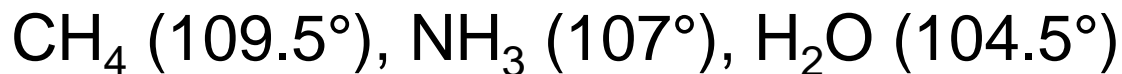


**Table 2.6** The basic arrangement of regions of electron density according to the VSEPR model

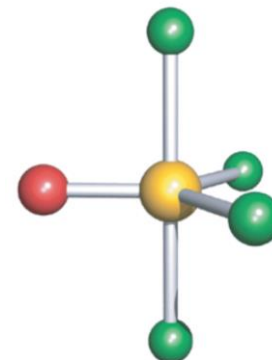
Number of electron regions	Arrangement
2	Linear
3	Trigonal planar
4	Tetrahedral
5	Trigonal bipyramidal
6	Octahedral

# Repulsione

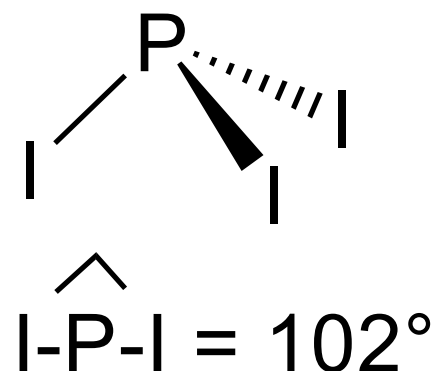
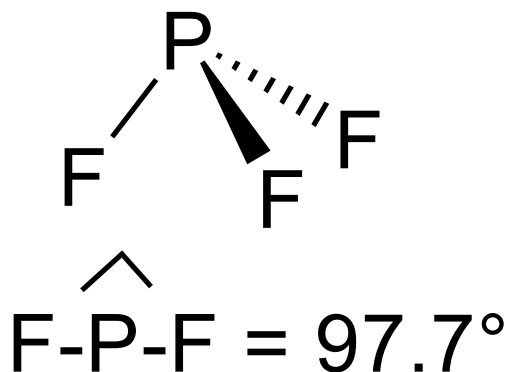
coppia solitaria – coppia solitaria > coppia solitaria – coppia di legame > coppia di legame – coppia di legame



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



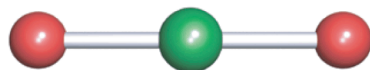
**numero sterico** = numero di coppie di legame e di non legame intorno all'atomo centrale

**n.s.** = elettroni di valenza ( $\pm$  carica)/8 + resto/2

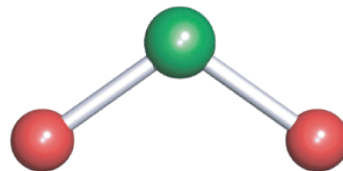


*Il numero sterico determina la **geometria delle coppie**, che non necessariamente coincide con la **geometria molecolare***

**2-Coordinate**

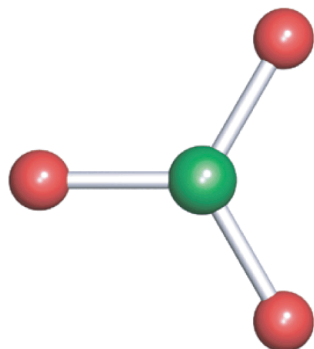


Linear

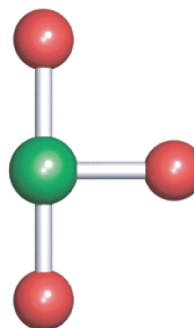


Bent

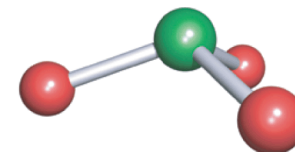
**3-Coordinate**



Trigonal planar



T-shaped

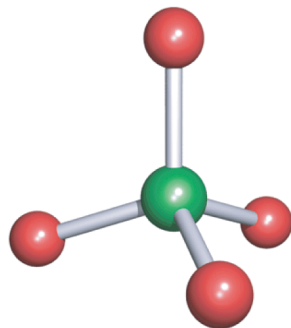


Trigonal pyramidal

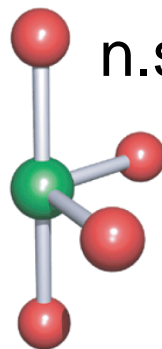


n.s. = 5

4-Coordinate

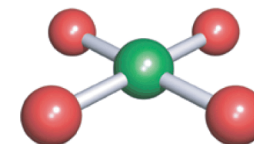
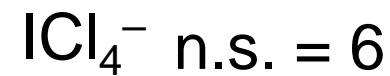


Tetrahedral



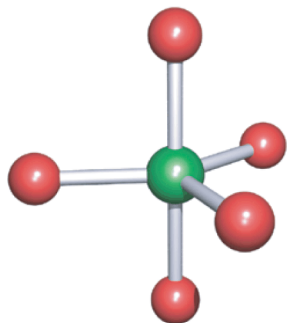
n.s. = 5

Disphenoidal

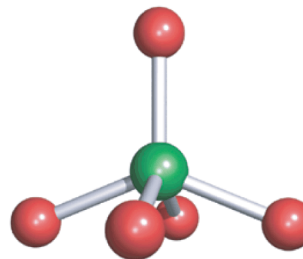


Square planar

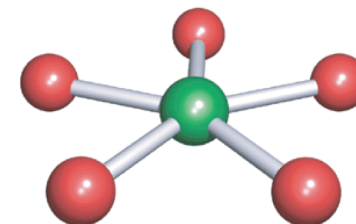
5-Coordinate



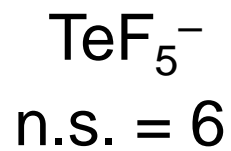
Trigonal bipyramidal



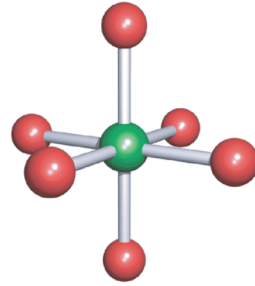
Square-based pyramidal



Pentagonal planar

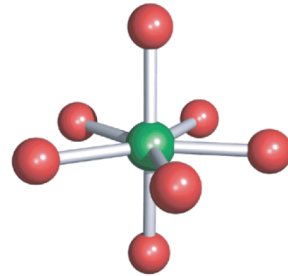


**6-Coordinate**



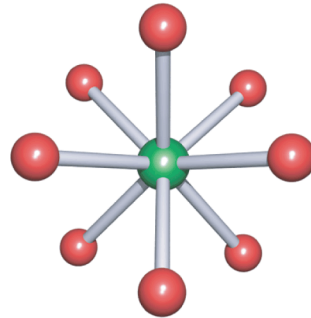
Octahedral

**7-Coordinate**



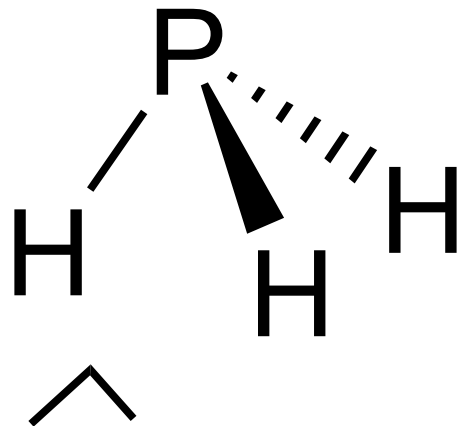
Pentagonal bipyramidal

**8-Coordinate**



Square antiprismatic

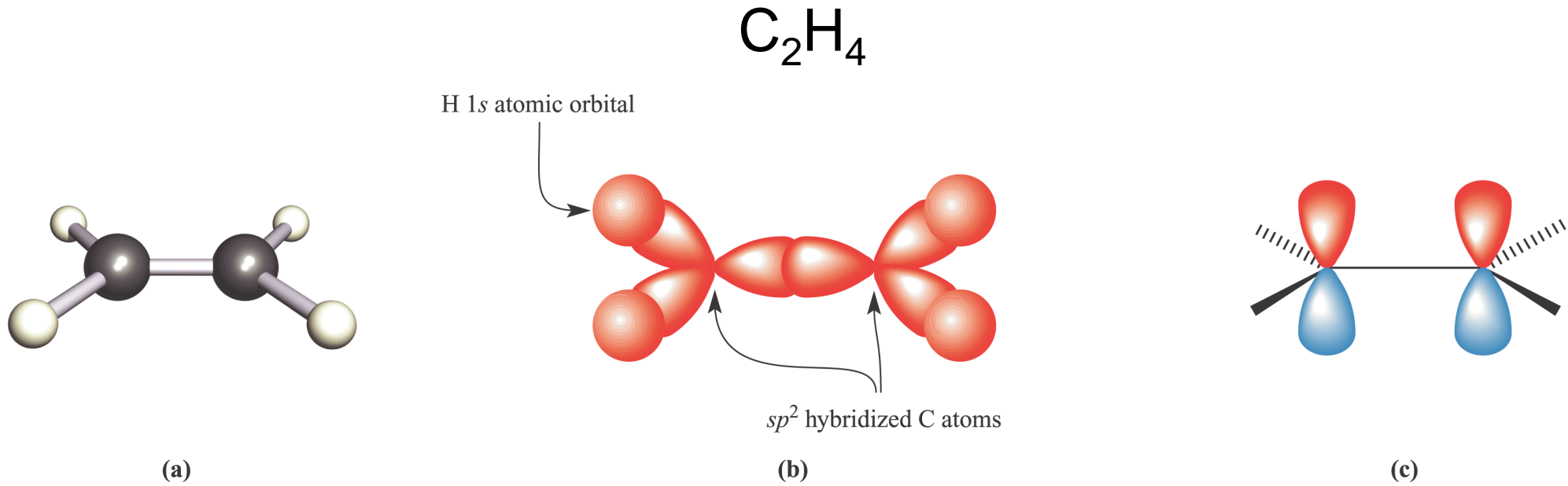
Coppie solitarie stereochimicamente inattive



H-P-H ca. 90°



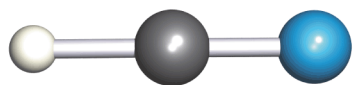
# Molecole poliatomiche secondo la teoria VB



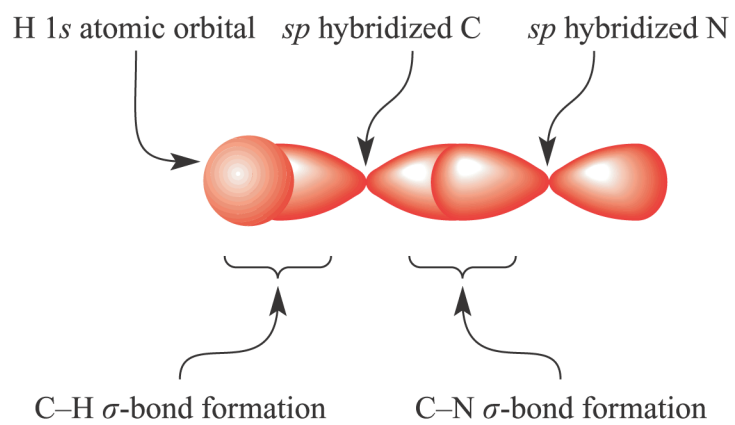
$598 \text{ kJ mol}^{-1}$  vs  $2 \times 346 \text{ kJ mol}^{-1}$



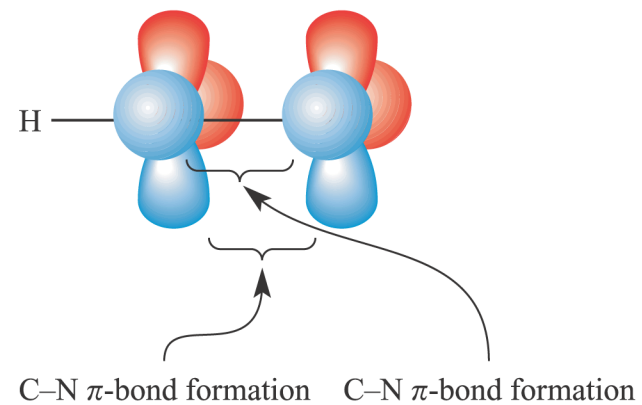
# HCN



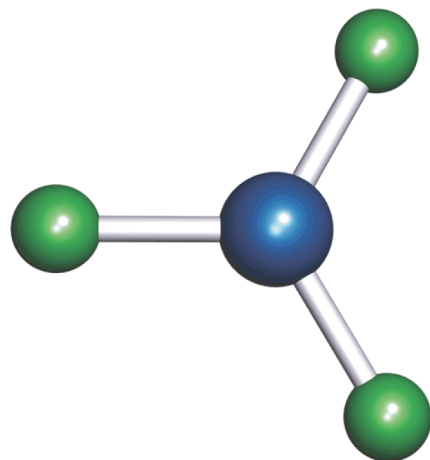
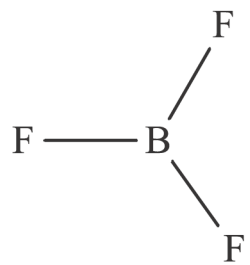
(a)



