Simetria e Orbitais Moleculares

Roberto B. Faria
faria@iq.ufrj.br
www.iq.ufrj.br/~faria
Universidade Federal do Rio de Janeiro
Departamento de Química Inorgânica

Aula 3 - Moléculas lineares

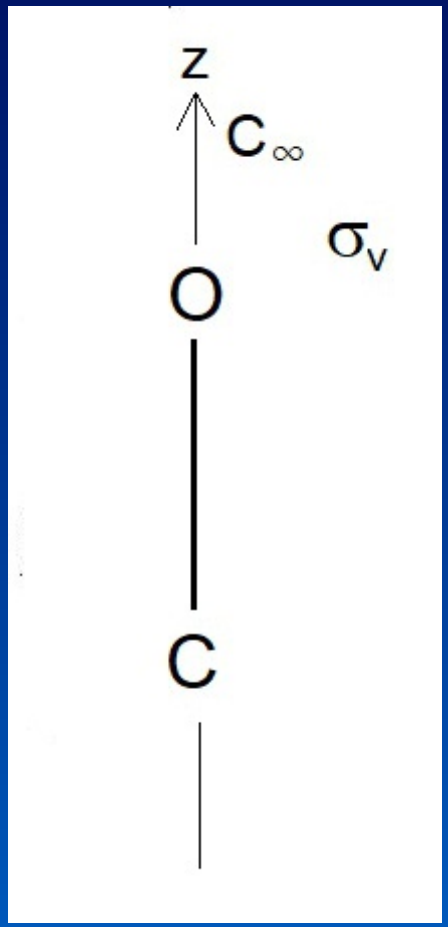
Diatômicas heteronucleares - $C_{\infty v}$

Diatômicas homonucleares - $D_{\infty h}$

08/08/2022

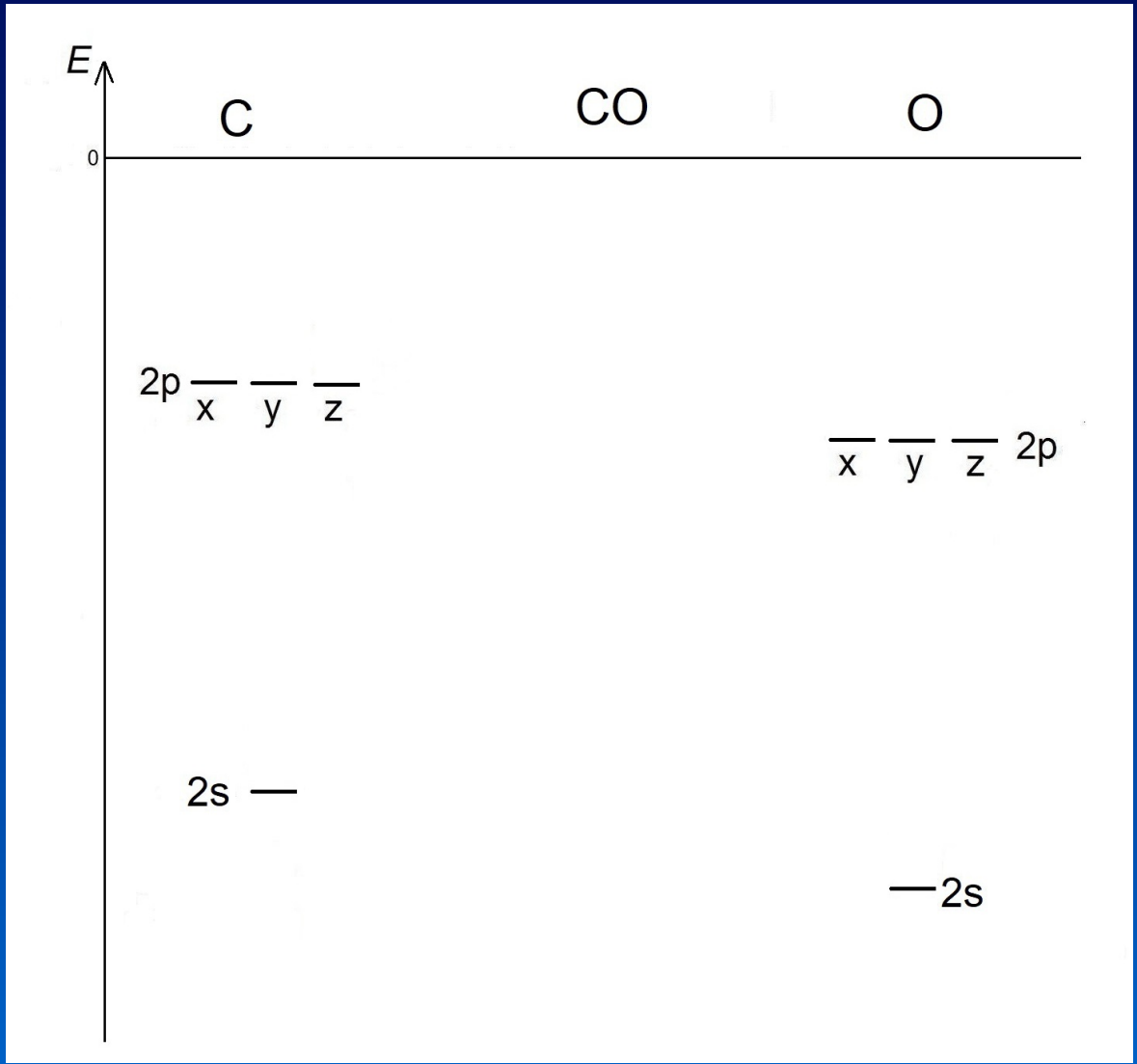
Diatômicas heteronucleares - $C_{\infty v}$

