

Química de Coordenação (IQG-241)

Química Inorgânica II (IQG-364)

QAT - Química - Licenciatura



Aula 6

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Departamento de Química Inorgânica



17/03/2024

Teoria de orbitais moleculares

Diagrama de orbitais moleculares da água (C_{2v})

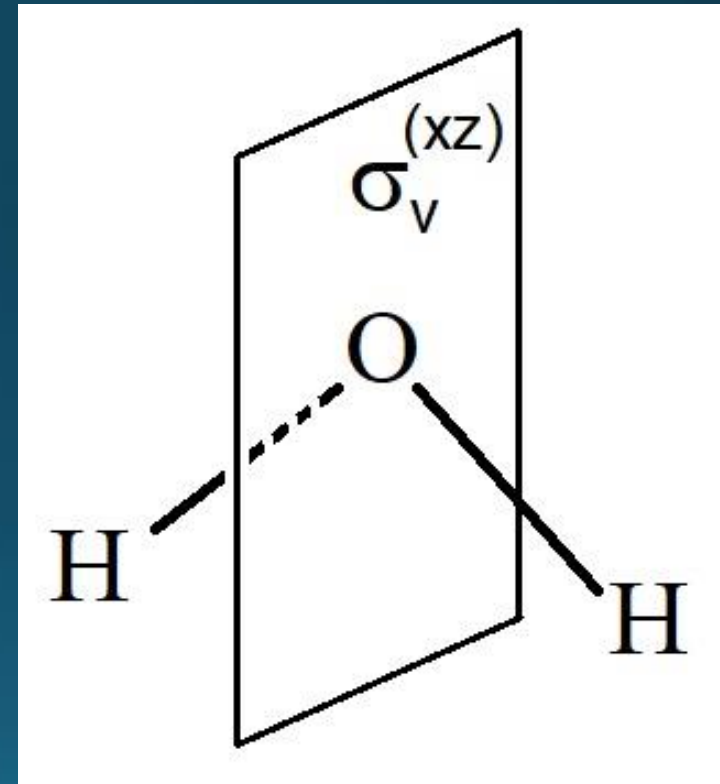
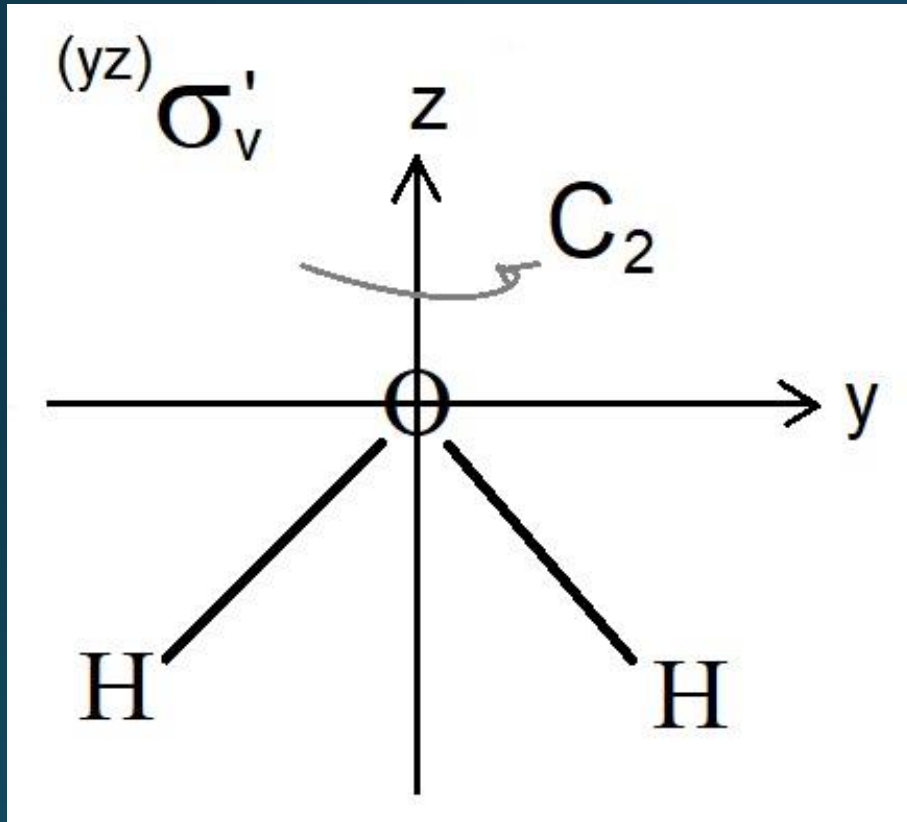


Diagrama de orbitais moleculares da água (C_{2v})

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma'_v(yz)$
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1

Diagrama de orbitais moleculares da água (C_{2v})

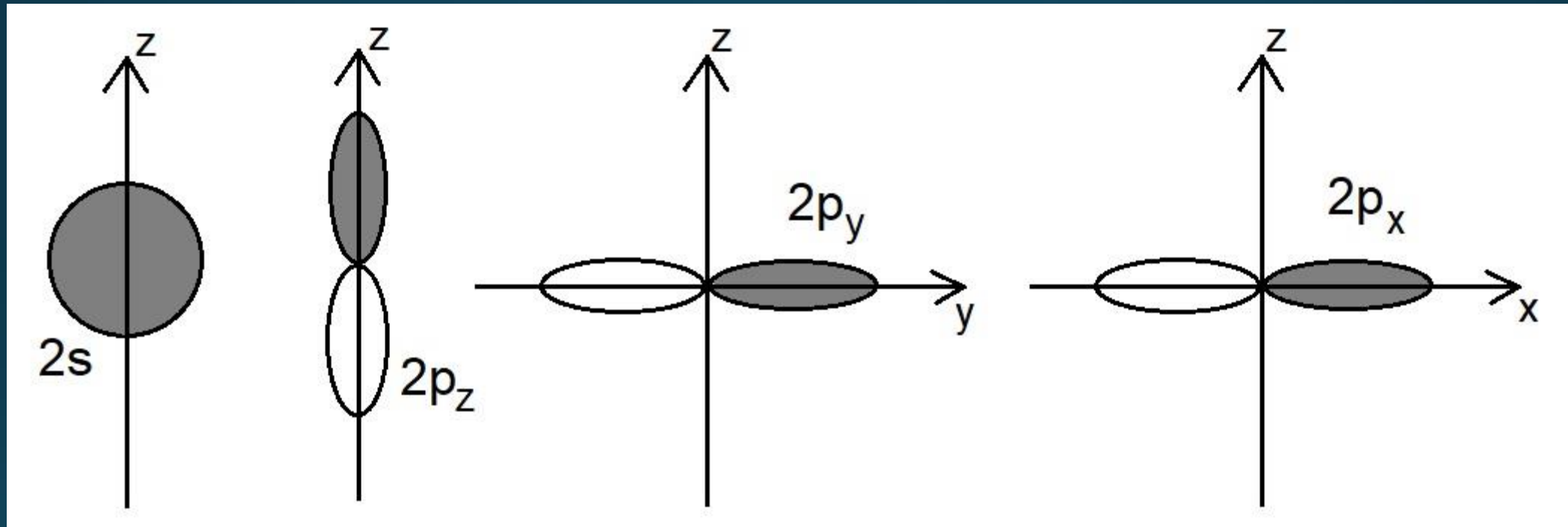


Diagrama de orbitais moleculares da água (C_{2v})

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A_1	1	1	1	1	
A_2	1	1	-1	-1	
B_1	1	-1	1	-1	
B_2	1	-1	-1	1	
<hr/>					
2s	1	1	1	1	A_1
$2p_z$	1	1	1	1	A_1
$2p_y$	1	-1	-1	1	B_2
$2p_x$	1	-1	1	-1	B_1

Diagrama de orbitais moleculares da água (C_{2v})

