

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

Le coppie elettroniche del guscio di valenza intorno all'atomo centrale si dispongono in modo da stare il più lontano possibile le une dalle altre

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

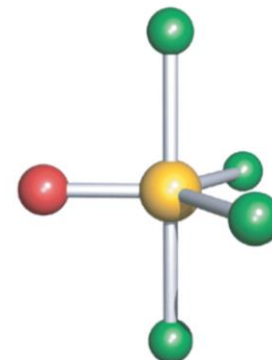
Number of electron regions	Arrangement
2	Linear
3	Trigonal planar
4	Tetrahedral
5	Trigonal bipyramidal
6	Octahedral

Repulsione fra le coppie

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

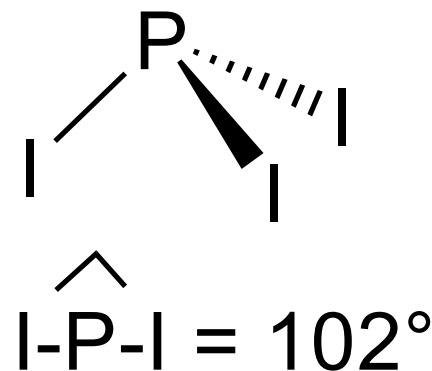
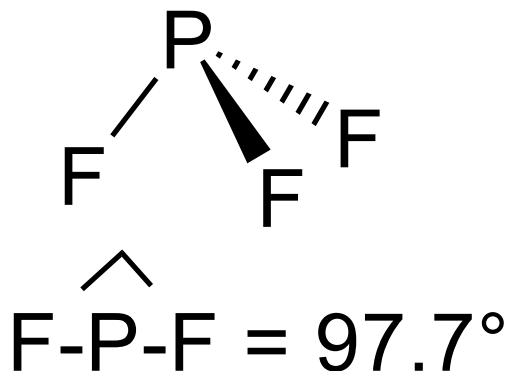
CH_4 (109.5°), NH_3 (107°), H_2O (104.5°)

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

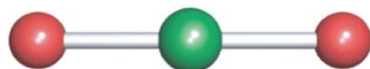


numero sterico = numero di coppie di legame e di non legame intorno all'atomo centrale. Se non ci sono legami E-H:

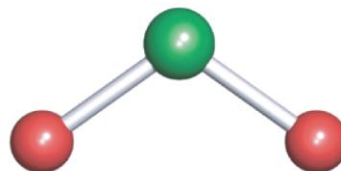
$$\text{n.s.} = \underbrace{\text{elettroni di valenza } (\pm \text{ carica}) / 8}_{\text{Legami}} + \underbrace{\text{resto} / 2}_{\text{Coppie solitarie}}$$

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

2-Coordinate

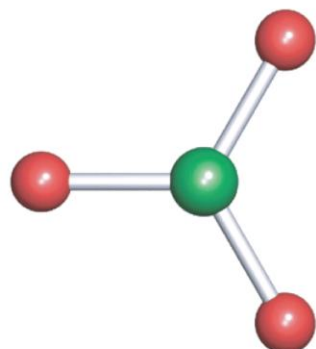


Linear

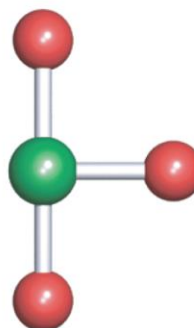


Bent

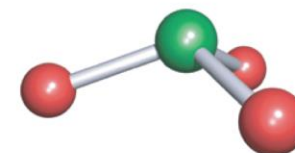
3-Coordinate



Trigonal planar



T-shaped

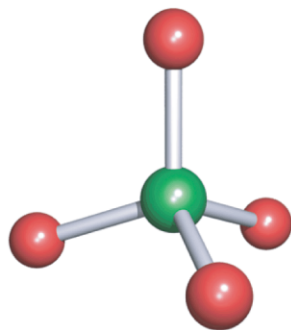


Trigonal pyramidal

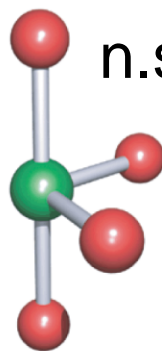


$n.s. = 5$

4-Coordinate

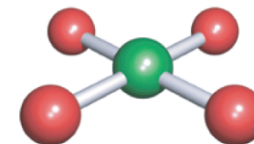


Tetrahedral



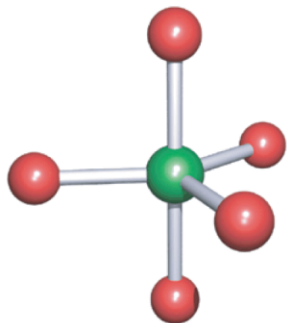
n.s. = 5

Disphenoidal

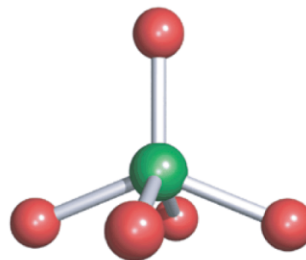


Square planar

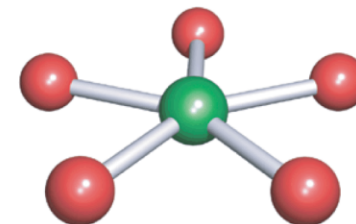
5-Coordinate



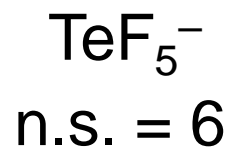
Trigonal bipyramidal



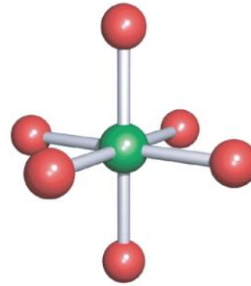
Square-based pyramidal



Pentagonal planar

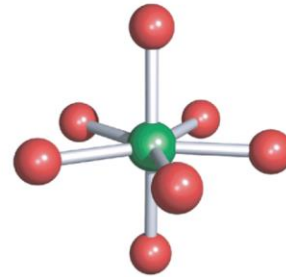


6-Coordinate



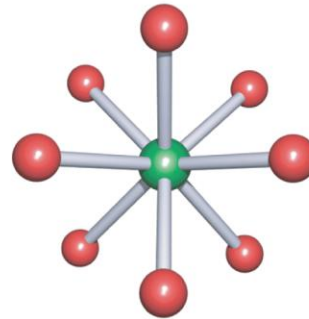
Octahedral

7-Coordinate



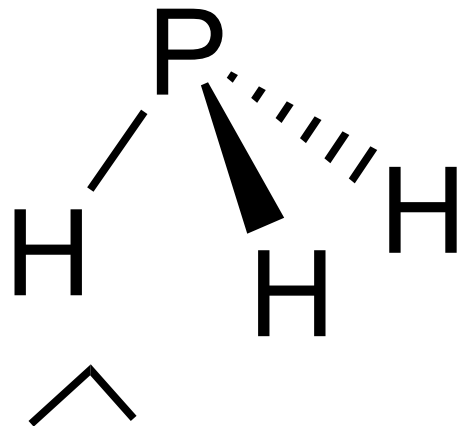
Pentagonal bipyramidal

8-Coordinate



Square antiprismatic

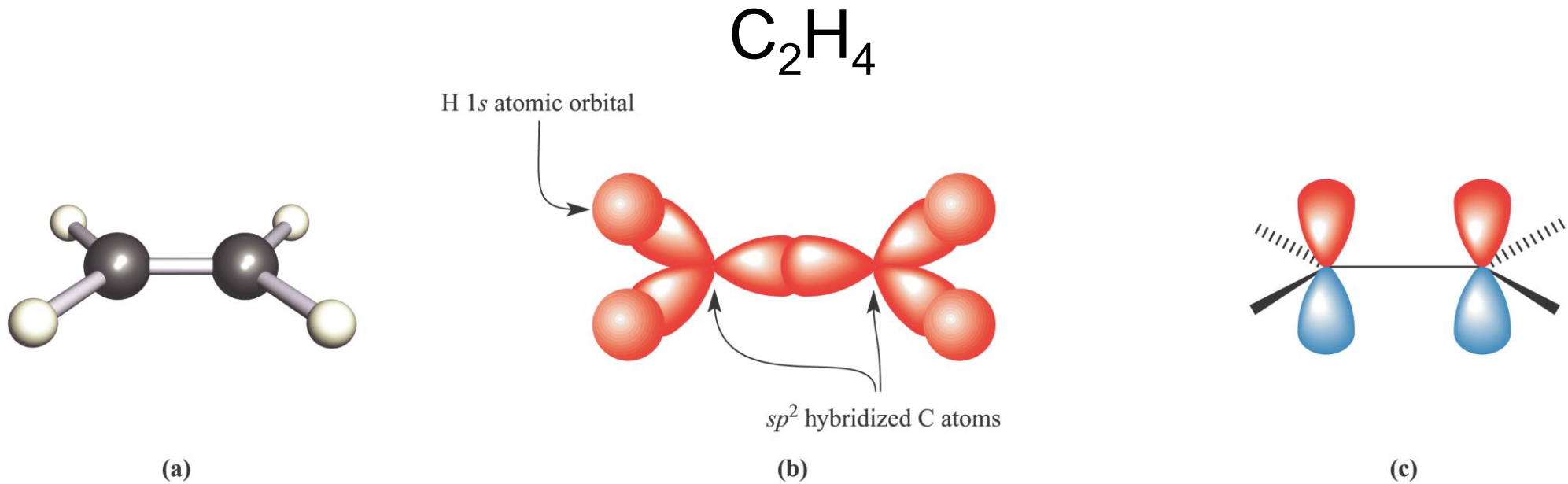
Coppie solitarie stereochimicamente inattive



$\text{H}-\text{P}-\text{H}$ ca. 90°



Molecole poliatomiche secondo la teoria VB

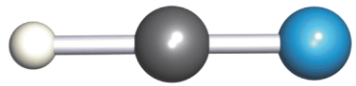


598 kJ mol^{-1} vs $2 \times 346 \text{ kJ mol}^{-1}$

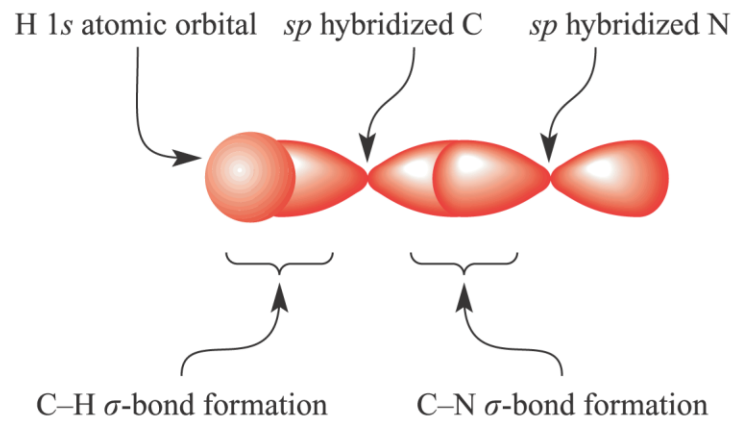
$\sigma + \pi$

2σ

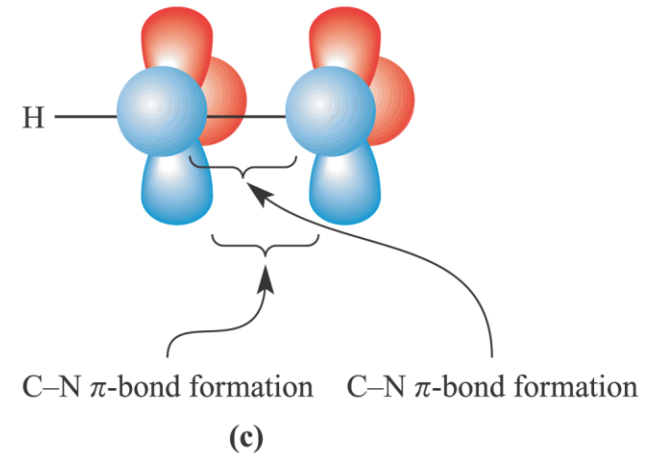
HCN



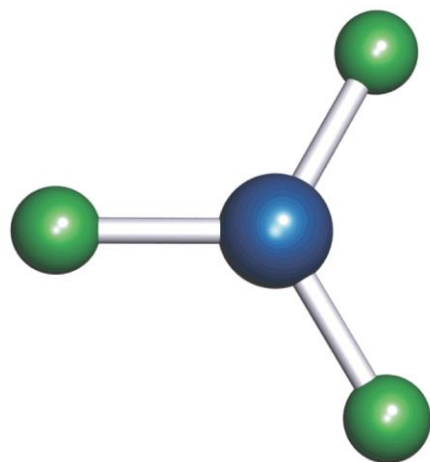
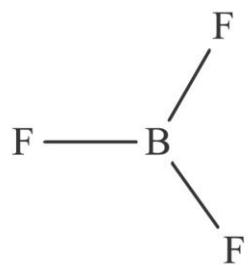
(a)



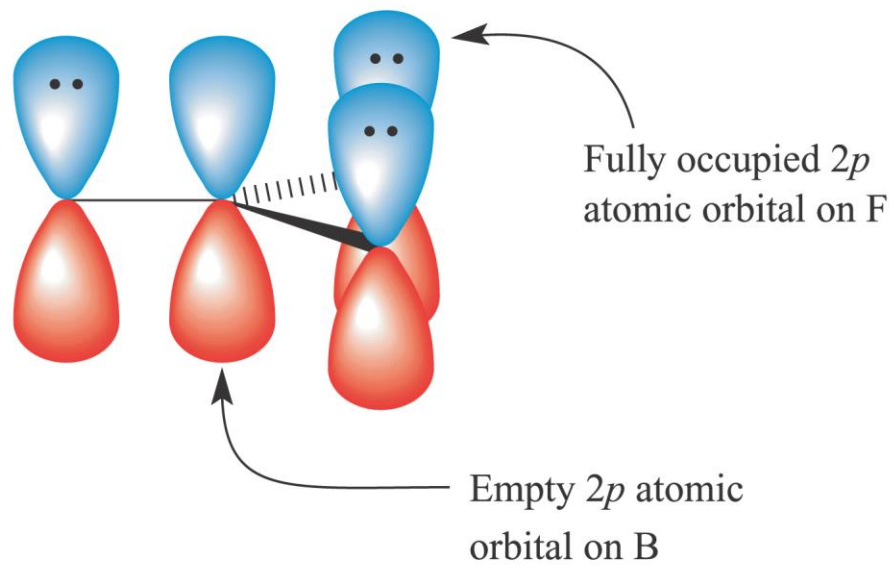
(b)