CO - $C_{\infty v}$



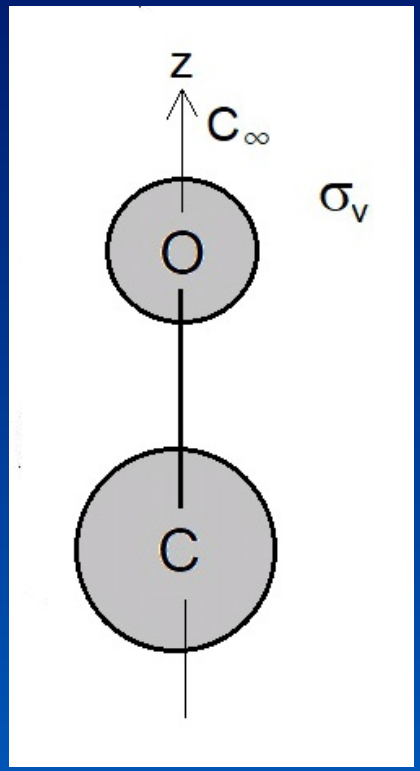
$C_{\infty v}$	E	$2C_{\infty}^{\varphi}$	$\infty\sigma_v$
Σ^+	1	1	1
Σ^-	1	1	-1
Π	2	$2\cos\varphi$	0
Δ	2	$2\cos2\varphi$	0
Φ	2	$2\cos3\varphi$	0