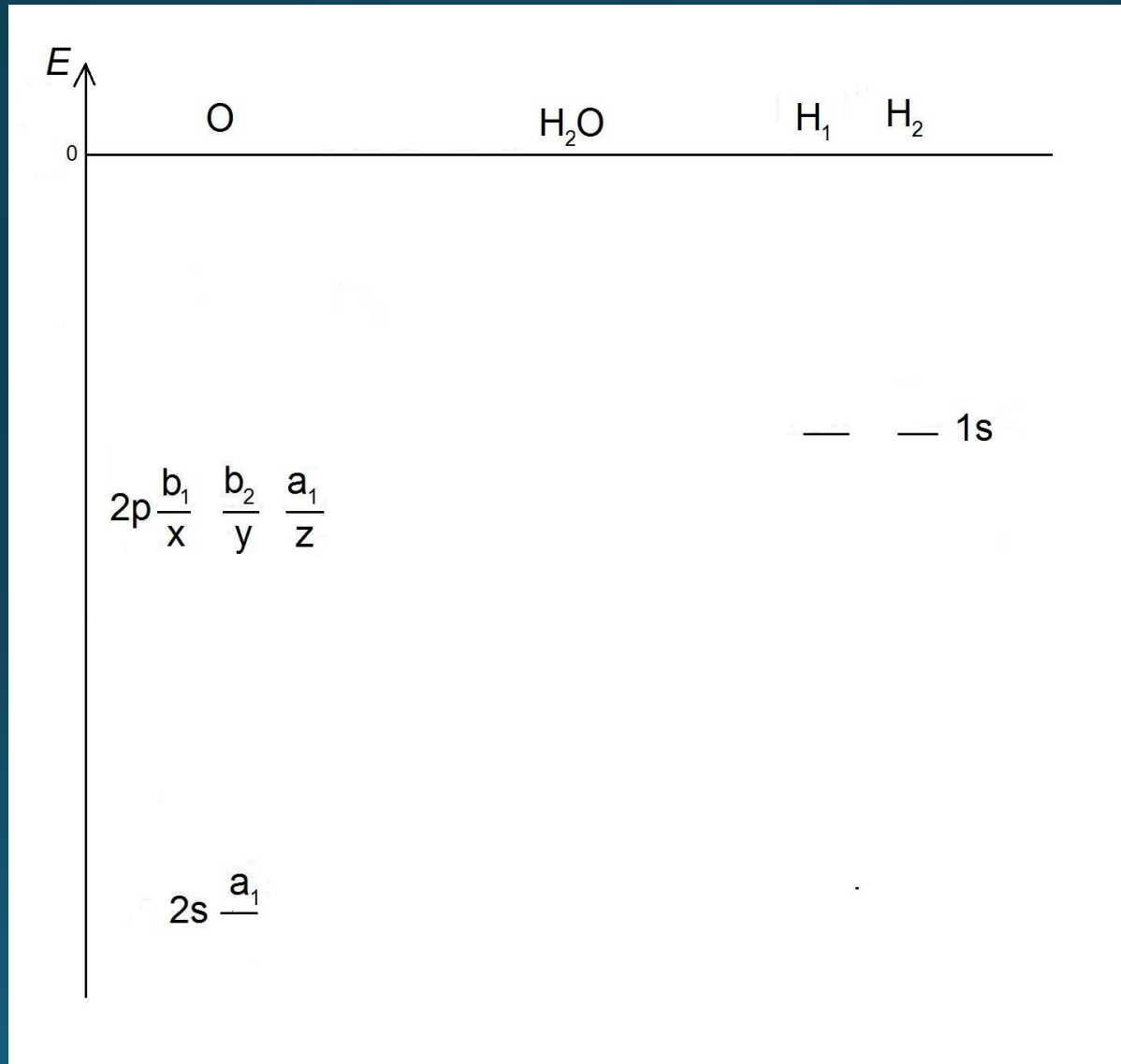


Diagrama de orbitais moleculares da água (C_{2v})

Classificando os orbitais 1s dos H, que são inseparáveis

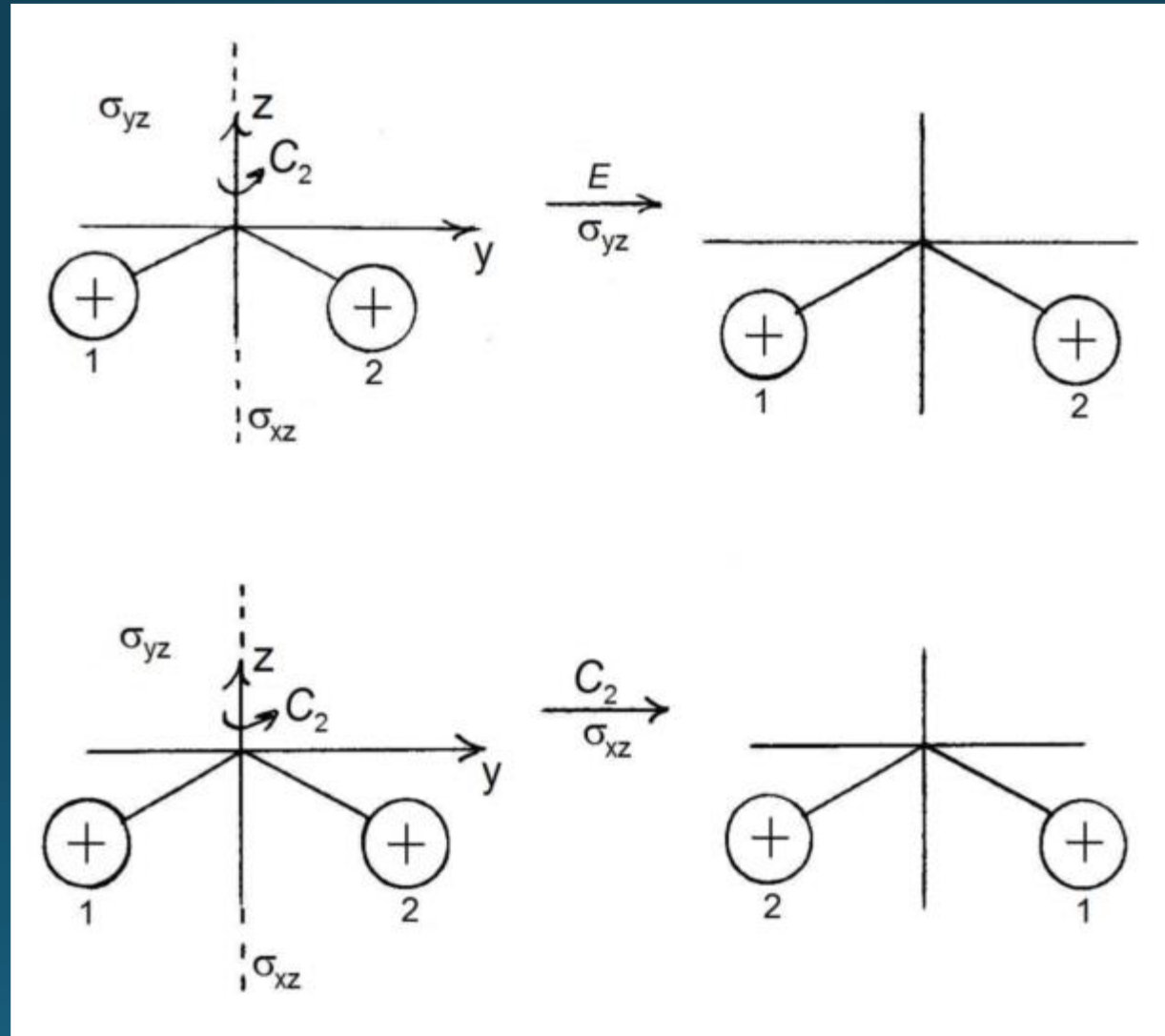


Diagrama de orbitais moleculares da água (C_{2v})

Classificando os orbitais 1s dos H, que são inseparáveis

	$1sH_1$	$1sH_2$			$1sH_1$	$1sH_2$
$1sH_1$	1	0	E	$1sH_1$	1	0
$1sH_2$	0	1	→	$1sH_2$	0	1
			$\sigma'_v(yz)$			
						$\chi = 2$

	$1sH_1$	$1sH_2$			$1sH_1$	$1sH_2$
$1sH_1$	1	0	C_2	$1sH_1$	0	1
$1sH_2$	0	1	→	$1sH_2$	1	0
			$\sigma_v(xz)$			
						$\chi = 0$