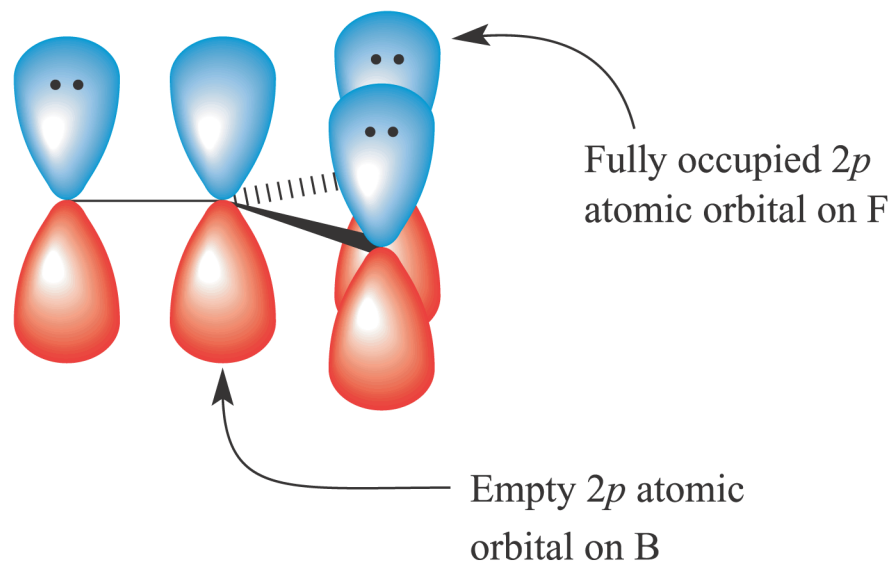
(b)



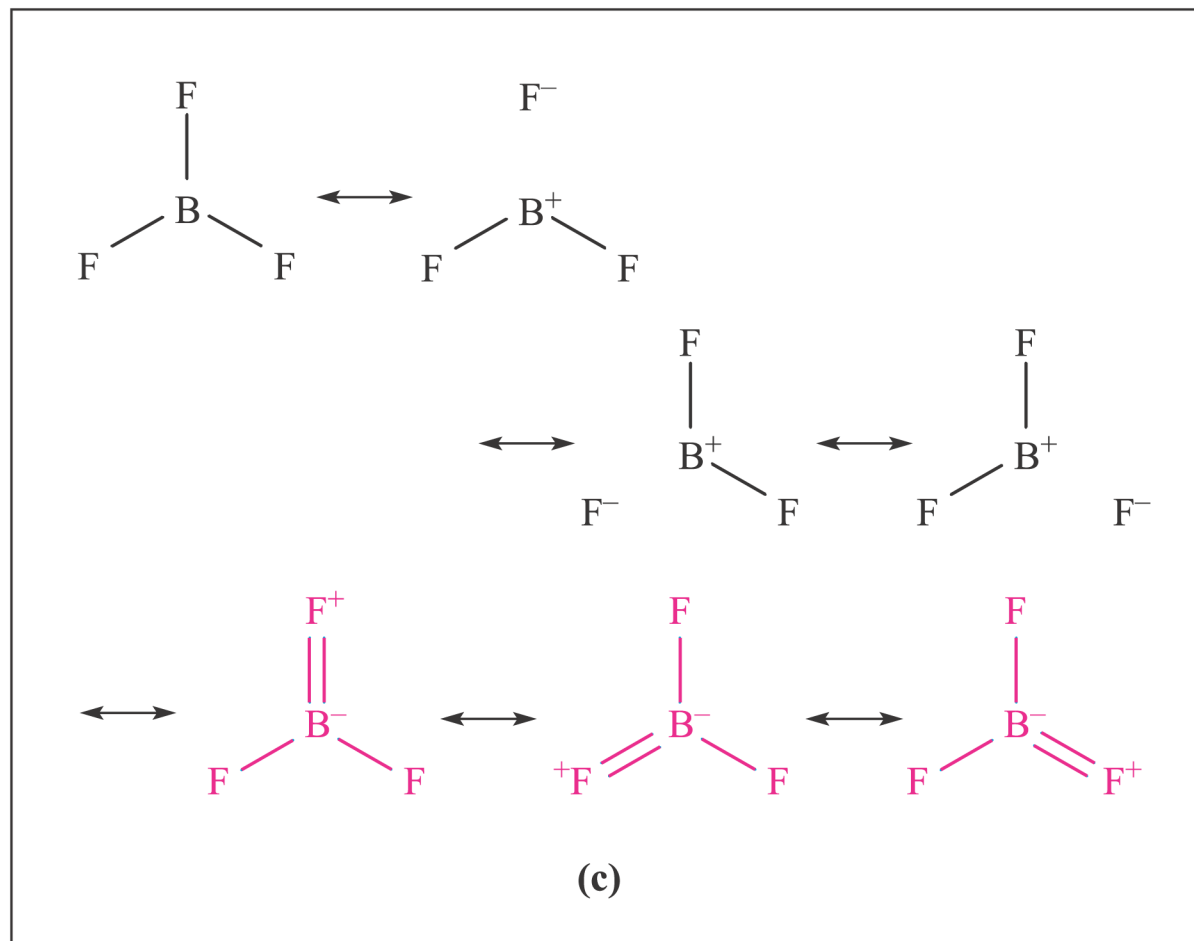
(c)



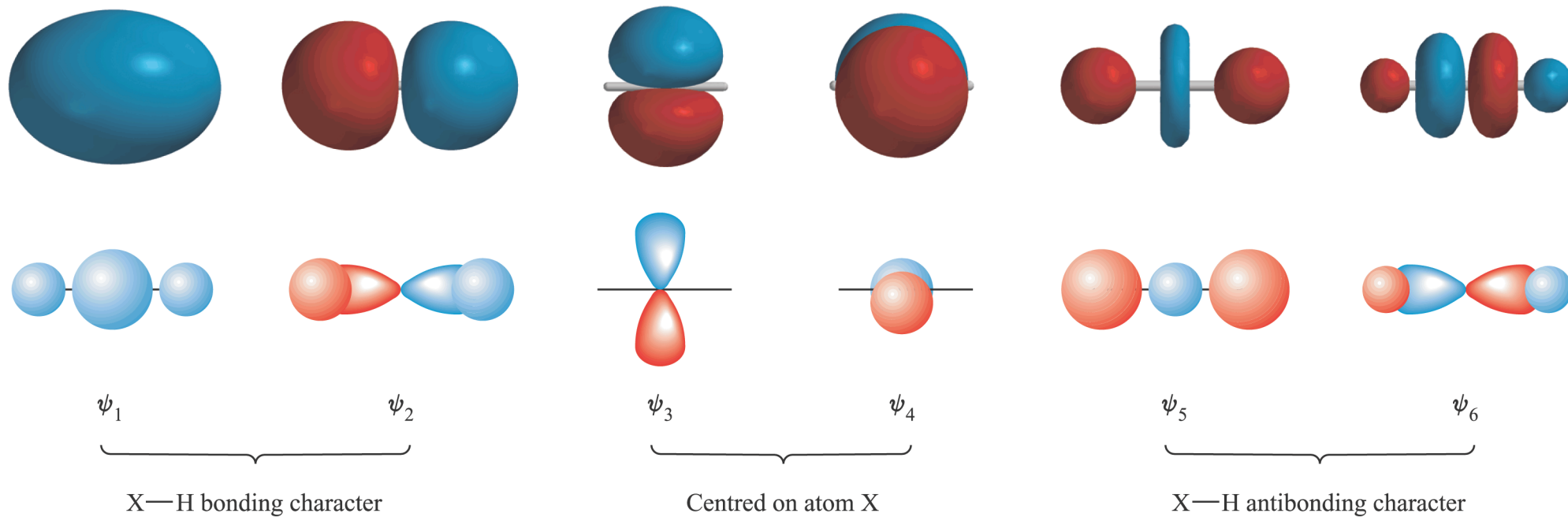
(a)



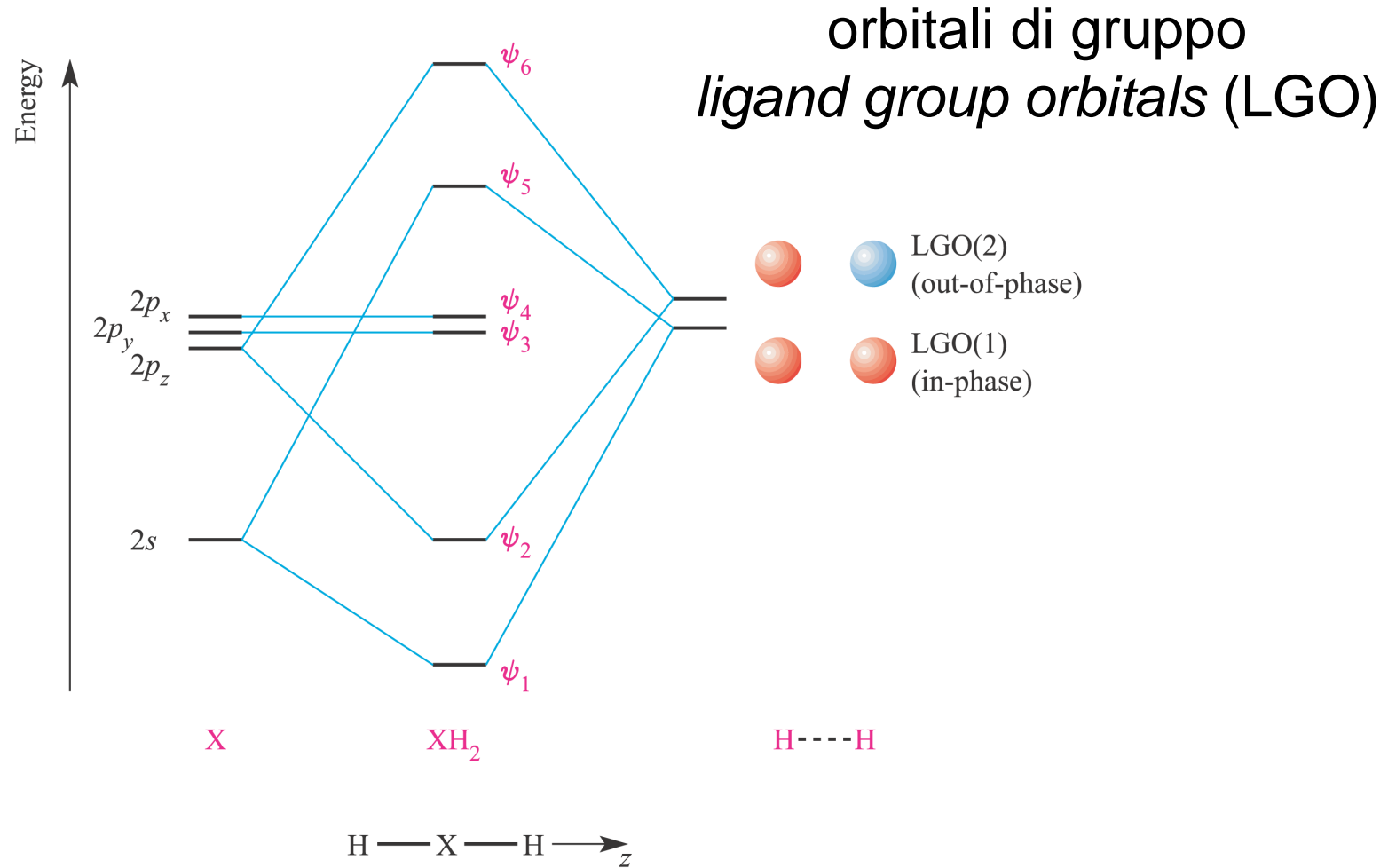
(b)

