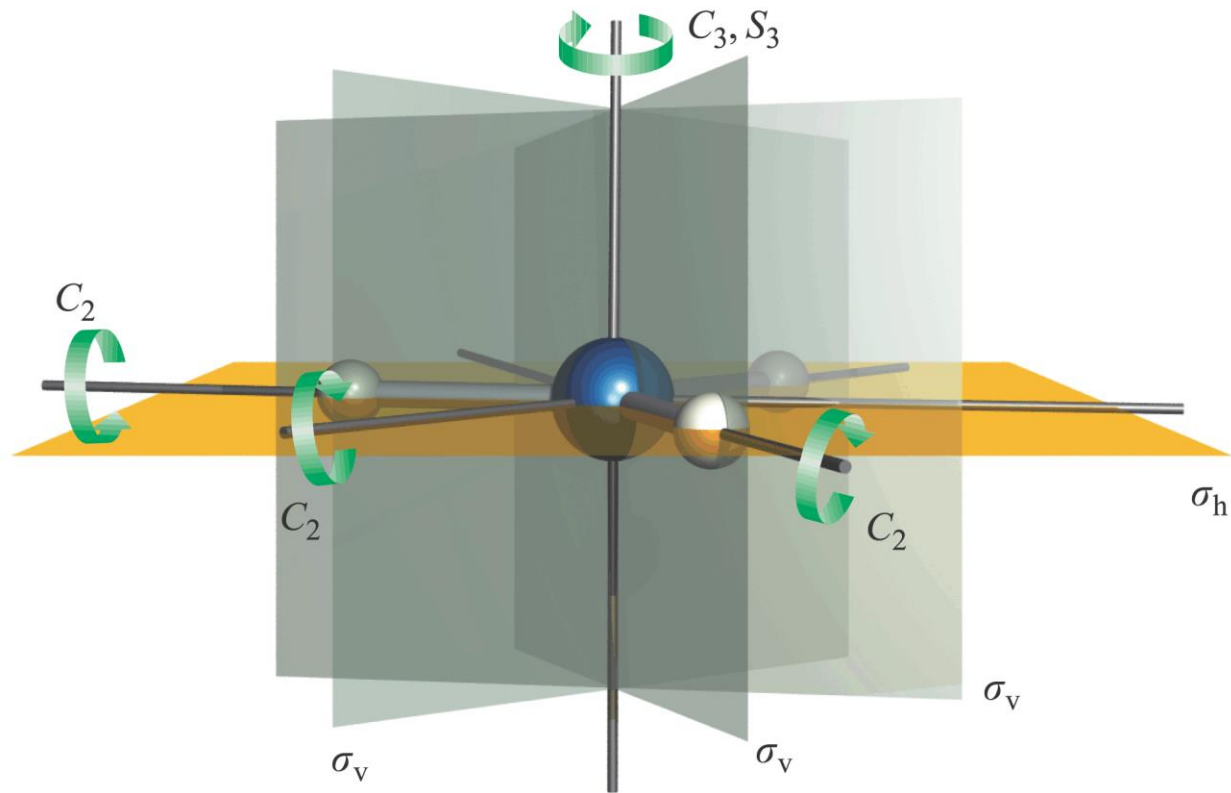


Combinazioni lineari di orbitali molecolari



Localizzate	Delocalizzate
Forza dei legami	Spettri elettronici
Costanti di forza	Fotoionizzazione
Lunghezze di legame	Affinità elettronica
Acidità di Brønsted*	Magnetismo
Descrizione VSEPR	Potenziali standard [†]

BH₃, gruppo puntuale D_{3h}

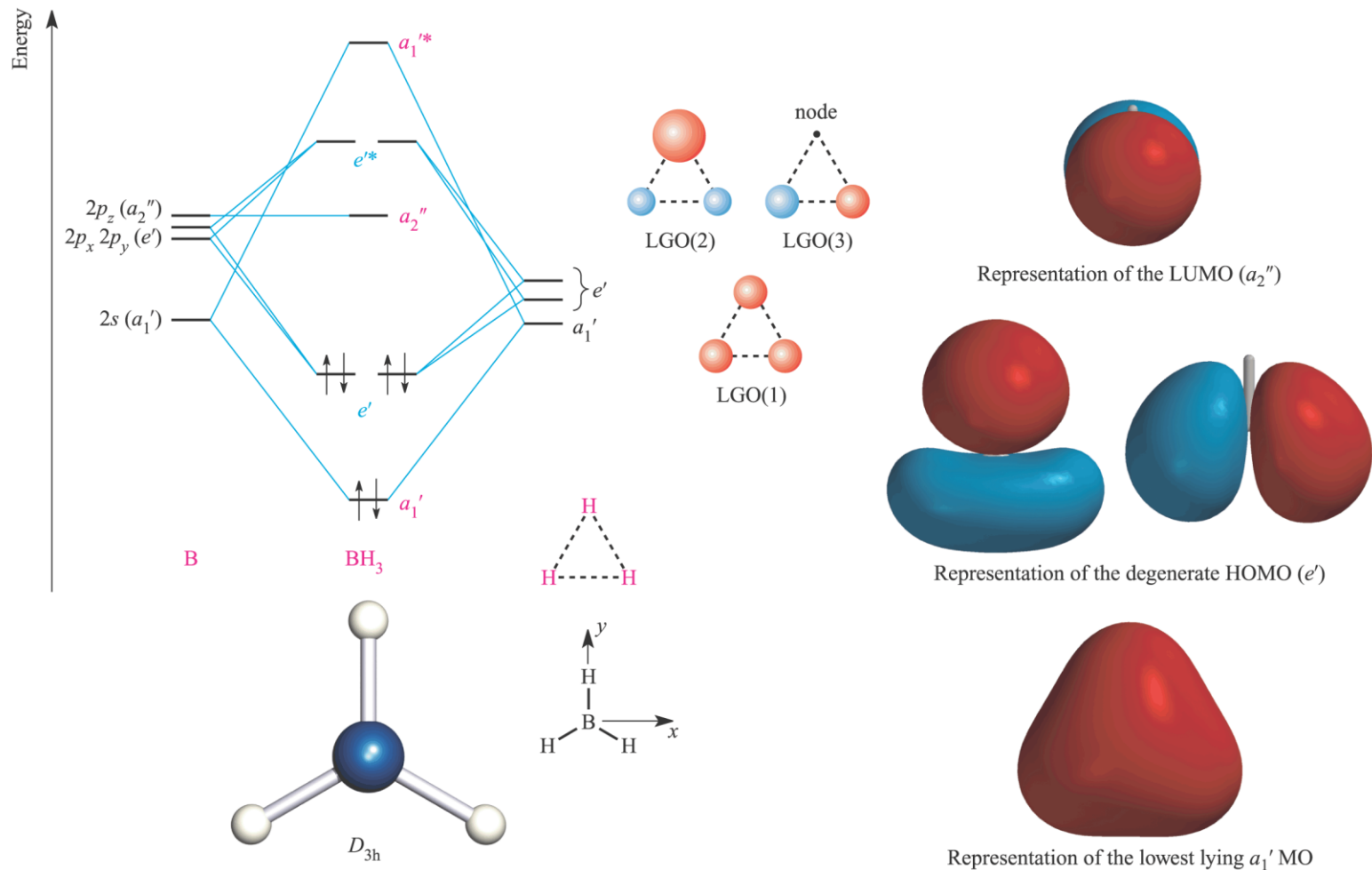


D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
A_1'	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2'	1	1	-1	1	1	-1	R_z	
E'	2	-1	0	2	-1	0	(x, y)	$(x^2 - y^2, xy)$
A_1''	1	1	1	-1	-1	-1		
A_2''	1	1	-1	-1	-1	1	z	
E''	2	-1	0	-2	1	0	(R_x, R_y)	(xz, yz)

3H

3	0	1	3	0	1
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$A_1' + E'$



$$\Psi(a_1') = 1/\sqrt{3} \times (\Psi_1 + \Psi_2 + \Psi_3)$$

(LGO1)

