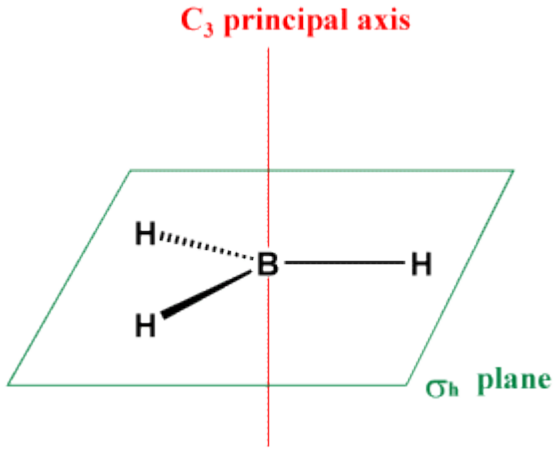
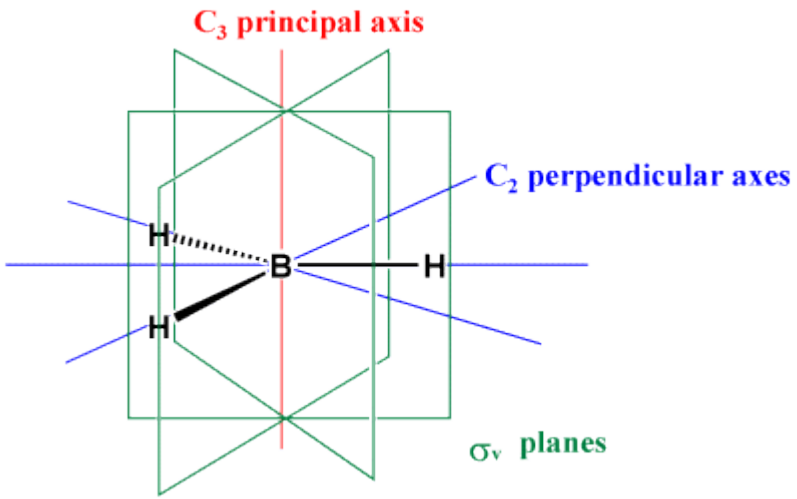
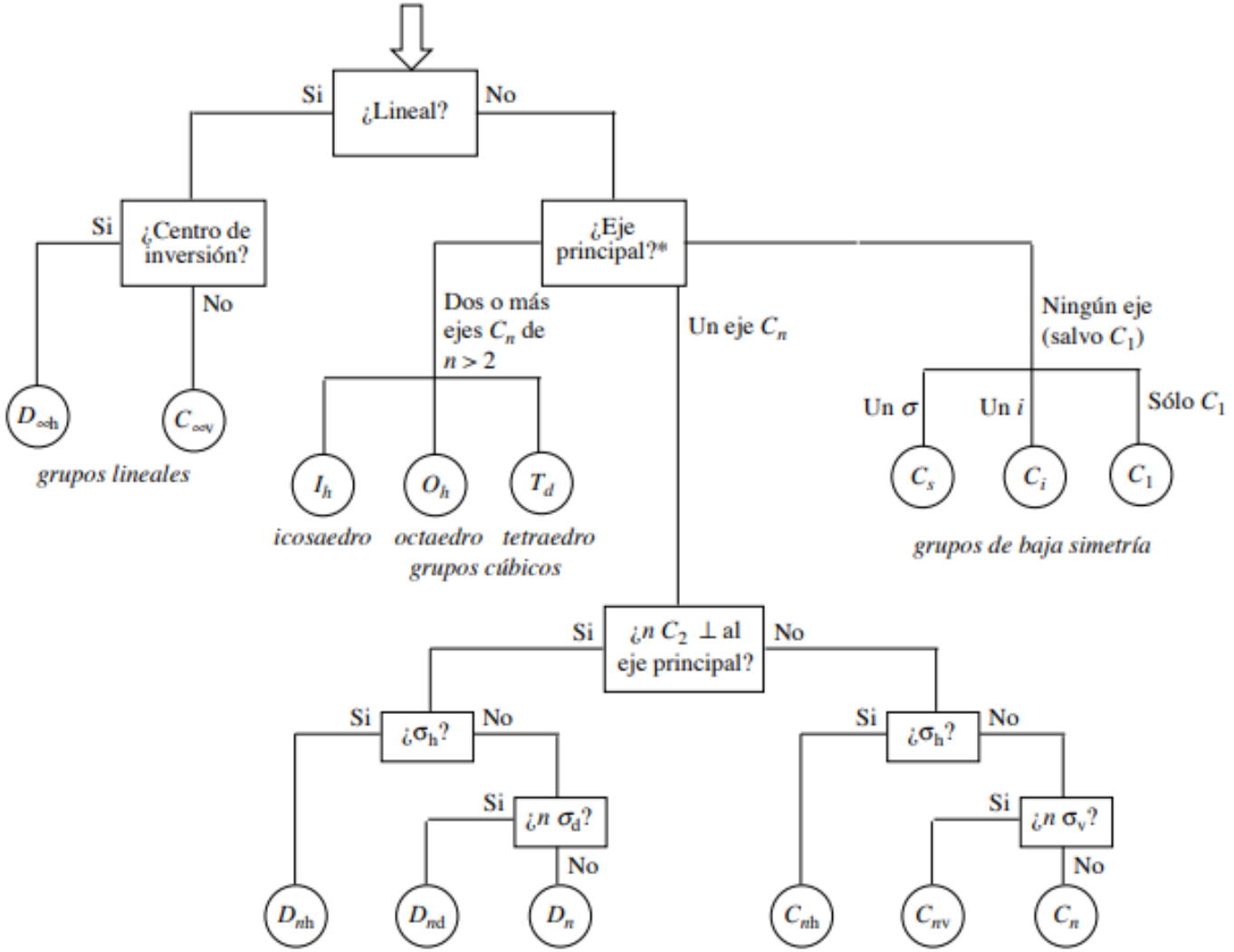
Orbital Molecular BH_3