Diagrama de orbitais moleculares da água (C_{2v})

C_{2v}	E	C_2	$\sigma_v^{(xz)}$	$\sigma'_v^{(yz)}$	
A_1	1	1	1	1	
A_2	1	1	-1	-1	
B_1	1	-1	1	-1	
B_2	1	-1	-1	1	
<hr/>					
$1s(H_{1'}, H_2)$	2	0	0	2	$A_1 + B_2$

Diagrama de orbitais moleculares da água (C_{2v})

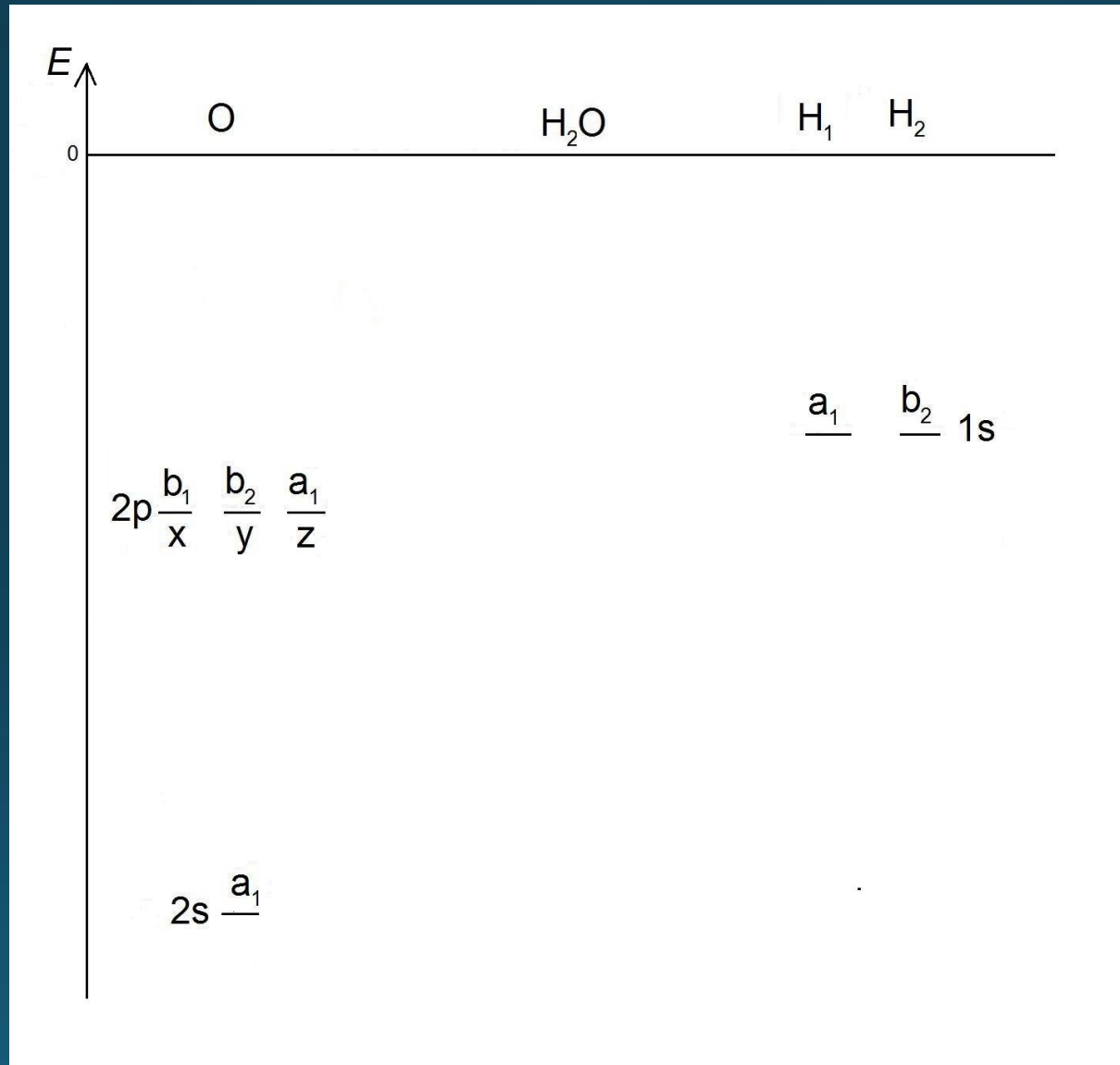


Diagrama de orbitais moleculares da água (C_{2v})

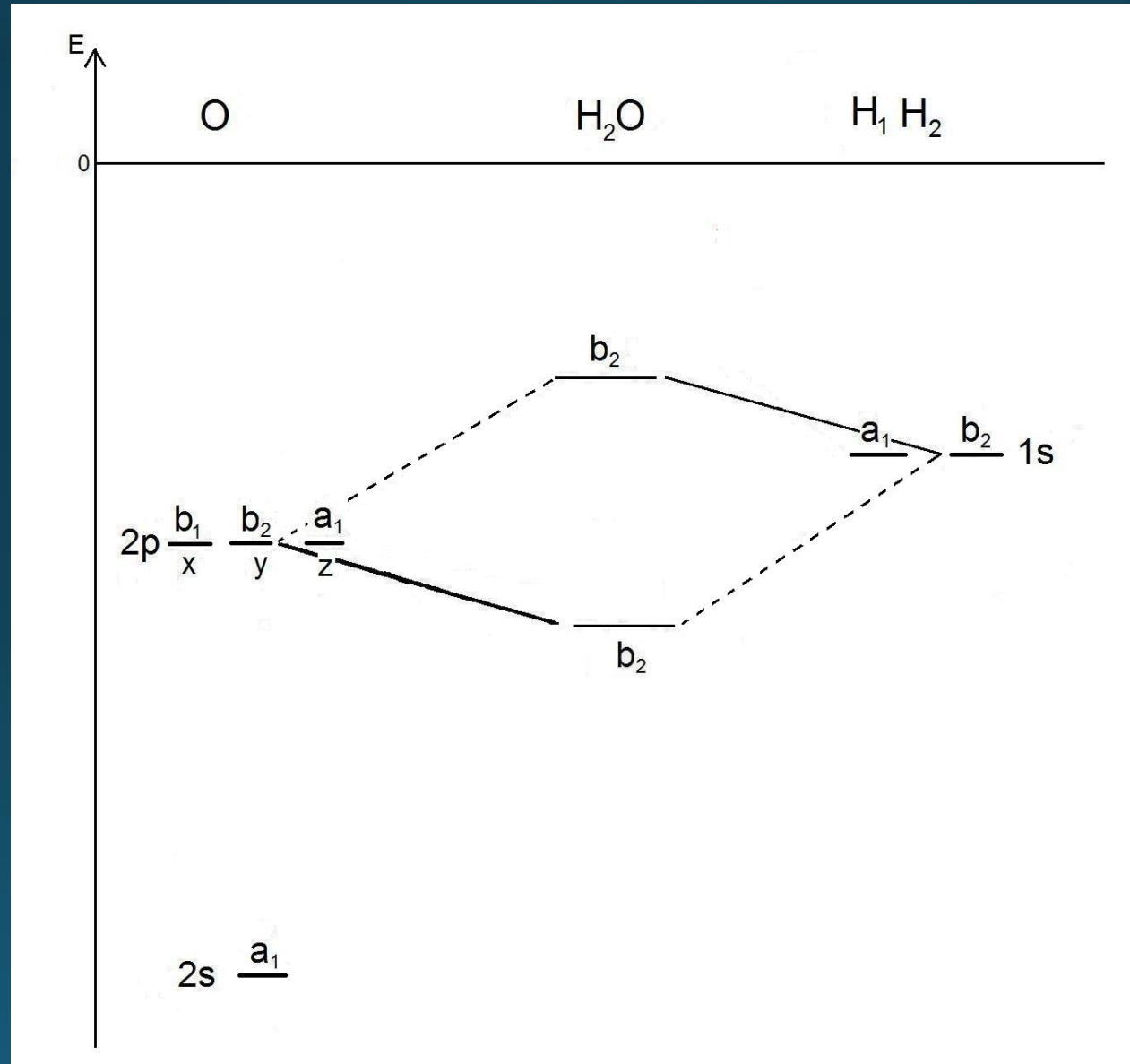


Diagrama de orbitais moleculares da água (C_{2v})