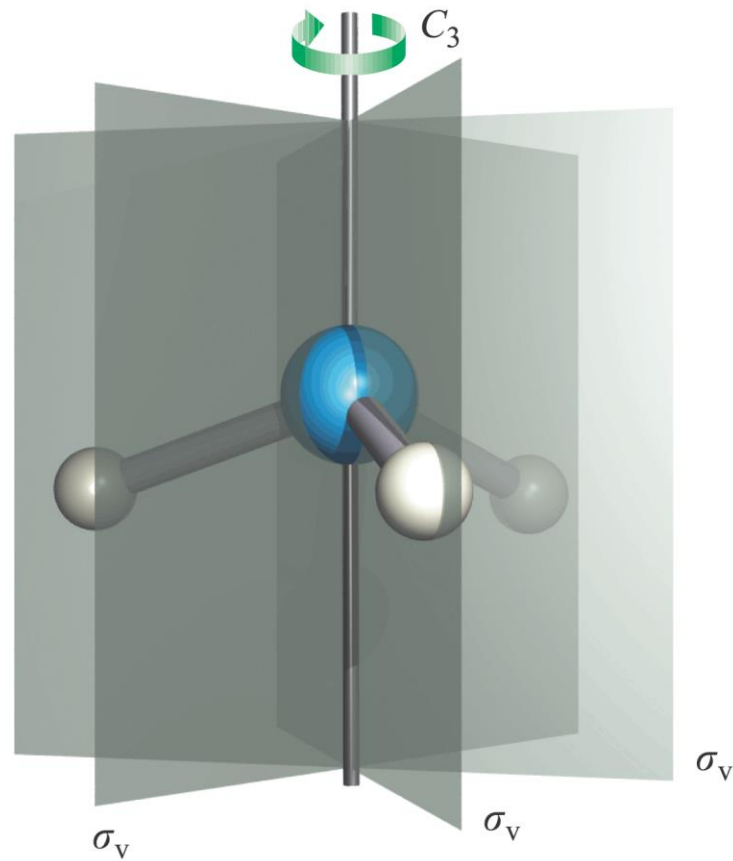
$$\Psi(e')_1 = 1/\sqrt{6} \times (2\Psi_1 - \Psi_2 - \Psi_3)$$

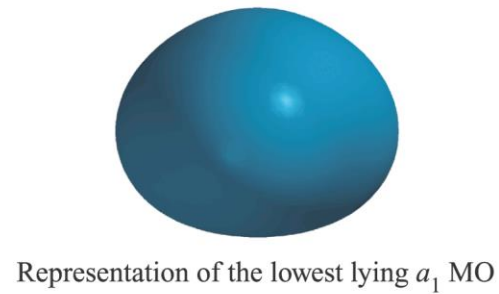
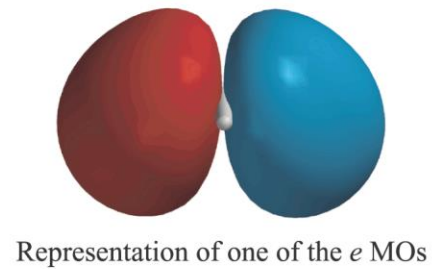
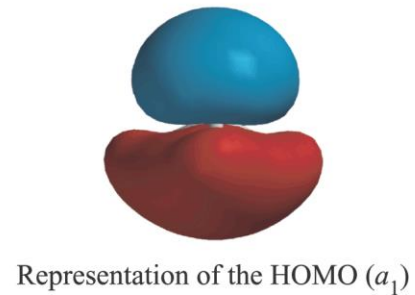
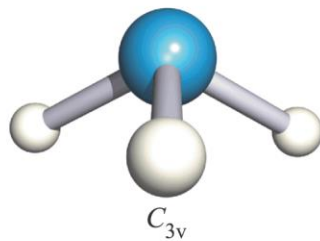
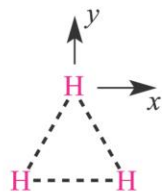
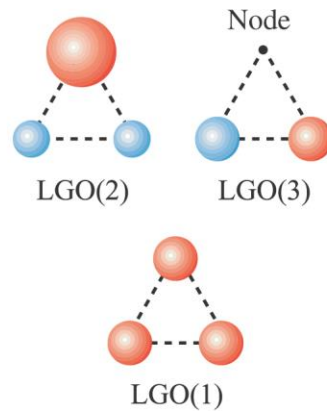
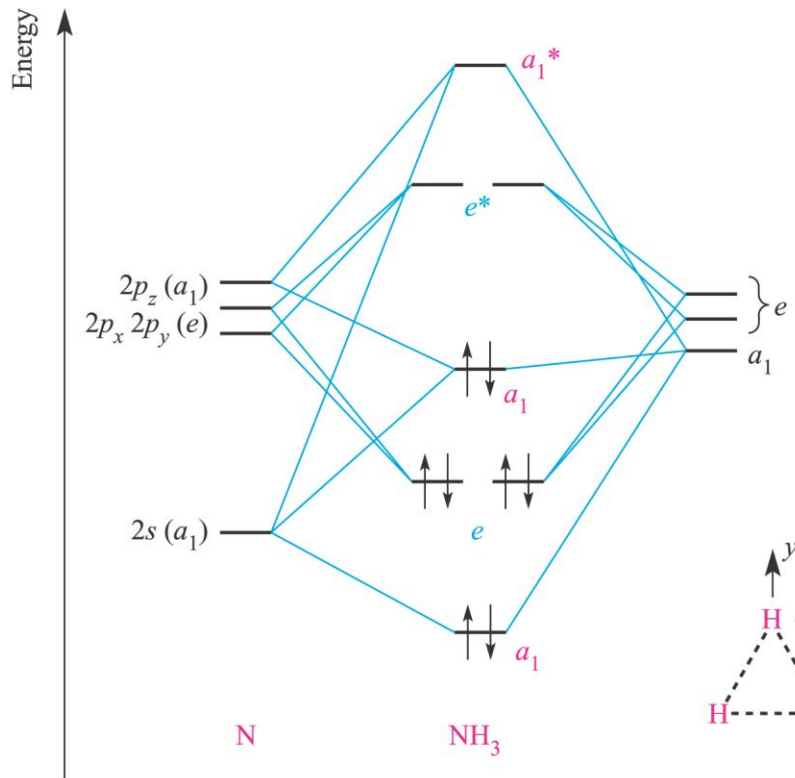
(LGO2)

$$\Psi(e')_2 = 1/\sqrt{2} \times (\Psi_2 - \Psi_3)$$

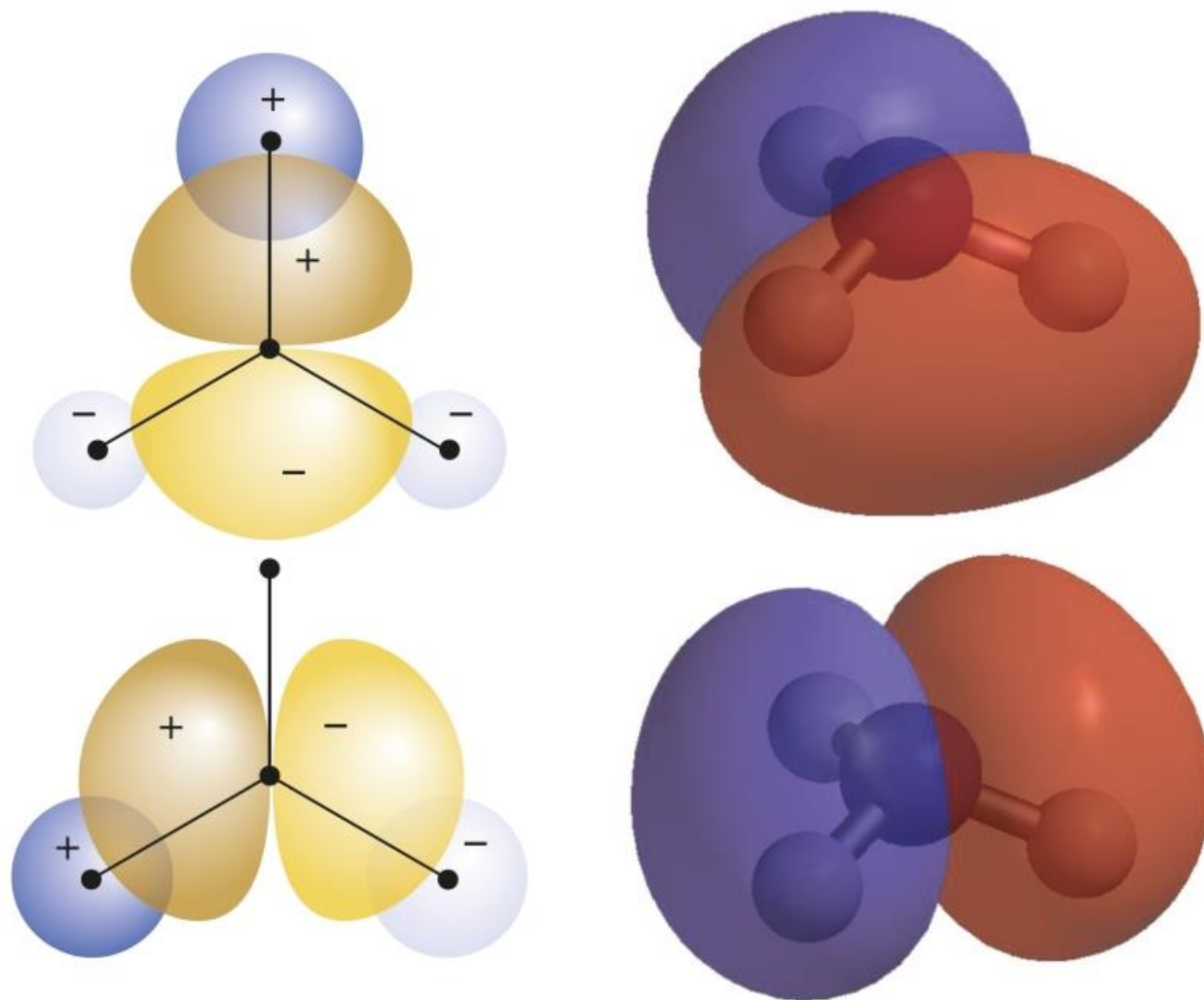
(LGO3)