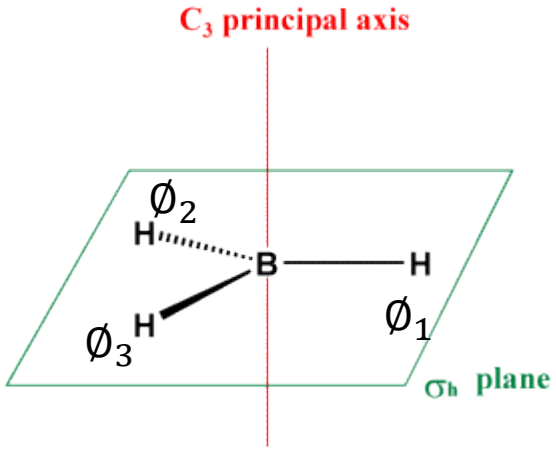


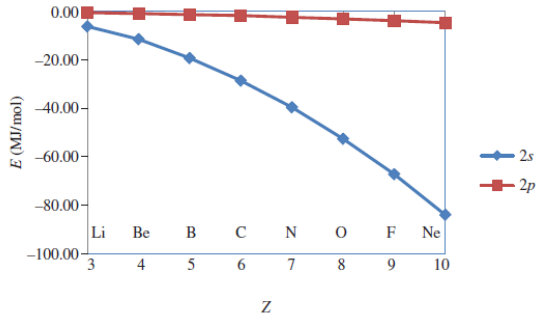




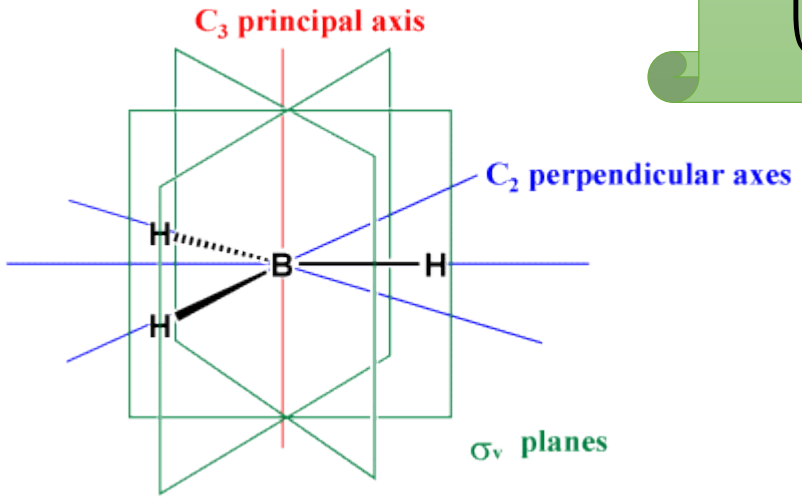
D_{3h}

$$OM = OA_{ac} + CLAS$$





$$OA_B$$
$$2s = A_1^{'}$$
$$2p \begin{cases} p_z = A_2^{''} \\ p_{x=E^{'}} \\ p_{yE^{'}} \end{cases}$$



Combinación Lineal Adaptada por Simetría (CLAS-SALC)

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$
Γ_{3H}	3	0	1	3	0	1

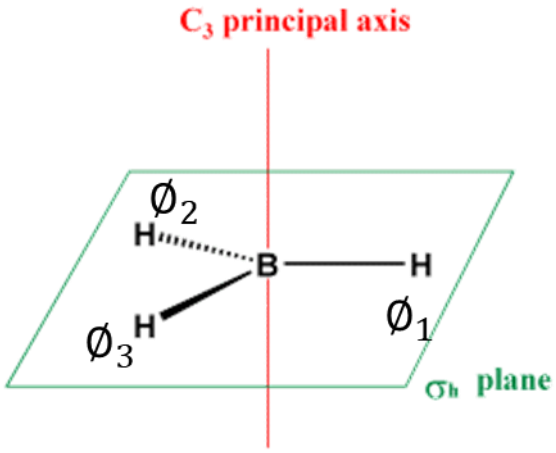
$$\Gamma_{3H} = A_1^{'} + E^{'} \Rightarrow n_i = \frac{1}{h}\Sigma g_r X_v(R) X_i(R)$$