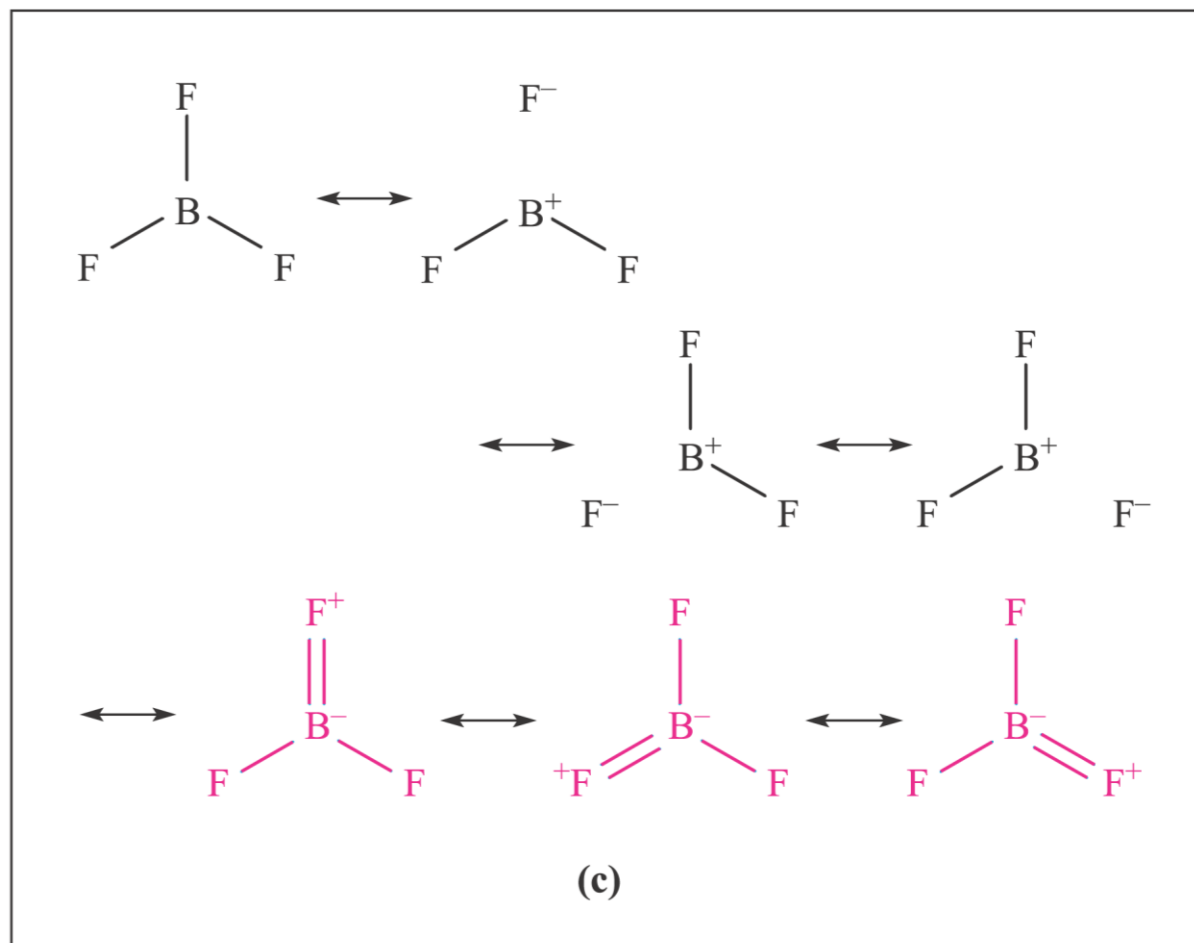
(c)



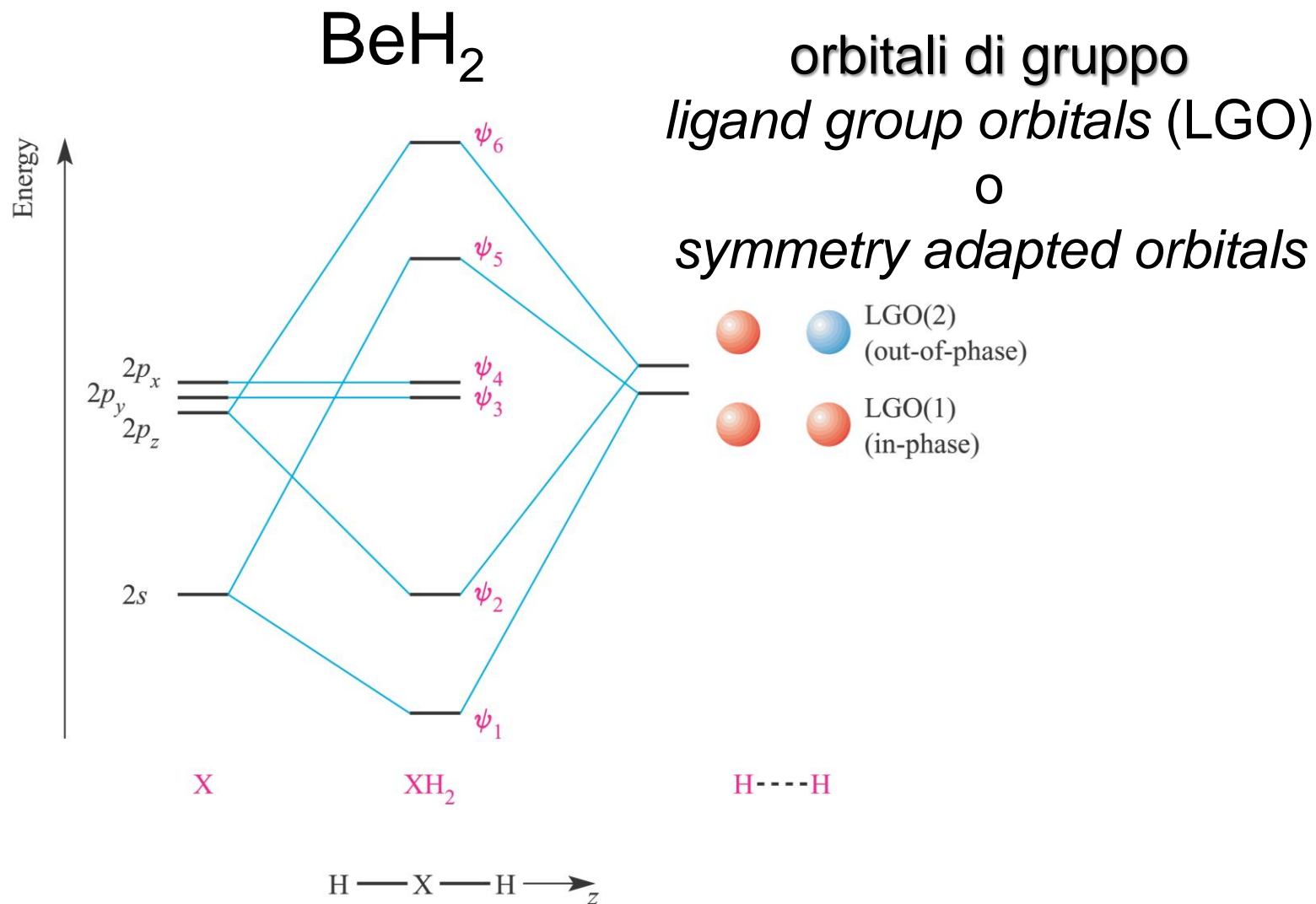
(a)



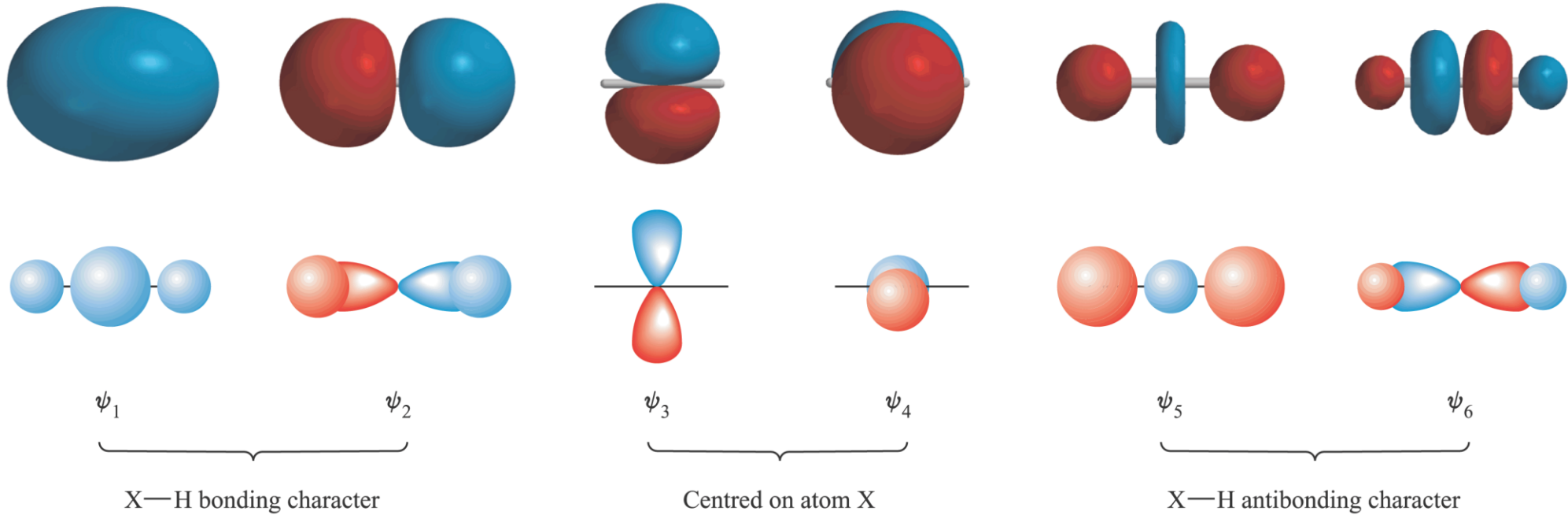
(b)

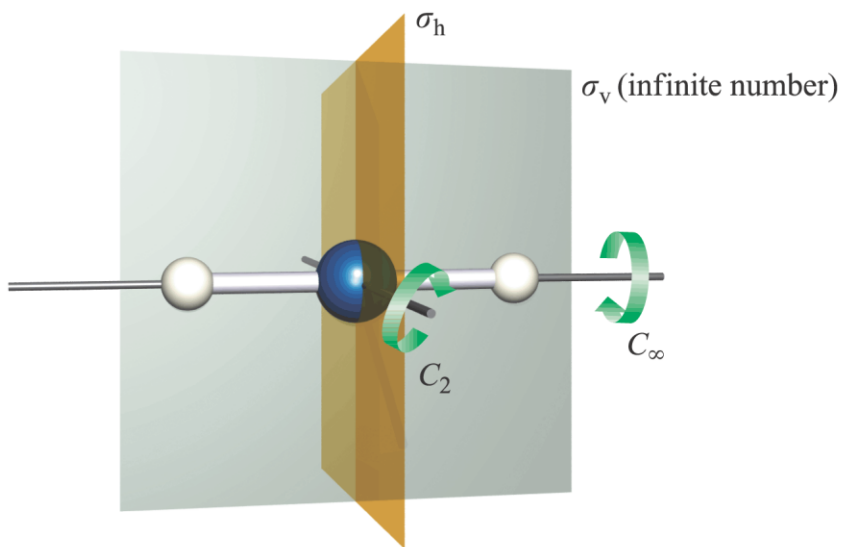


Molecole poliatomiche secondo la teoria MO



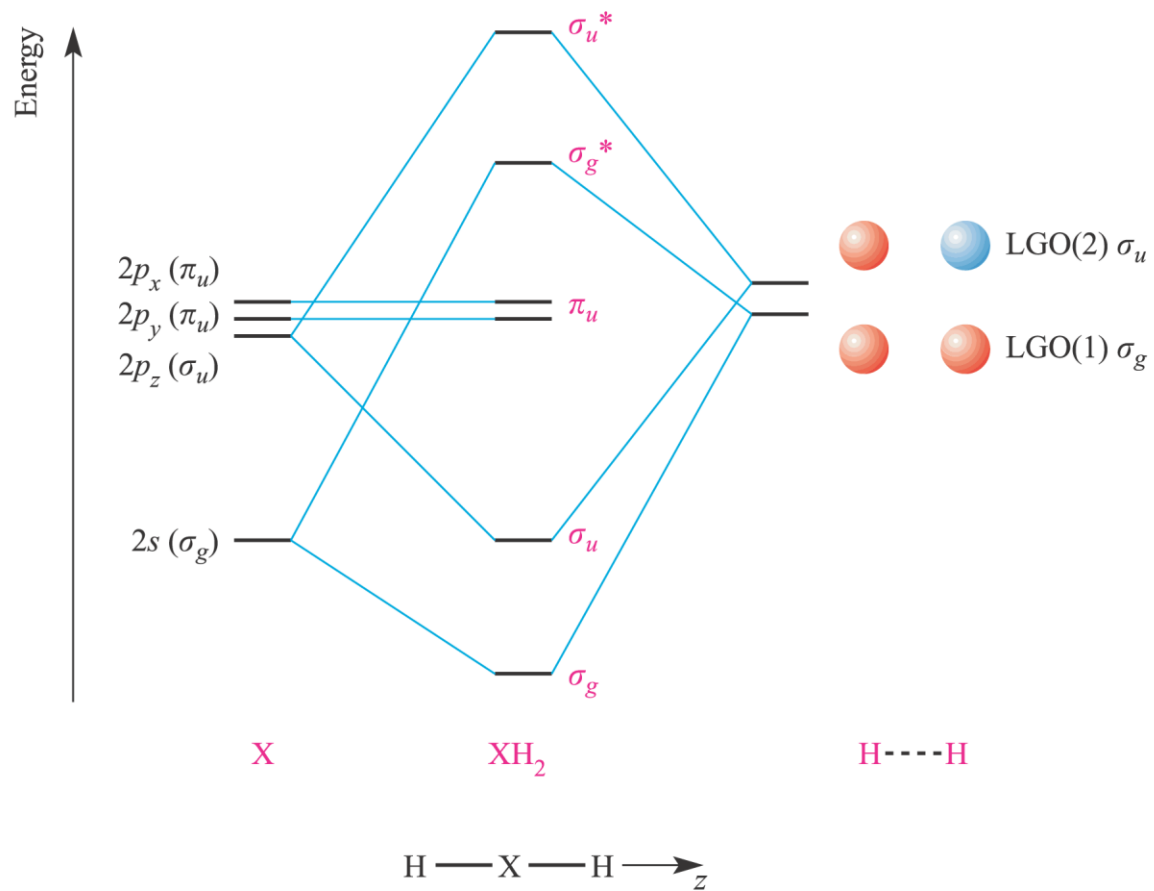
Molecole poliatomiche secondo la teoria MO