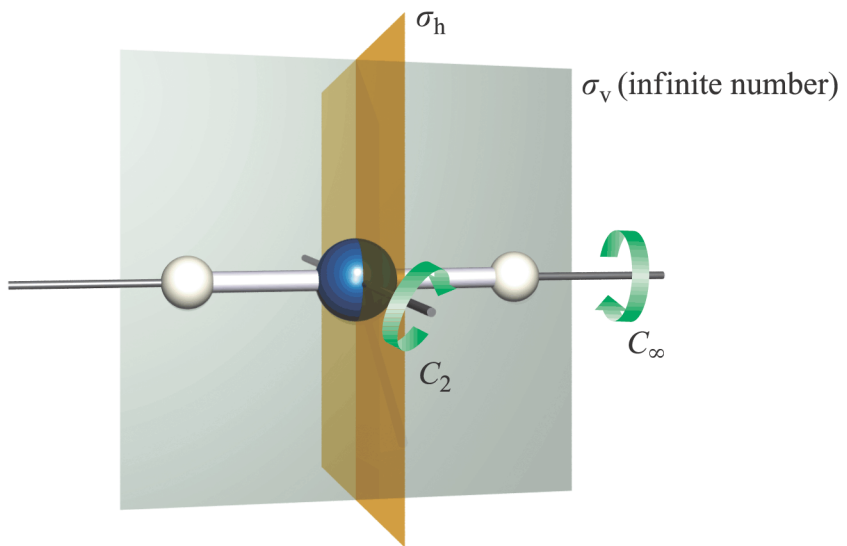


# Molecole poliatomiche secondo la teoria MO



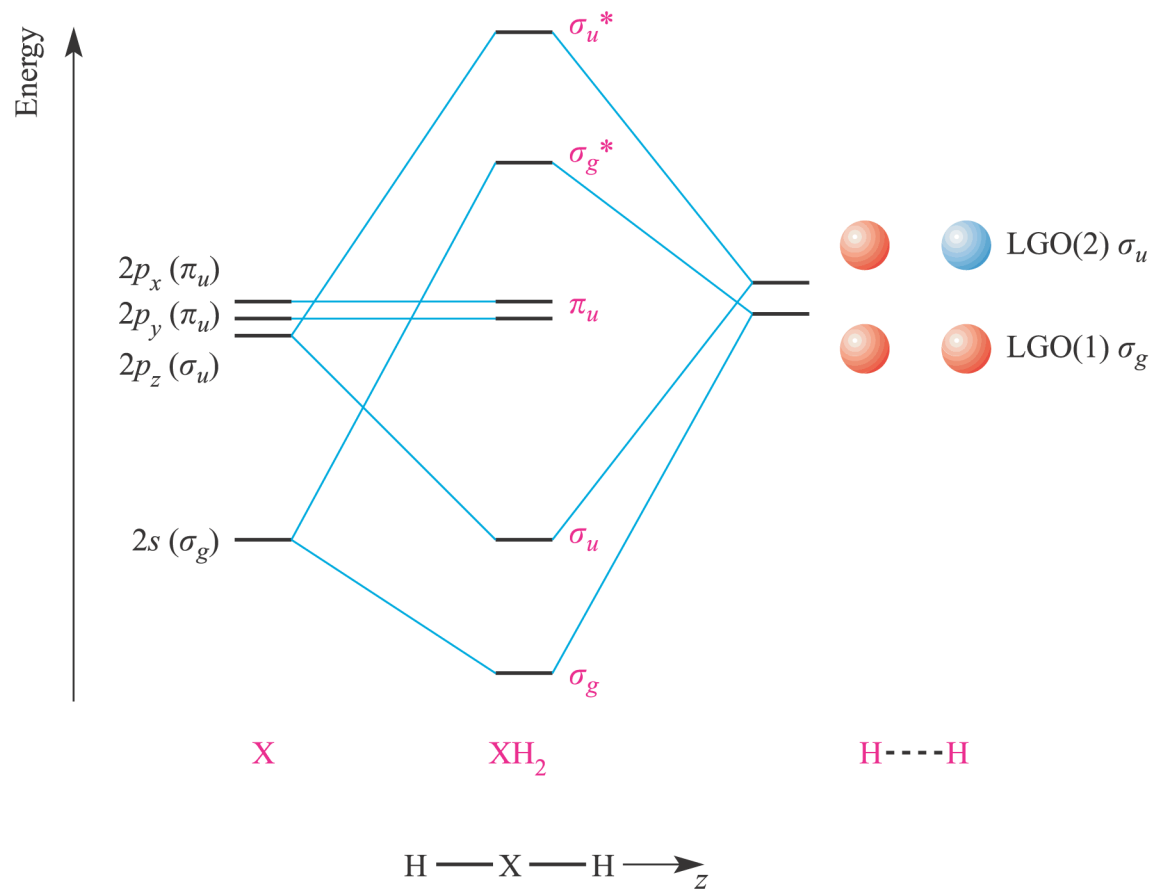
# Molecole poliatomiche secondo la teoria MO



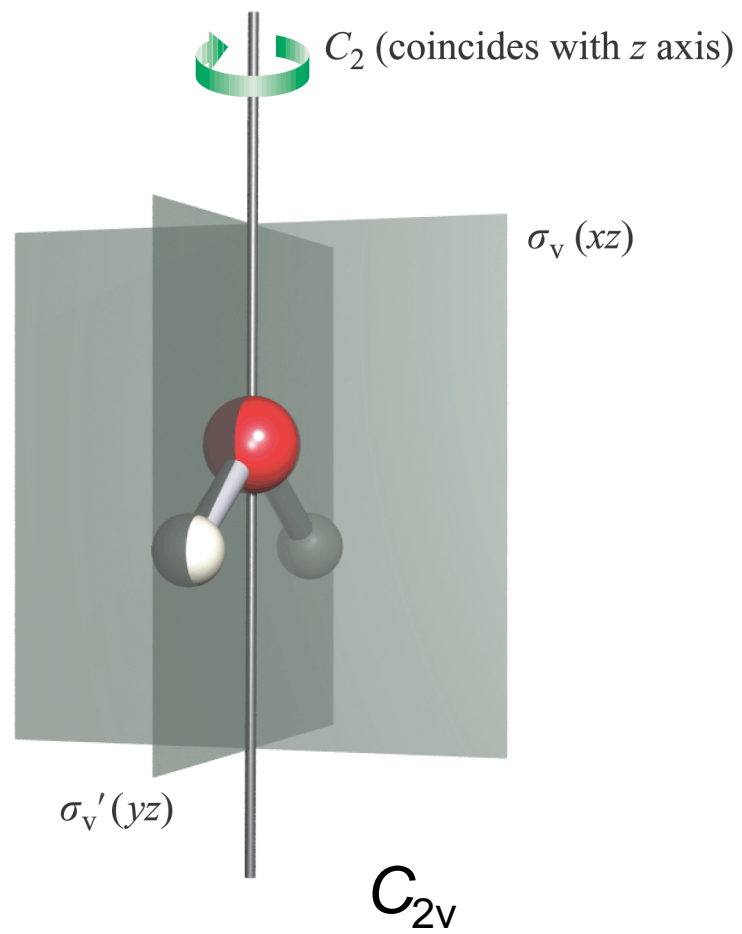


$D_{\infty h}$

(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	$y, R_x$	$yz$

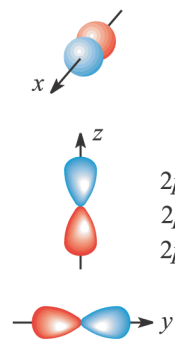
2H

2	0	0	2
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$A_1 + B_2$
-------------



Energy



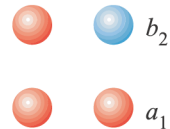
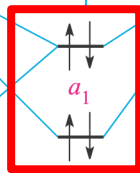
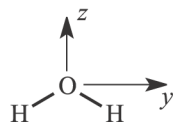
$2p_x (b_1)$   
 $2p_z (a_1)$   
 $2p_y (b_2)$

$2s (a_1)$

O

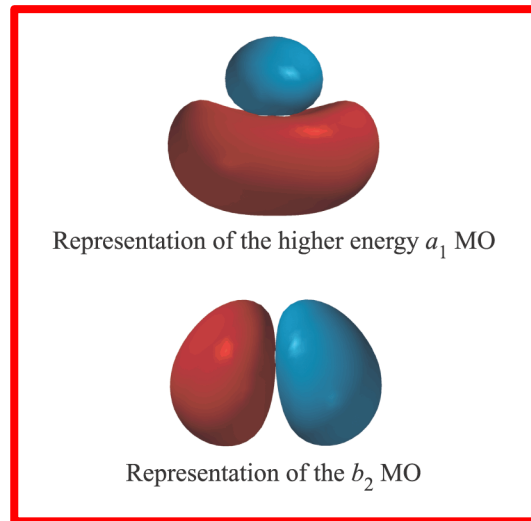
$H_2O$

H-----H



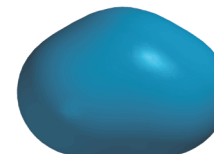
Representation of the  $b_1$  MO

n.l.