CO - $C_{\infty v}$



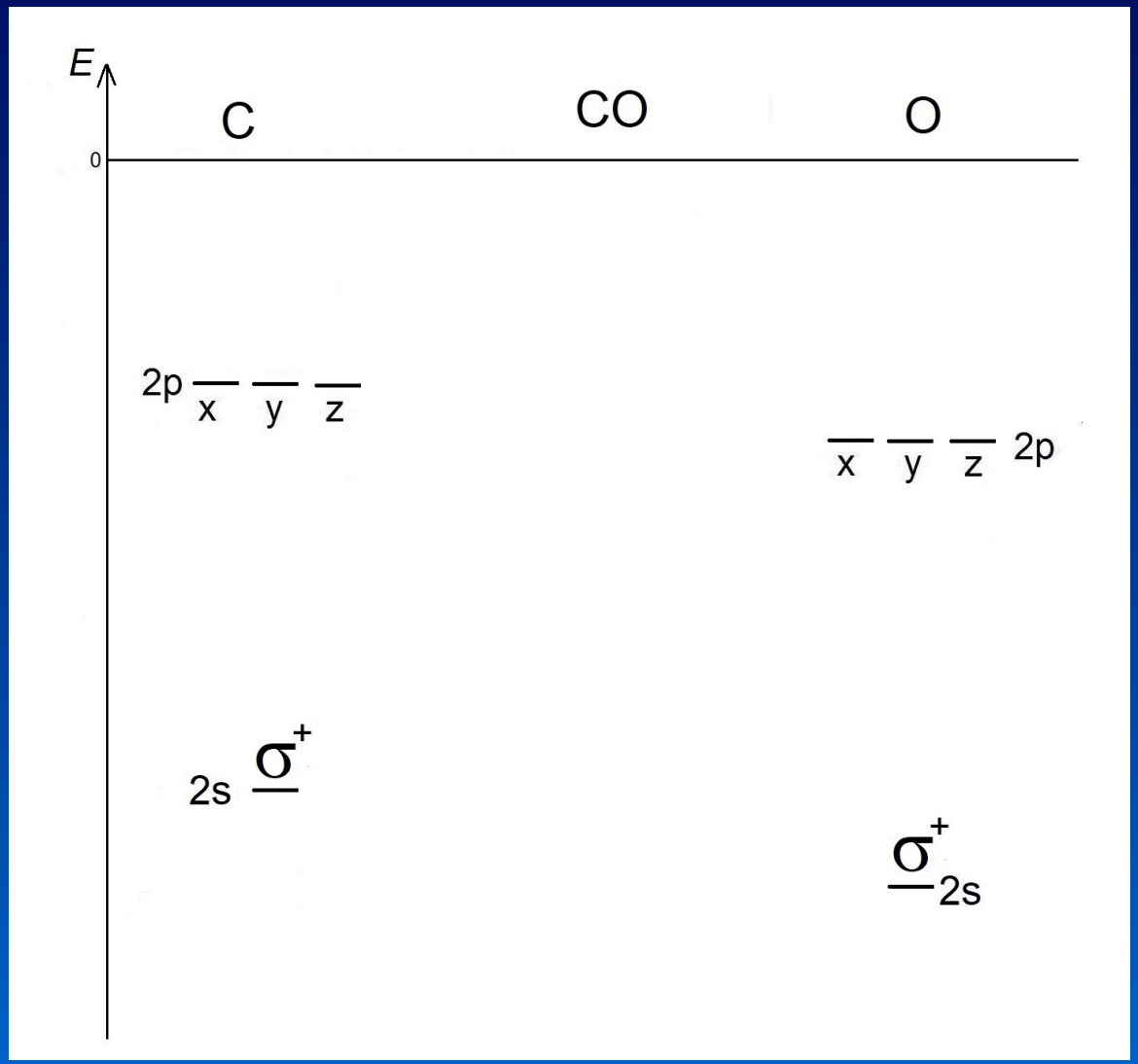
CO - $C_{\infty v}$

Orbitais 2s -independentes



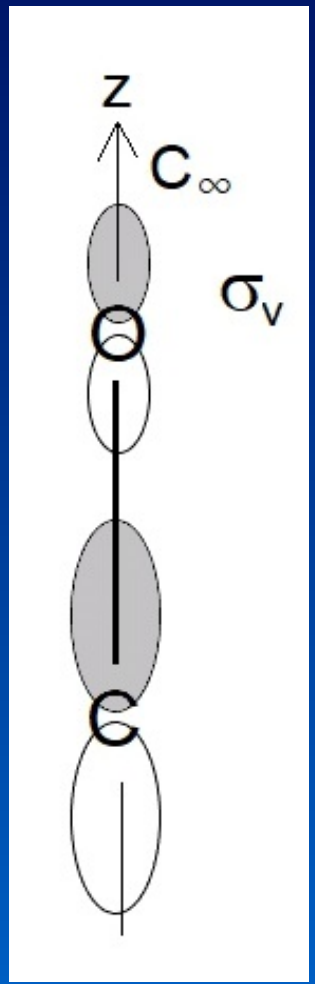
$C_{\infty v}$	E	$2C_{\infty}^{\varphi}$	$\infty\sigma_v$	
Σ^+	1	1	1	
Σ^-	1	1	-1	
Π	2	$2\cos\varphi$	0	
Δ	2	$2\cos2\varphi$	0	
Φ	2	$2\cos3\varphi$	0	
2s(C)	1	1	1	Σ^+
2s(O)	1	1	1	Σ^+