Tabla de caracteres para el grupo puntual D_{3h}

	E	$2C_3$	$3C'_2$	σ_h	$2S_3$	$3\sigma_v$	linear, rotations	quadratic
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)

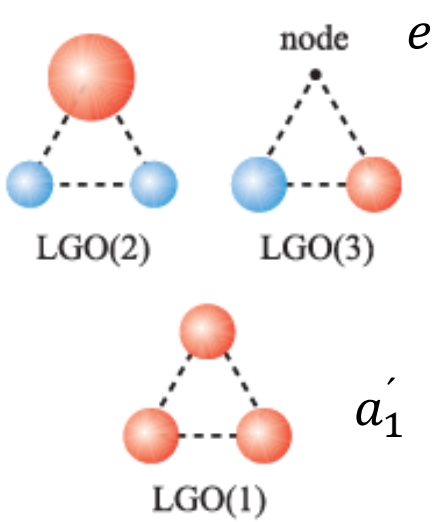
$$E^{'} = \frac{1}{12}(1*3*2 + 2*0*-1 + 3*1*0 + 1*3*2 + 2*0*-1 + 3*1*0) = 1E^{'}$$

Operador de Proyección



D_{3h}	E	C_3^1	C_3^{-1}	C_2'	C_2''	C_2'''	σ_h	S_3	S_3^{-1}	σ_v'	σ_v''	σ_v'''
Φ_1	Φ_1	Φ_2	Φ_3	Φ_1	Φ_2	Φ_3	Φ_1	Φ_2	Φ_3	Φ_1	Φ_2	Φ_3
a_1'	1	1	1	1	1	1	1	1	1	1	1	1
e'	2	-1	-1	0	0	0	2	-1	-1	0	0	0

$$a_1' = 4(\Phi_1 + \Phi_2 + \Phi_3)$$

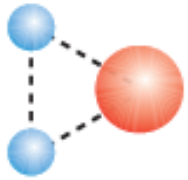


e'

a_1'

$$e' = 2\,(2\Phi_1 - \Phi_2 - \Phi_3)$$

Como es bidimensional debe tener dos representaciones

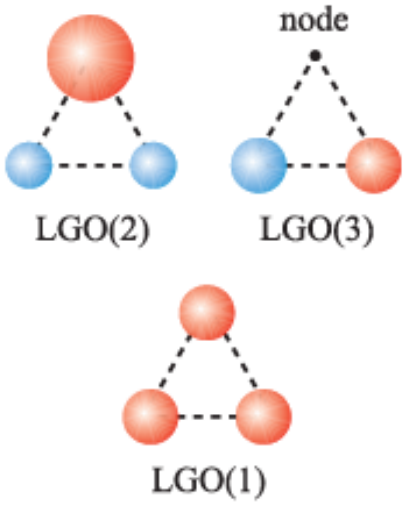


$$C_3(2\Phi_1 - \Phi_2 - \Phi_3)$$
$$-(-\Phi_1 + 2\Phi_2 - \Phi_3)$$
$$3\Phi_1 - 3\Phi_2 - 0$$
$$3(\Phi_1 - \Phi_2)$$

Tabla de caracteres para el grupo puntual D_{3h}

	E	$2C_3$	$3C'_2$	σ_h	$2S_3$	$3\sigma_v$	linear, rotations	quadratic
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)