Representation of the higher energy  $a_1$  MO

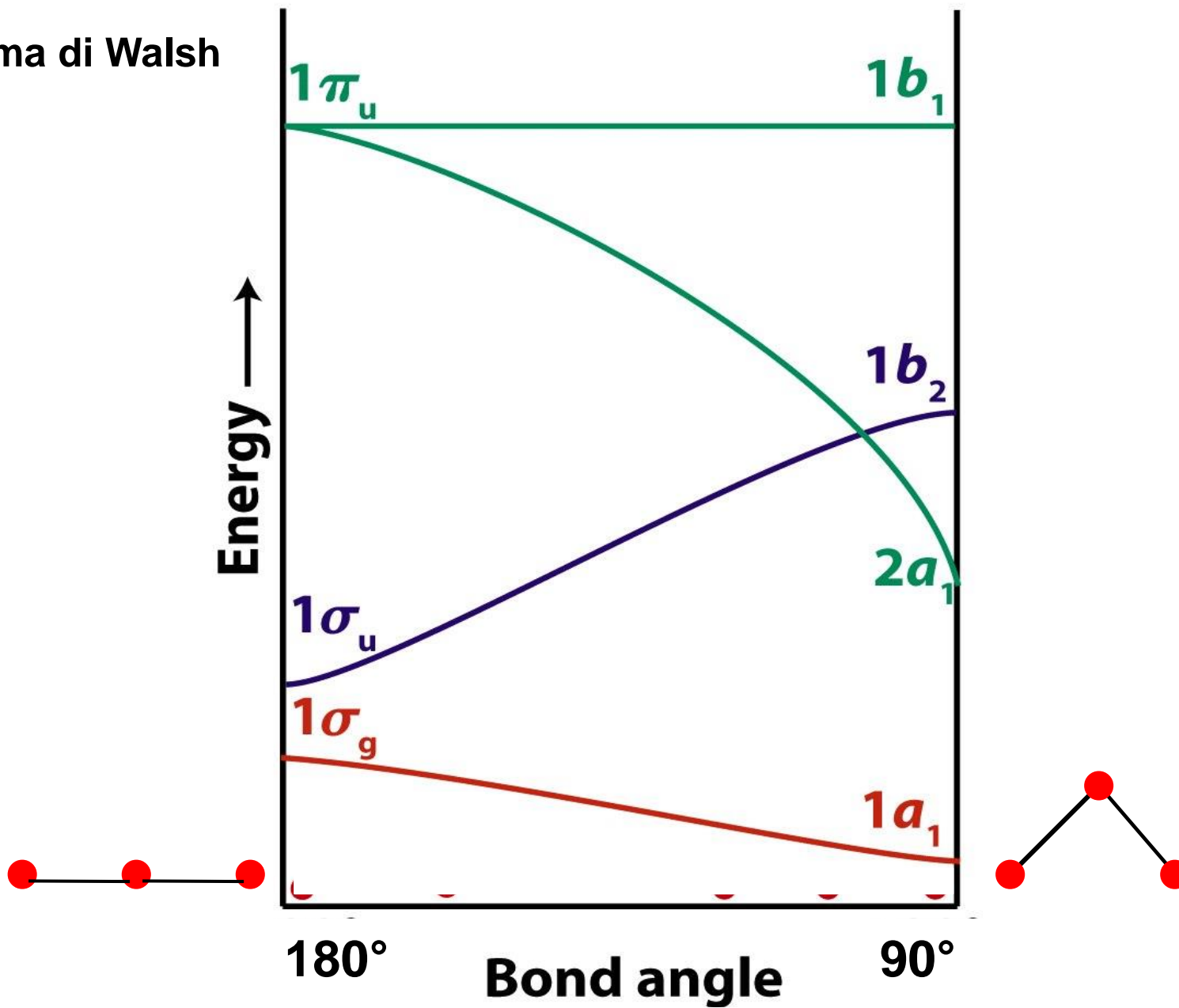
Representation of the  $b_2$  MO

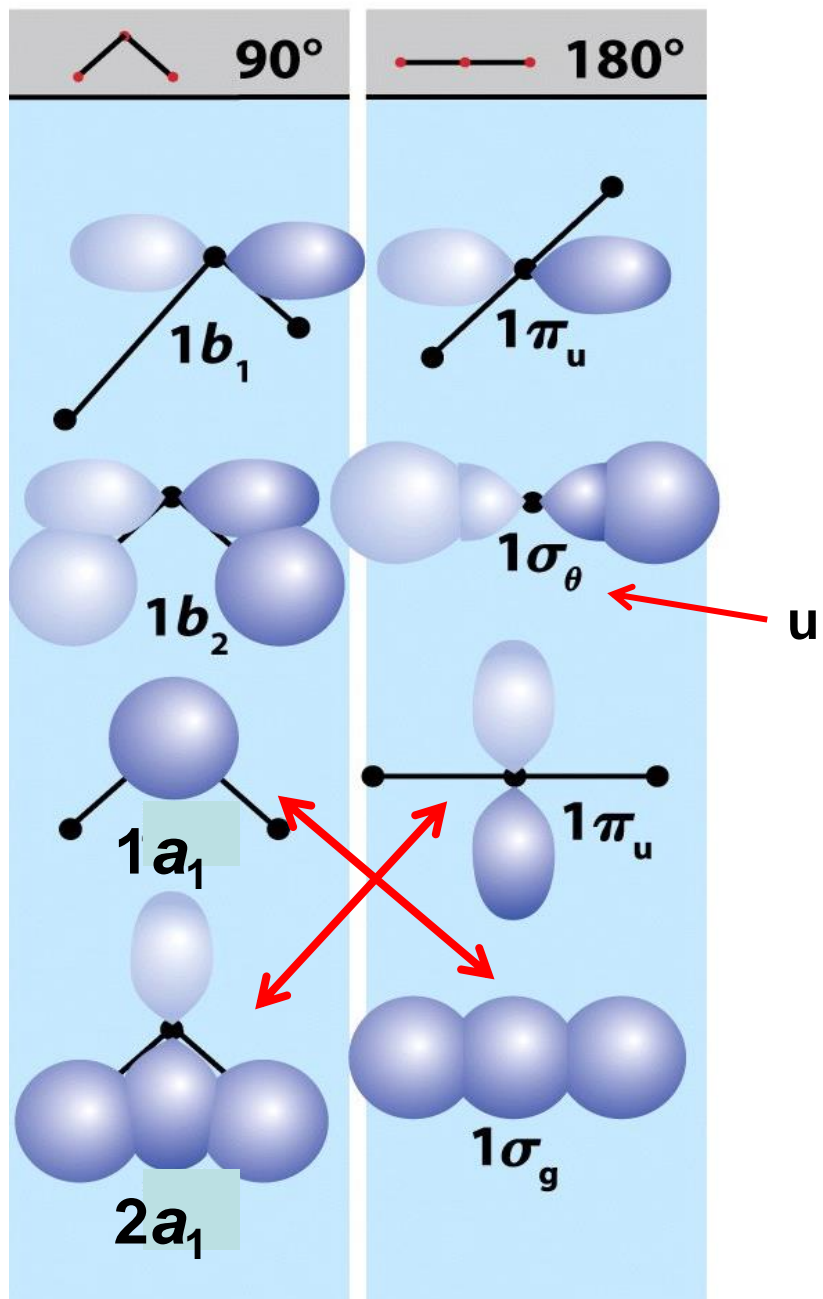


Representation of the lower energy  $a_1$  MO

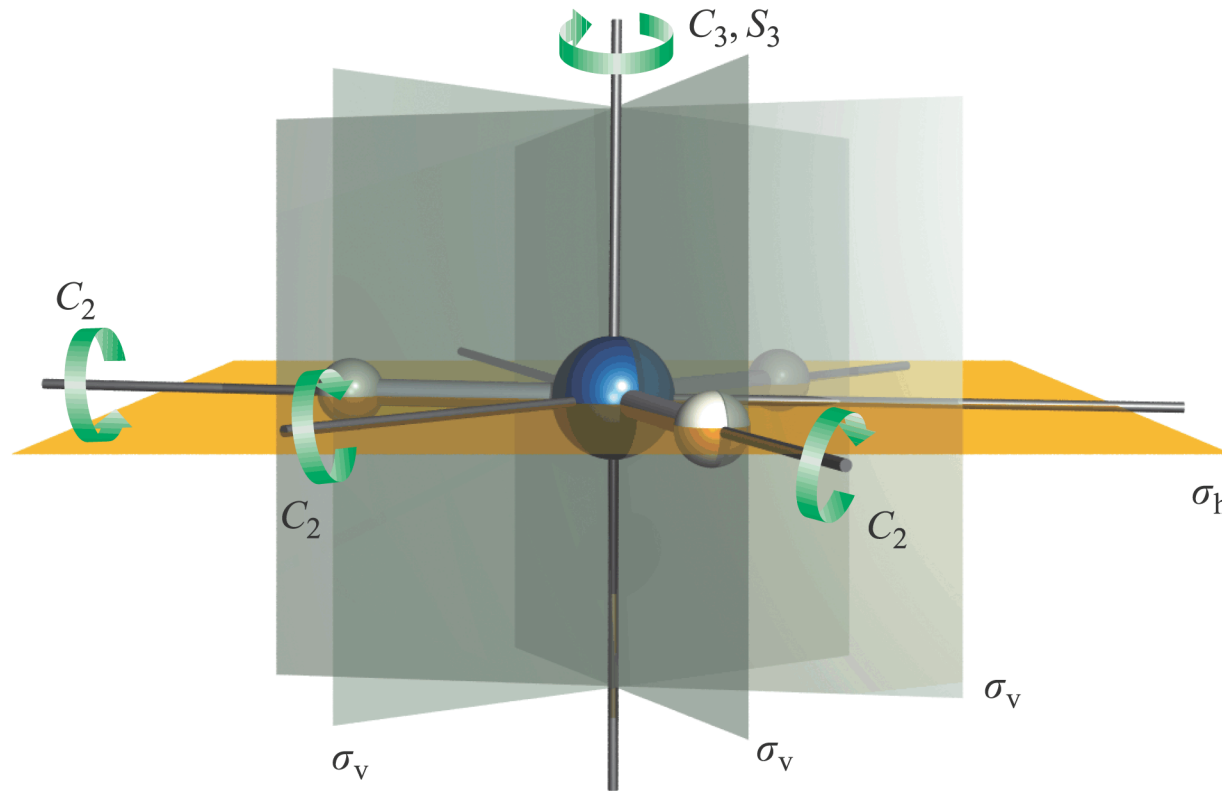
n.l.

# Diagramma di Walsh





# BH<sub>3</sub>, gruppo puntuale D<sub>3h</sub>

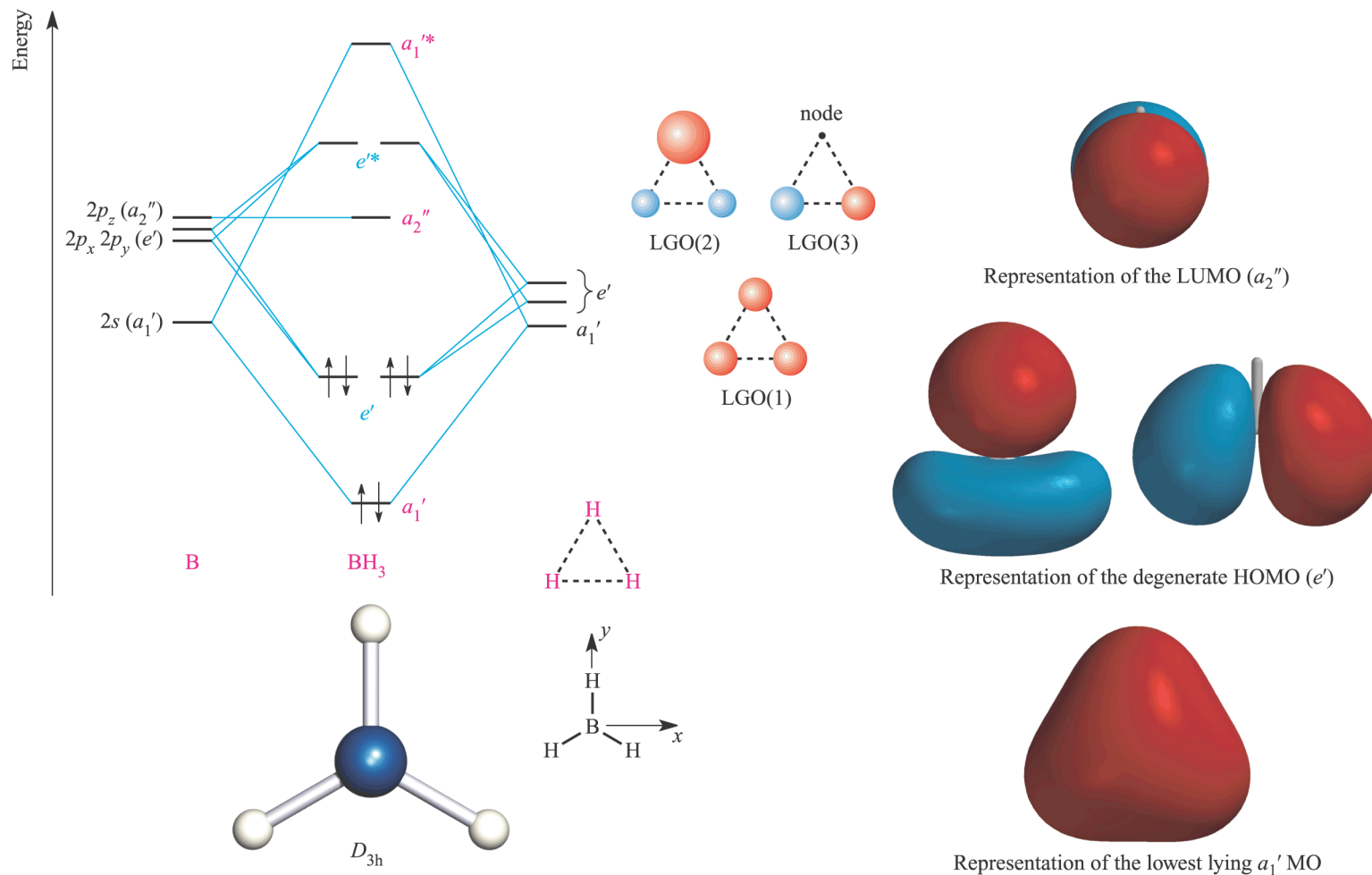


$D_{3h}$	$E$	$2C_3$	$3C_2$	$\sigma_h$	$2S_3$	$3\sigma_v$		
$A_1'$	1	1	1	1	1	1		$x^2 + y^2, z^2$
$A_2'$	1	1	-1	1	1	-1	$R_z$	
$E'$	2	-1	0	2	-1	0	$(x, y)$	$(x^2 - y^2, xy)$
$A_1''$	1	1	1	-1	-1	-1		
$A_2''$	1	1	-1	-1	-1	1	$z$	
$E''$	2	-1	0	-2	1	0	$(R_x, R_y)$	$(xz, yz)$