$CO - C_{\infty v}$



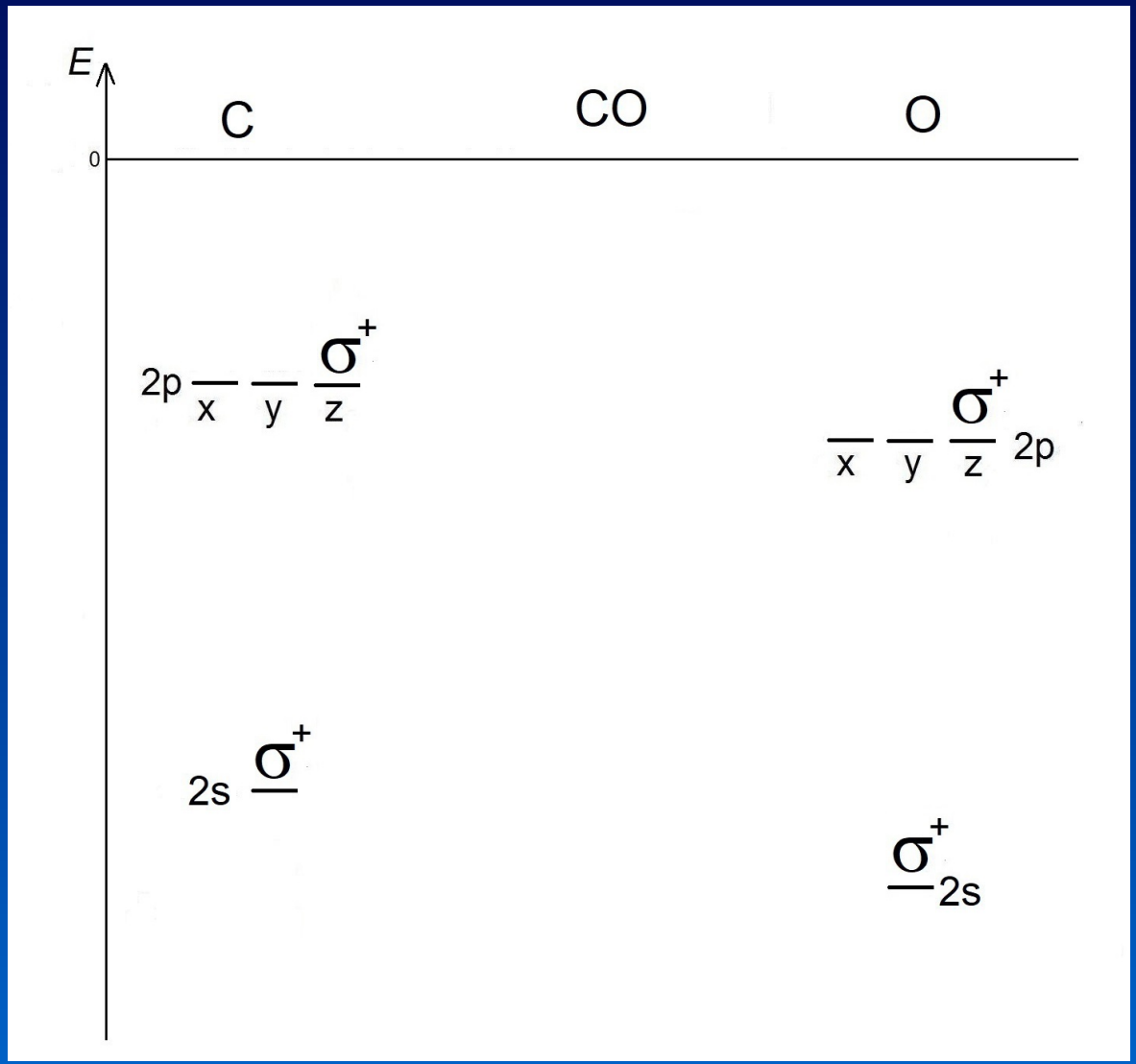
CO - $C_{\infty v}$

Orbitais $2p_z$ - independentes



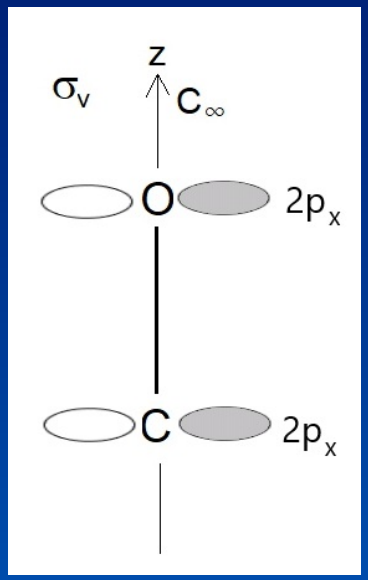
$C_{\infty v}$	E	$2C_\infty^{\varphi}$	$\infty\sigma_v$	
Σ^+	1	1	1	
Σ^-	1	1	-1	
Π	2	$2\cos\varphi$	0	
Δ	2	$2\cos2\varphi$	0	
Φ	2	$2\cos3\varphi$	0	
$2p_z(C)$	1	1	1	Σ^+
$2p_z(O)$	1	1	1	Σ^+

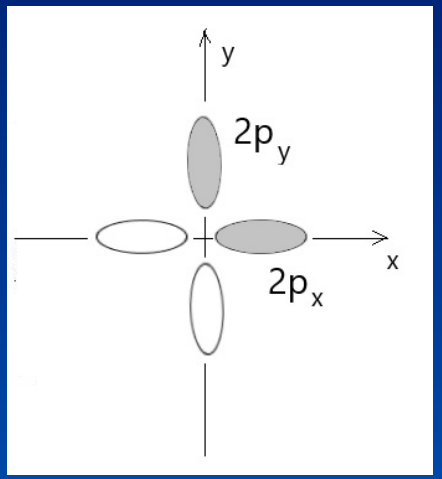
$CO - C_{\infty v}$



CO - $C_{\infty v}$

Orbitais do carbono ou do oxigênio
$2p_x$ e $2p_y$ - inseparáveis





Escolhendo $\varphi = 90°$