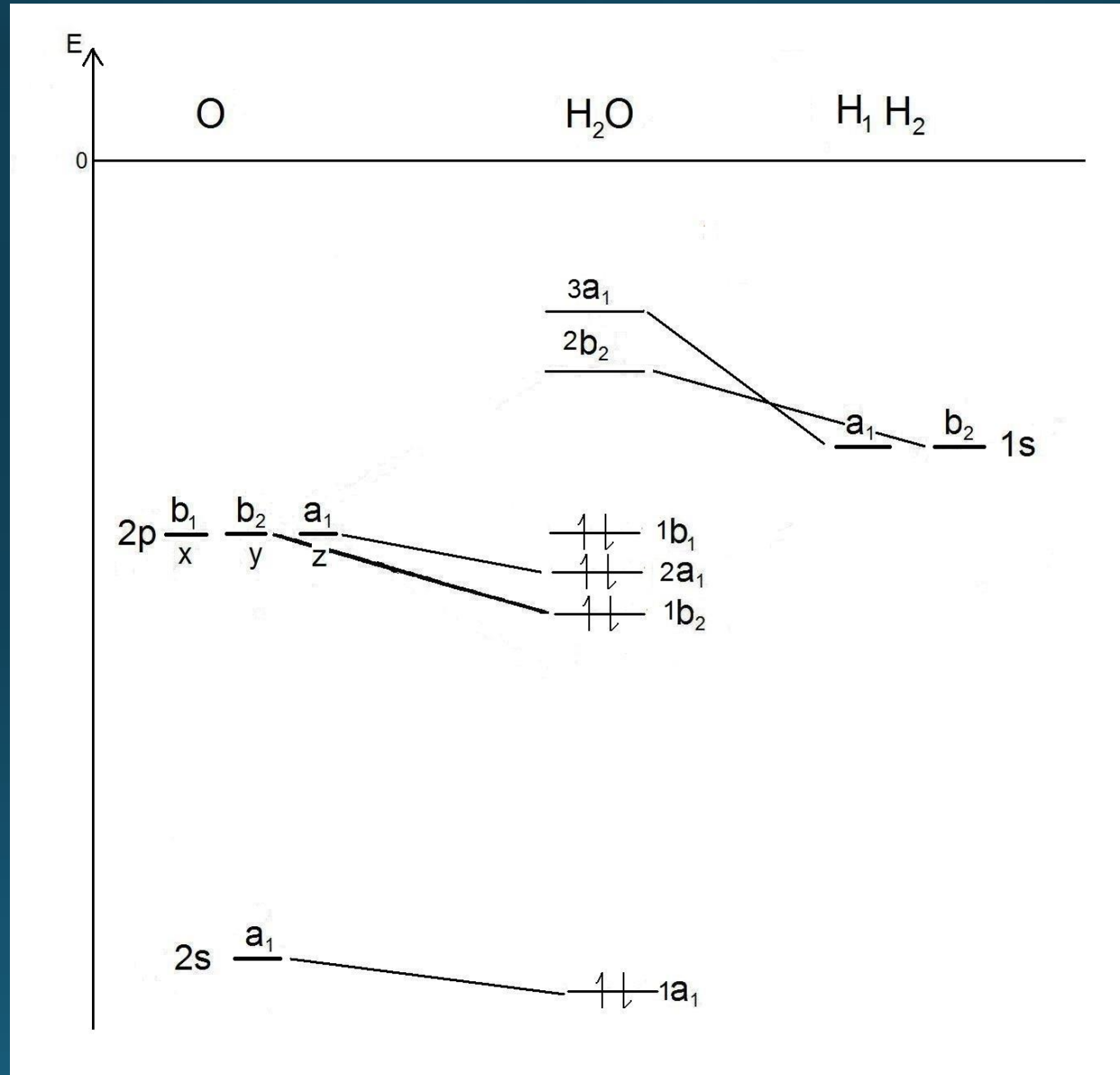


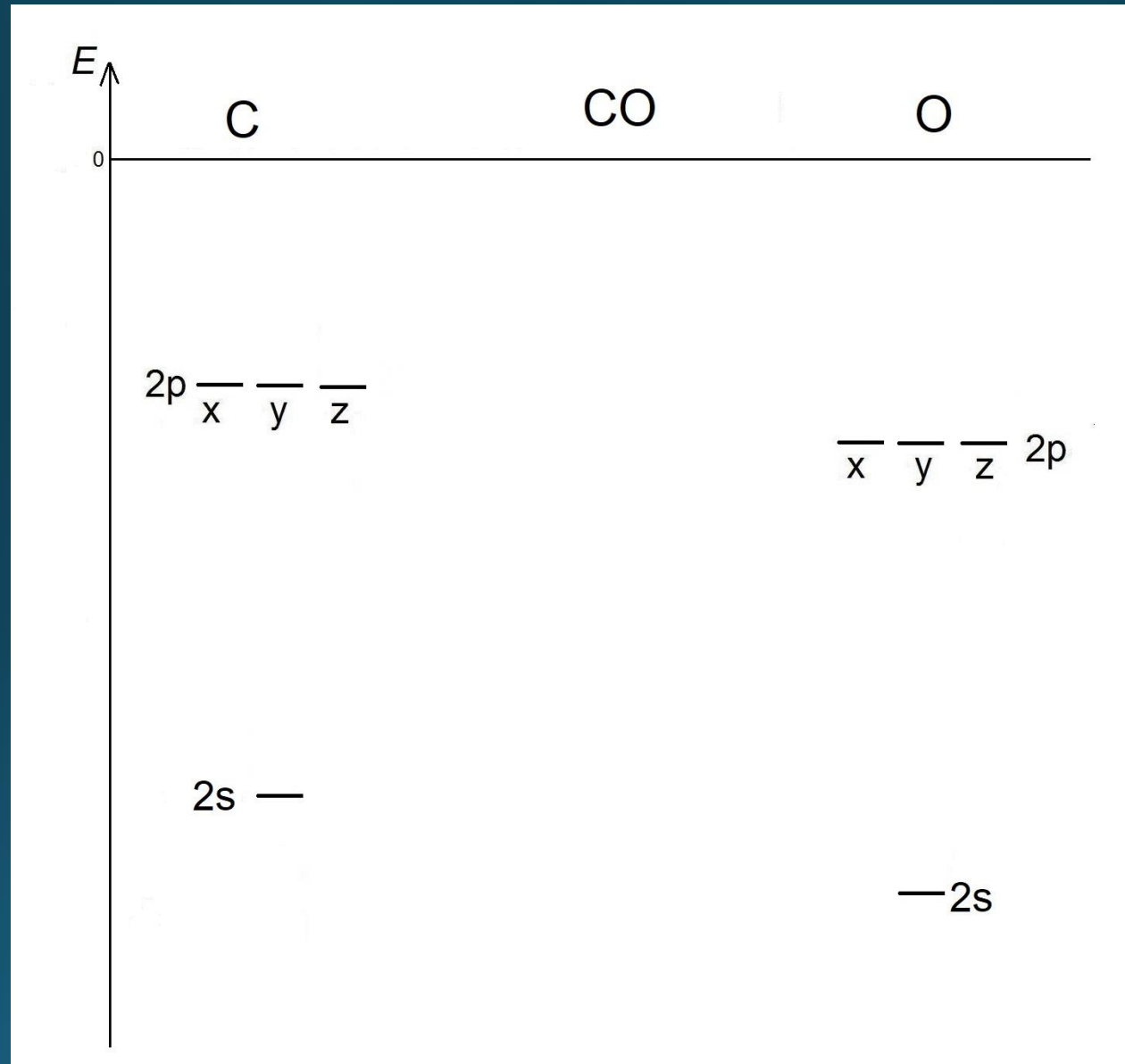
Diagrama de orbitais moleculares do
monóxido de carbono
CO