3H

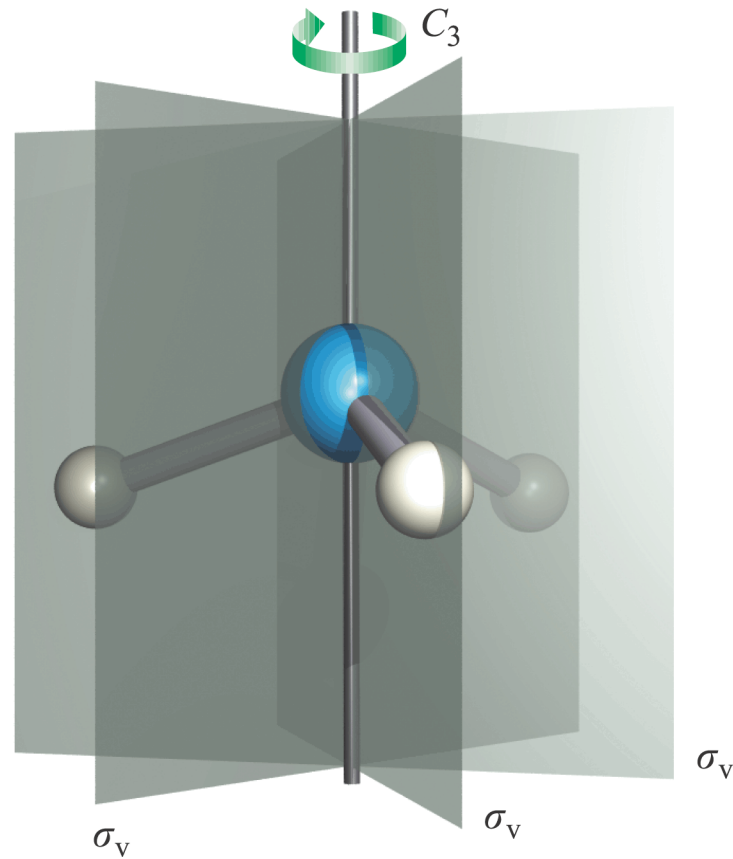
3	0	1	3	0	1
---	---	---	---	---	---

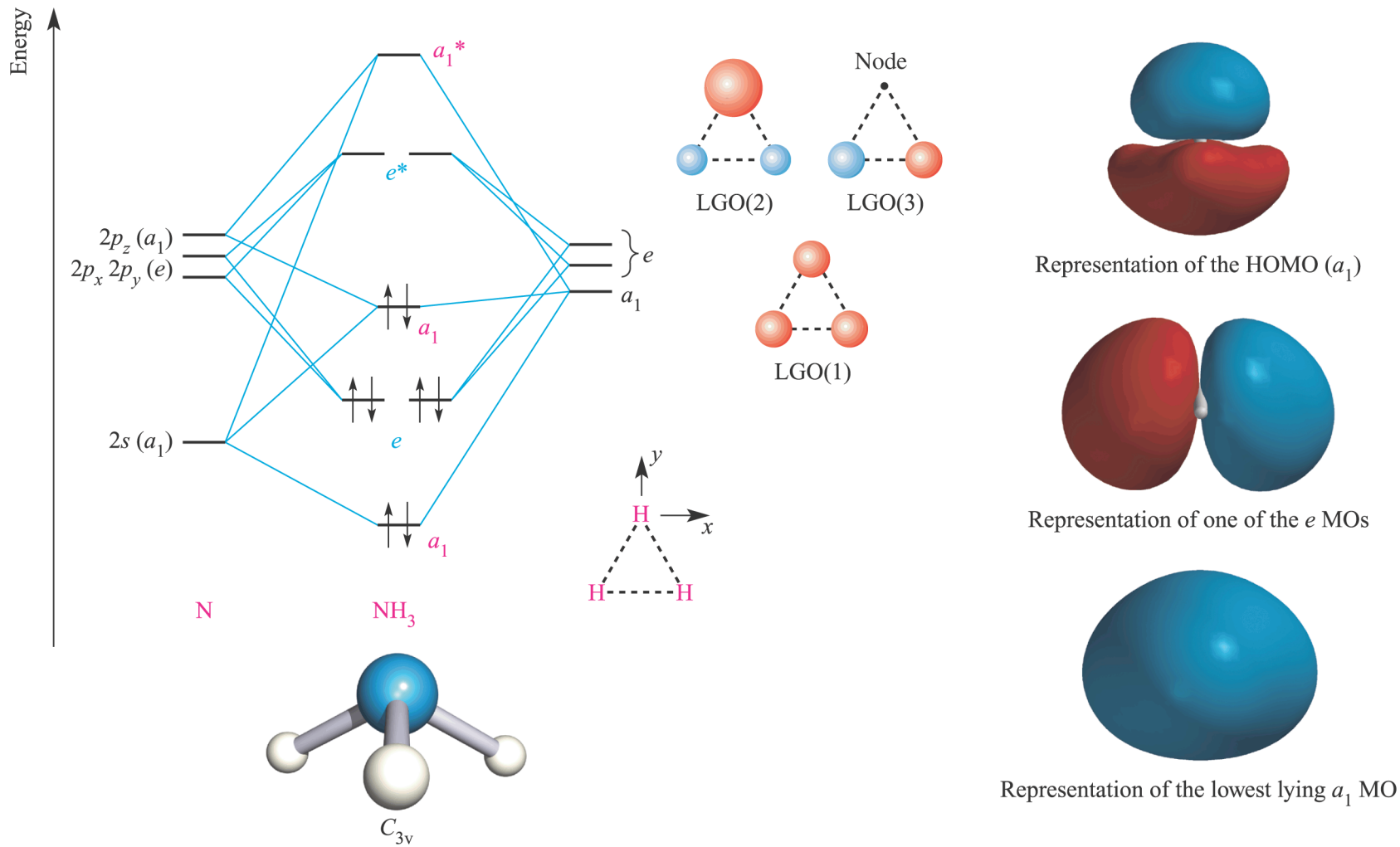
$A_1' + E'$
-------------



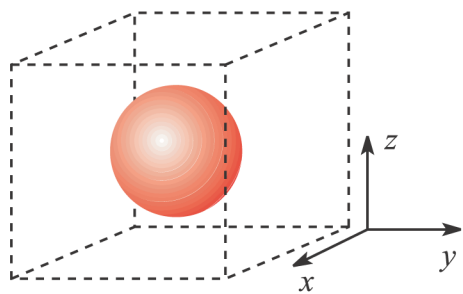
$$\begin{aligned} \Psi(a_1') &= 1/\sqrt{3} \times (\Psi_1 + \Psi_2 + \Psi_3) && \text{(LGO1)} \\ \Psi(e')_1 &= 1/\sqrt{6} \times (2\Psi_1 - \Psi_2 - \Psi_3) && \text{(LGO2)} \\ \Psi(e')_2 &= 1/\sqrt{2} \times (\Psi_2 - \Psi_3) && \text{(LGO3)} \end{aligned}$$

# $\text{NH}_3$ , gruppo puntuale $C_{3v}$

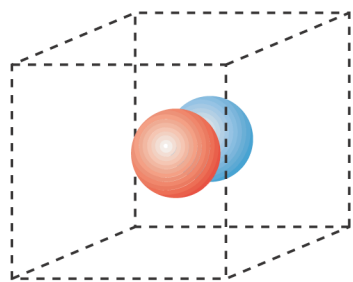




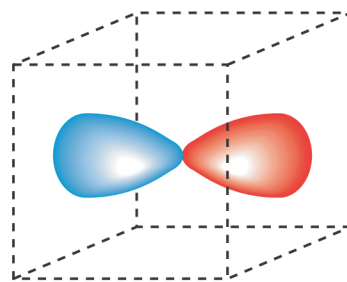




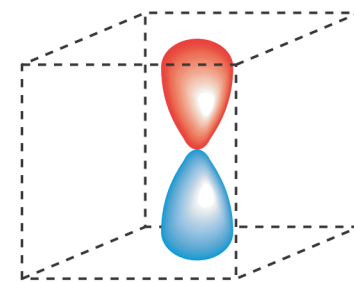
$2s (a_1)$



$2p_x (t_2)$

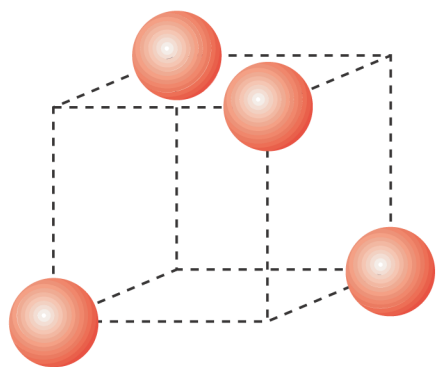


$2p_y (t_2)$

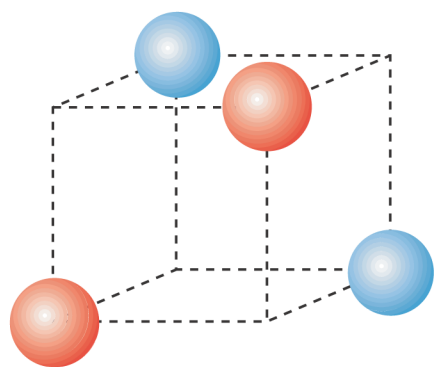


$2p_z (t_2)$

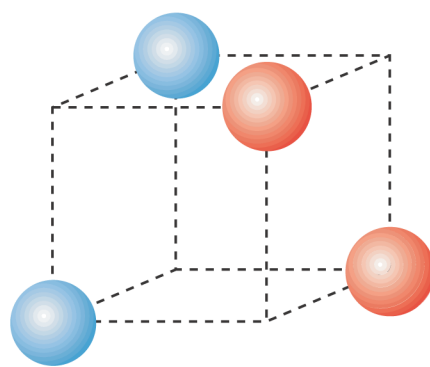
(a)



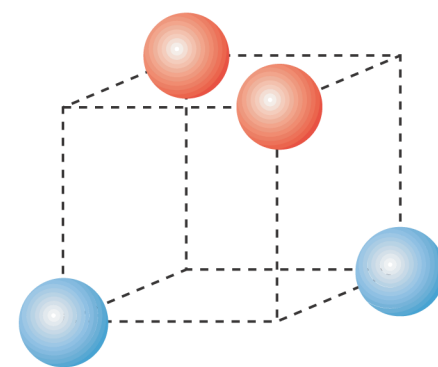
LGO(1) ( $a_1$ )



LGO(2) ( $t_2$ )

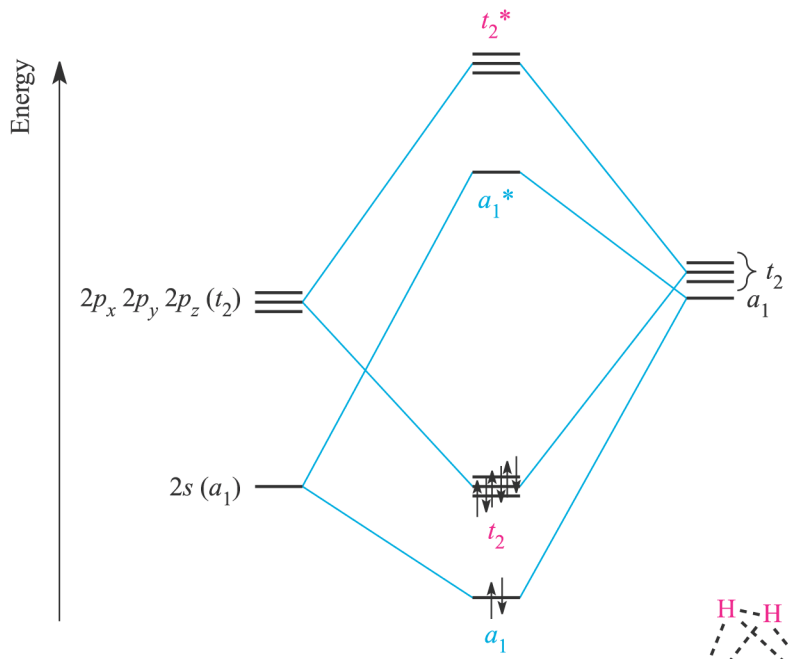


LGO(3) ( $t_2$ )



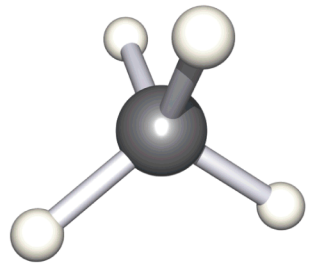
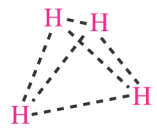
LGO(4) ( $t_2$ )

(b)