NH₃, gruppo puntuale C_{3v}

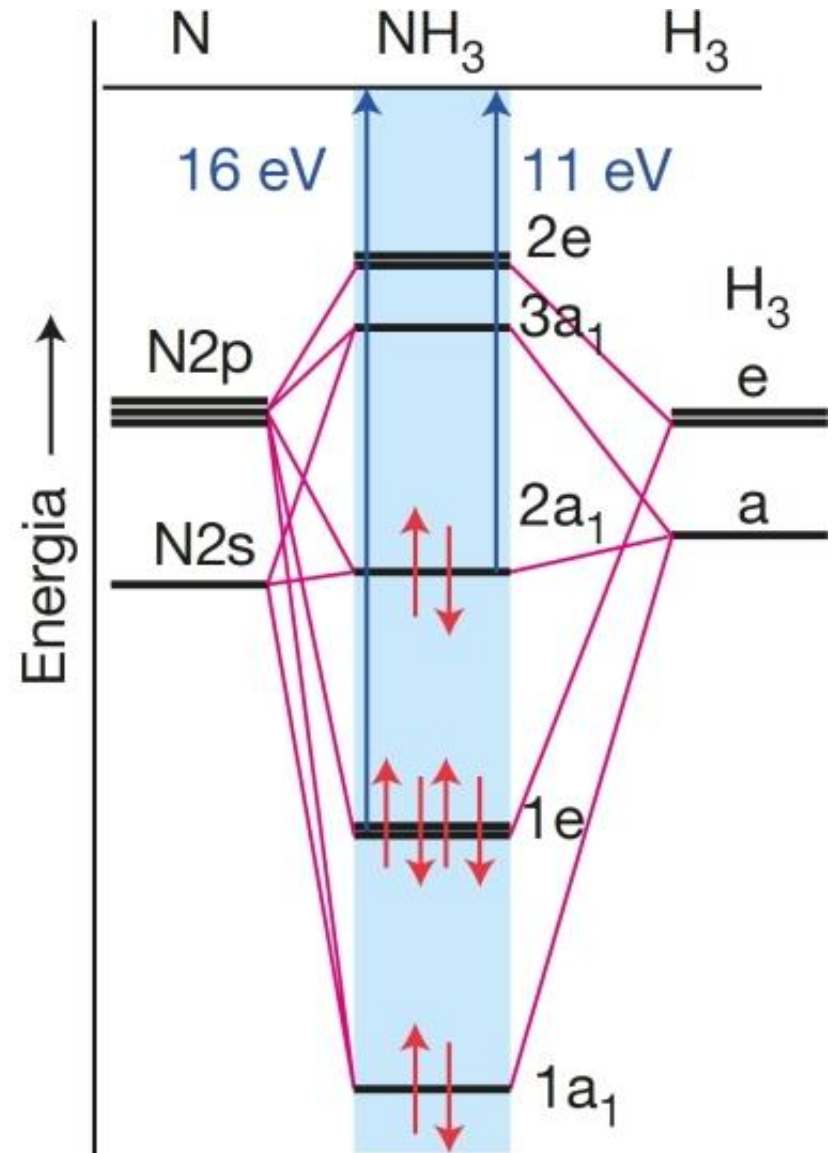
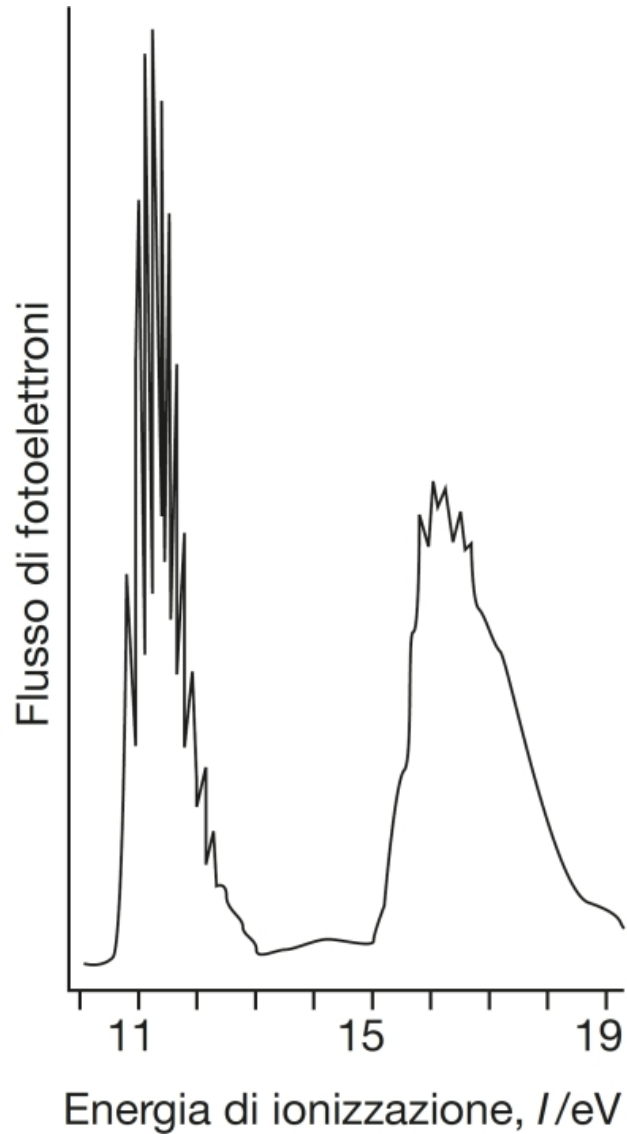


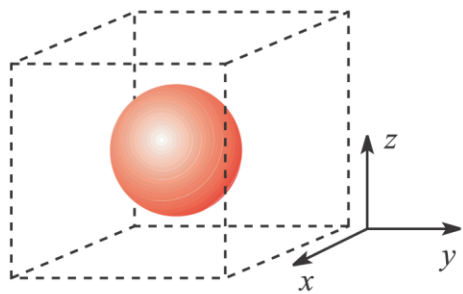


Formazione degli orbitali molecolari leganti e

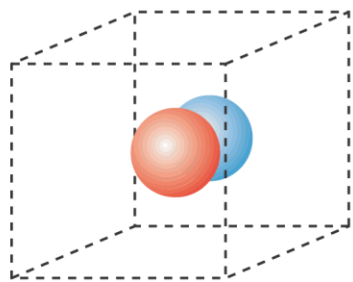


Spettro di fotoelettroni di NH_3

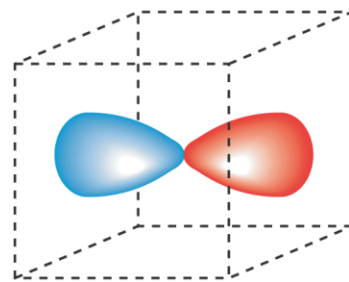




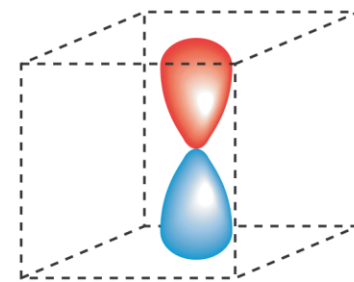
$2s (a_1)$



$2p_x (t_2)$

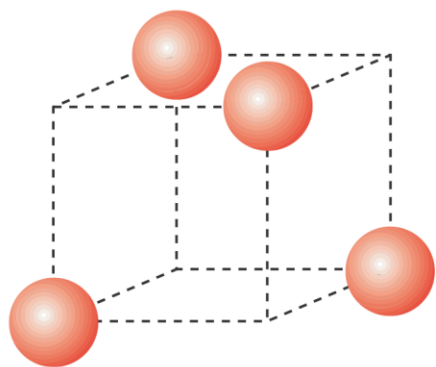


$2p_y (t_2)$

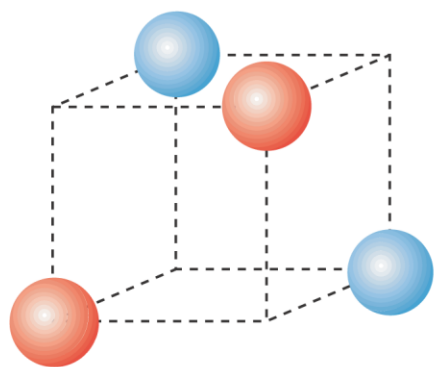


$2p_z (t_2)$

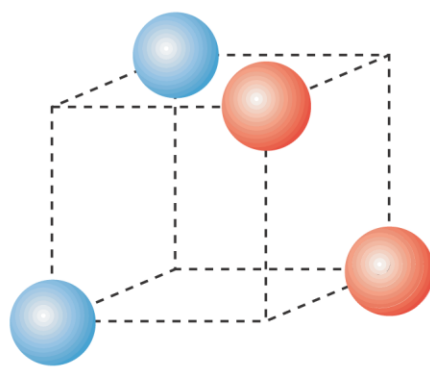
(a)