$CLAS\ 3H$ $OM\ BH_3$ OA_{Boro}



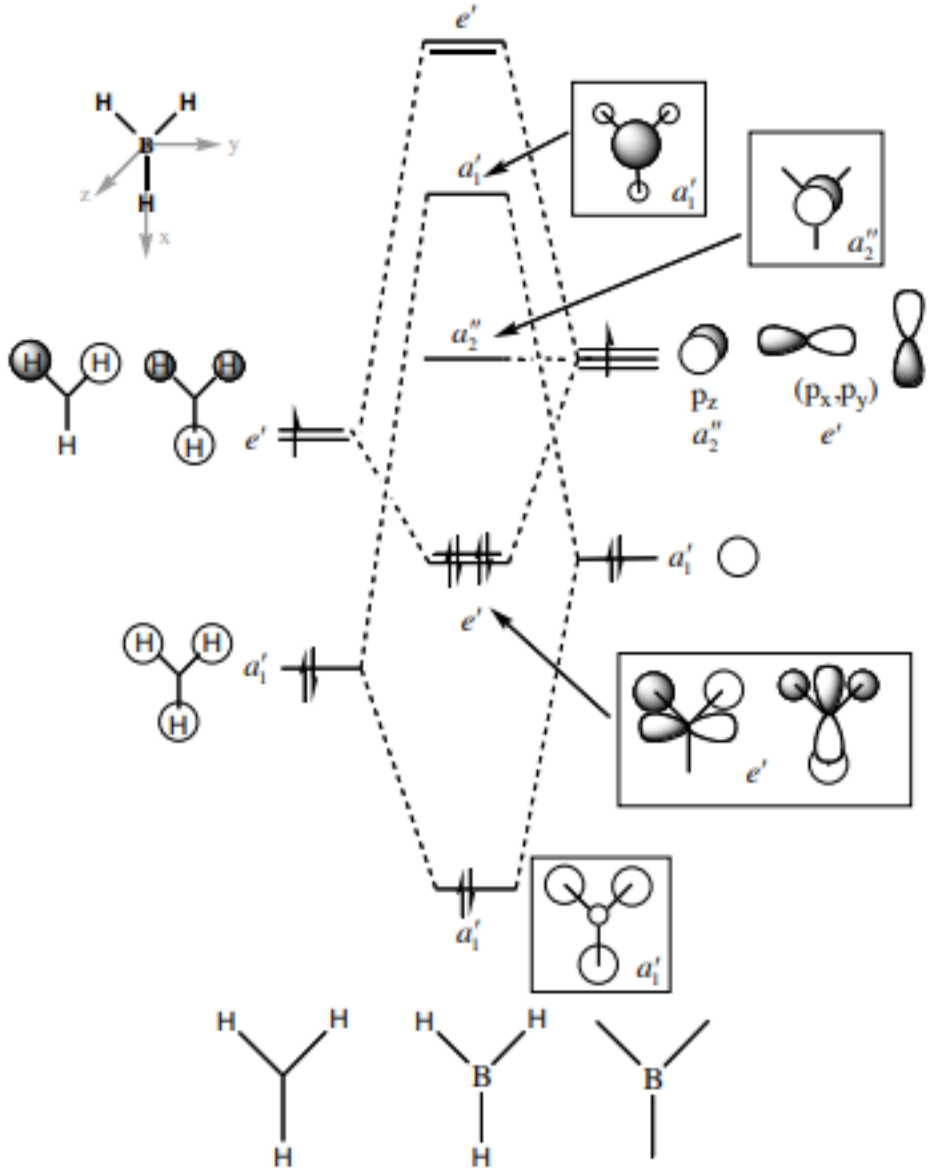
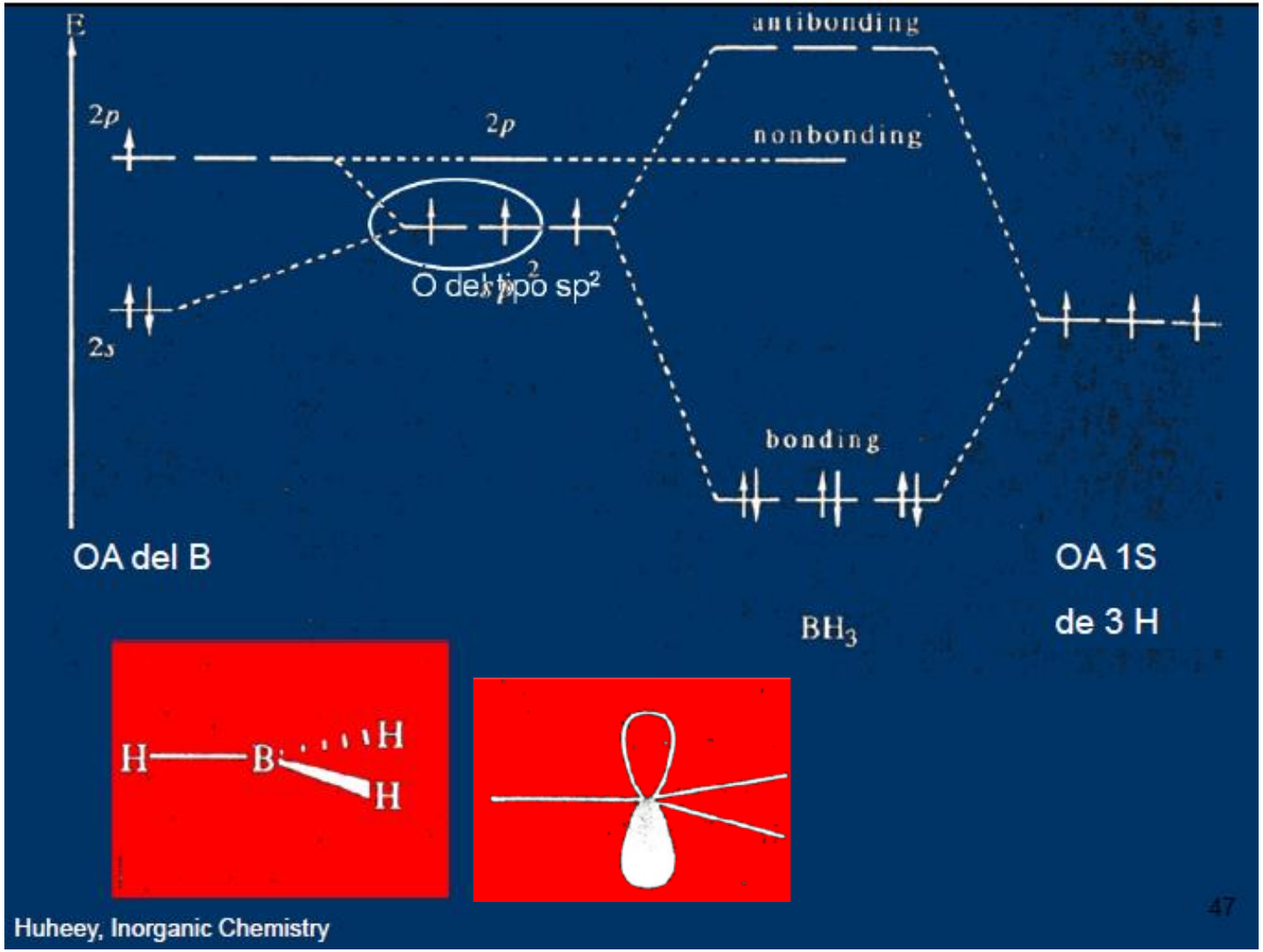