$C_\infty{}^{\varphi} = C_4$

$p_x \rightarrow p_y$

$p_y \rightarrow -p_x$

CO - $C_{\infty v}$

Orbitais do carbono $2p_x$ e $2p_y$ -inseparáveis

$C_{\infty v}$	E	$2C_\infty^{\varphi}$	$\infty\sigma_v$
Σ^+	1	1	1
Σ^-	1	1	-1
Π	2	$2\cos\varphi$	0
Δ	2	$2\cos2\varphi$	0
Φ	2	$2\cos3\varphi$	0

φ	$2\cos\varphi$	$2\cos2\varphi$	$2\cos3\varphi$
90°	0	-2	0
180°	-2	2	-2
45°	$\sqrt{2}$	0	$-\sqrt{2}$

CO - $C_{\infty v}$

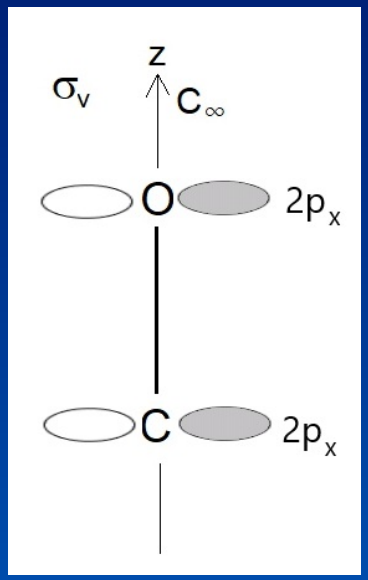
Orbitais do carbono $2p_x$ e $2p_y$ -inseparáveis