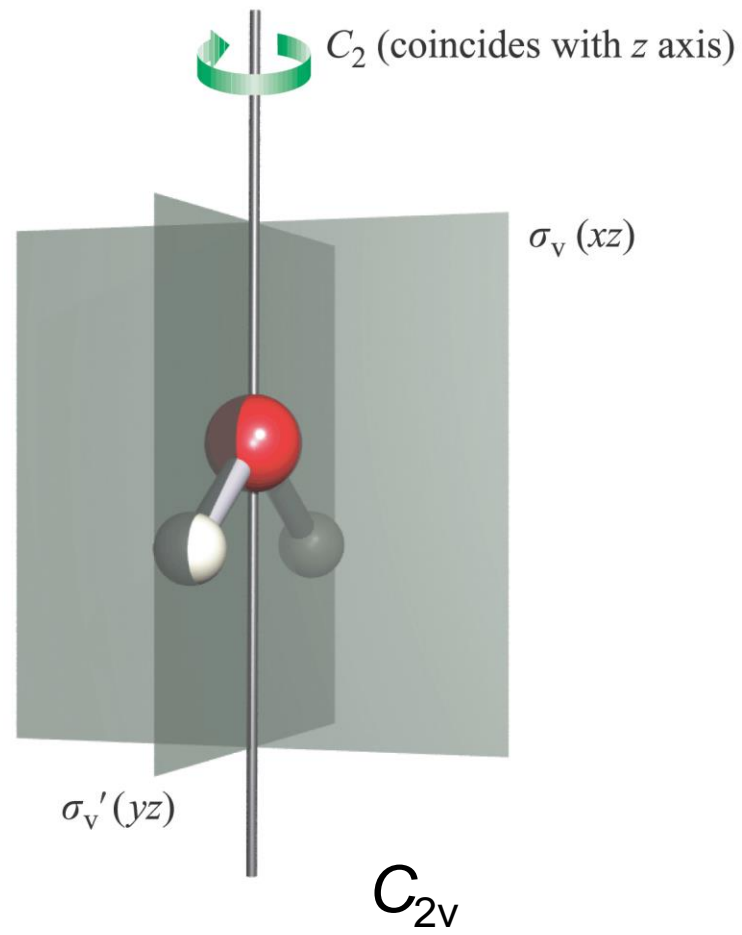


$D_{\infty h}$

(a)



(b)

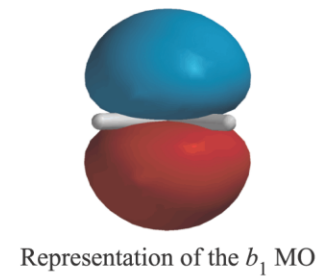
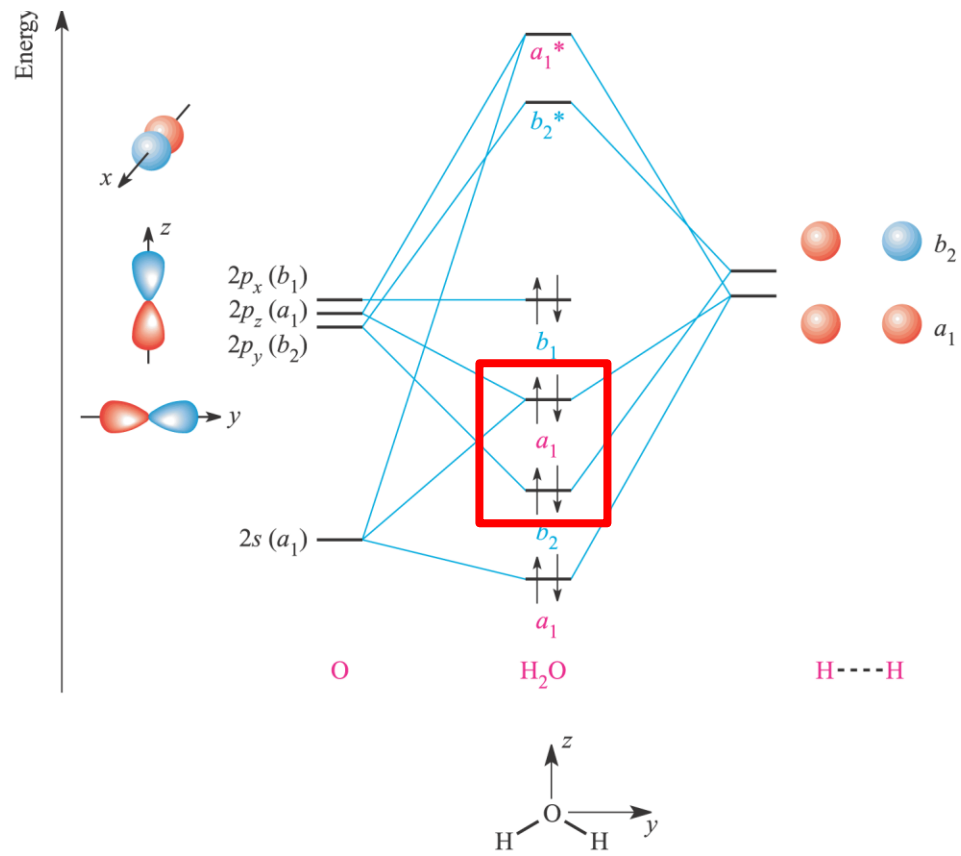


C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	1	y, R_x	yz

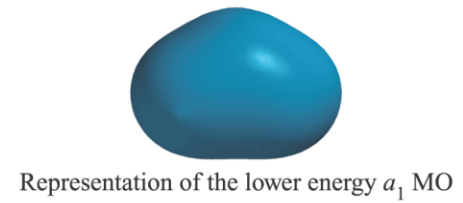
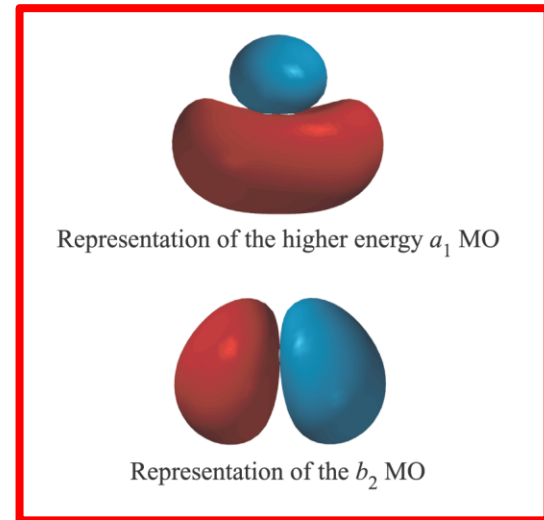
2H

2	0	0	2
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$A_1 + B_2$

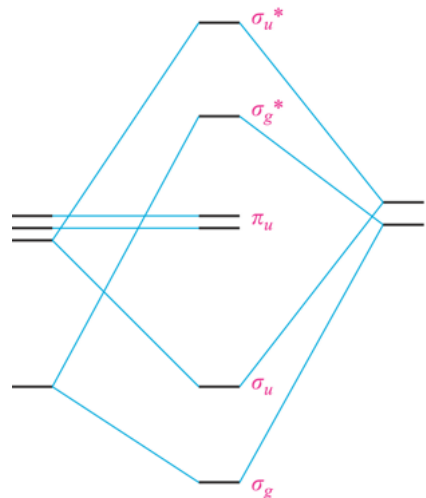


n.l.

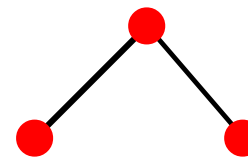
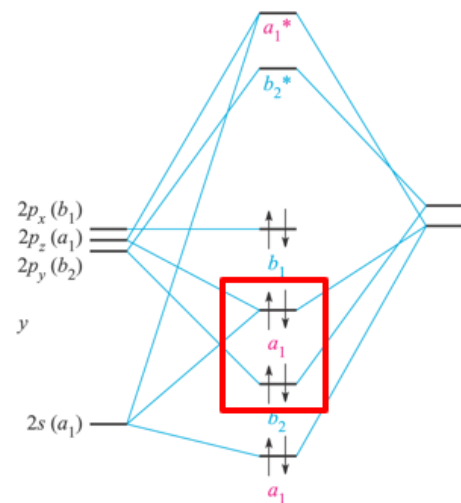
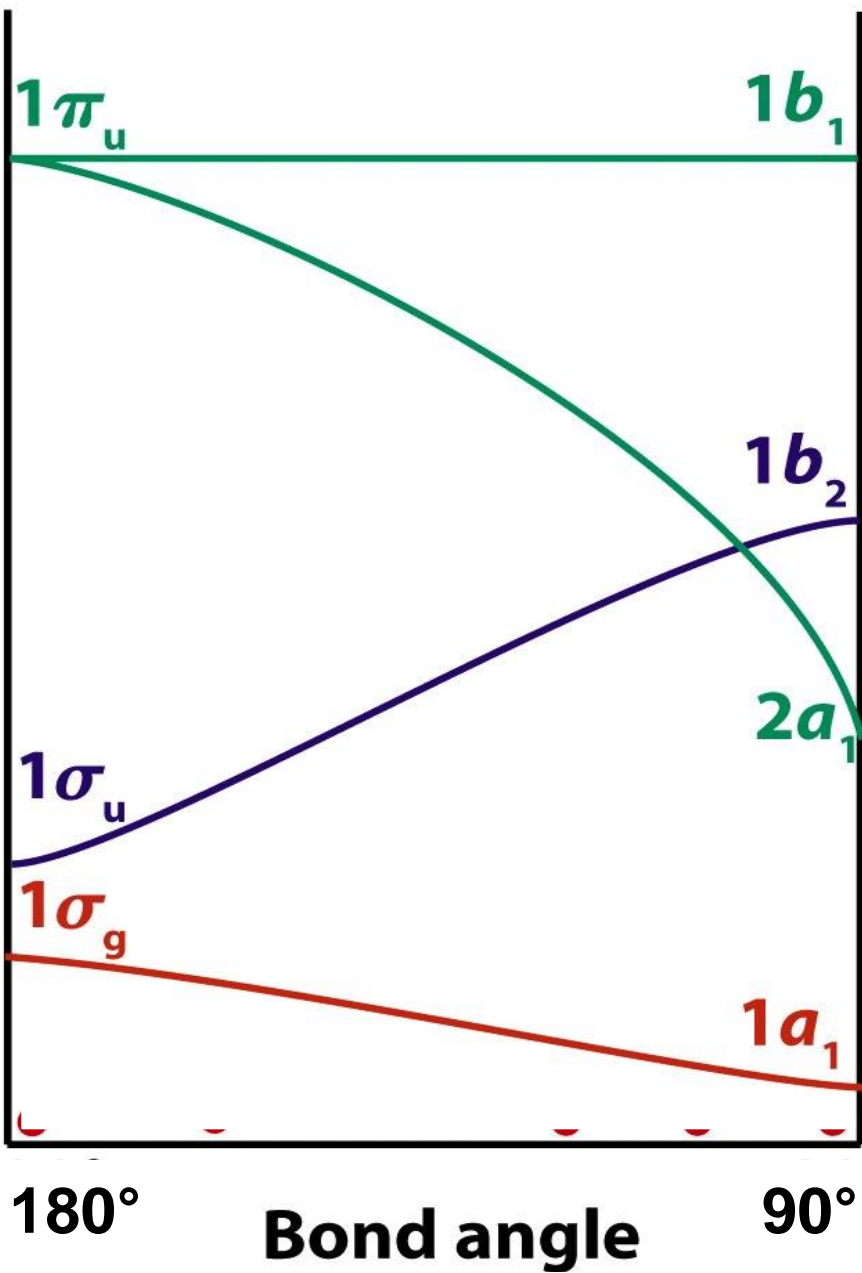


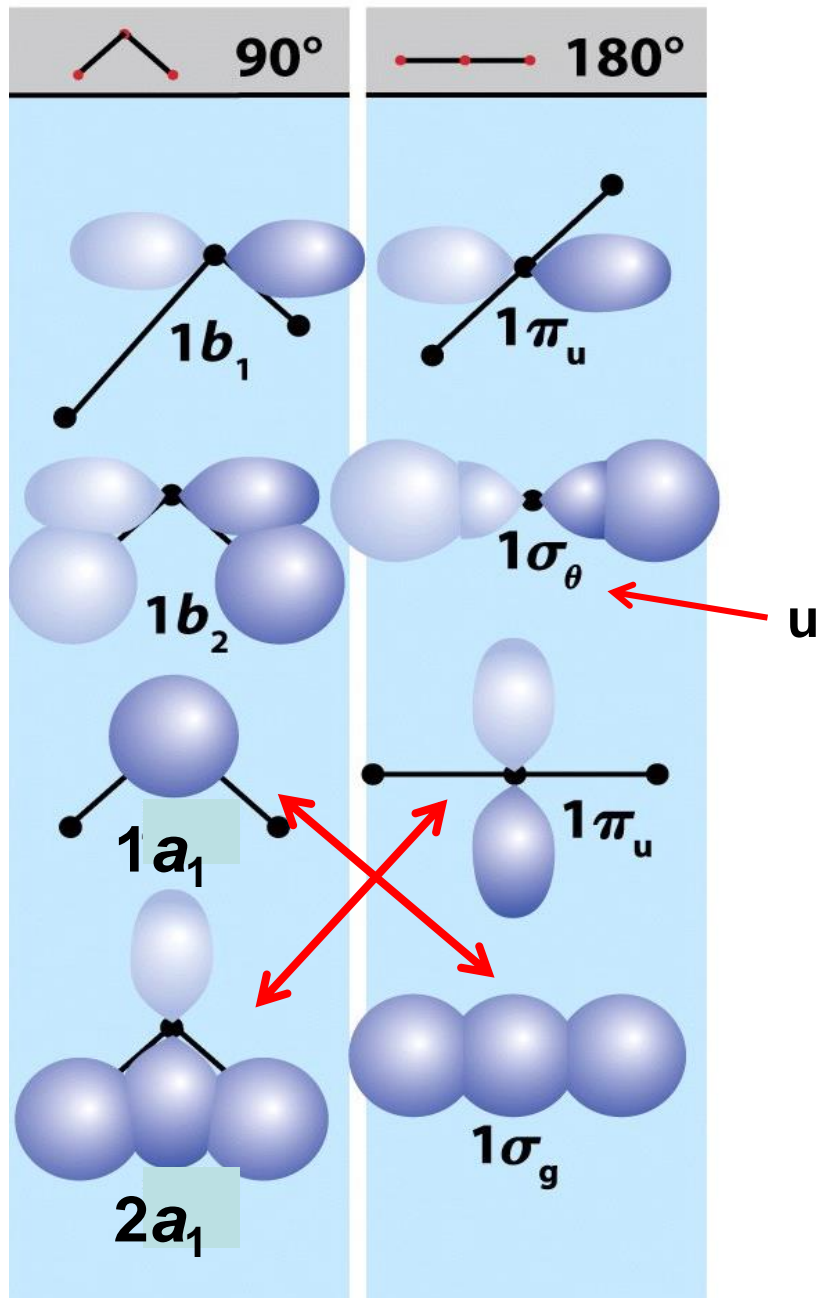
n.l.