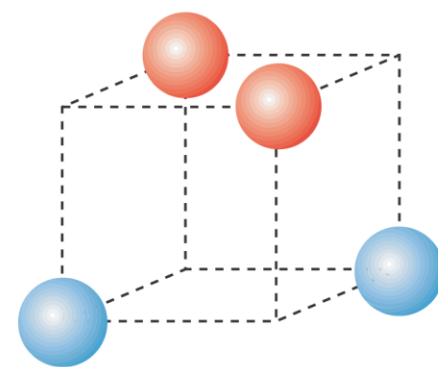
LGO(1) (a_1)



LGO(2) (t_2)

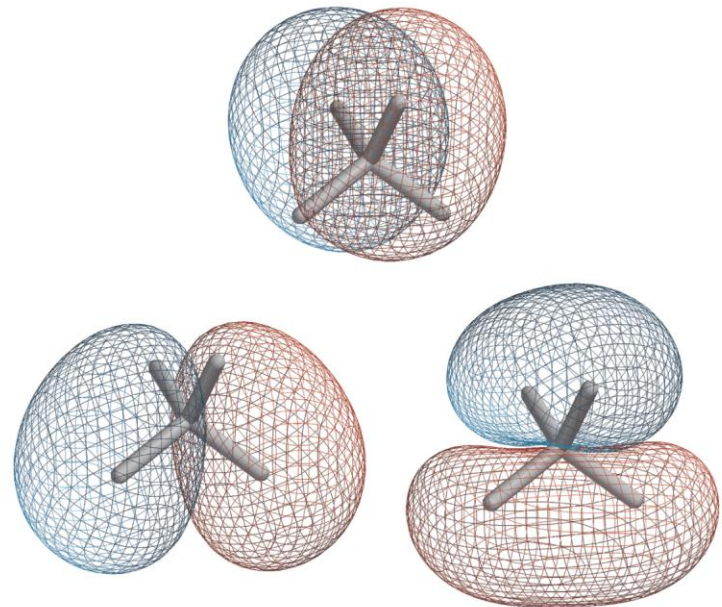
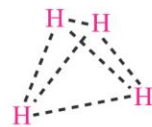
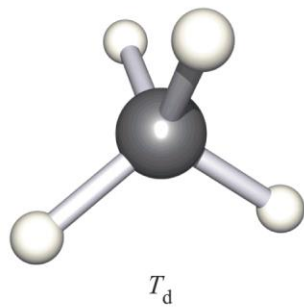
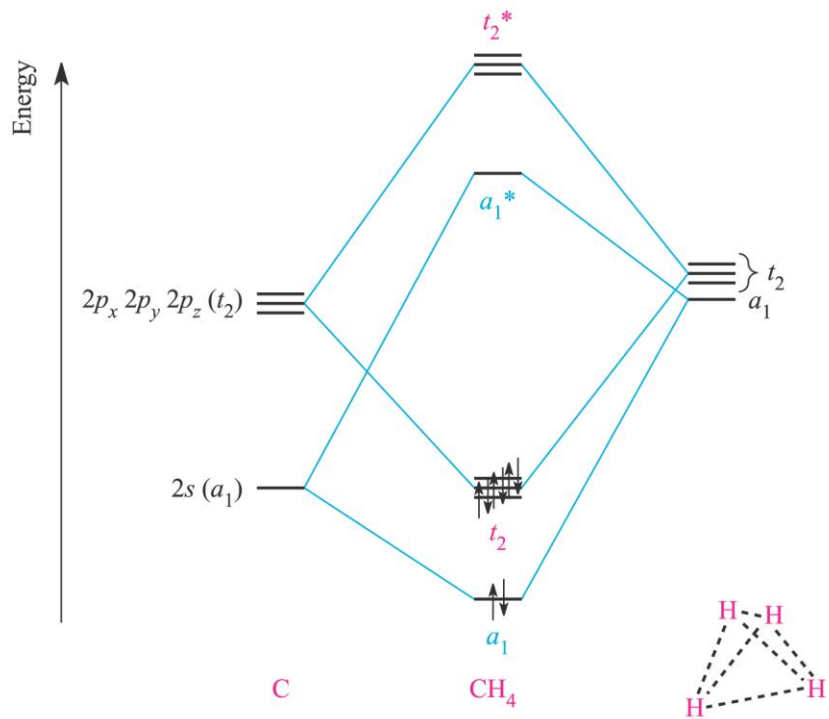


LGO(3) (t_2)

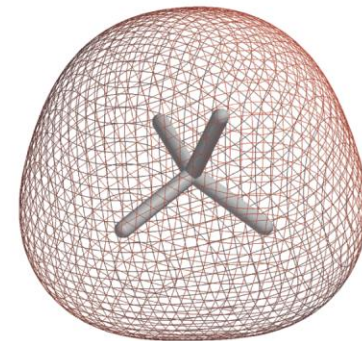


LGO(4) (t_2)

(b)



Representations of the triply degenerate (t_2) bonding MOs

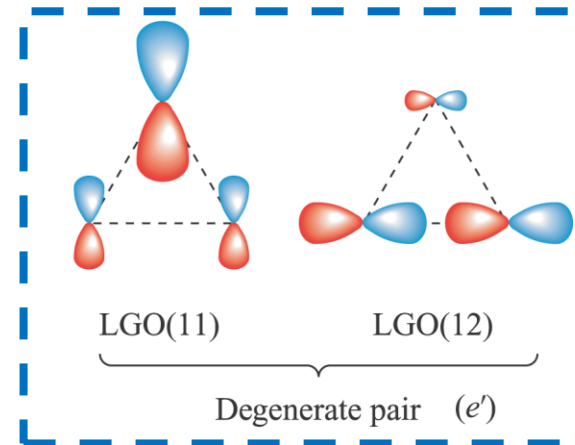
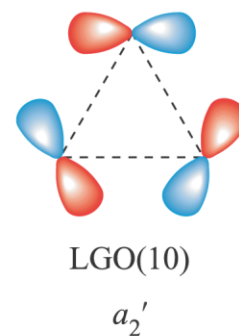
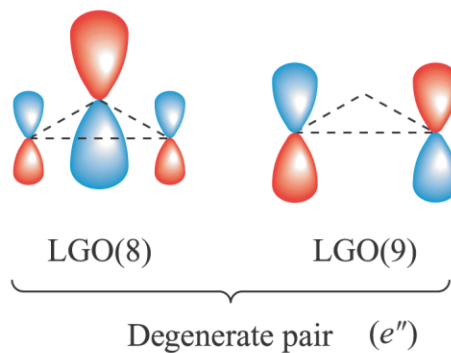
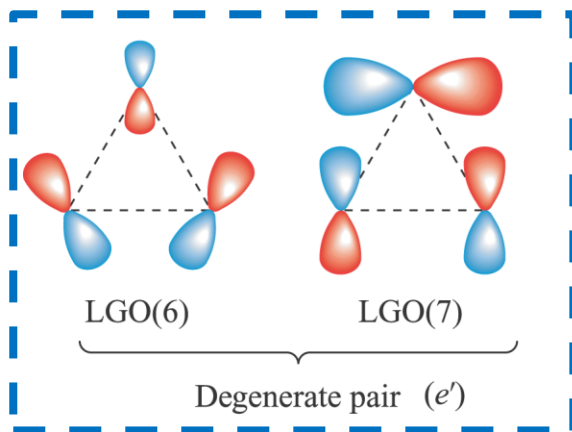
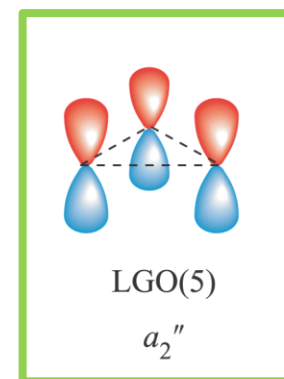
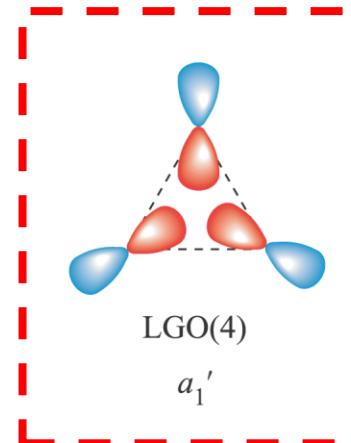
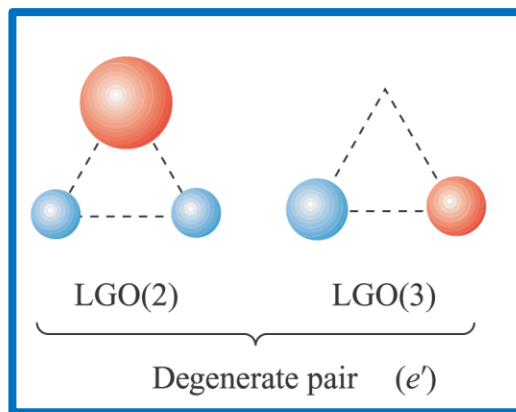
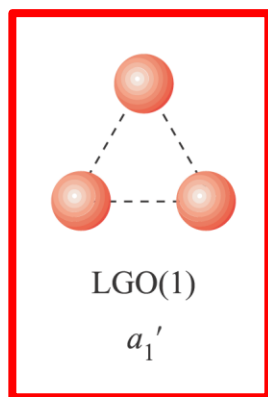
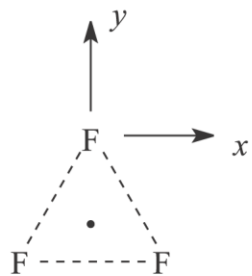