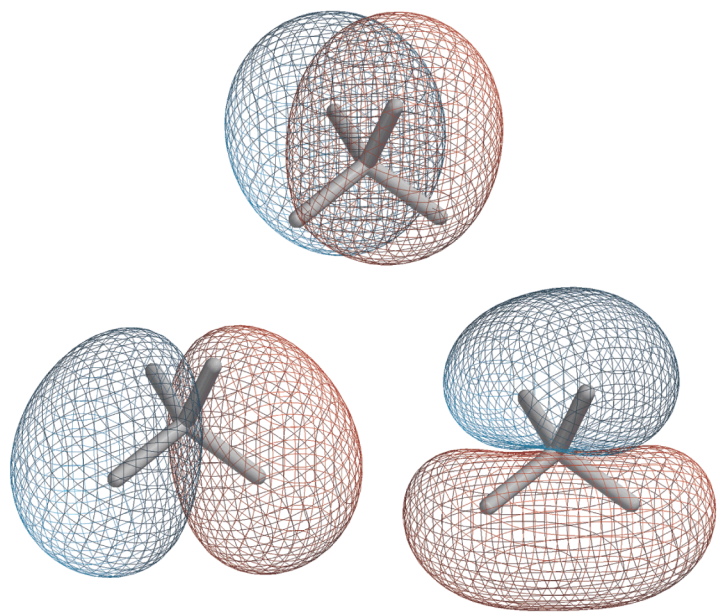


C

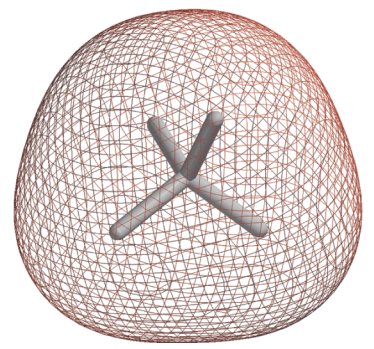
CH<sub>4</sub>



T<sub>d</sub>



Representations of the triply degenerate (*t*<sub>2</sub>) bonding MOs

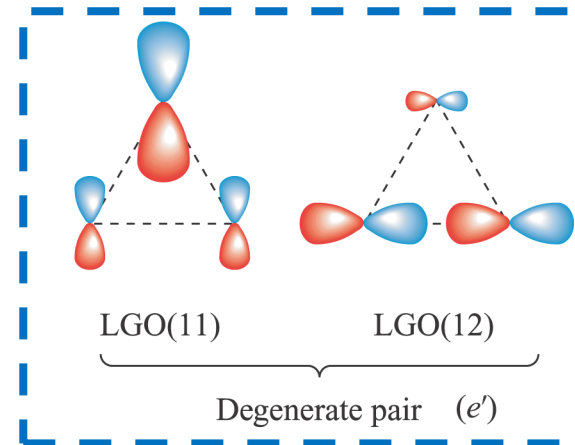
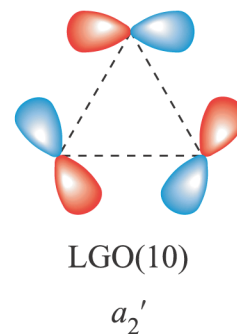
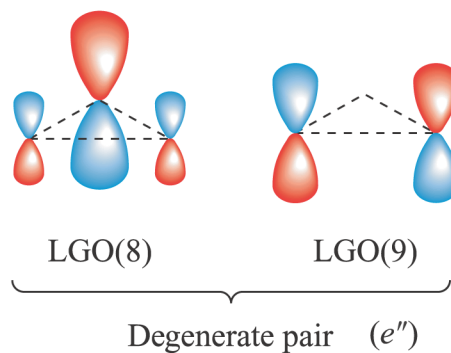
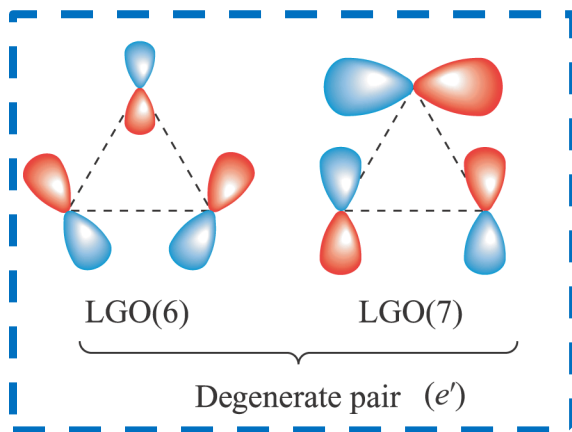
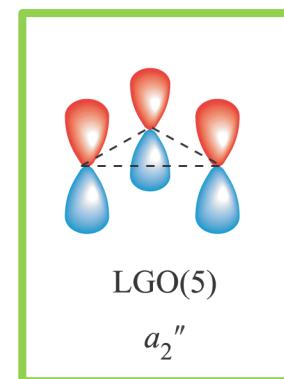
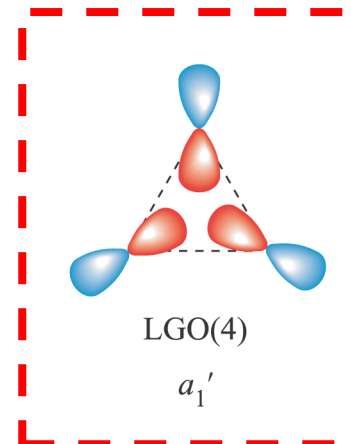
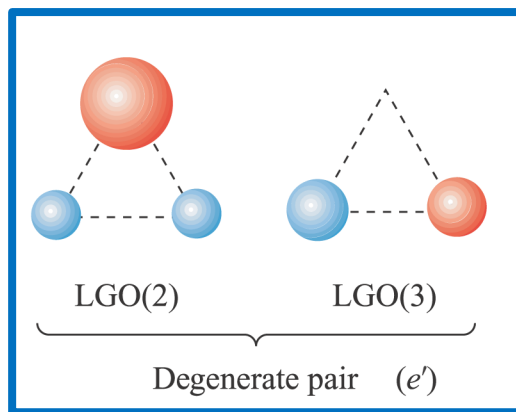
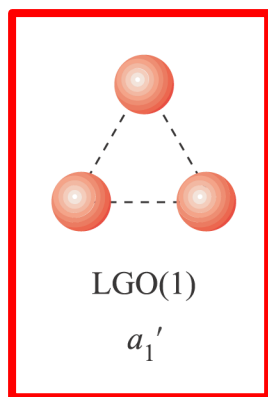
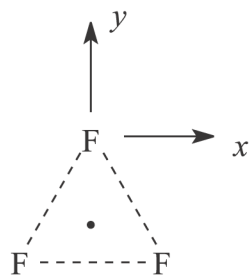


Representation of the *a*<sub>1</sub> bonding MO



<i>D</i> <sub>3h</sub>	<i>E</i>	<i>2C</i> <sub>3</sub>	<i>3C</i> <sub>2</sub>	<i>σ</i> <sub>h</sub>	<i>2S</i> <sub>3</sub>	<i>3σ</i> <sub>v</sub>		
<i>A</i> <sub>1</sub> '	1	1	1	1	1	1		<i>x</i> <sup>2</sup> + <i>y</i> <sup>2</sup> , <i>z</i> <sup>2</sup>
<i>A</i> <sub>2</sub> '	1	1	-1	1	1	-1	<i>R</i> <sub>z</sub>	
<i>E</i> '	2	-1	0	2	-1	0	( <i>x</i> , <i>y</i> )	( <i>x</i> <sup>2</sup> - <i>y</i> <sup>2</sup> , <i>xy</i> )
<i>A</i> <sub>1</sub> ''	1	1	1	-1	-1	-1		
<i>A</i> <sub>2</sub> ''	1	1	-1	-1	-1	1	<i>z</i>	
<i>E</i> ''	2	-1	0	-2	1	0	( <i>R</i> <sub>x</sub> , <i>R</i> <sub>y</sub> )	( <i>xz</i> , <i>yz</i> )

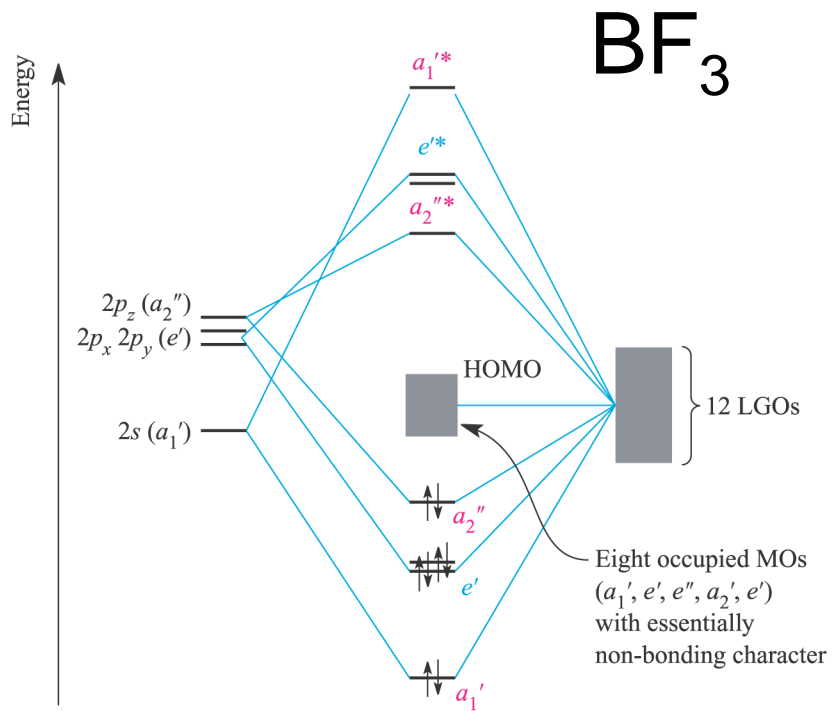
# BF<sub>3</sub>



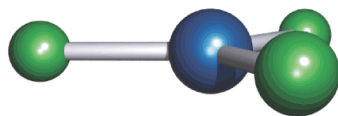
tre  $2p_z$

$E$	$C_3$	$C_2$	$\sigma_h$	$S_3$	$\sigma_v$
3	0	-1	-3	0	1

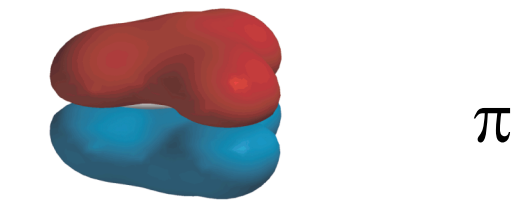
$A_2'' + E''$



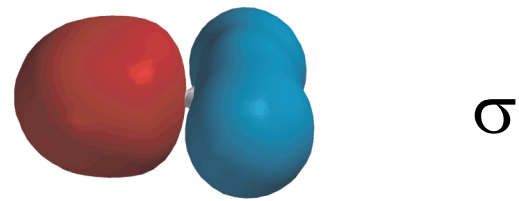
B                      BF<sub>3</sub>                      F<sub>3</sub> fragment



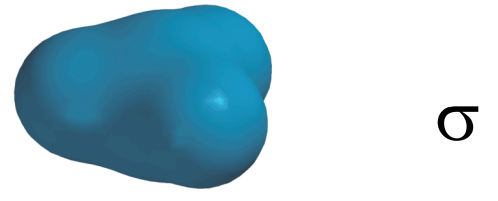
$D_{3h}$



Representation of the  $a_2''$  MO



Representation of one of the  $e'$  MOs



Representation of the  $a_1'$  MO

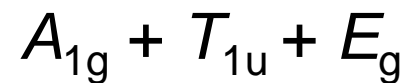
Ordine di legame 4/3

# Molecole ipervalenti: SF<sub>6</sub> (gruppo O<sub>h</sub>)

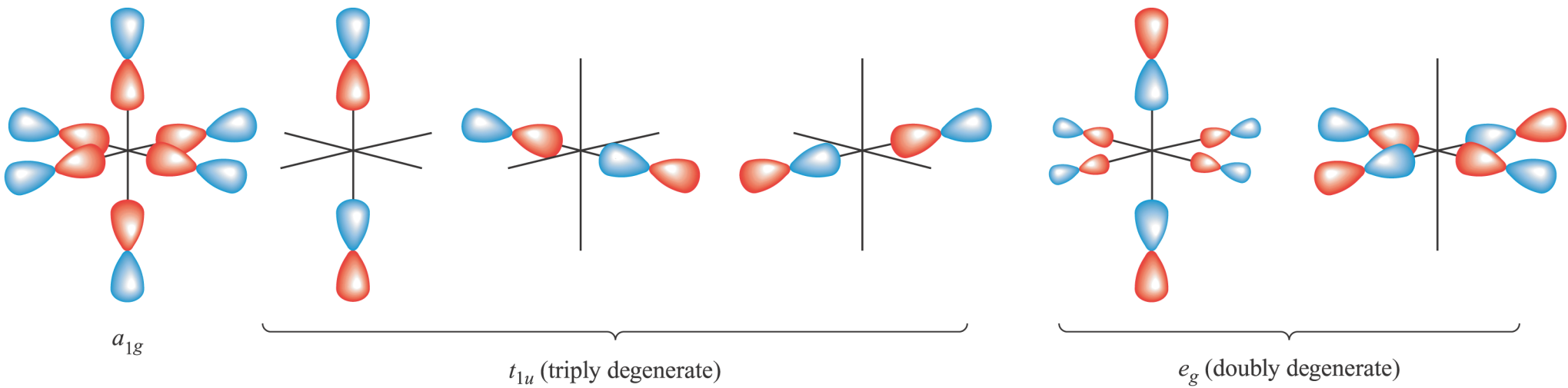
O <sub>h</sub>	E	8C <sub>3</sub>	6C <sub>2</sub>	6C <sub>4</sub>	3C <sub>2</sub> (= C <sub>4</sub> <sup>2</sup> )	i	6S <sub>4</sub>	8S <sub>6</sub>	3σ <sub>h</sub>	6σ <sub>d</sub>
A <sub>1g</sub>	1	1	1	1	1	1	1	1	1	1
A <sub>2g</sub>	1	1	-1	-1	1	1	-1	1	1	-1
E <sub>g</sub>	2	-1	0	0	2	2	0	-1	2	0
T <sub>1g</sub>	3	0	-1	1	-1	3	1	0	-1	-1
T <sub>2g</sub>	3	0	1	-1	-1	3	-1	0	-1	1
A <sub>1u</sub>	1	1	1	1	1	-1	-1	-1	-1	-1
A <sub>2u</sub>	1	1	-1	-1	1	-1	1	-1	-1	1
E <sub>u</sub>	2	-1	0	0	2	-2	0	1	-2	0
T <sub>1u</sub>	3	0	-1	1	-1	-3	-1	0	1	1
T <sub>2u</sub>	3	0	1	-1	-1	-3	1	0	1	-1

sei 2p<sub>z</sub> radiali

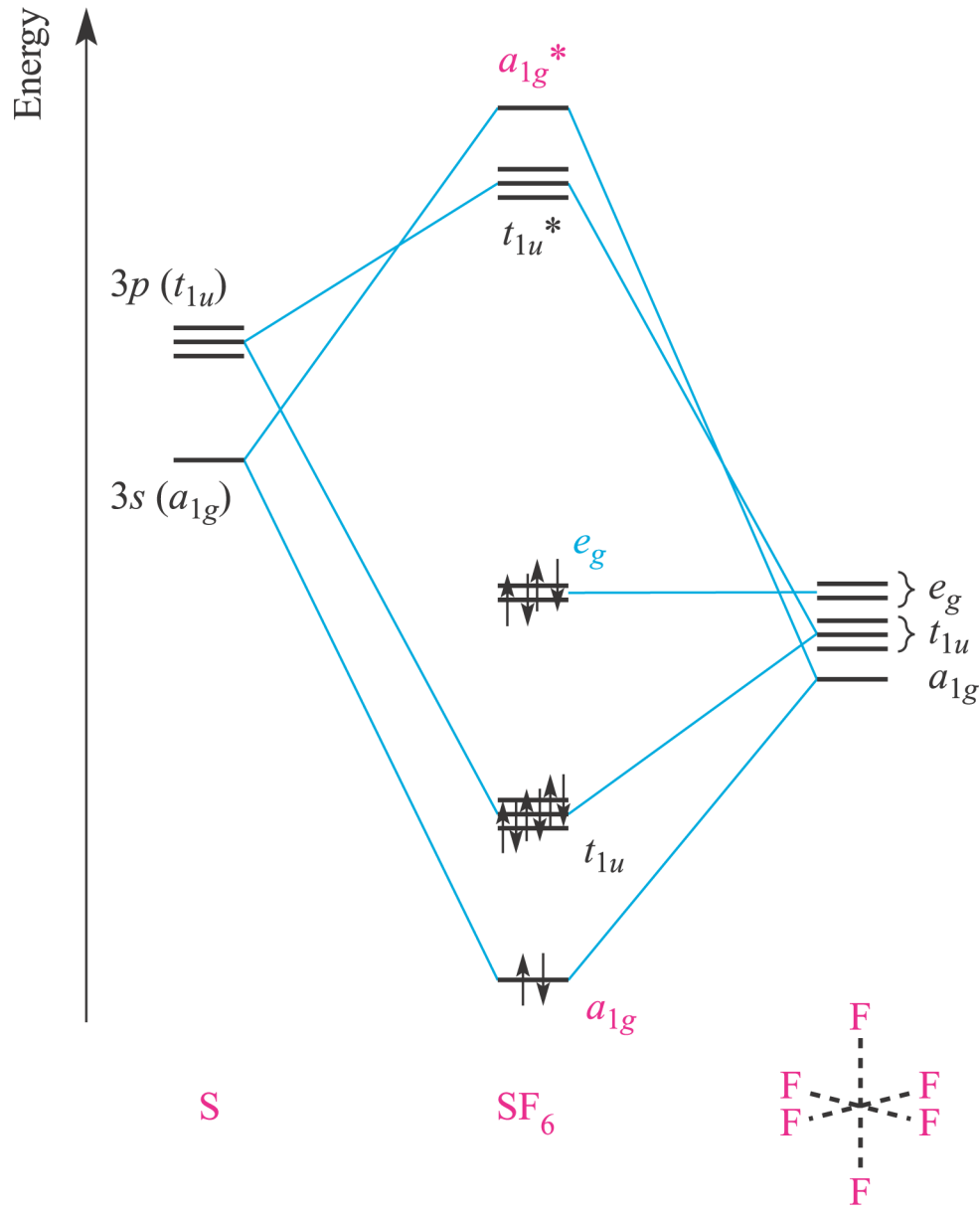
E	8C <sub>3</sub>	6C <sub>2</sub>	6C <sub>4</sub>	3C <sub>2</sub>	i	6S <sub>4</sub>	8S <sub>6</sub>	3σ <sub>h</sub>	6σ <sub>d</sub>
6	0	0	2	2	0	0	0	4	2