Diagramma di Walsh

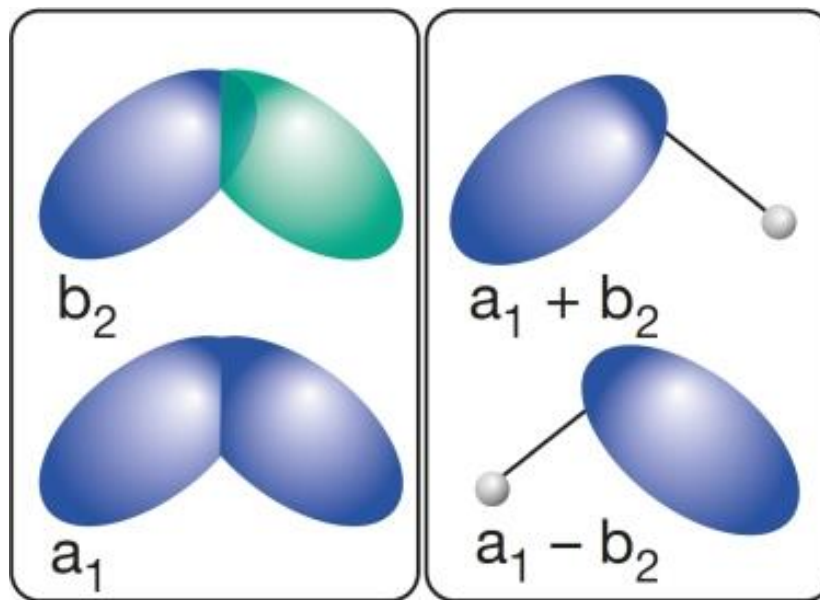


Energy ↑



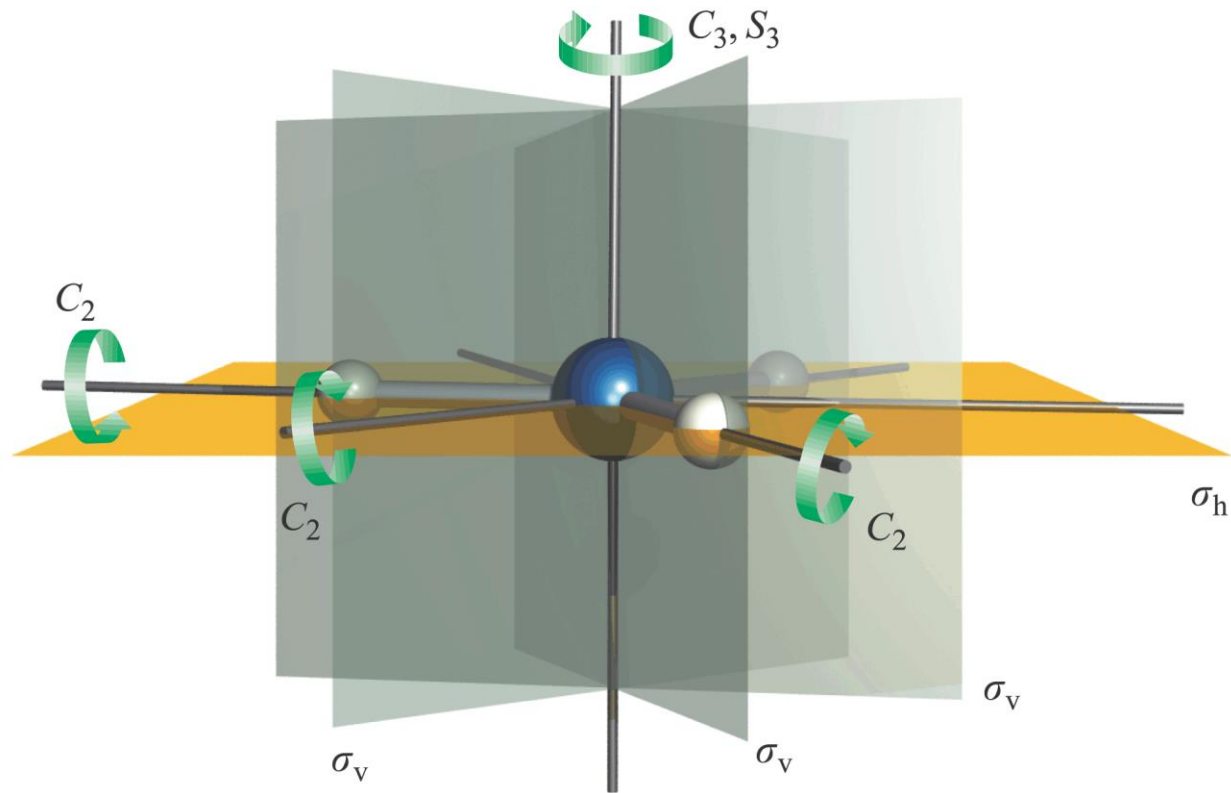


Combinazioni lineari di orbitali molecolari



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}

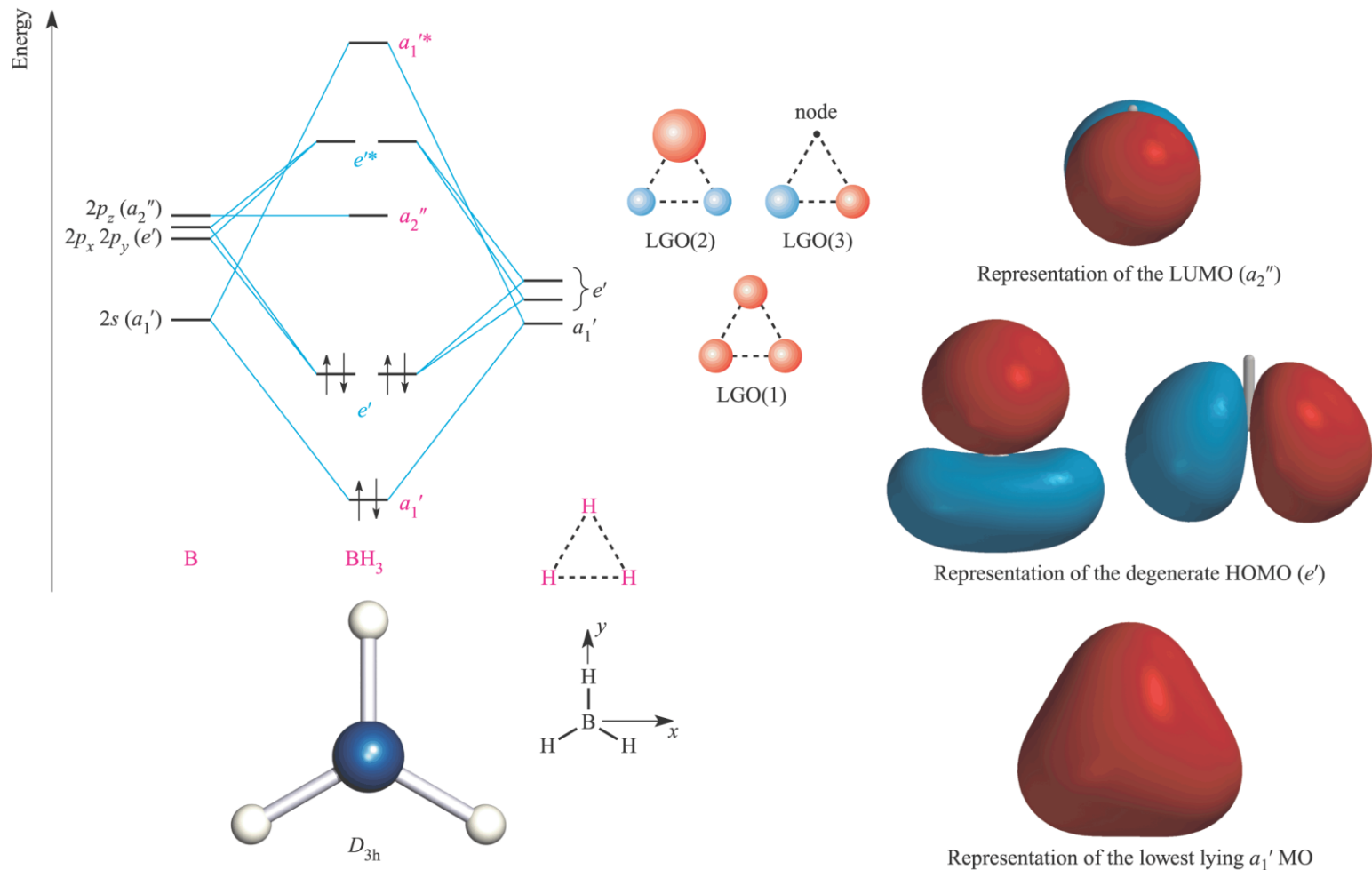


D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
A_1'	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2'	1	1	-1	1	1	-1	R_z	
E'	2	-1	0	2	-1	0	(x, y)	$(x^2 - y^2, xy)$
A_1''	1	1	1	-1	-1	-1		
A_2''	1	1	-1	-1	-1	1	z	
E''	2	-1	0	-2	1	0	(R_x, R_y)	(xz, yz)

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)

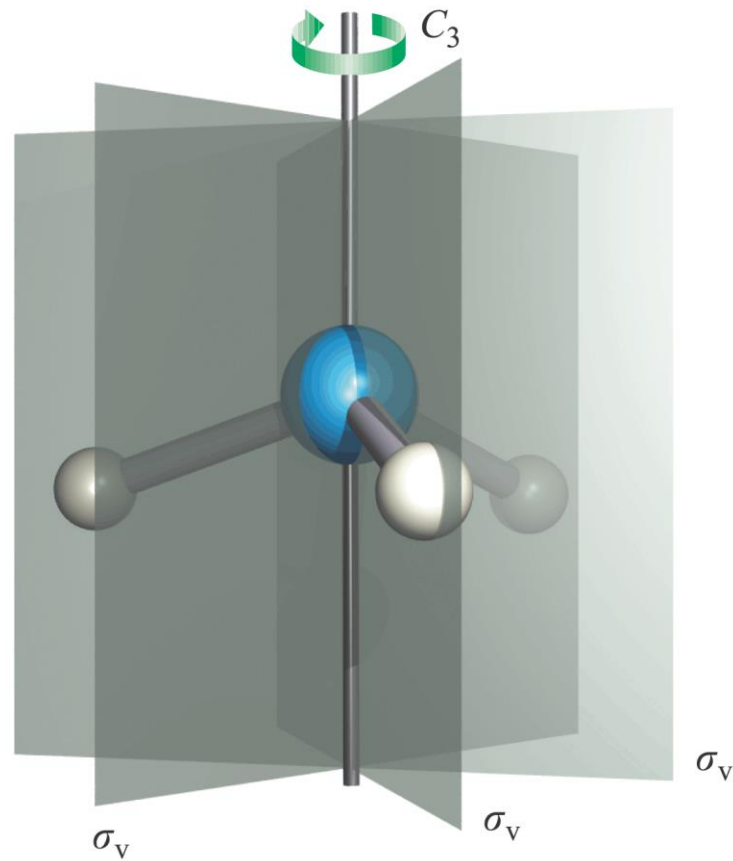
$$\Psi(e')_1 = 1/\sqrt{6} \times (2\Psi_1 - \Psi_2 - \Psi_3)$$

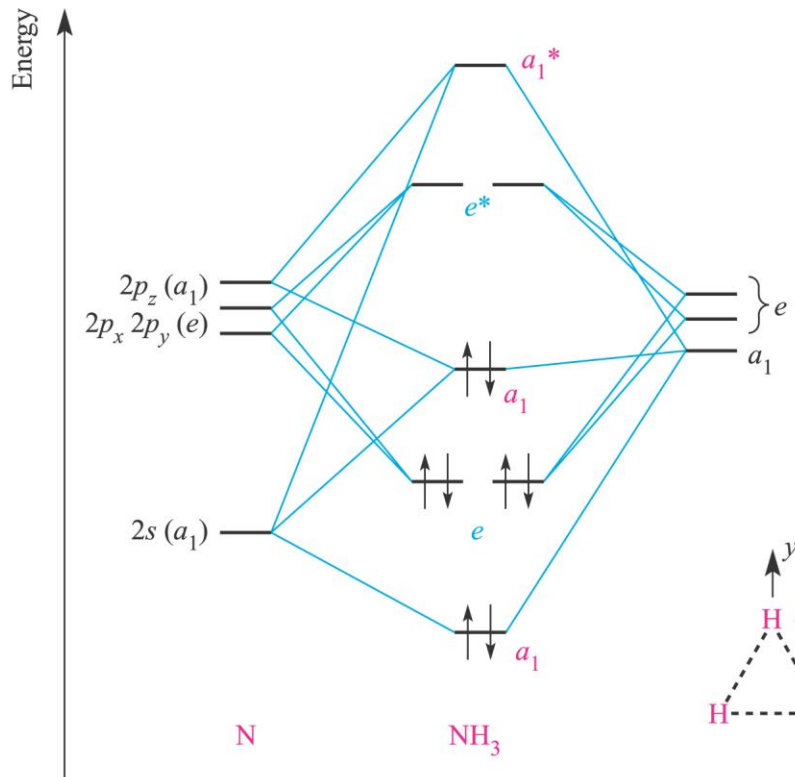
(LGO2)