Representation of the a_1 bonding MO



<i>D</i> _{3h}	<i>E</i>	<i>2C</i> ₃	<i>3C</i> ₂	<i>σ</i> _h	<i>2S</i> ₃	<i>3σ</i> _v		
<i>A</i> ₁ '	1	1	1	1	1	1		<i>x</i> ² + <i>y</i> ² , <i>z</i> ²
<i>A</i> ₂ '	1	1	-1	1	1	-1	<i>R</i> _z	
<i>E</i> '	2	-1	0	2	-1	0	(<i>x</i> , <i>y</i>)	(<i>x</i> ² - <i>y</i> ² , <i>xy</i>)
<i>A</i> ₁ ''	1	1	1	-1	-1	-1		
<i>A</i> ₂ ''	1	1	-1	-1	-1	1	<i>z</i>	
<i>E</i> ''	2	-1	0	-2	1	0	(<i>R</i> _x , <i>R</i> _y)	(<i>xz</i> , <i>yz</i>)

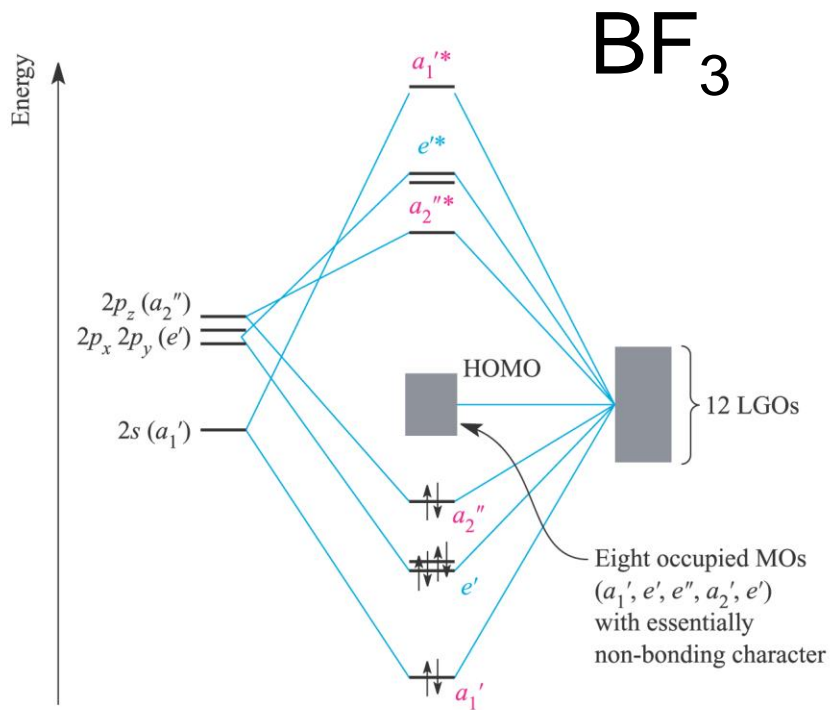
BF₃



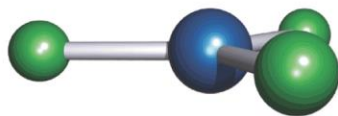
tre $2p_z$

E	C_3	C_2	σ_h	S_3	σ_v
3	0	-1	-3	0	1

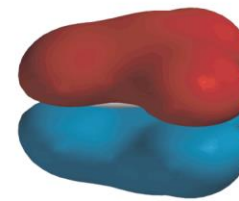
$A_2'' + E''$



B BF₃ F₃ fragment

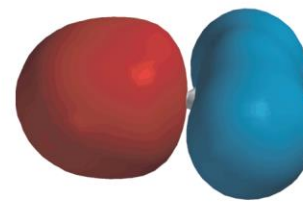


D_{3h}



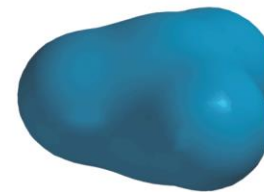
Representation of the a_2'' MO

π



Representation of one of the e' MOs

σ



Representation of the a_1' MO

σ

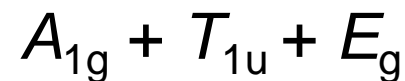
Ordine di legame 4/3

Molecole ipervalenti: SF₆ (gruppo O_h)

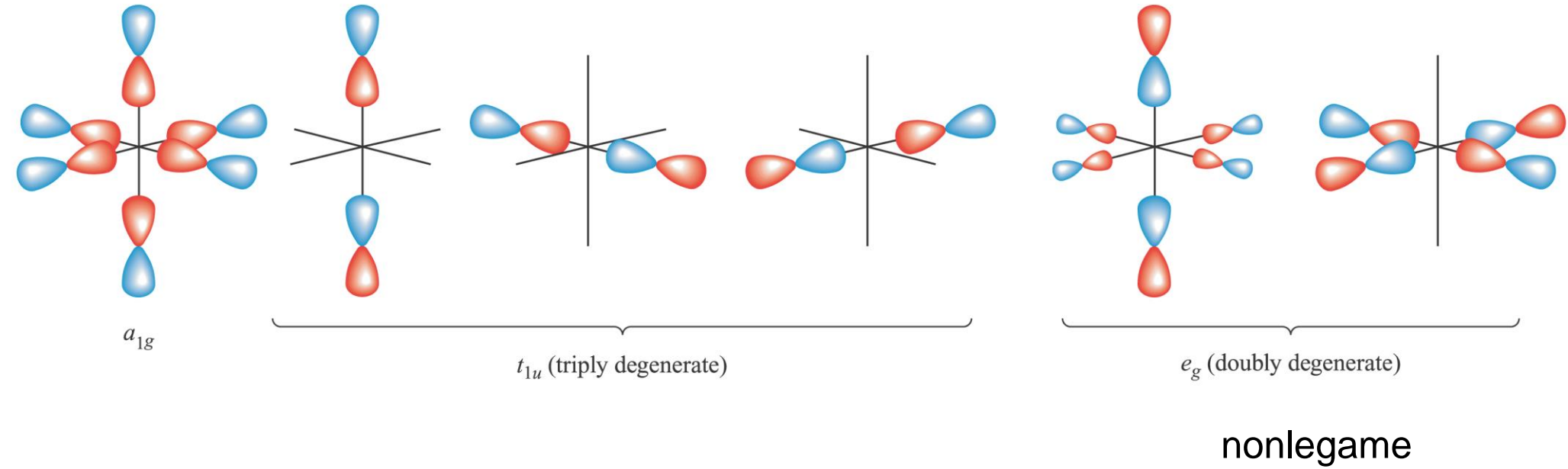
O _h	E	8C ₃	6C ₂	6C ₄	3C ₂ (= C ₄ ²)	i	6S ₄	8S ₆	3σ _h	6σ _d
A _{1g}	1	1	1	1	1	1	1	1	1	1
A _{2g}	1	1	-1	-1	1	1	-1	1	1	-1
E _g	2	-1	0	0	2	2	0	-1	2	0
T _{1g}	3	0	-1	1	-1	3	1	0	-1	-1
T _{2g}	3	0	1	-1	-1	3	-1	0	-1	1
A _{1u}	1	1	1	1	1	-1	-1	-1	-1	-1
A _{2u}	1	1	-1	-1	1	-1	1	-1	-1	1
E _u	2	-1	0	0	2	-2	0	1	-2	0
T _{1u}	3	0	-1	1	-1	-3	-1	0	1	1
T _{2u}	3	0	1	-1	-1	-3	1	0	1	-1