# LGO del frammento $F_6$ in $SF_6$



nonlegame

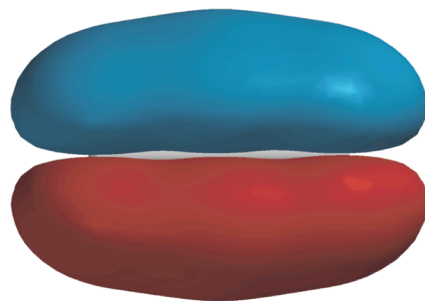
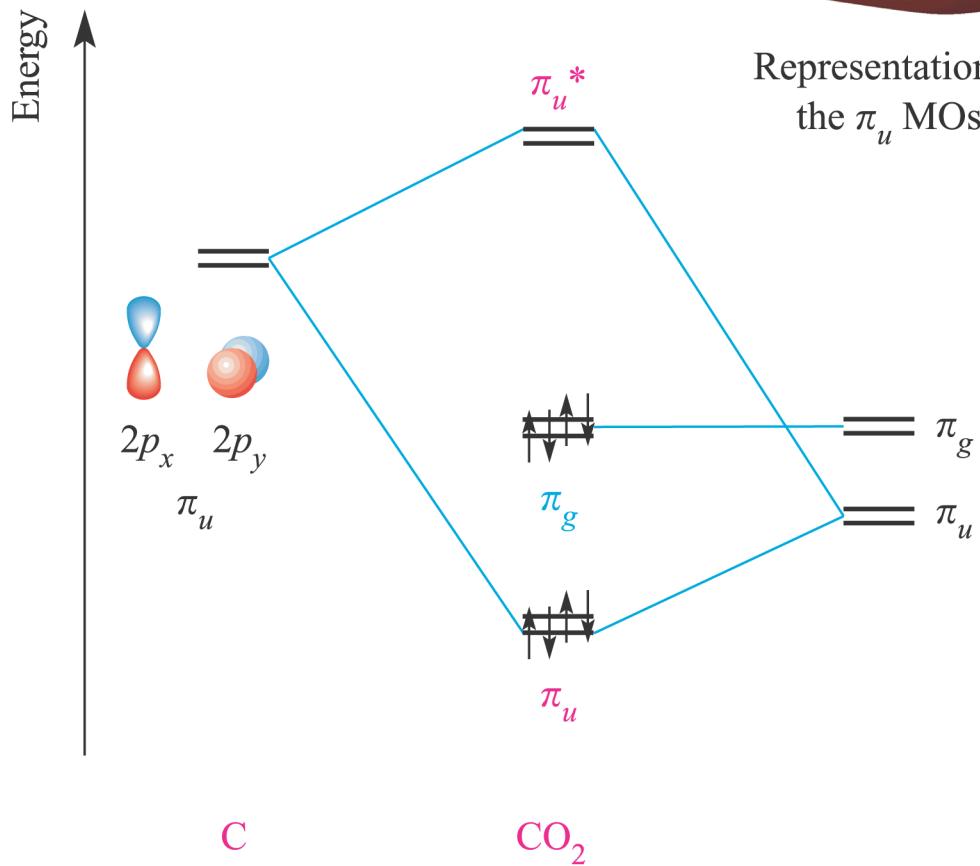


Ordine di legame 2/3,  
nessun orbitale d

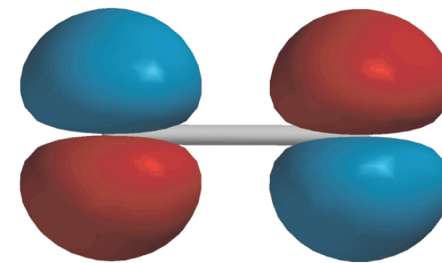


# CO<sub>2</sub>

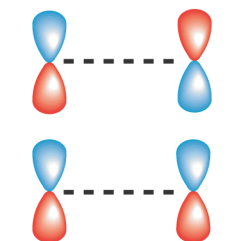
## Diagrammi MO parziali



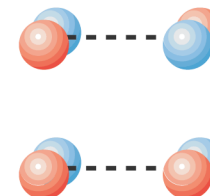
Representation of one of the  $\pi_u$  MOs in CO<sub>2</sub>



Representation of one of the  $\pi_g$  MOs in CO<sub>2</sub>



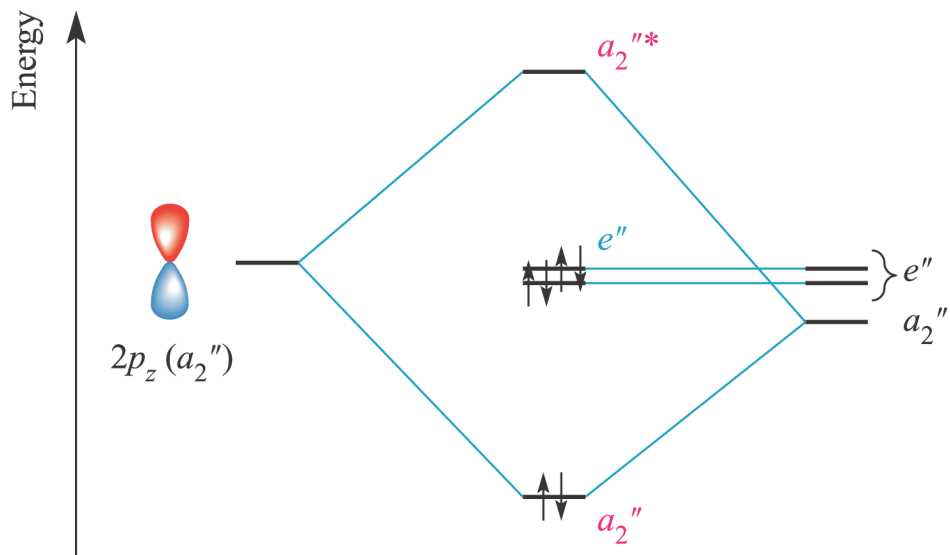
Combination of  $2p_x$  orbitals



Combination of  $2p_y$  orbitals

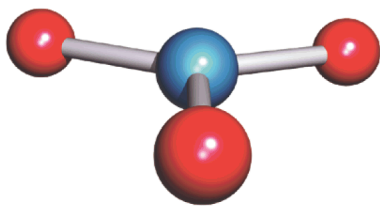


# NO<sub>3</sub><sup>-</sup>

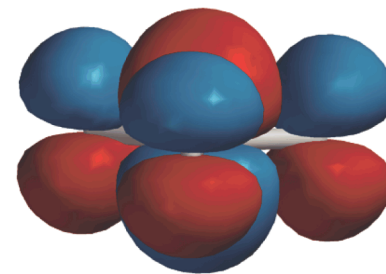
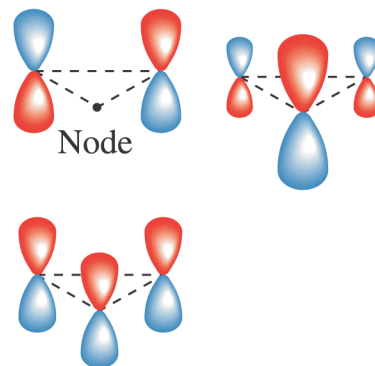