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

(LGO3)

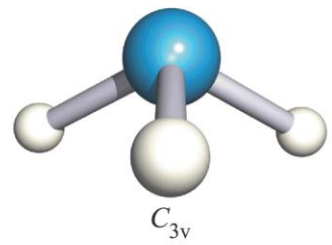
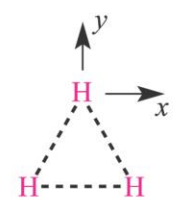
NH₃, gruppo puntuale C_{3v}



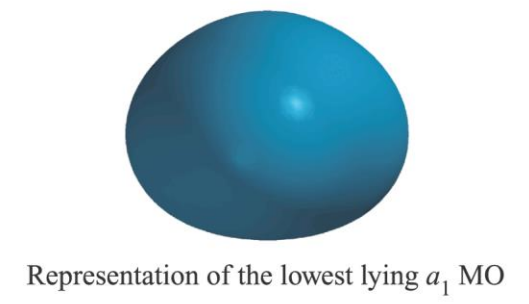
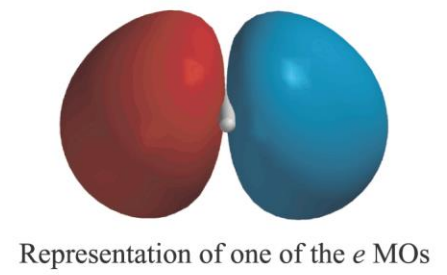
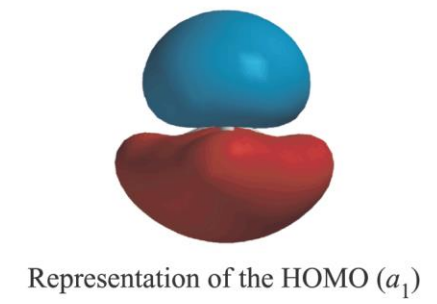
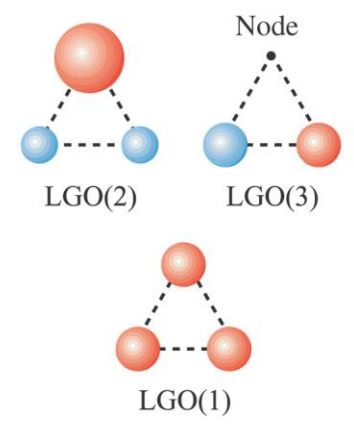


N

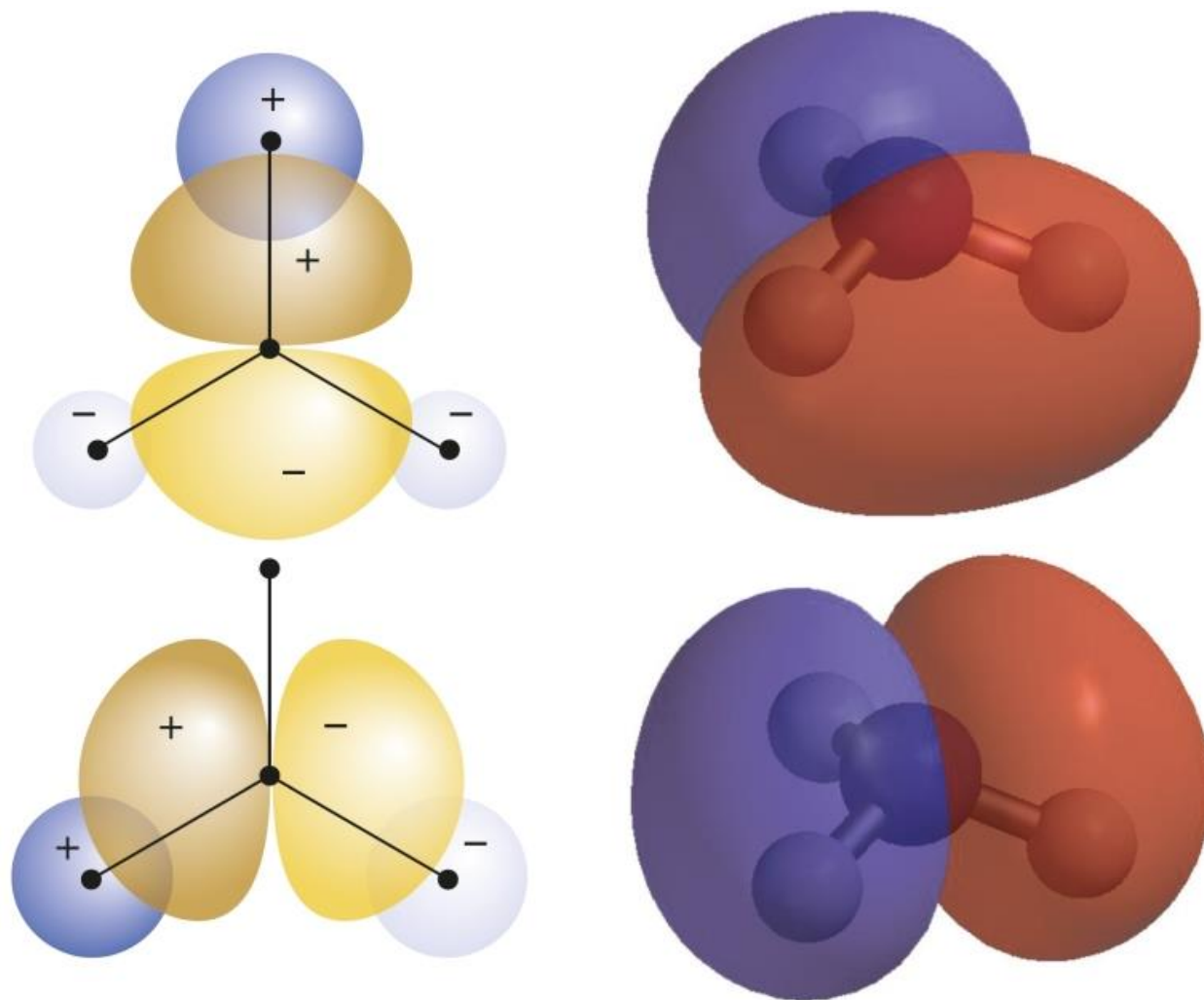
NH_3



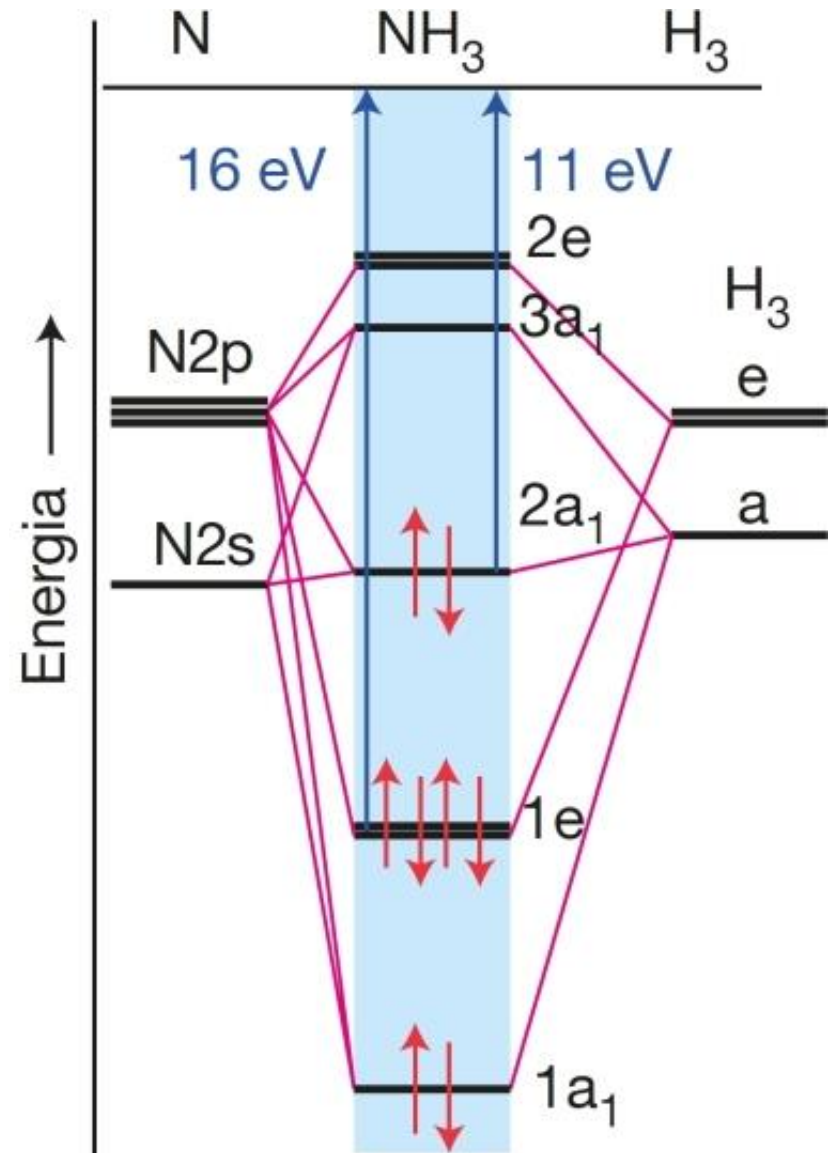
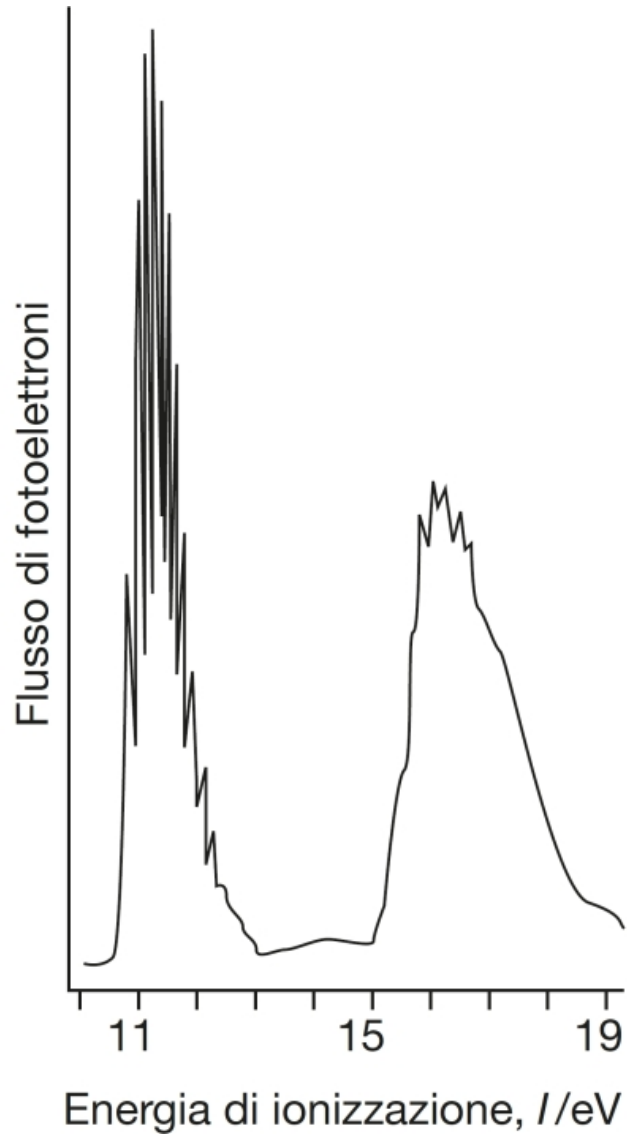
C_{3v}

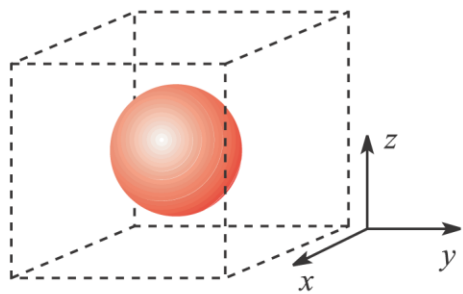


Formazione degli orbitali molecolari leganti e

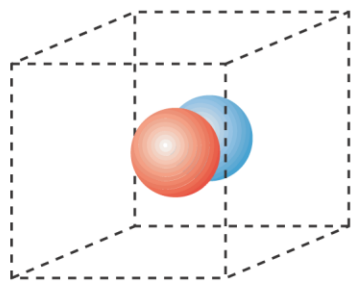


Spettro di fotoelettroni di NH_3

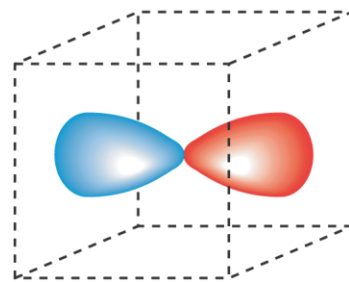




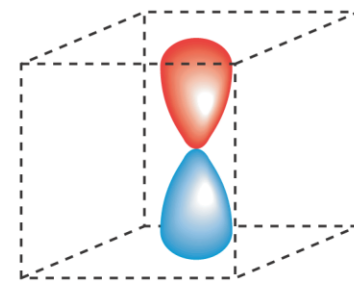
$2s (a_1)$



$2p_x (t_2)$

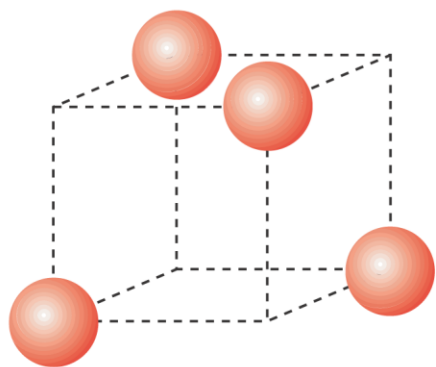


$2p_y (t_2)$

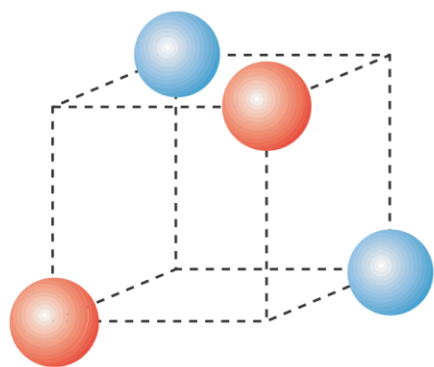


$2p_z (t_2)$

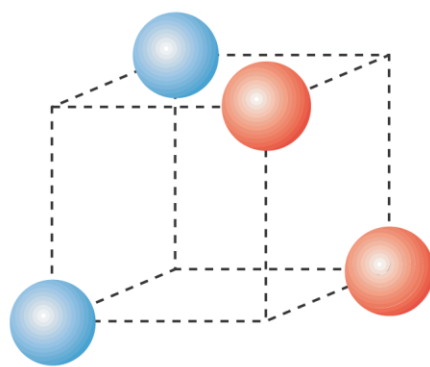
(a)