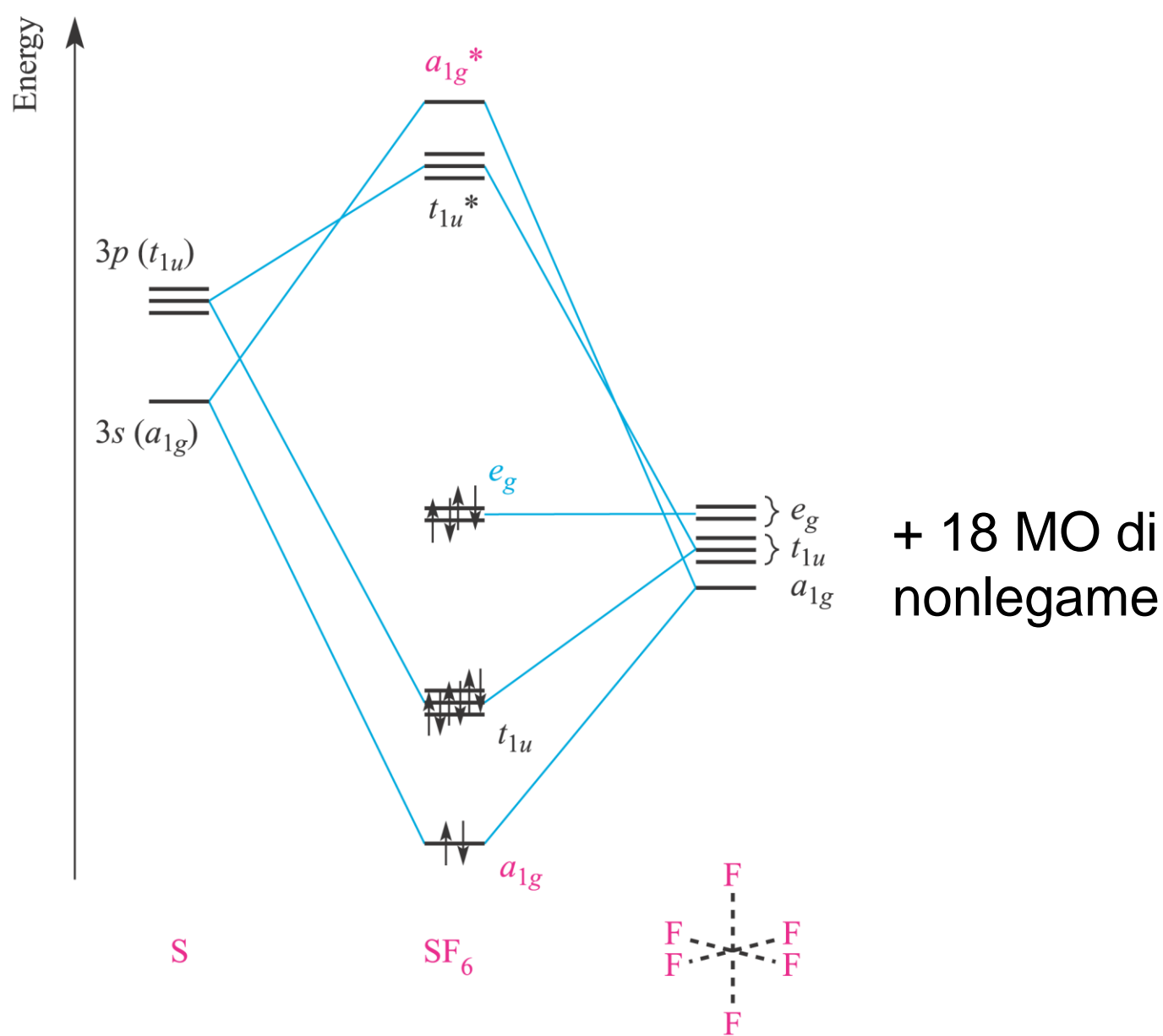
sei 2p_z radiali

E	8C ₃	6C ₂	6C ₄	3C ₂	i	6S ₄	8S ₆	3σ _h	6σ _d
6	0	0	2	2	0	0	0	4	2



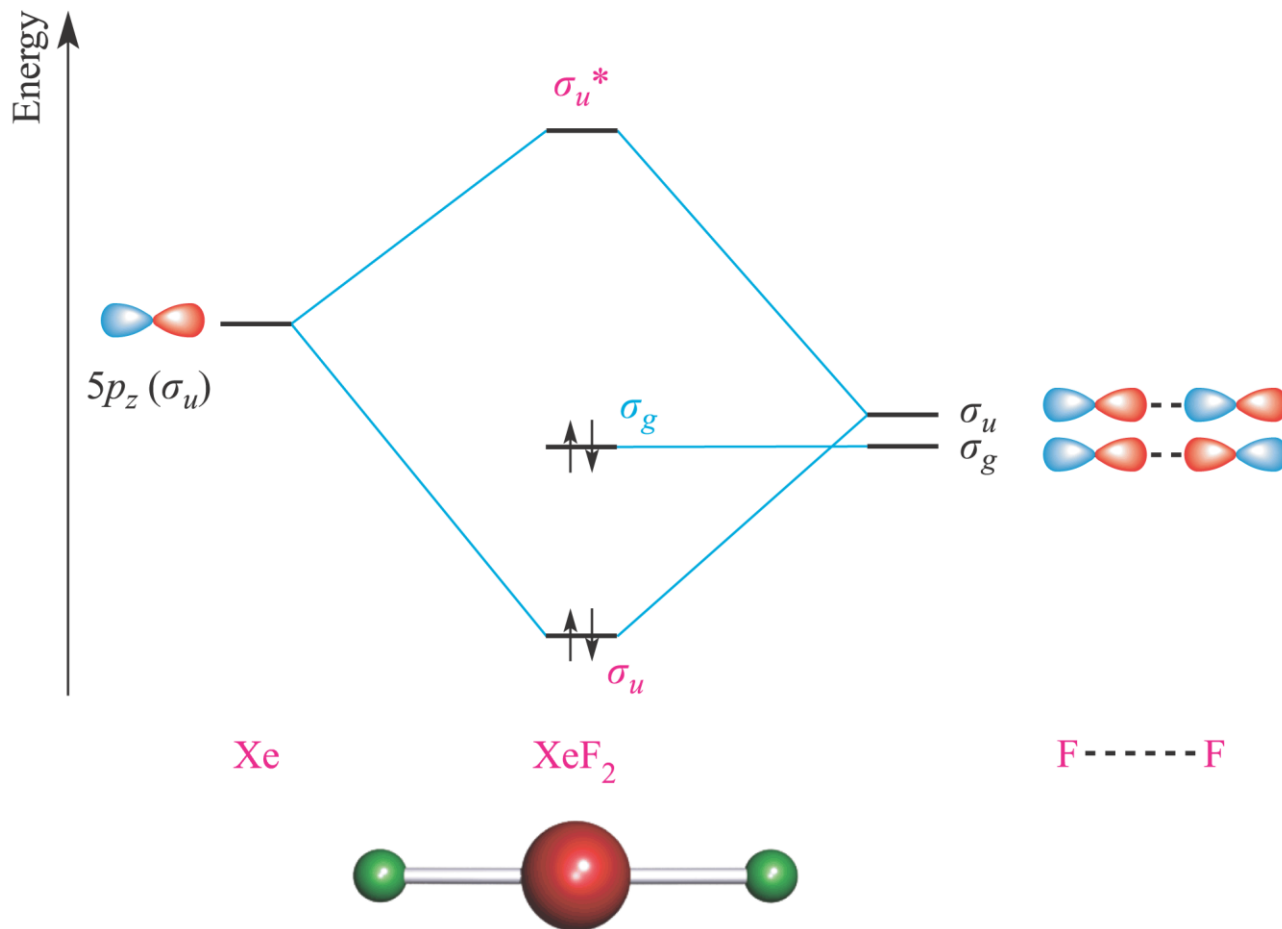
LGO del frammento F_6 in SF_6



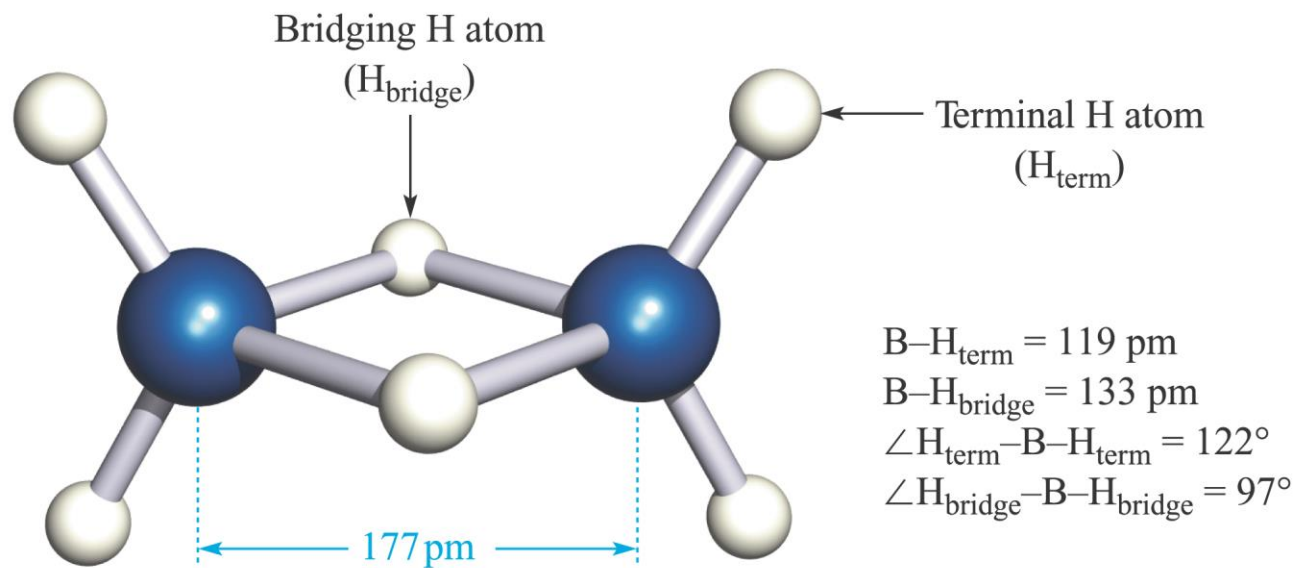


Ordine di legame 2/3,