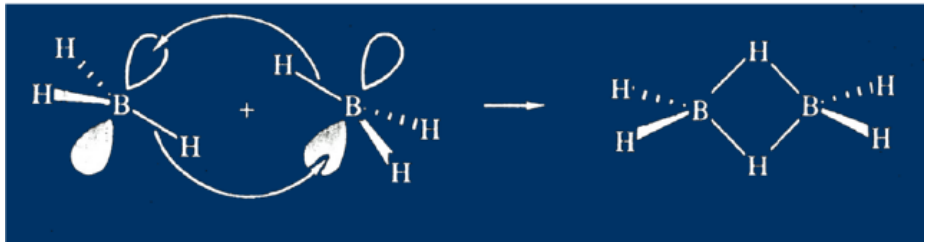
Figure 3 MO diagram for BH_3

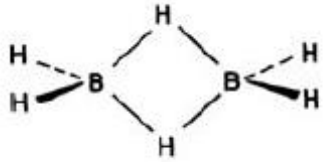
$$OA_B$$
$$2s = A_1^{'}$$
$$2p \begin{cases} p_z = A_2^{''} \\ p_{x=E^{'}} \\ p_{yE^{'}} \end{cases}$$

BH_3 ácido de Lewis

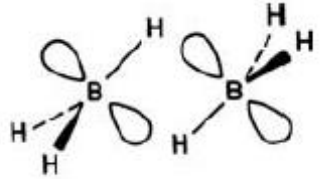


BH_3 dimeriza