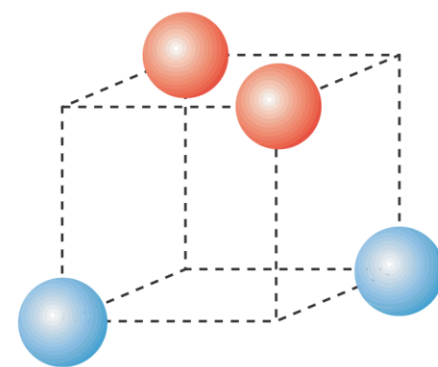
$LGO(1) (a_1)$



$LGO(2) (t_2)$

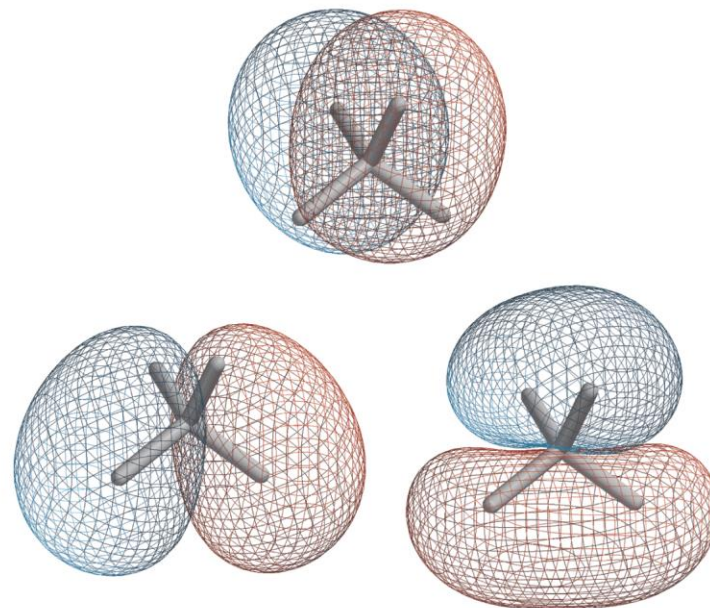
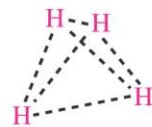
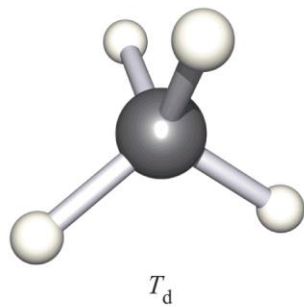
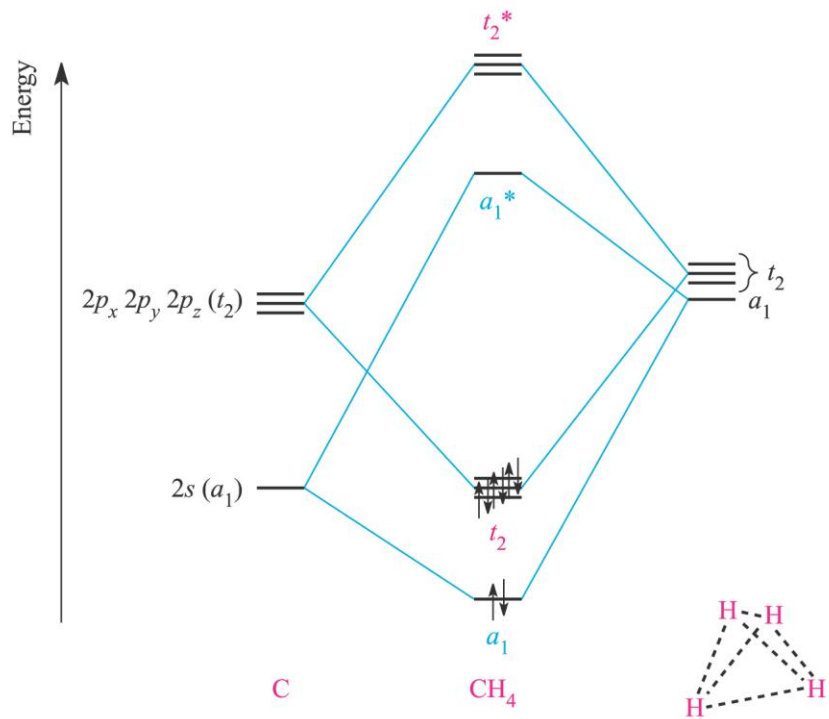


$LGO(3) (t_2)$

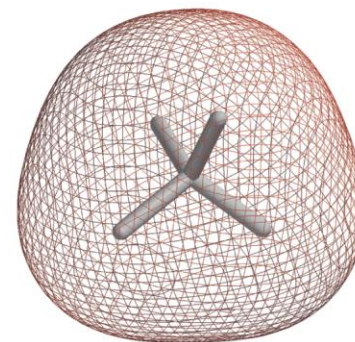


$LGO(4) (t_2)$

(b)



Representations of the triply degenerate (t_2) bonding MOs

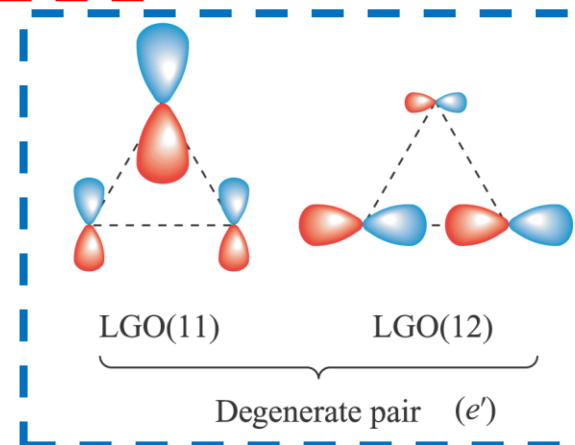
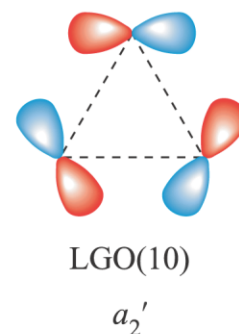
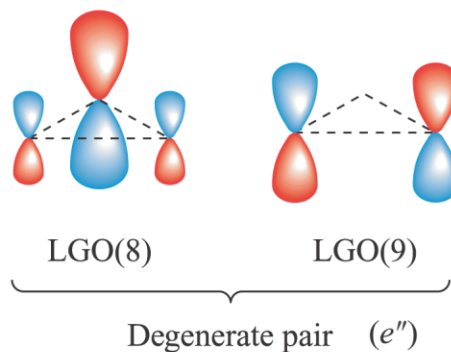
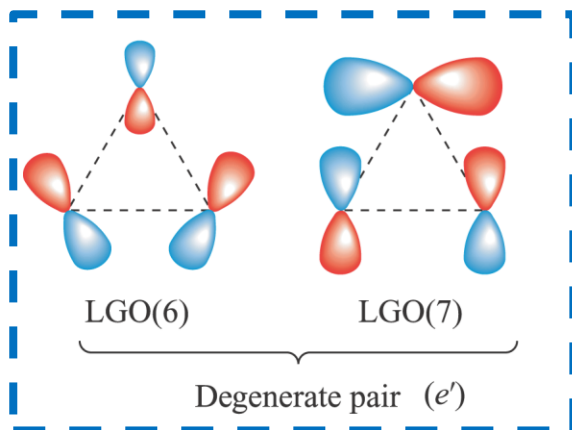
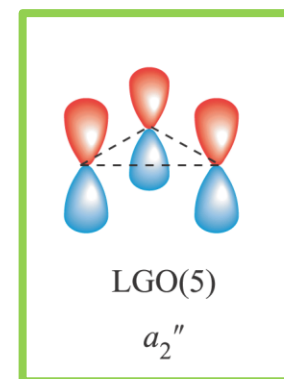
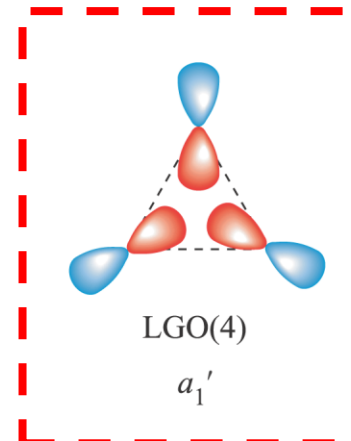
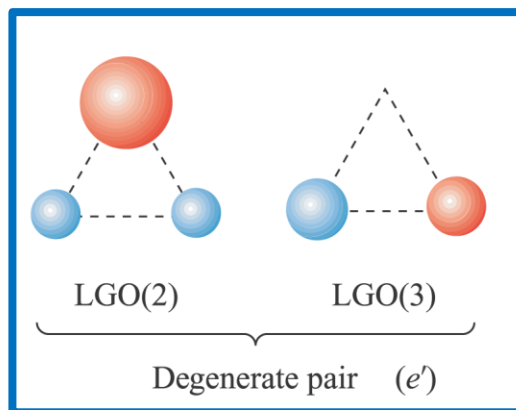
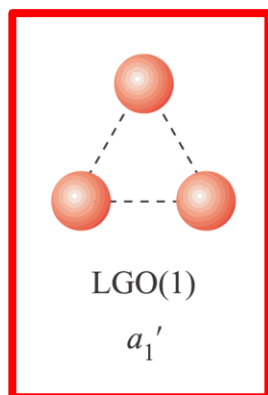
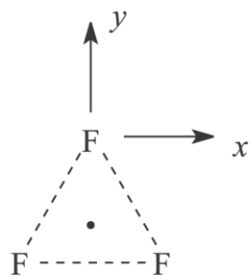


Representation of the a_1 bonding MO



<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>)

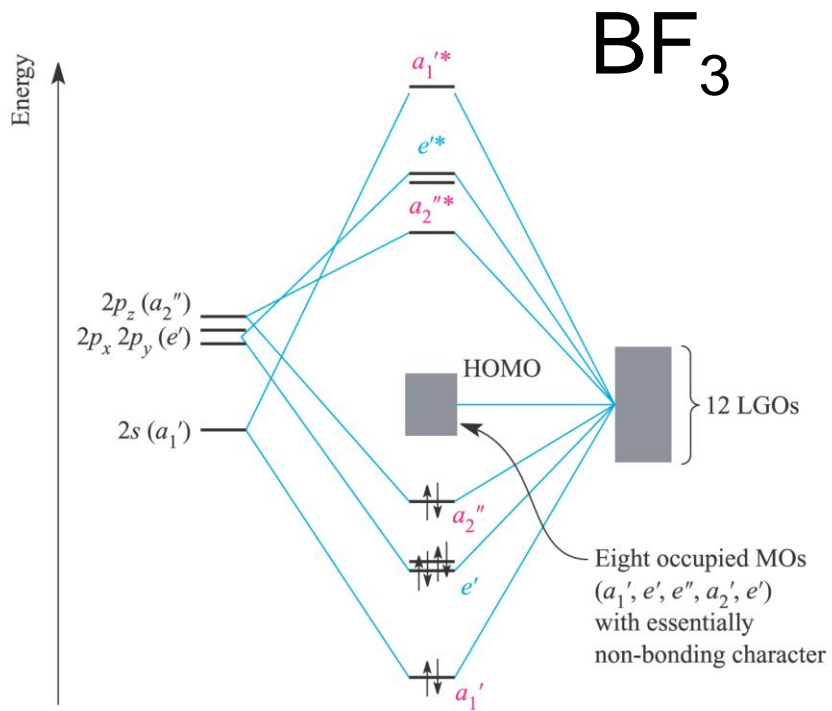
BF₃



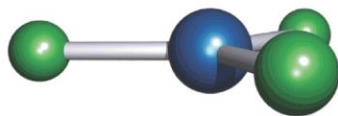
tre $2p_z$

E	C_3	C_2	σ_h	S_3	σ_v
3	0	-1	-3	0	1

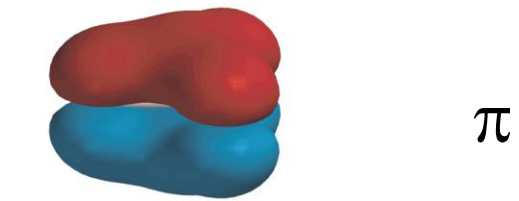
$A_2'' + E''$



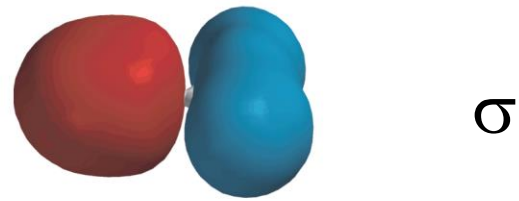
B BF₃ F₃ fragment



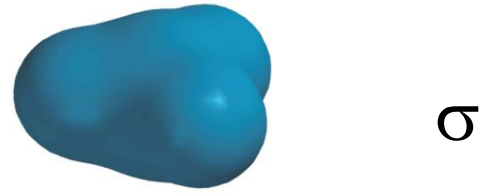
D_{3h}



Representation of the a_2'' MO



Representation of one of the e' MOs



Representation of the a_1' MO

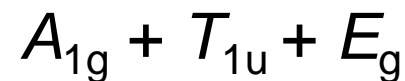
Ordine di legame 4/3

Molecole ipervalenti: SF₆ (gruppo O_h)