Monóxido de carbono

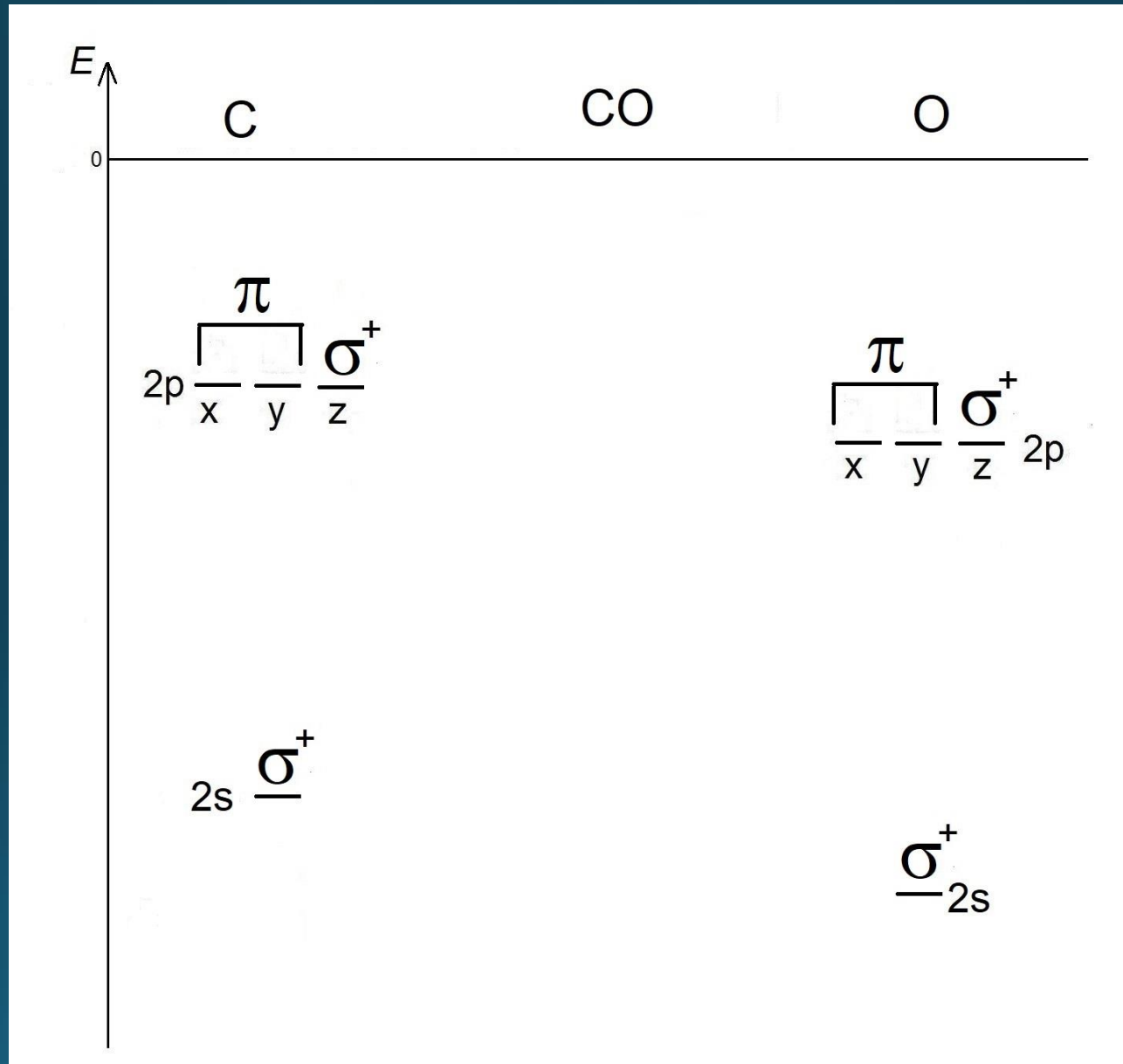


$\text{C}_{\infty v}$	E	$2\text{C}_{\infty}^{\phi}$	$\infty\sigma_v$
Σ^+	1	1	1
Σ^-	1	1	-1
Π	2	$2\cos\phi$	0
Δ	2	$2\cos 2\phi$	0
Φ	2	$2\cos 3\phi$	0

CO ($C_{\infty V}$)



CO ($C_{\infty V}$)



CO ($C_{\infty V}$)