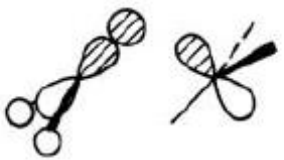




9.9



9.10

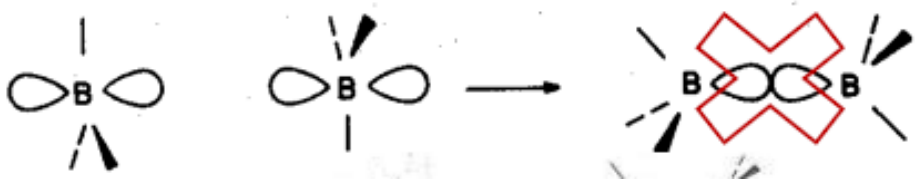


HOMO — LUMO

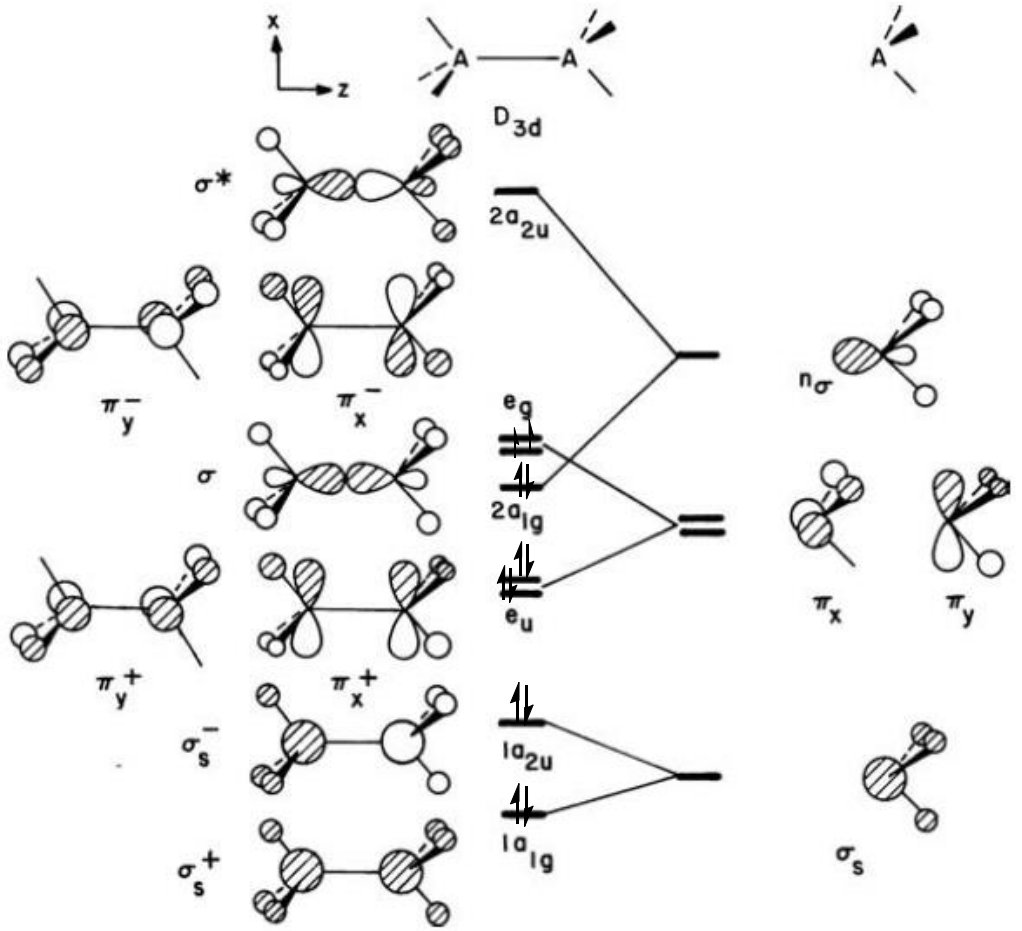
LUMO — HOMO

DIMERIZACIÓN

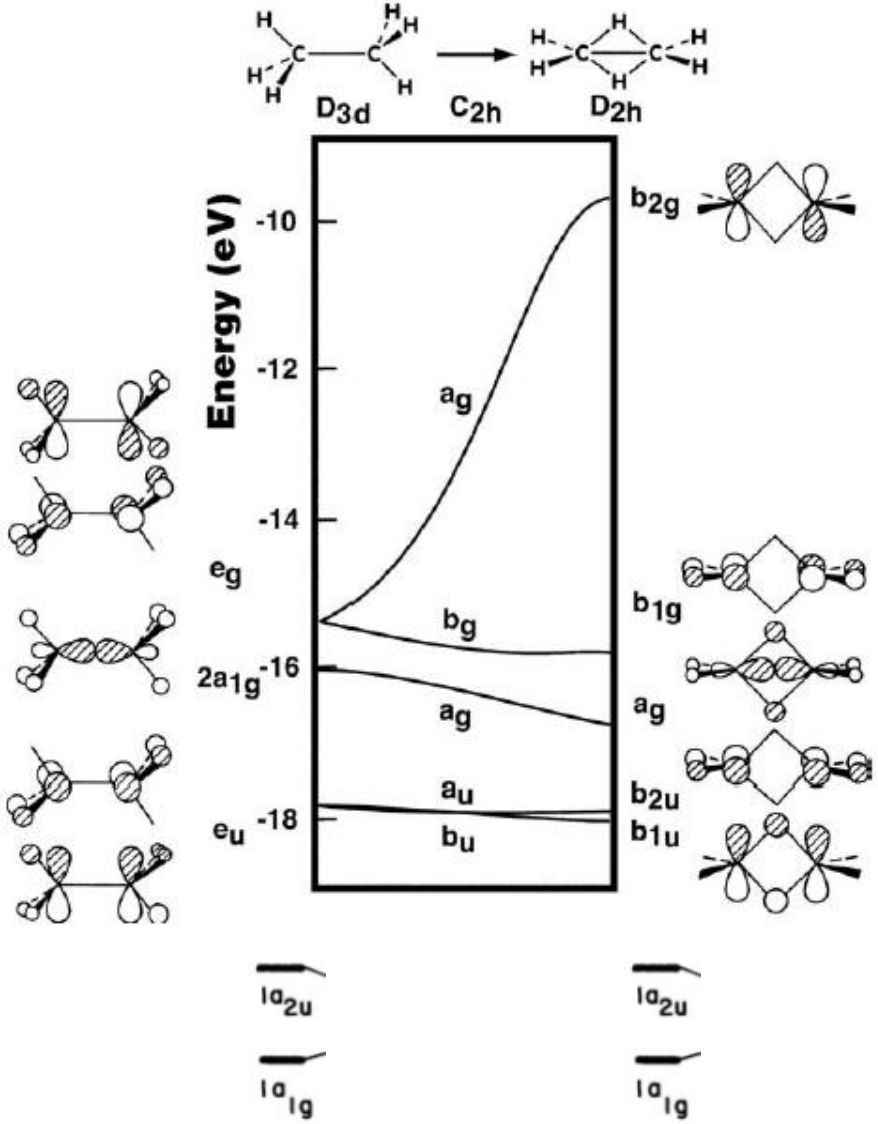
14 ELECTRONES

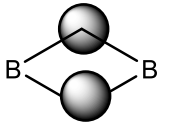


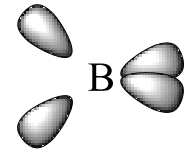