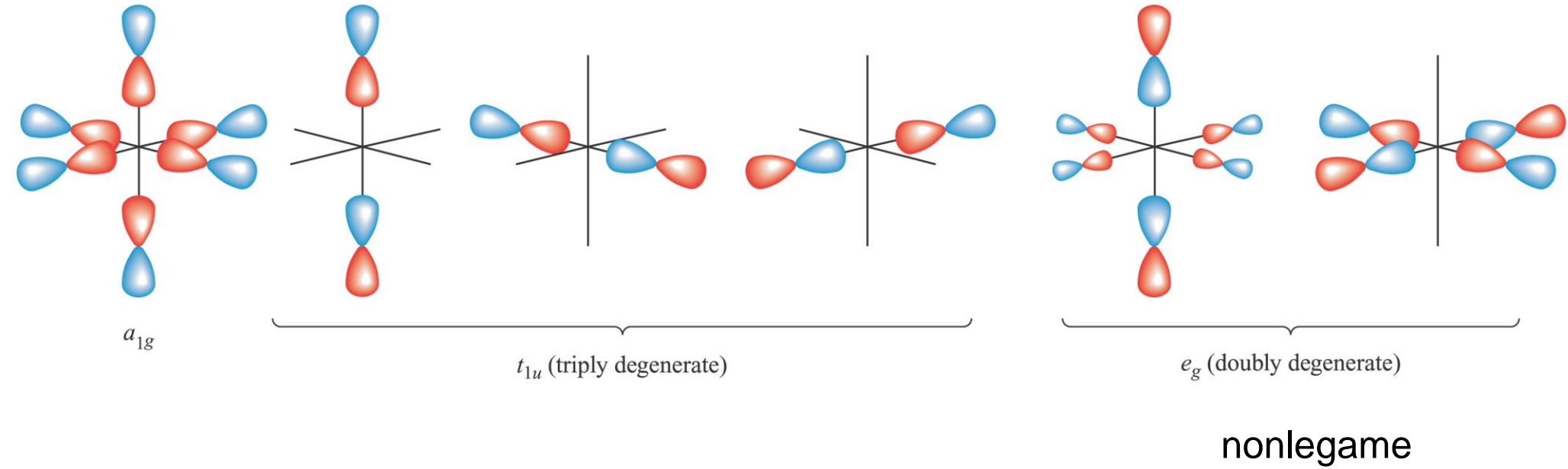
O _h	E	8C ₃	6C ₂	6C ₄	3C ₂ (= C ₄ ²)	i	6S ₄	8S ₆	3σ _h	6σ _d
A _{1g}	1	1	1	1	1	1	1	1	1	1
A _{2g}	1	1	-1	-1	1	1	-1	1	1	-1
E _g	2	-1	0	0	2	2	0	-1	2	0
T _{1g}	3	0	-1	1	-1	3	1	0	-1	-1
T _{2g}	3	0	1	-1	-1	3	-1	0	-1	1
A _{1u}	1	1	1	1	1	-1	-1	-1	-1	-1
A _{2u}	1	1	-1	-1	1	-1	1	-1	-1	1
E _u	2	-1	0	0	2	-2	0	1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