nessun orbitale d

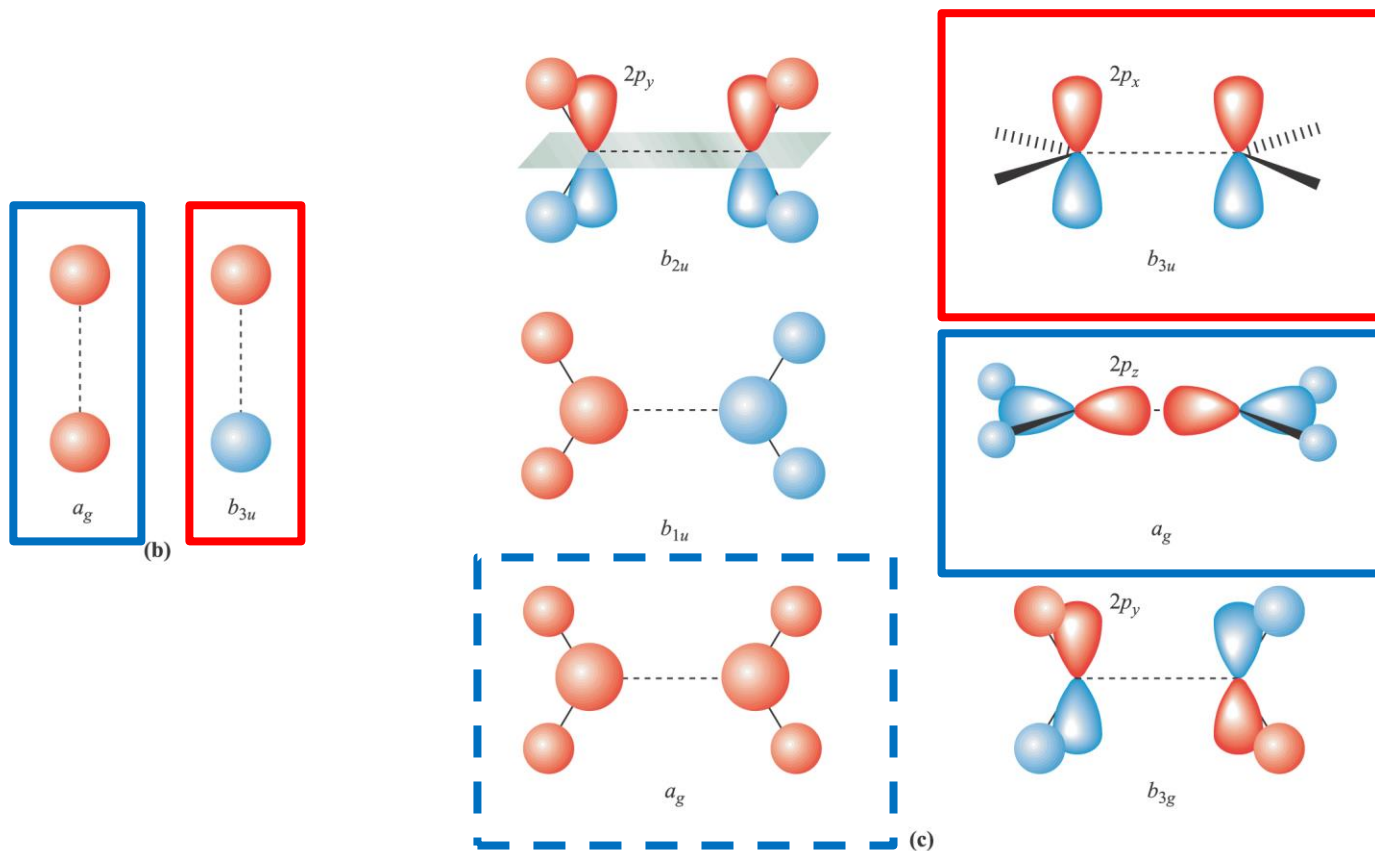
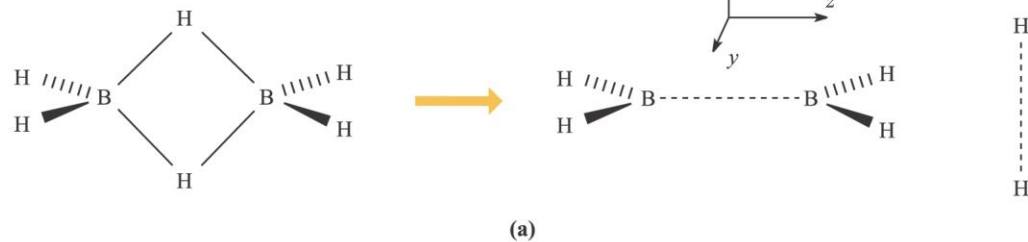
XeF₂: Interazione 3c – 2e



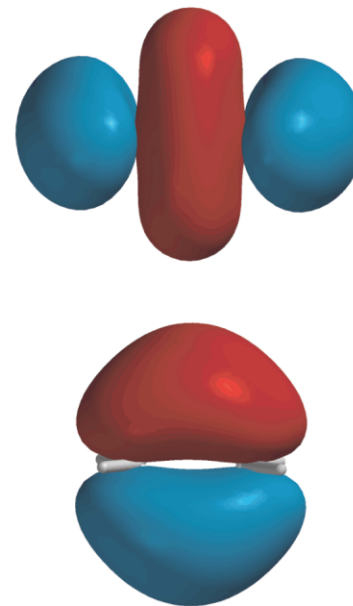
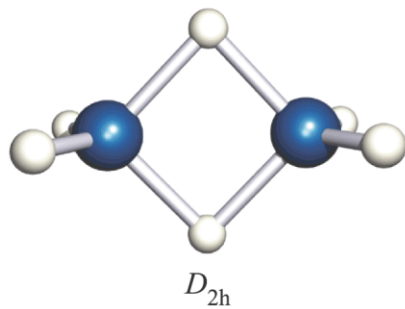
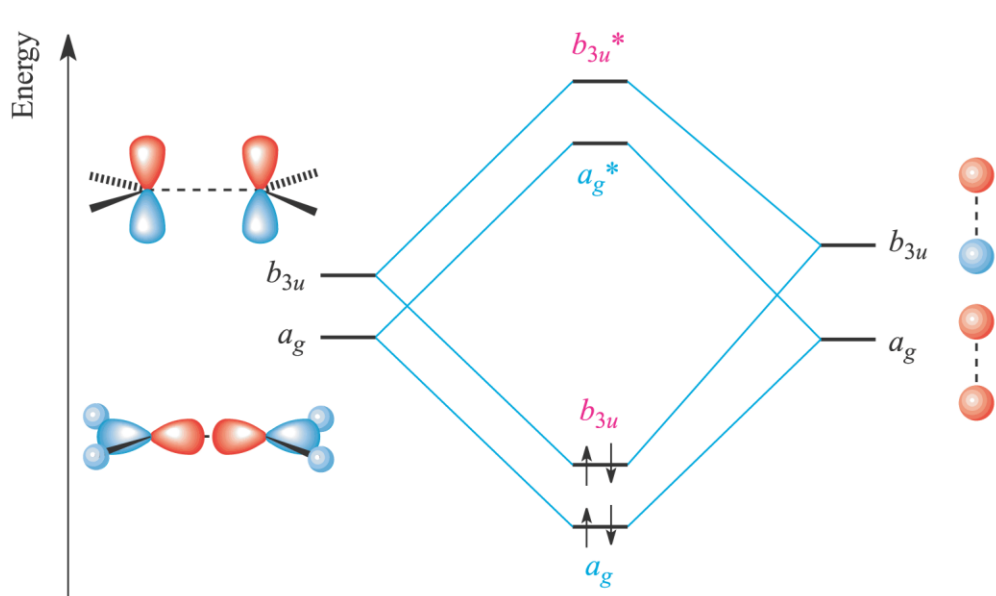
Diborano, B₂H₆