12 ELECTRONES



ORBITAL MOLECULAR DEL DIBORANO







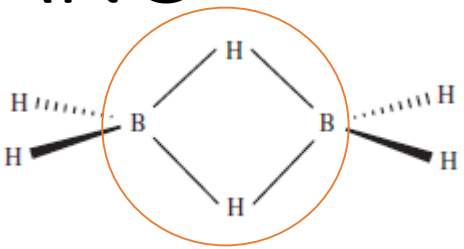
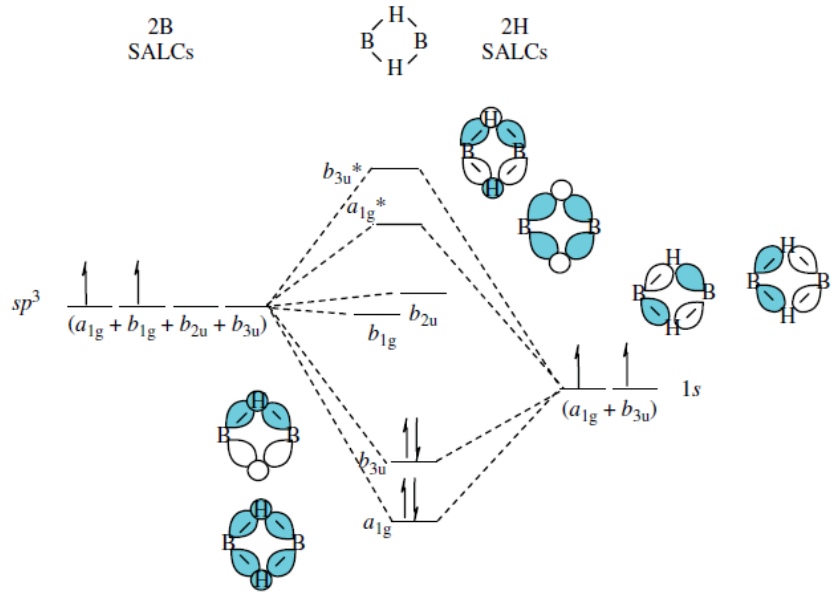
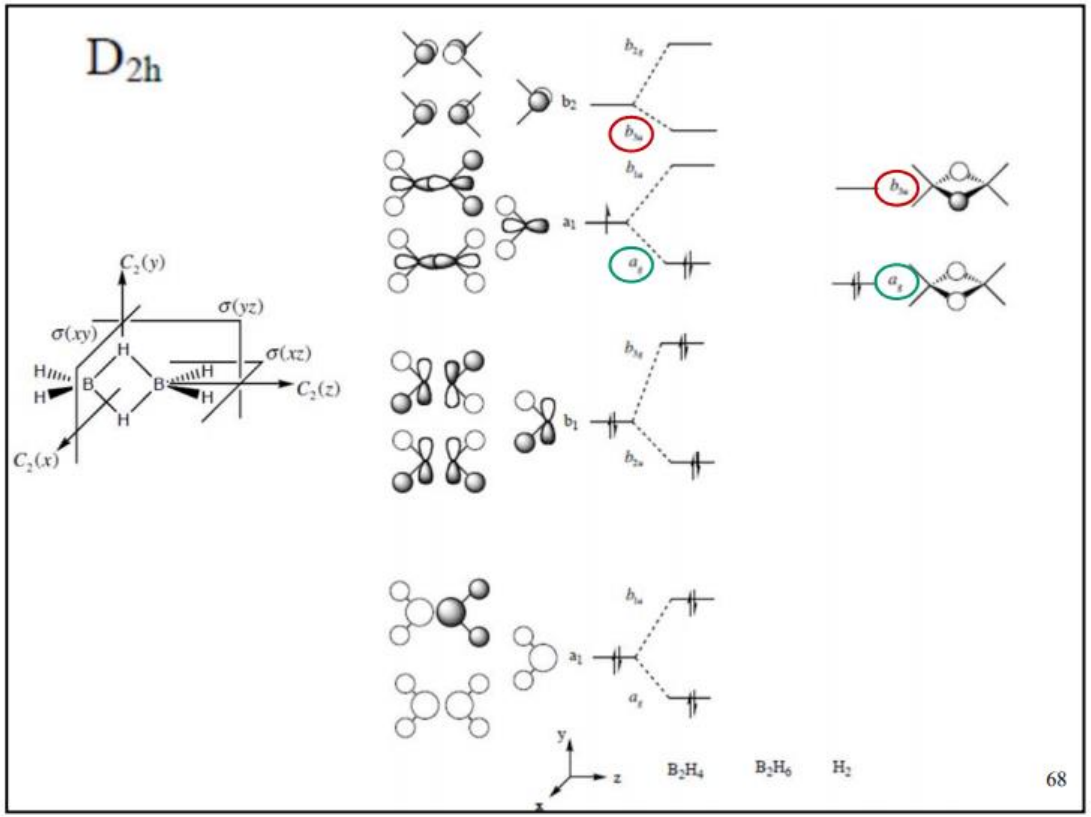


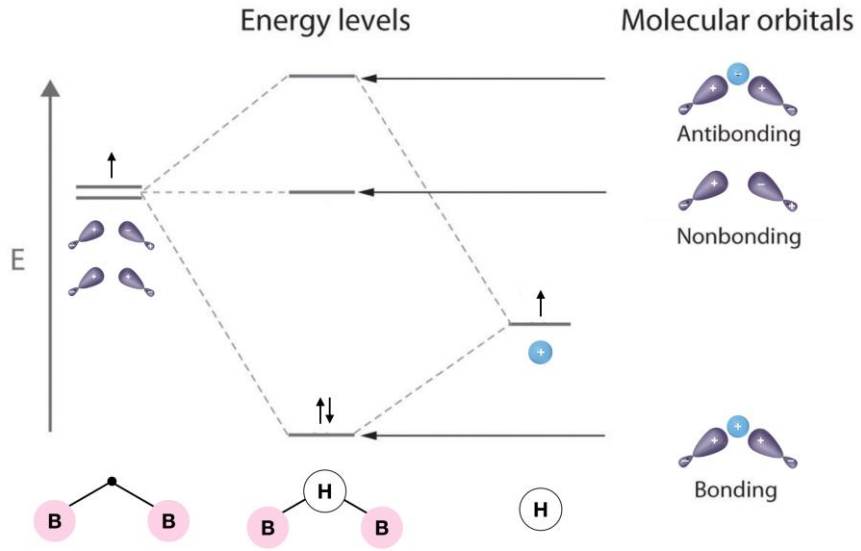
TABLE 10.17 Representations for the H and B orbitals involved in the B–H–B portion of diborane.