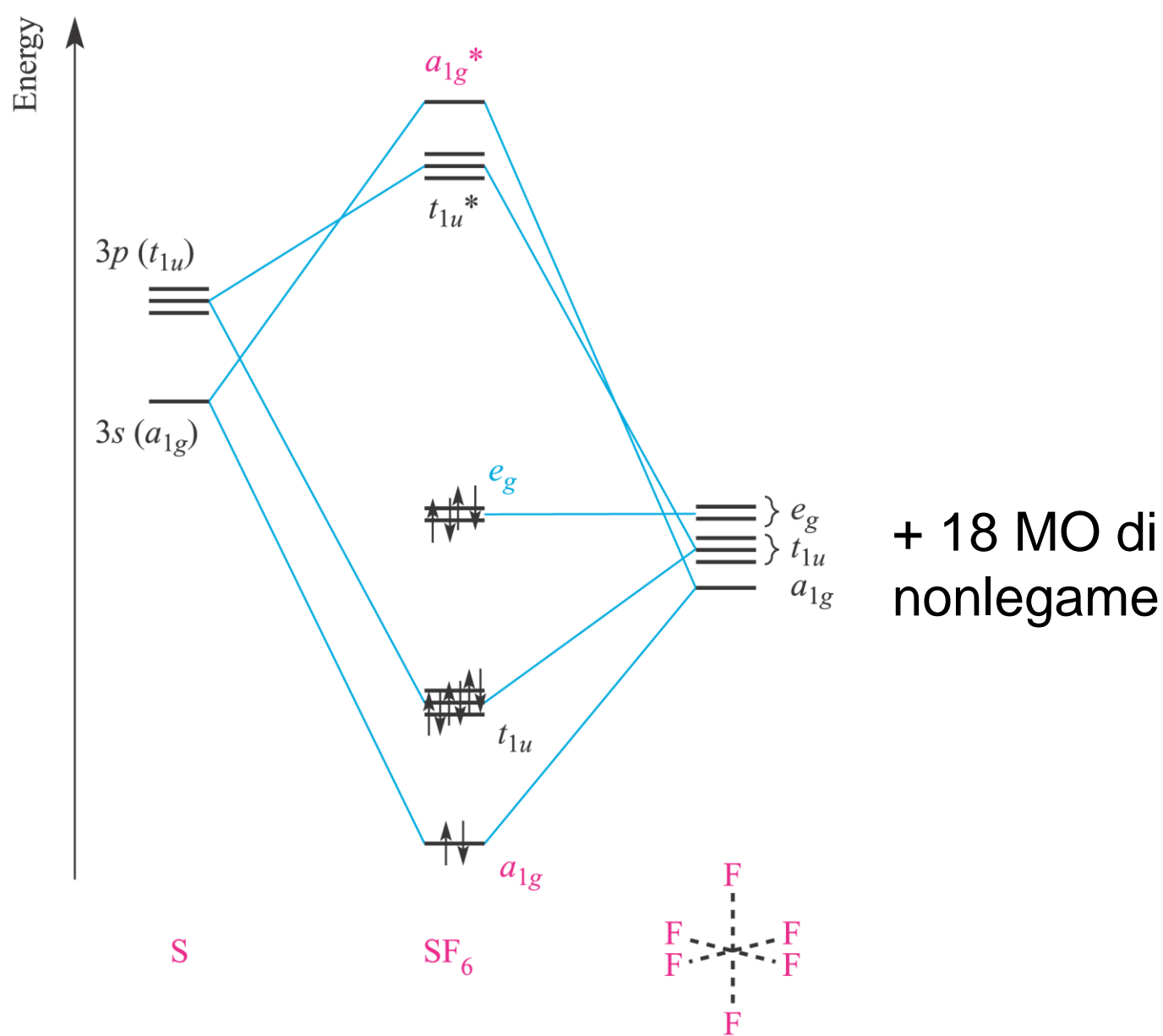
sei 2p_z radiali

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



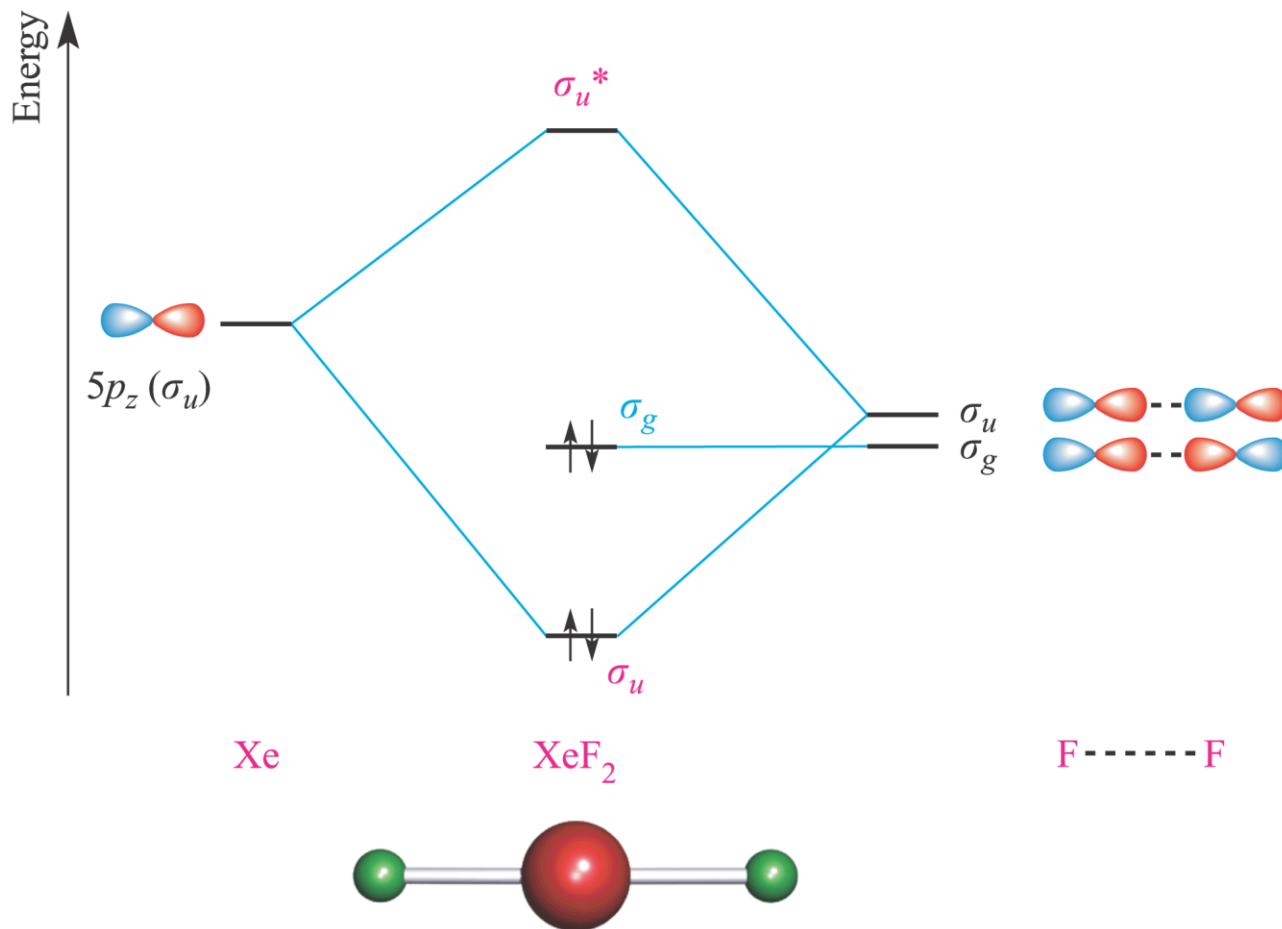
LGO del frammento F_6 in SF_6



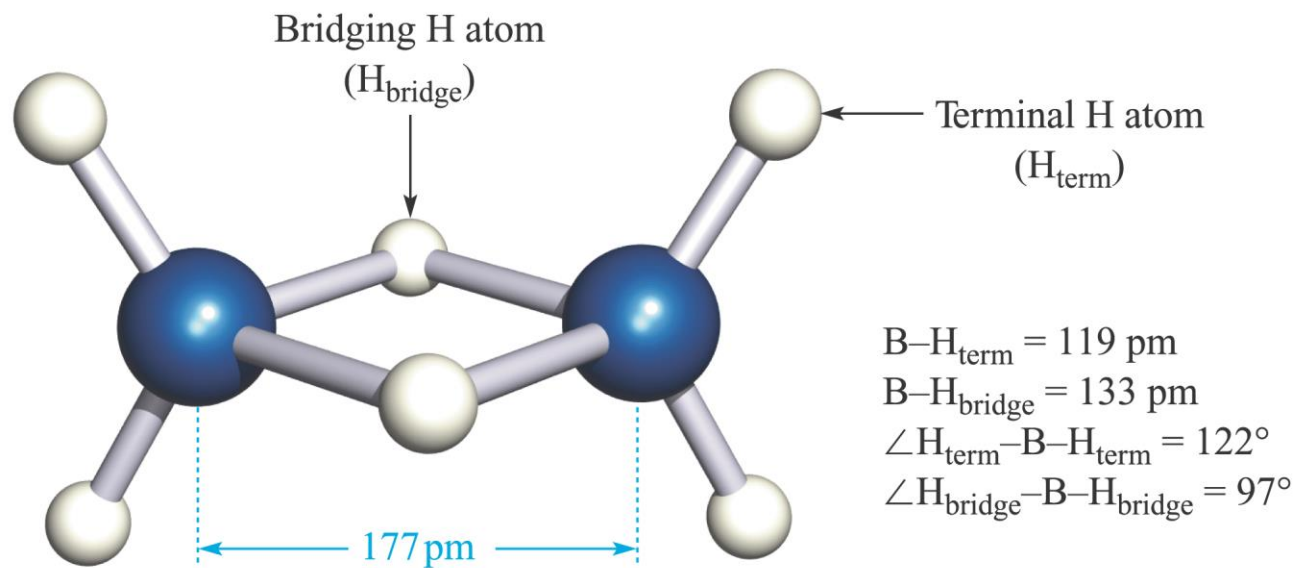


Ordine di legame $2/3$,
nessun orbitale d

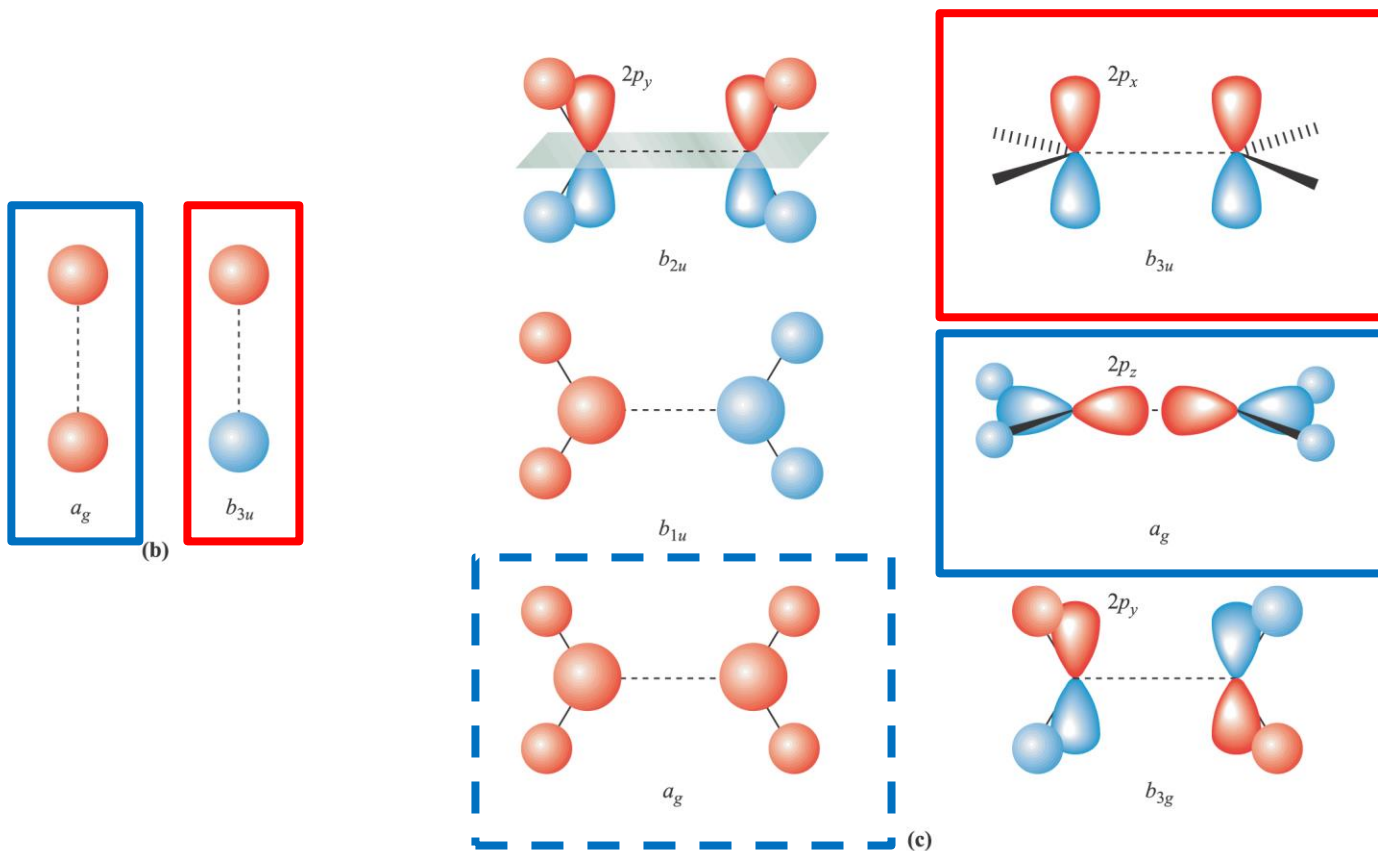
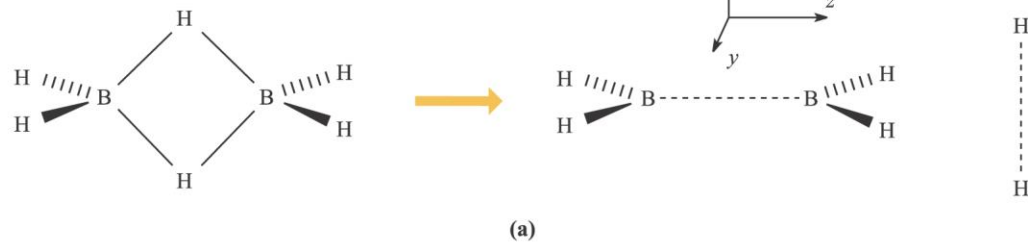
XeF₂: Interazione 3c – 2e



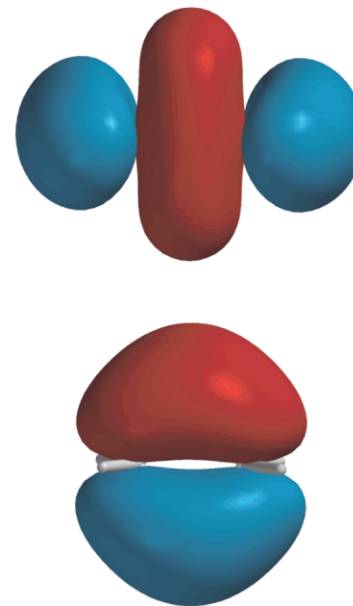
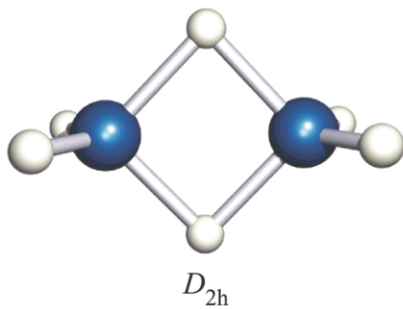
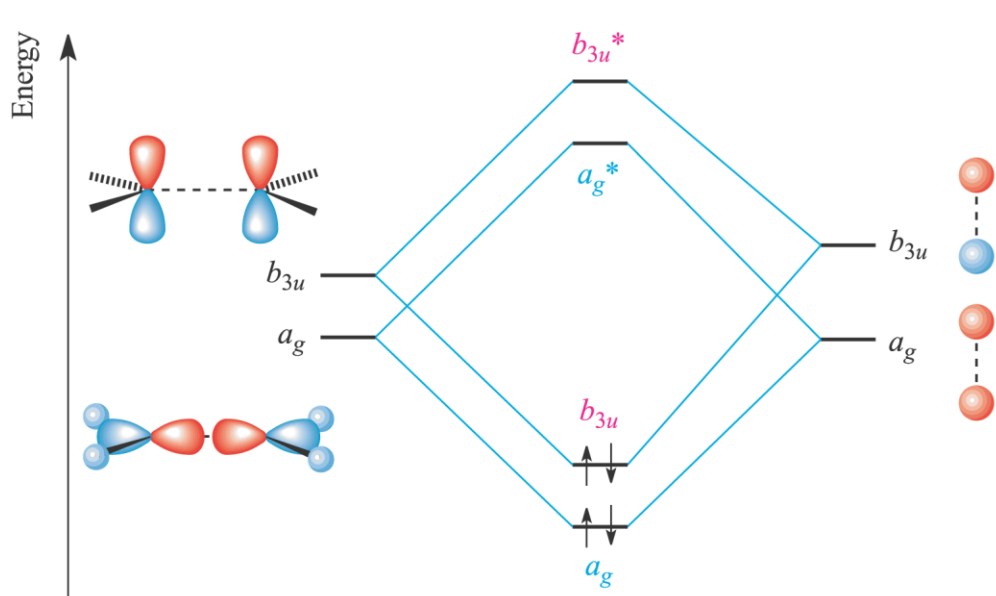
Diborano, B_2H_6



D_{2h}

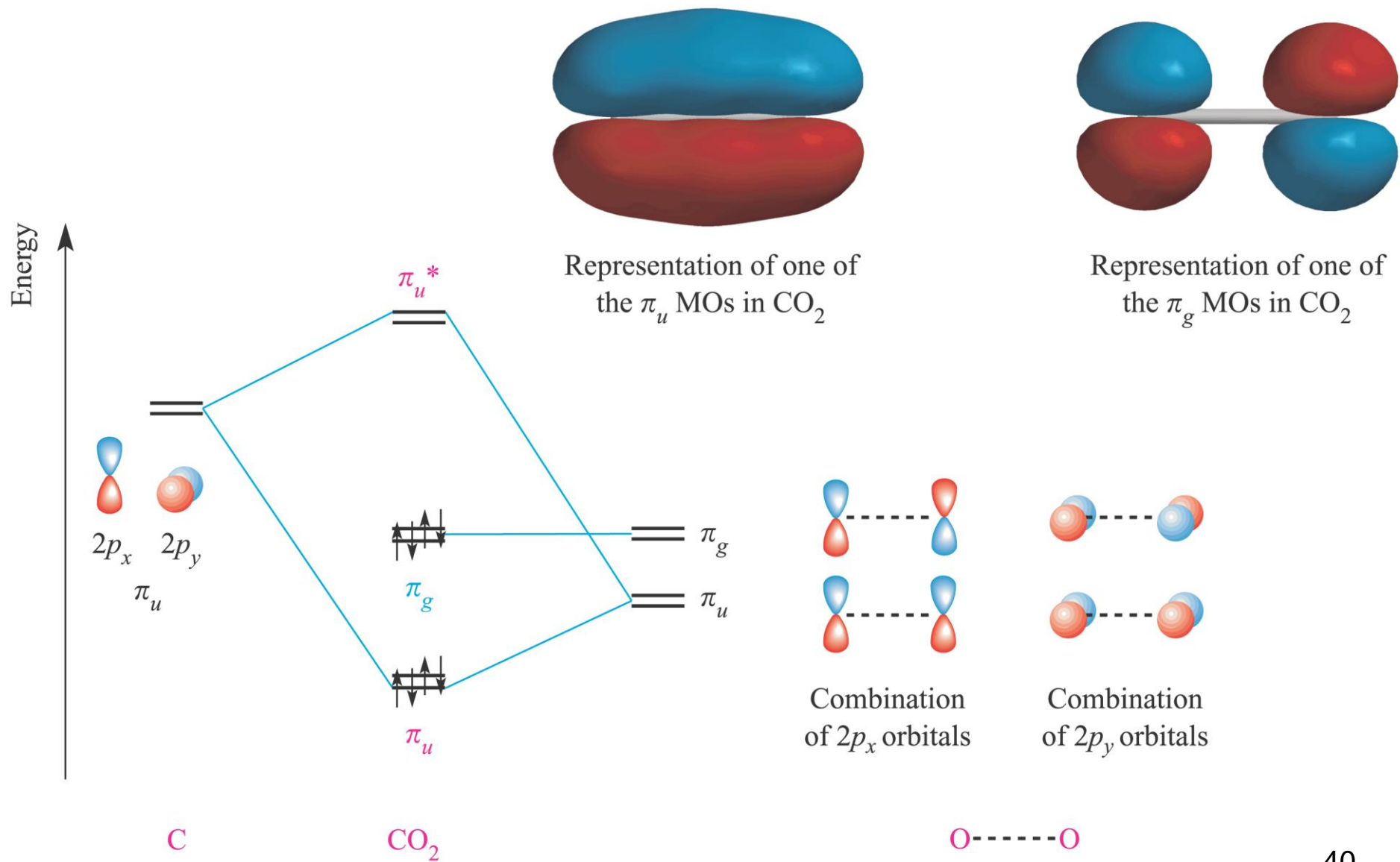


6 LGO (su 12) a energia più bassa del frammento B_2H_4

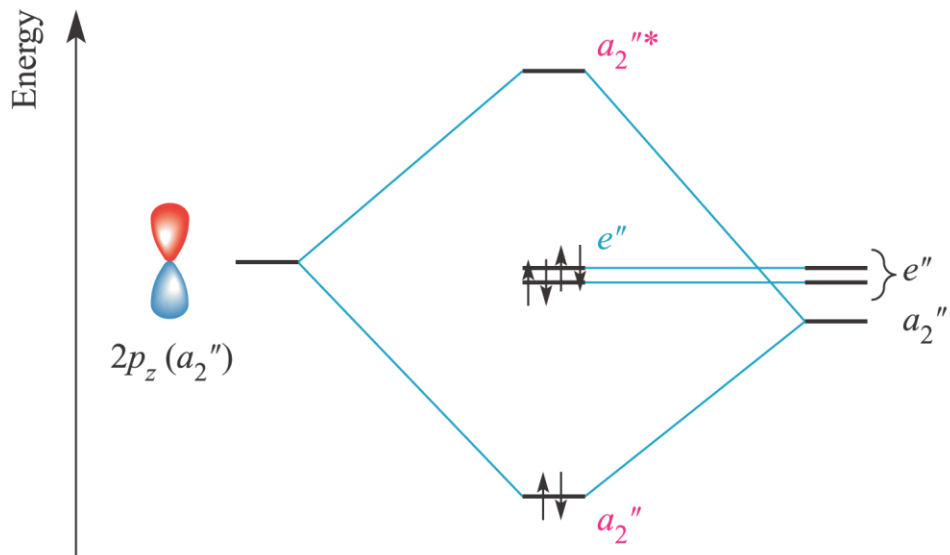


Representation of the a_g (top) and b_{3u} MOs which contain B–H–B bonding character

Diagrammi MO parziali: CO₂

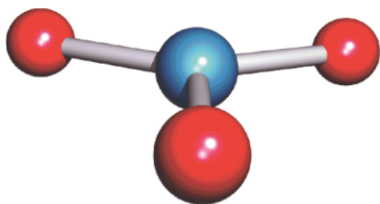


NO₃⁻

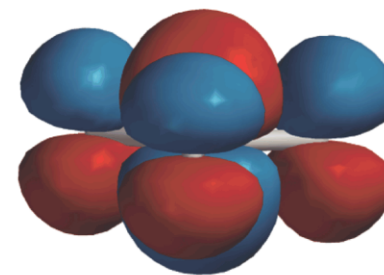
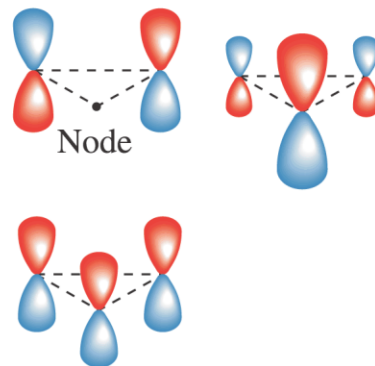


N

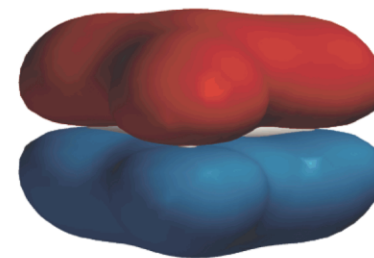
[NO₃]⁻



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