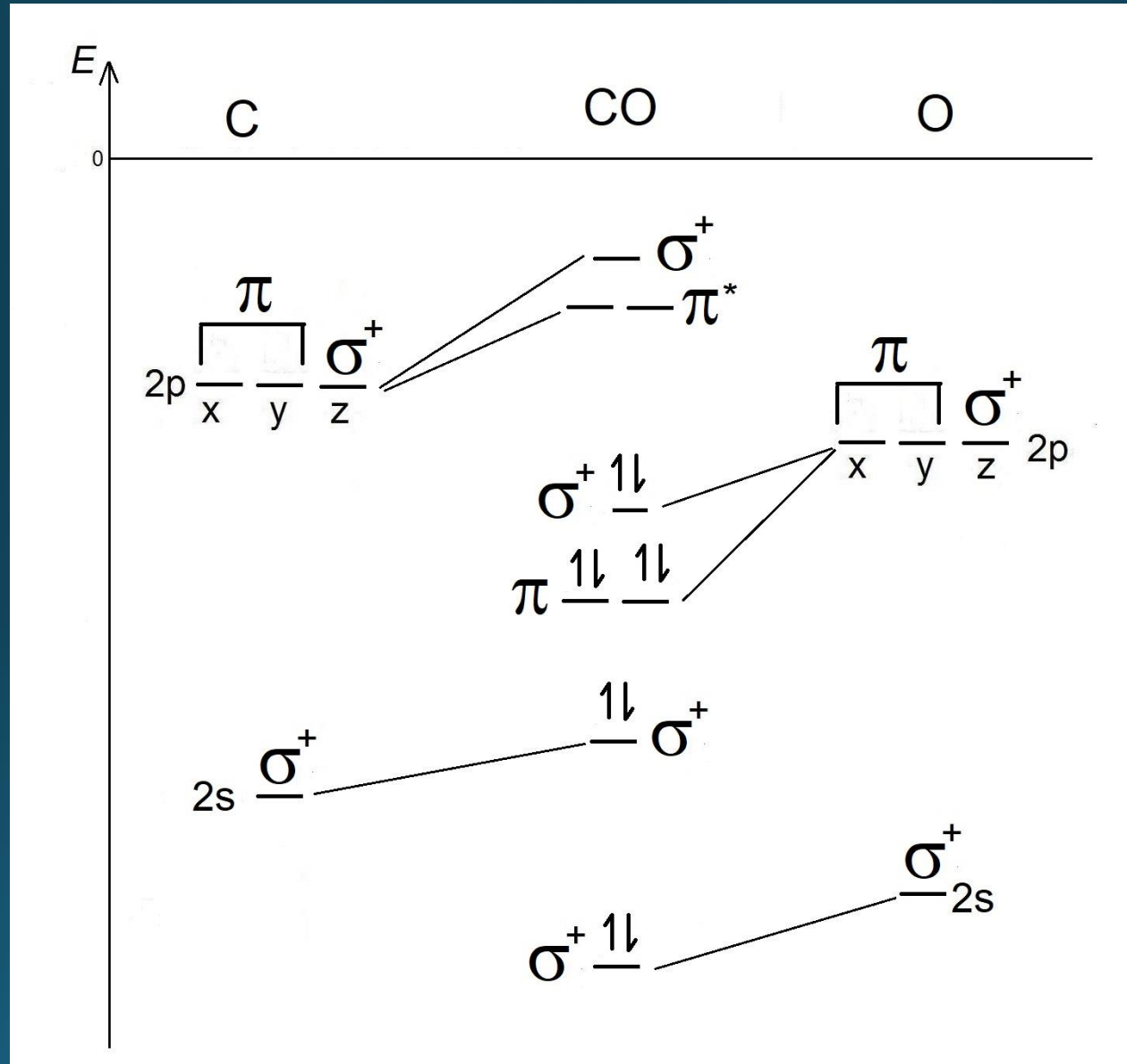
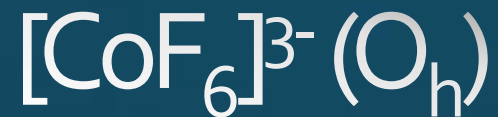
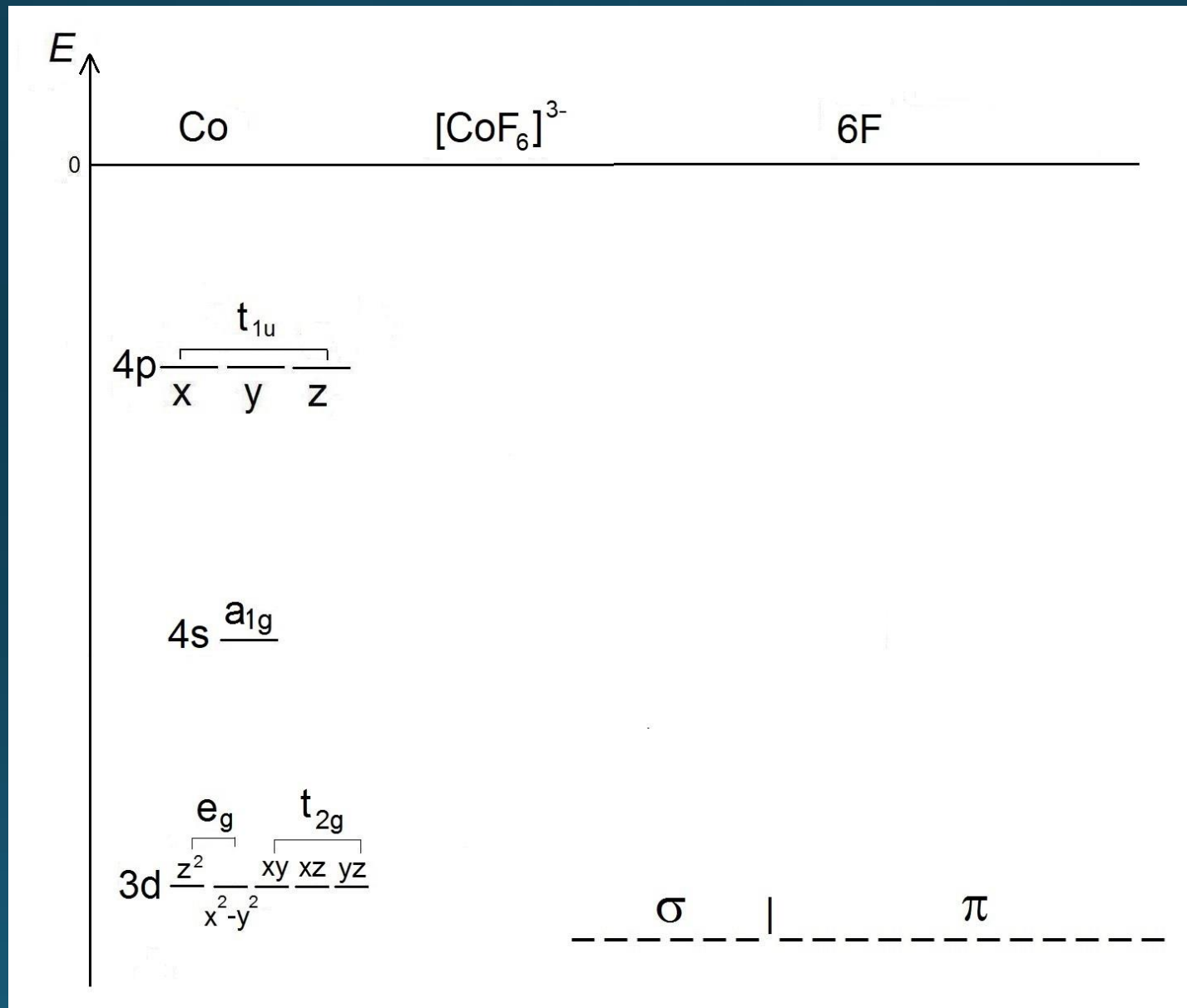
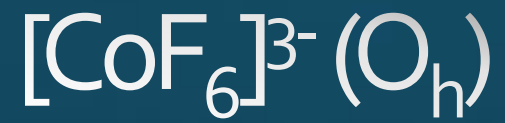
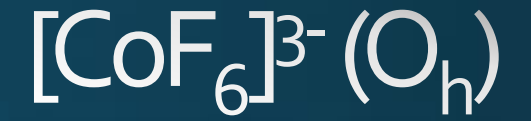
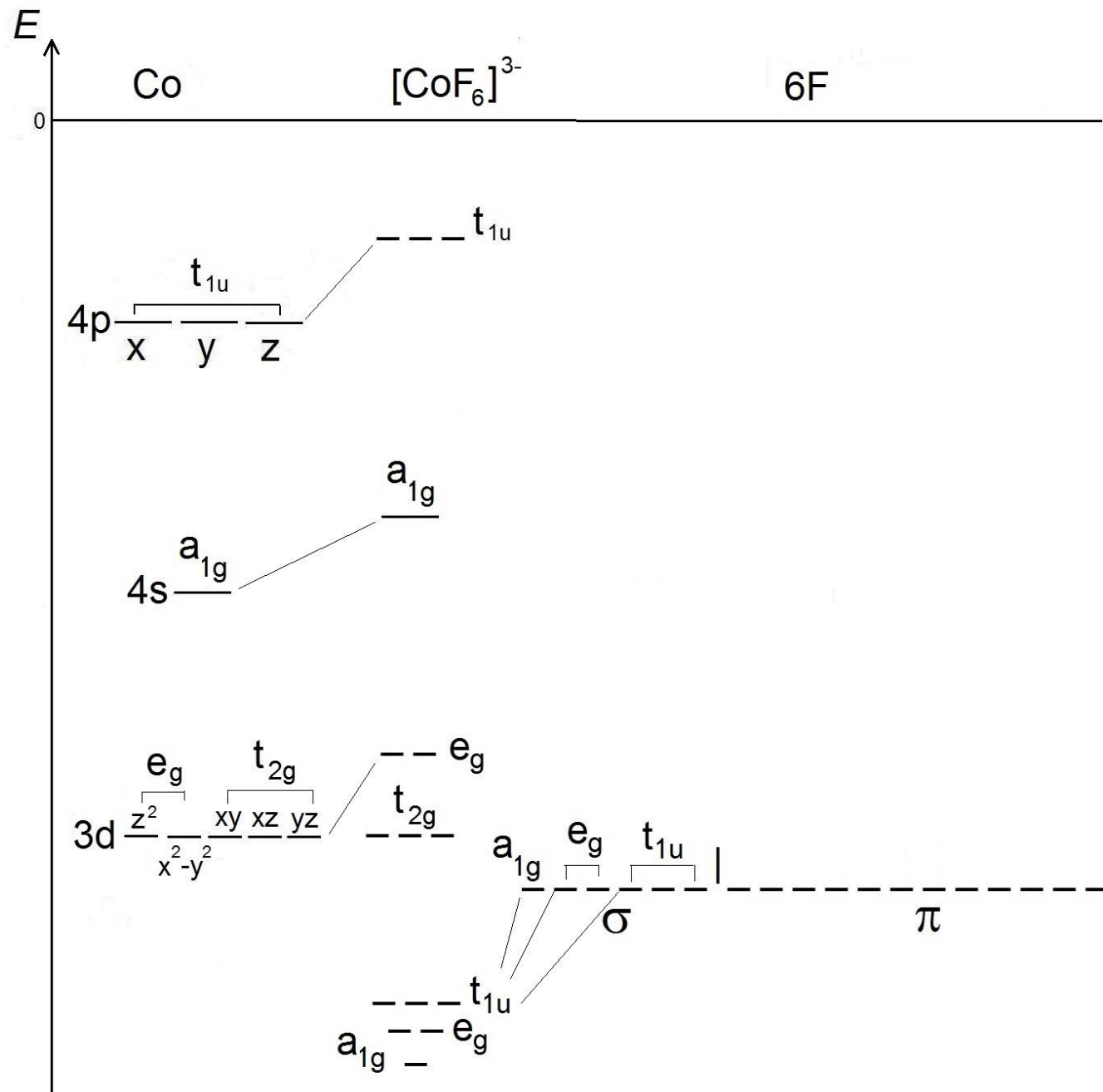