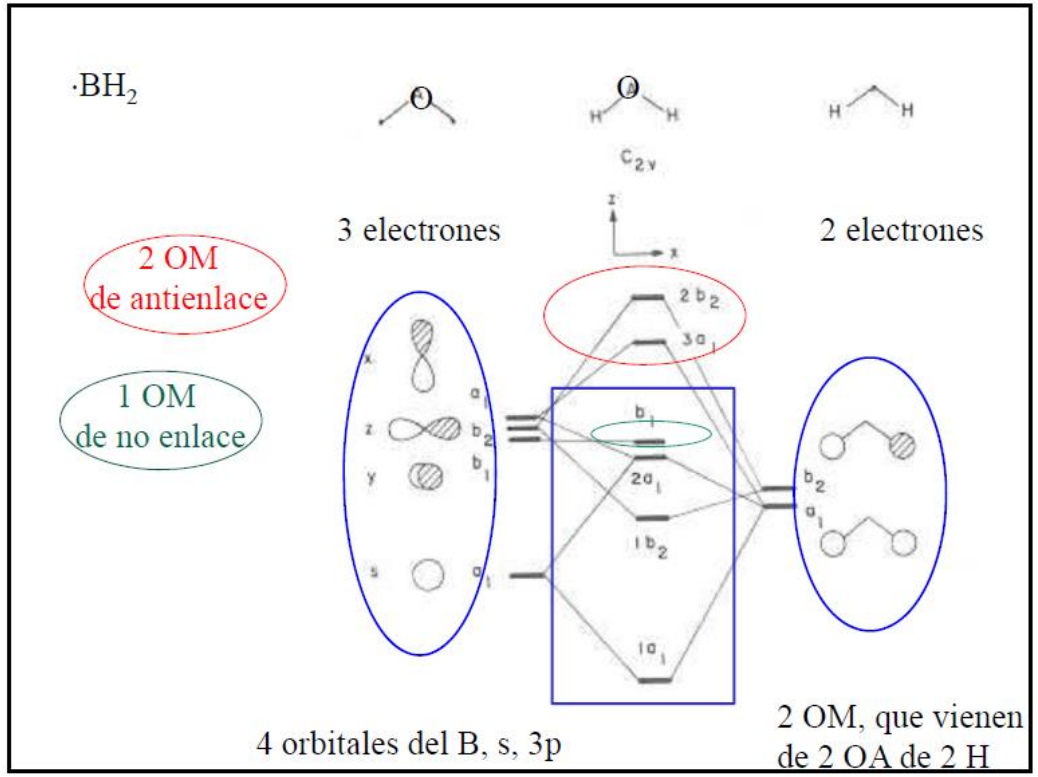
D_{2h}	E	C_2^z	C_2^y	C_2^x	i	σ_{xy}	σ_{xz}	σ_{yz}	IRRs:
Γ_H	2	0	0	2	0	2	2	0	$a_g + b_{3u}$
Γ_B	4	0	0	0	0	4	0	0	$a_g + b_{1g} + b_{2u} + b_{3u}$



FRAGMENTOS


D2h
$C_2(y)$
$\sigma(yz)$
$\sigma(xy)$
$\sigma(xz)$
$C_2(z)$
$C_2(x)$
b_2
a_1
b_1
a_1
B_2H_4
B_2H_6
H_2
68


Energy levels
Molecular orbitals
E
Antibonding
Nonbonding
Bonding
B
B
H
B
B
H


·BH_2
C_{2v}
3 electrones
2 electrones
2 OM
de antienlace
1 OM
de no enlace
$2b_2$
$3a_1$
b_1
$2a_1$
$1b_2$
$1a_1$
4 orbitales del B, s, 3p
2 OM, que vienen
de 2 OA de 2 H

Hidruros

Tabla 3.- Clasificación de hidruros de los bloques s y p

1	2	13	14	15	16	17
LiH	$(BeH_2)_n$	$(BH_3)_n$	CH_4	NH_3	H_2O	HF
NaH	MgH_2	$(AlH_3)_n$	SiH_4	PH_3	H_2S	HCl
KH	CaH_2	"GaH_3"	GeH_4	AsH_3	H_2Se	HBr
RbH	SrH_2		SnH_4	SbH_3	H_2Te	HI
CsH	BaH_2		PbH_4	BiH_3		
Iónicos		Poliméricos	Covalentes moleculares