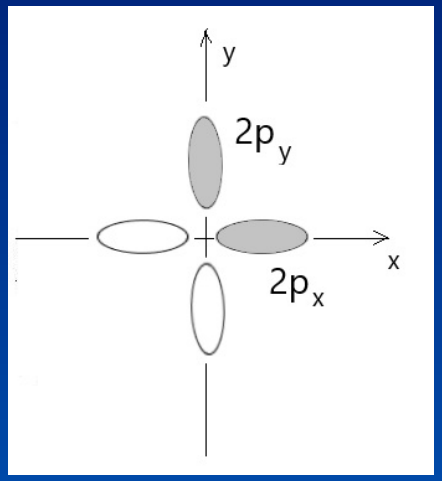
Escolhendo $\varphi = 45°$

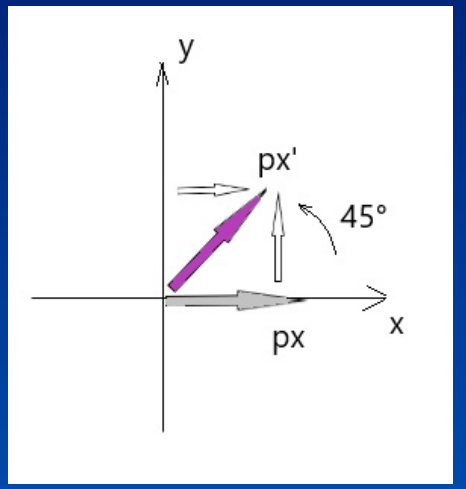
$C_{\infty v}$	E	$2C_{\infty}^{\varphi}$	$\infty\sigma_v$
Σ^+	1	1	1
Σ^-	1	1	-1
Π	2	$\sqrt{2}$	0
Δ	2	0	0
Φ	2	$-\sqrt{2}$	0

CO - $C_{\infty v}$

Orbitais do carbono ou do oxigênio
$2p_x$ e $2p_y$ - inseparáveis
Escolhendo $\varphi = 45°$



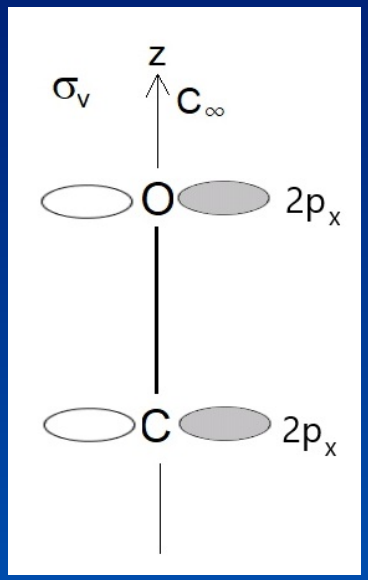


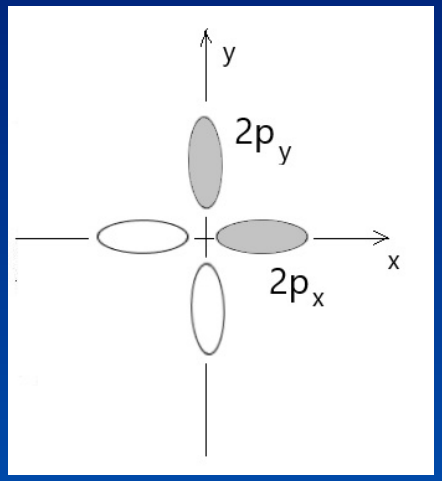


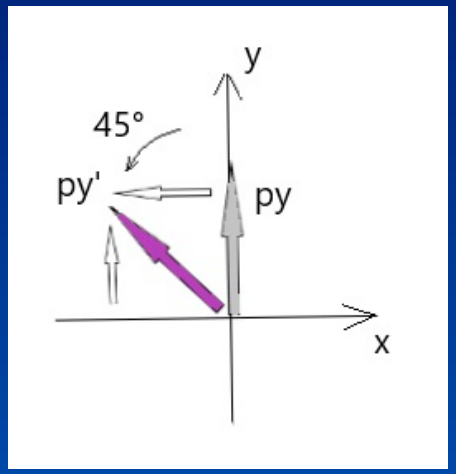
$$(C_8)p_x \rightarrow p_x' = \cos(45°)p_x + \text{sen}(45°)p_y$$
$$= (\sqrt{2}/2)p_x + (\sqrt{2}/2)p_y$$