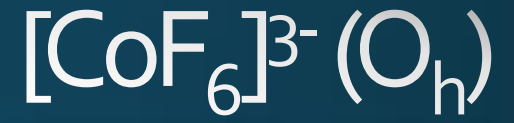
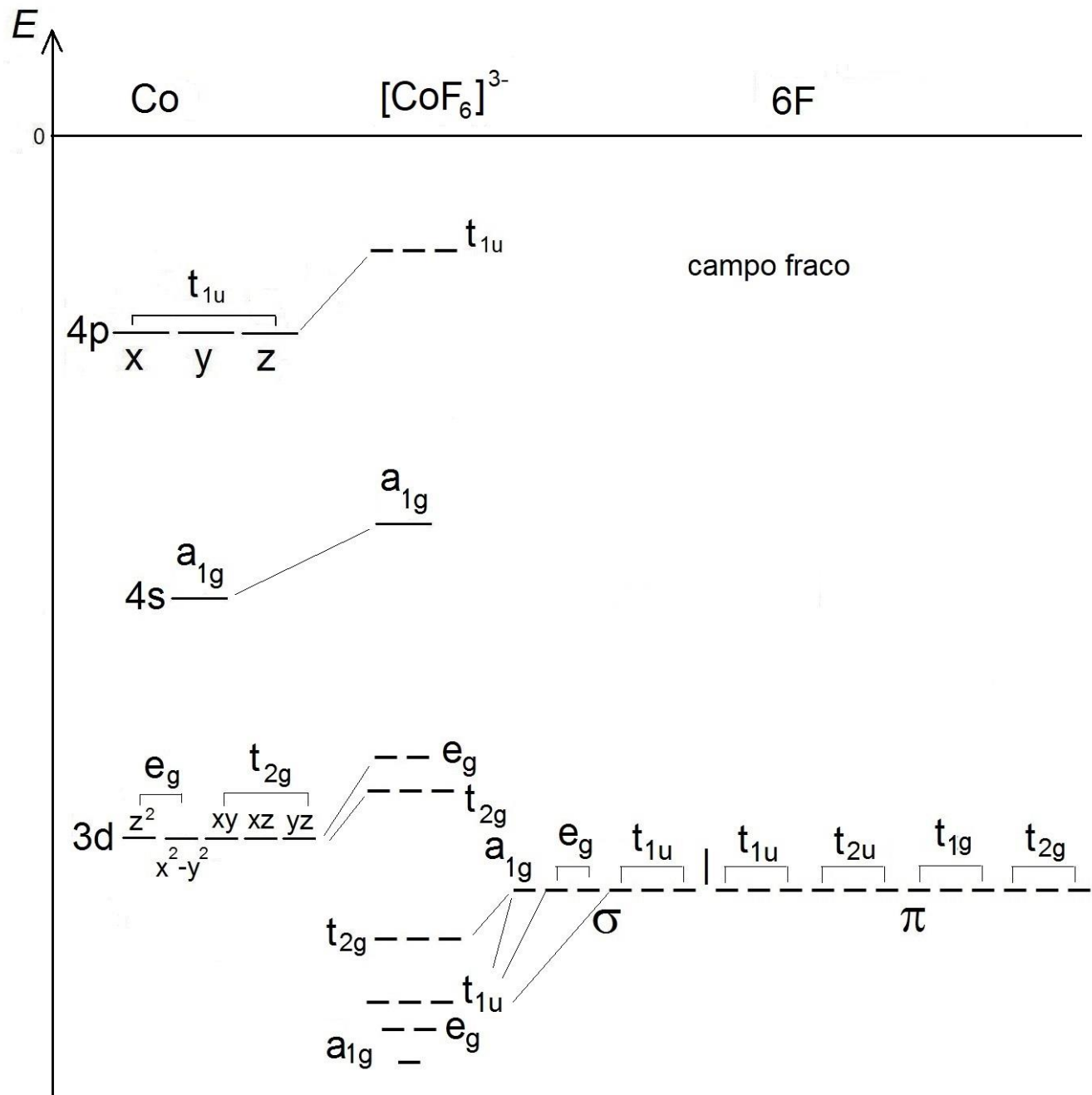
Diagrama de orbitais moleculares
para um complexo octaédrico
com ligantes de **campo fraco**



	(x,y,z)									
O_h	E	$8C_3$	$6C_2$	$6C_4$	$3C_2(=C_4^2)$	i	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$
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