N

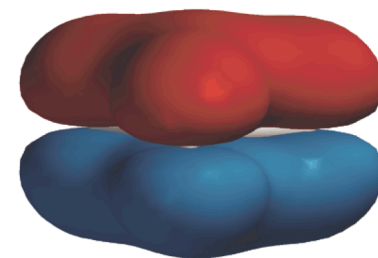
[NO<sub>3</sub>]<sup>-</sup>



$D_{3h}$

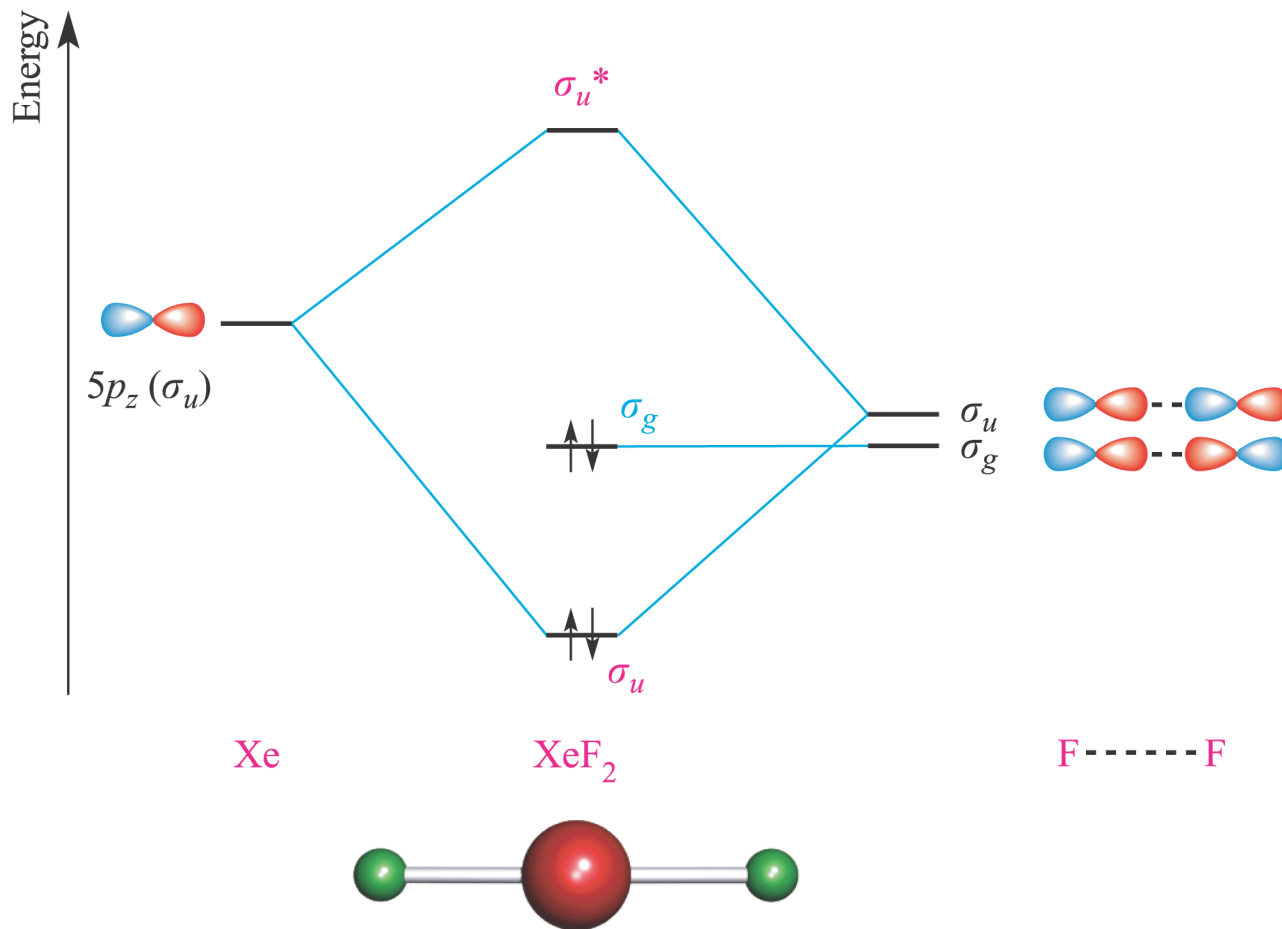


A representation of the  $a_2''^*$  MO

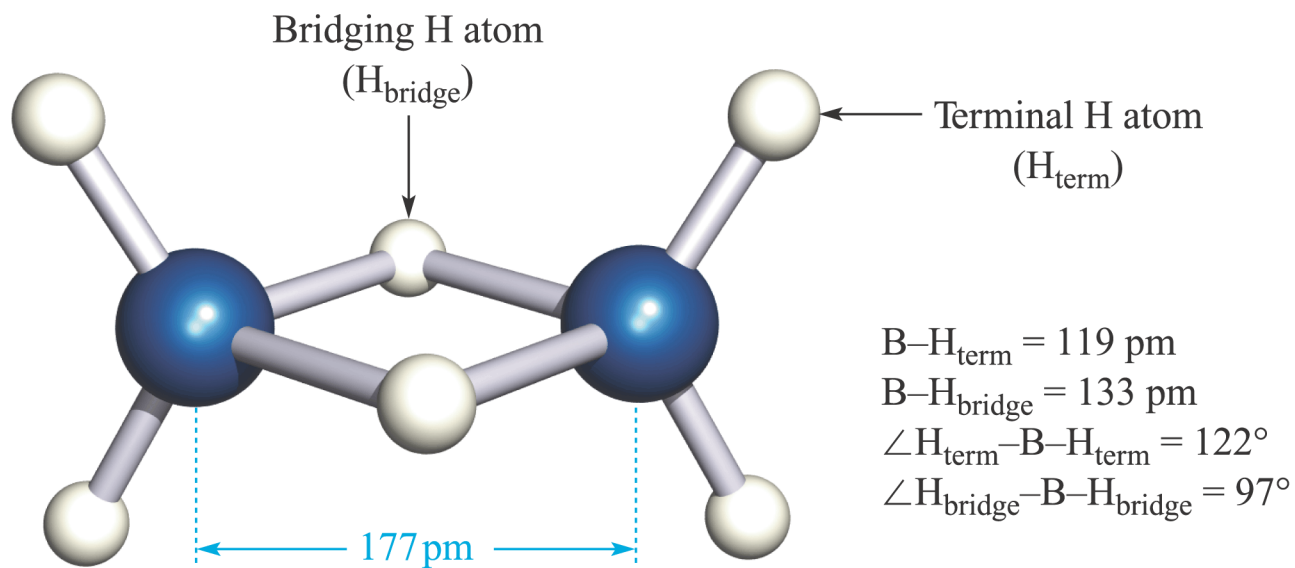


A representation of the  $a_2''$  MO showing the delocalization of  $\pi$ -character over the N and O centres

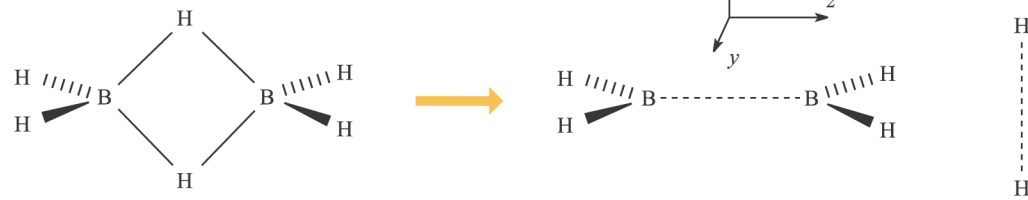
# Interazione 3c – 2e



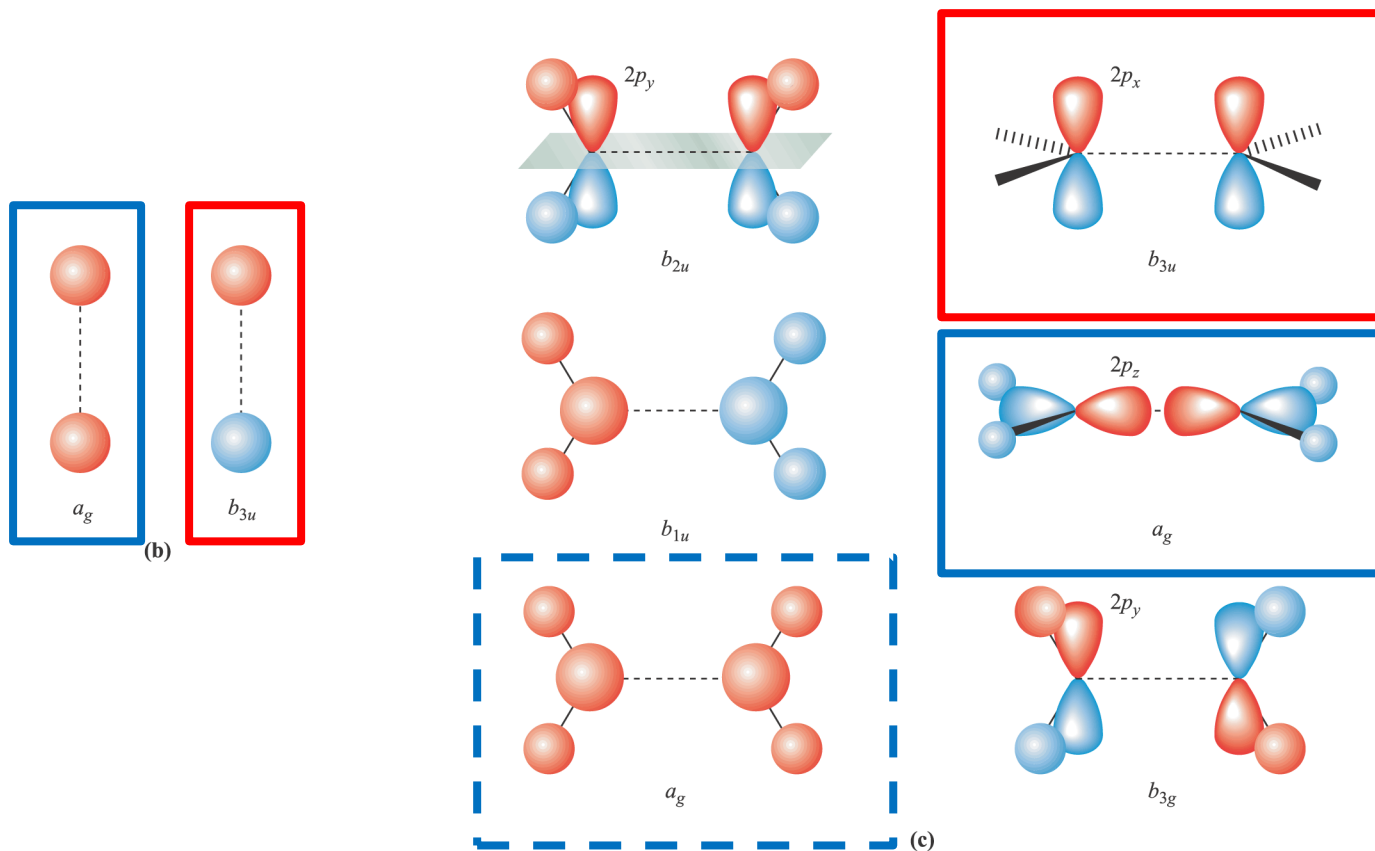
# Diborano, B<sub>2</sub>H<sub>6</sub>



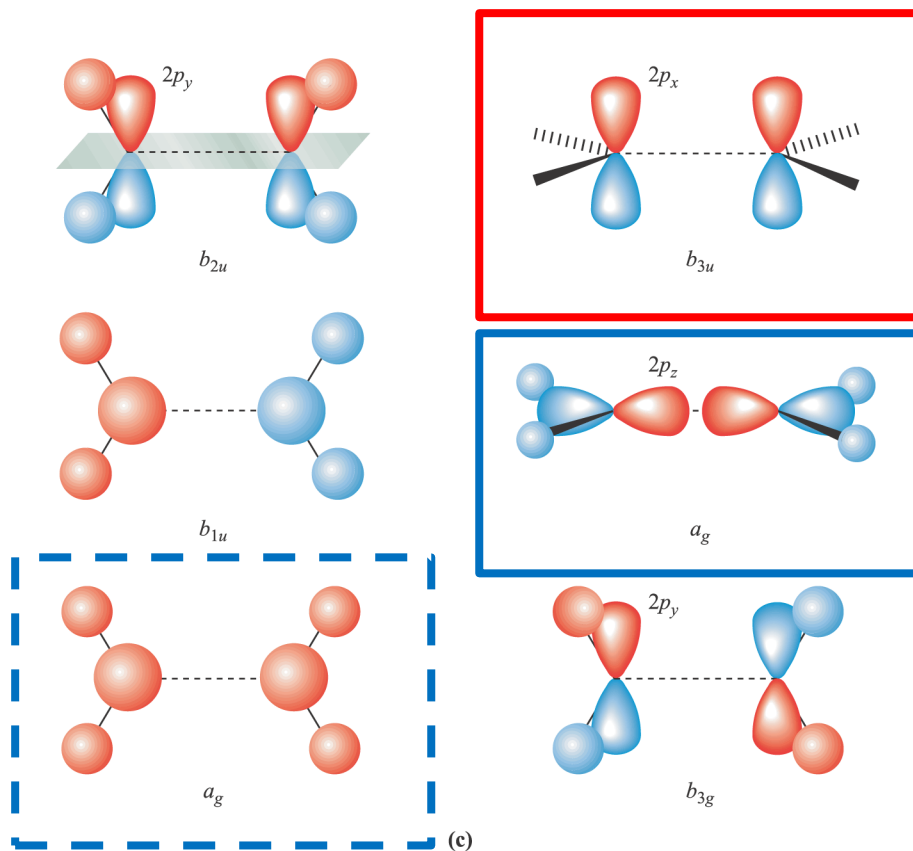
$D_{2h}$



(a)

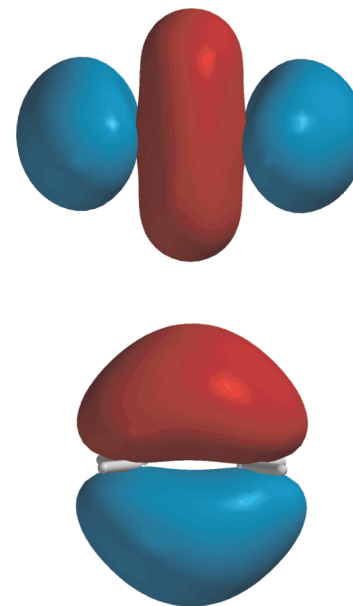
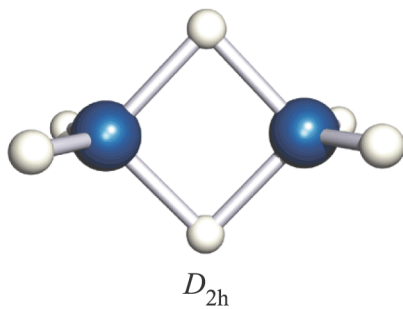
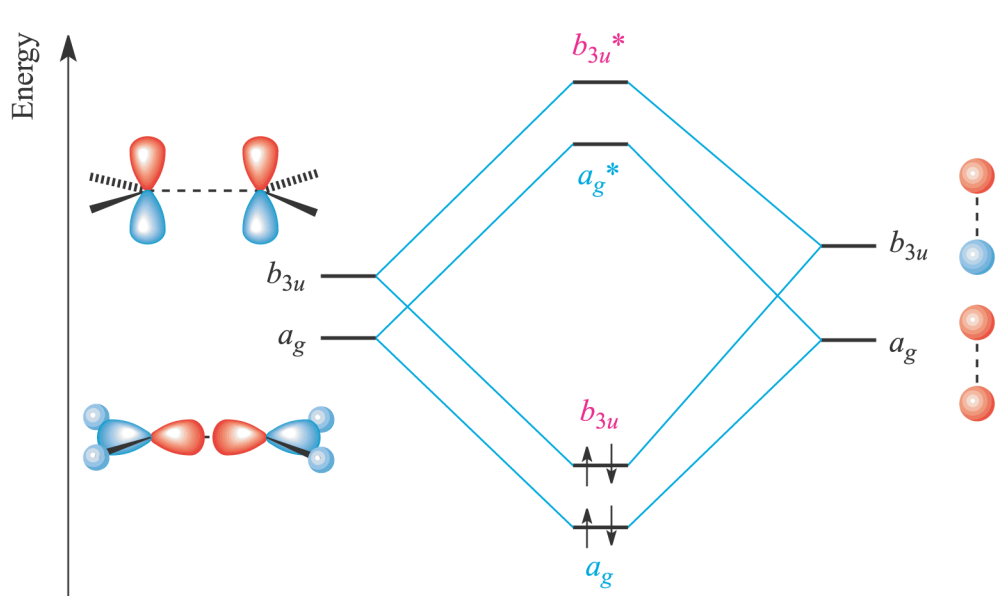


(b)



(c)

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