CO - $C_{\infty v}$

Orbitais do carbono ou do oxigênio
$2p_x$ e $2p_y$ - inseparáveis
Escolhendo $\varphi = 45°$







$$(C_8)p_y \rightarrow p_y' = -\text{sen}(45°)p_x + \cos(45°)p_y$$
$$= -(\sqrt{2}/2)p_x + (\sqrt{2}/2)p_y$$

CO - $C_{\infty v}$

Orbitais do carbono ou do oxigênio
$2p_x$ e $2p_y$ - inseparáveis
Escolhendo $\varphi = 45°$

$$(C_8)p_x \rightarrow p_x' = (\sqrt{2}/2)p_x + (\sqrt{2}/2)p_y$$
$$(C_8)p_y \rightarrow p_y' = -(\sqrt{2}/2)p_x + (\sqrt{2}/2)p_y$$

	$2p_x$	$2p_y$
$2p_x$	1	0
$2p_y$	0	1

C_8 →

	$2p_x$	$2p_y$
$2p_x$	$\sqrt{2}/2$	$\sqrt{2}/2$
$2p_y$	$-\sqrt{2}/2$	$\sqrt{2}/2$

$$\chi = \sqrt{2}$$

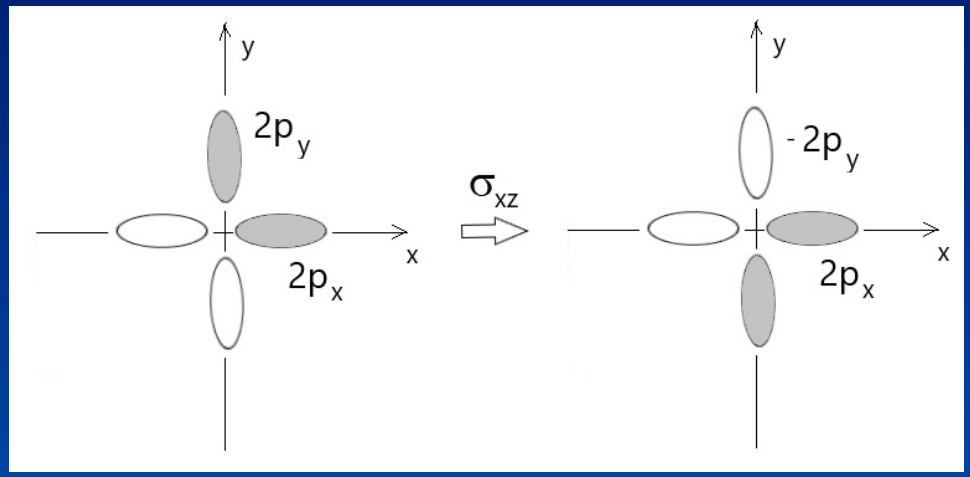
CO - $C_{\infty v}$

Orbitais do carbono $2p_x$ e $2p_y$ -inseparáveis
Orbitais do carbono ou do oxigênio
$2p_x$ e $2p_y$ - inseparáveis ($\varphi = 45°$)

$C_{\infty v}$	E	$2C_{\infty}^{\varphi}$	$\infty\sigma_v$
Σ^+	1	1	1
Σ^-	1	1	-1
Π	2	$\sqrt{2}$	0
Δ	2	0	0
Φ	2	$-\sqrt{2}$	0
$(p_x,p_y)_C$	2	$\sqrt{2}$	
$(p_x,p_y)_O$	2	$\sqrt{2}$	

CO - $C_{\infty v}$

Orbitais do carbono ou do oxigênio
$2p_x$ e $2p_y$ - inseparáveis
Escolhendo $\varphi = 45°$



	$2p_x$	$2p_y$
$2p_x$	1	0
$2p_y$	0	1

σ_{xz} →

	$2p_x$	$2p_y$
$2p_x$	1	0
$2p_y$	0	-1

$\chi = 0$

CO - $C_{\infty v}$

Orbitais do carbono $2p_x$ e $2p_y$ -inseparáveis
Orbitais do carbono ou do oxigênio
$2p_x$ e $2p_y$ - inseparáveis ($\varphi = 45°$)