D_{2h}

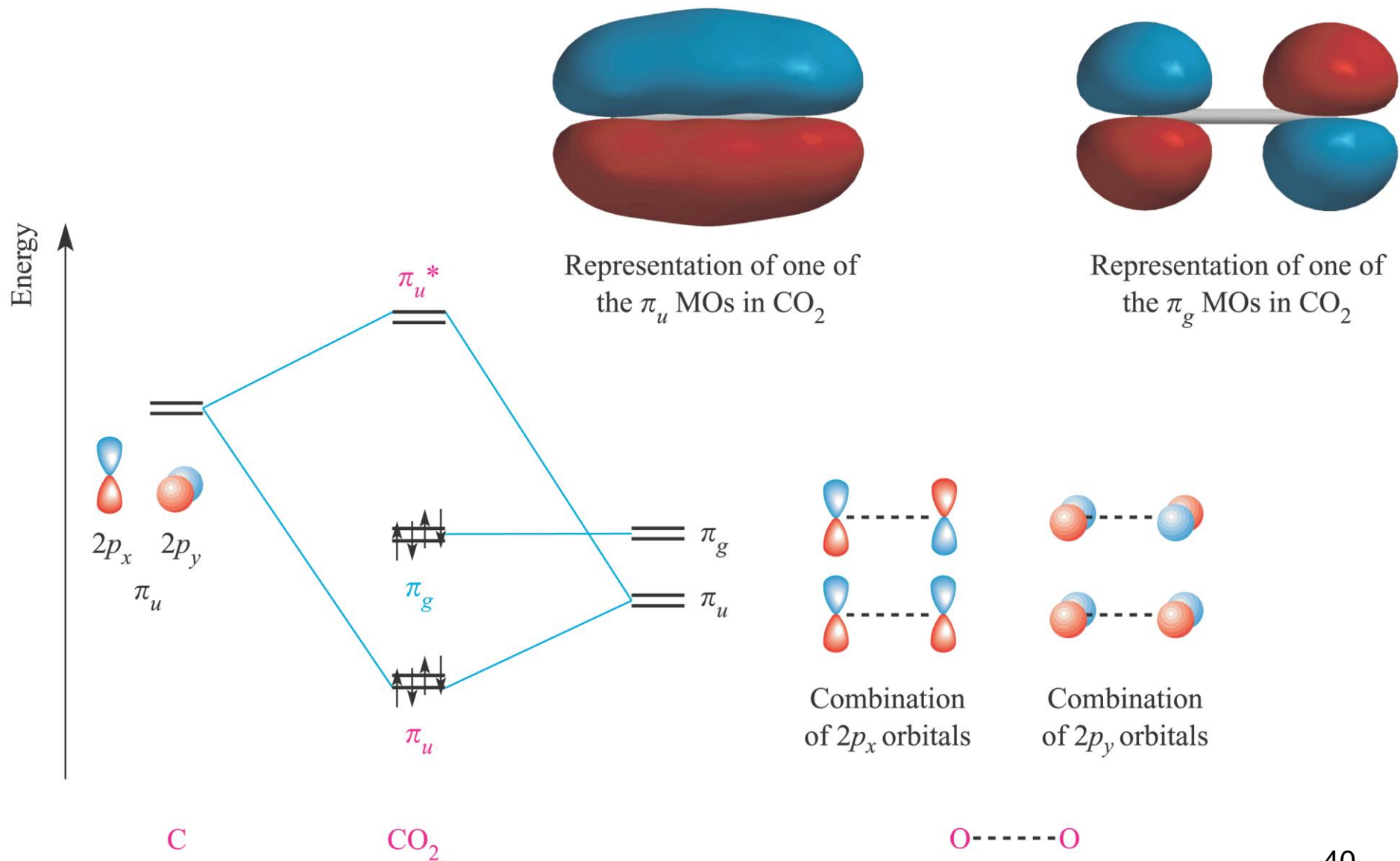


6 LGO (su 12) a energia più bassa del frammento B_2H_4

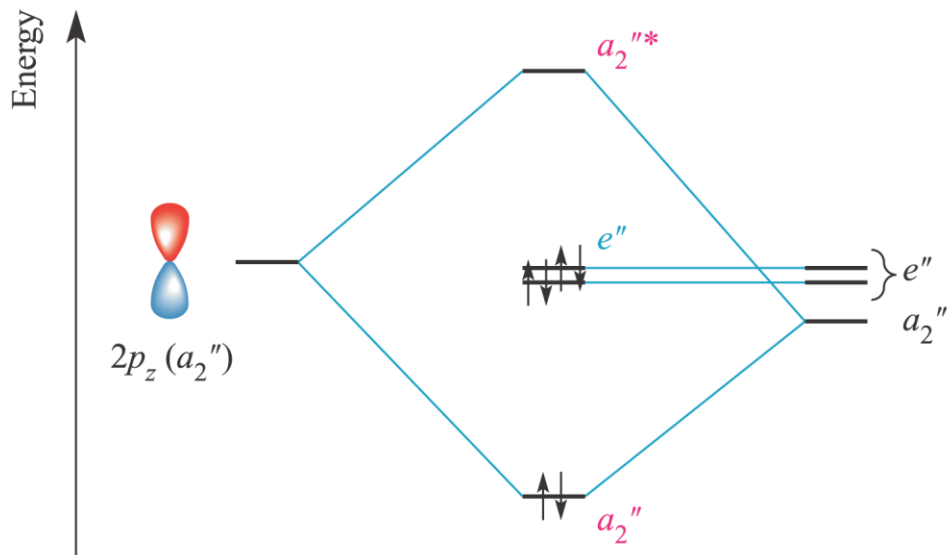


Representation of the a_g (top) and b_{3u} MOs which contain B–H–B bonding character

Diagrammi MO parziali: CO₂

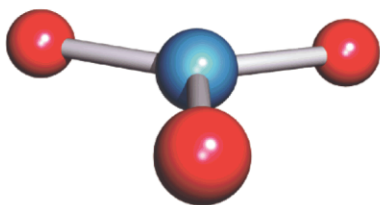


NO₃⁻

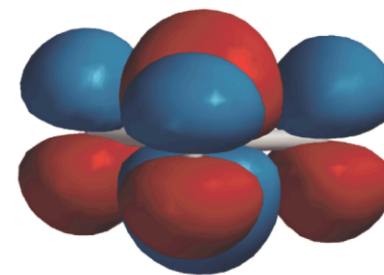
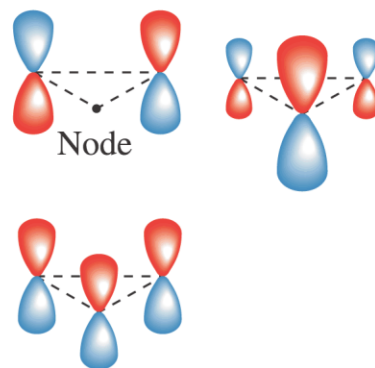


N

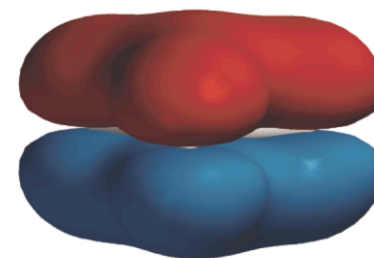
[NO₃]⁻



D_{3h}



A representation of the $a_2''^*$ MO



A representation of the a_2'' MO showing the delocalization of π -character over the N and O centres