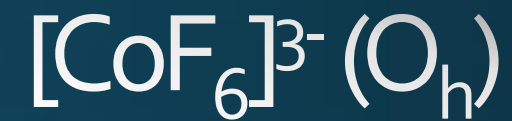
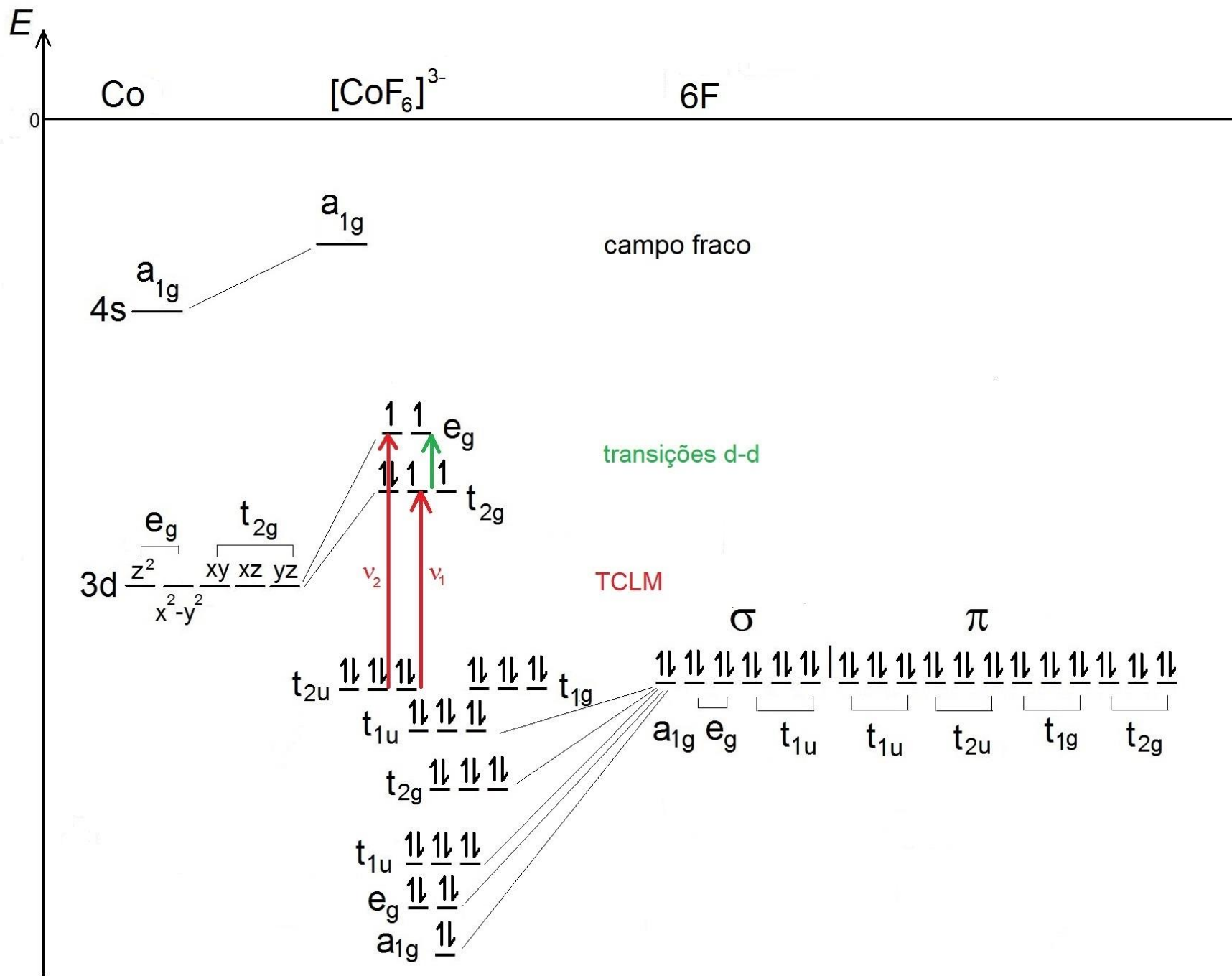
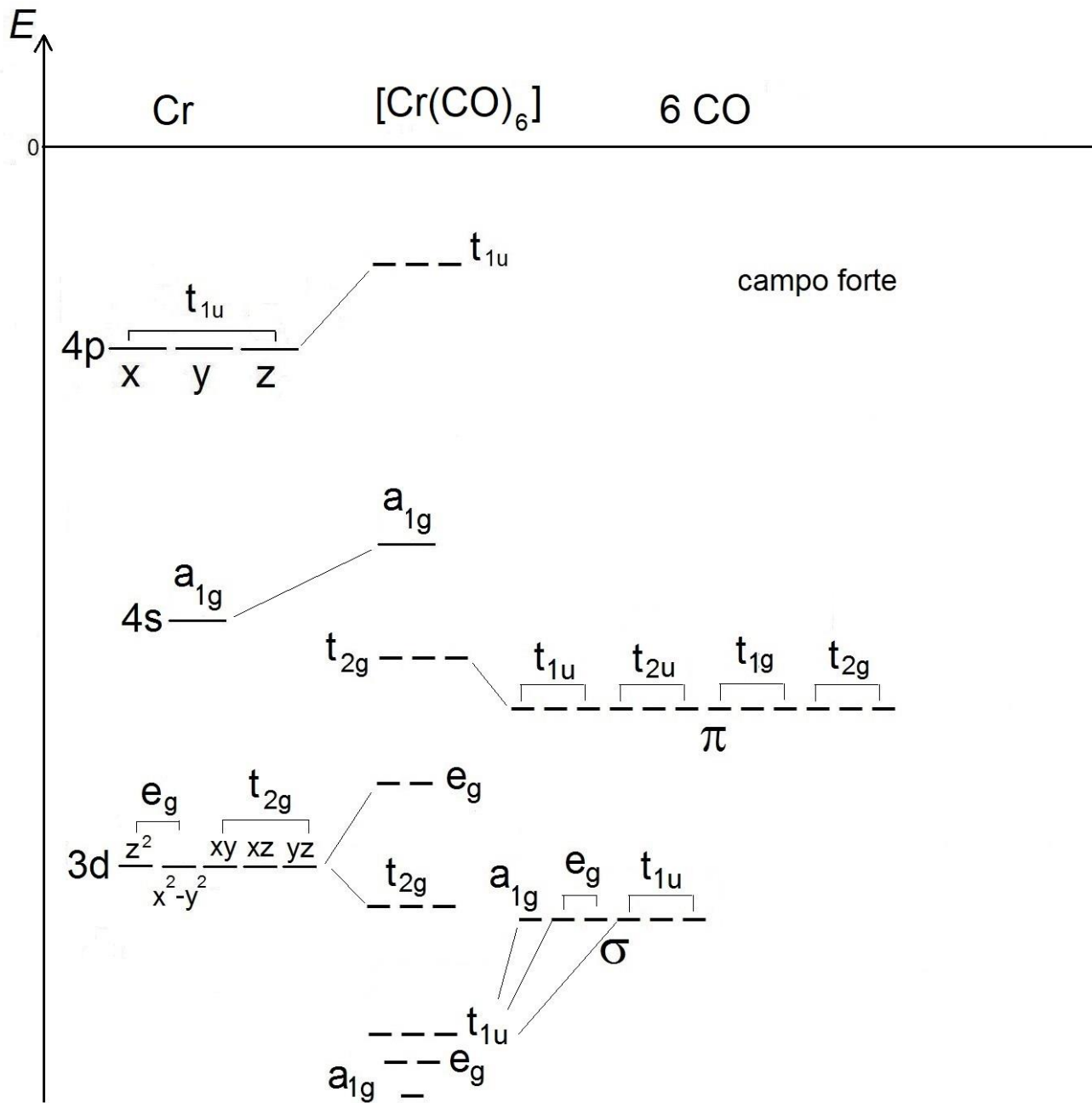


Diagrama de orbitais moleculares
para um complexo octaédrico
com ligantes de **campo forte**



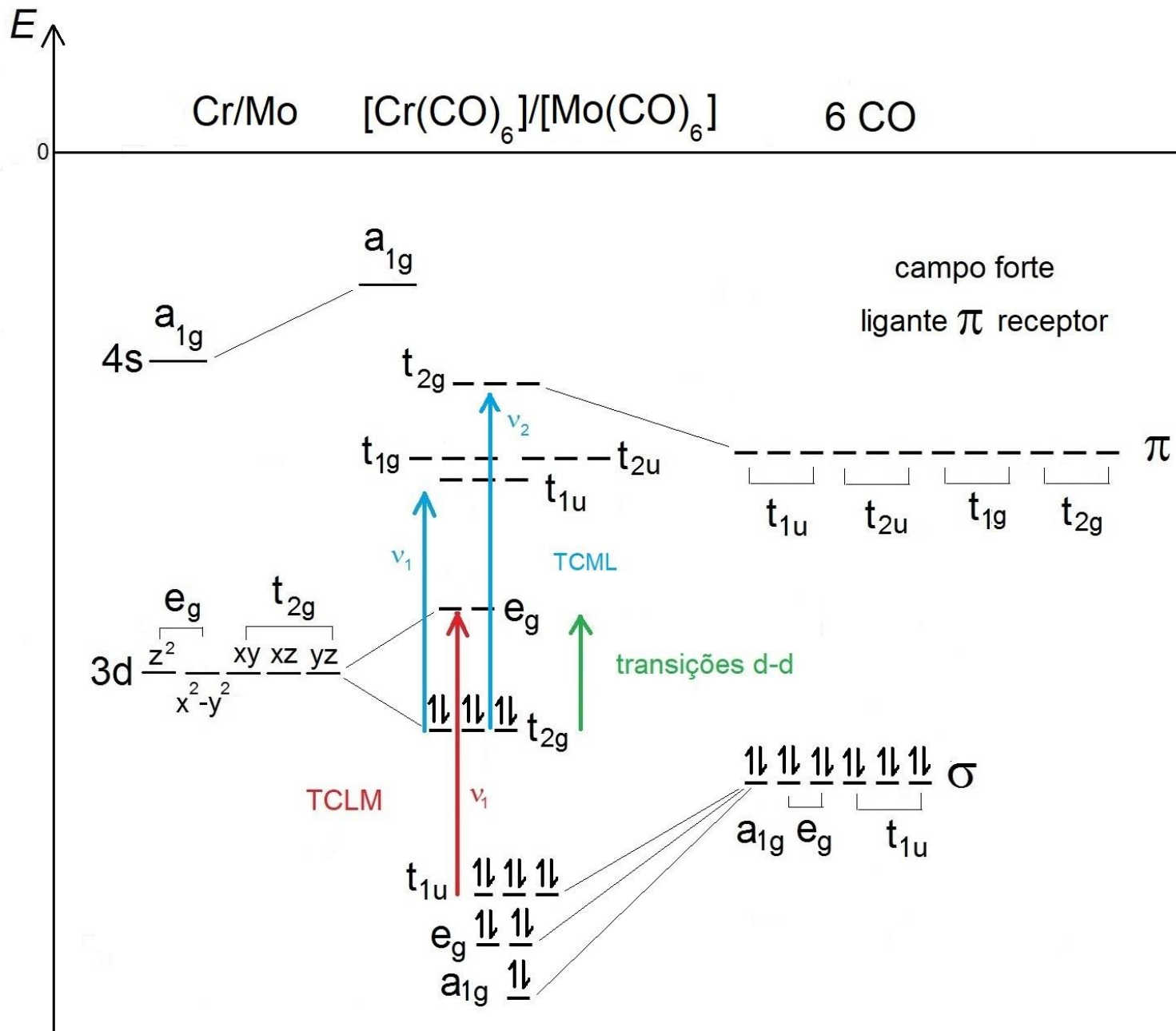


Diagrama de orbitais moleculares
para um complexo octaédrico
com ligantes de campo fraco
sem sistema π