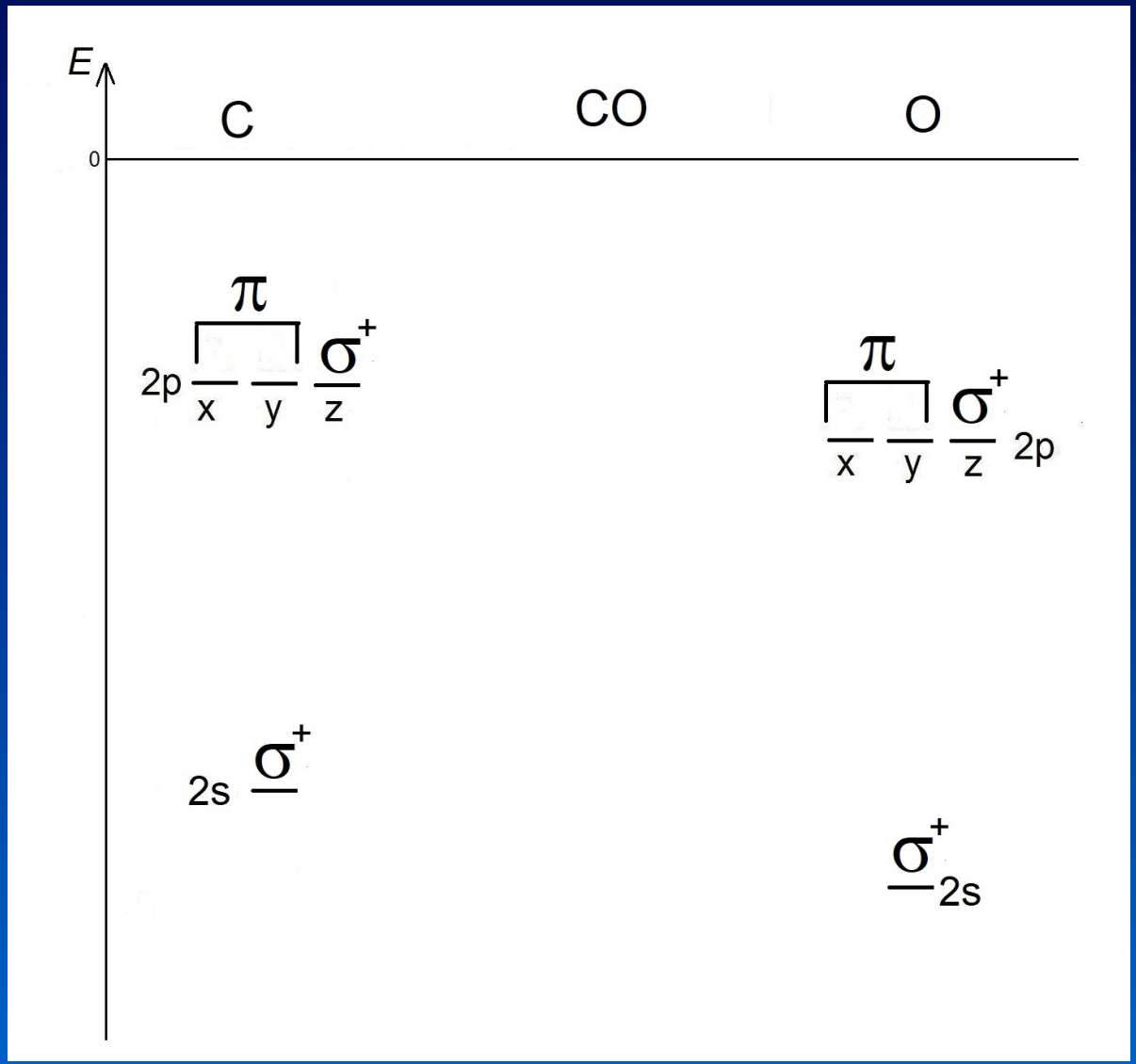
$C_{\infty v}$	E	$2C_\infty^{\varphi}$	$\infty\sigma_v$
Σ^+	1	1	1
Σ^-	1	1	-1
Π	2	$\sqrt{2}$	0
Δ	2	0	0
Φ	2	$-\sqrt{2}$	0
$(p_x,p_y)_C$	2	$\sqrt{2}$	0
$(p_x,p_y)_O$	2	$\sqrt{2}$	0

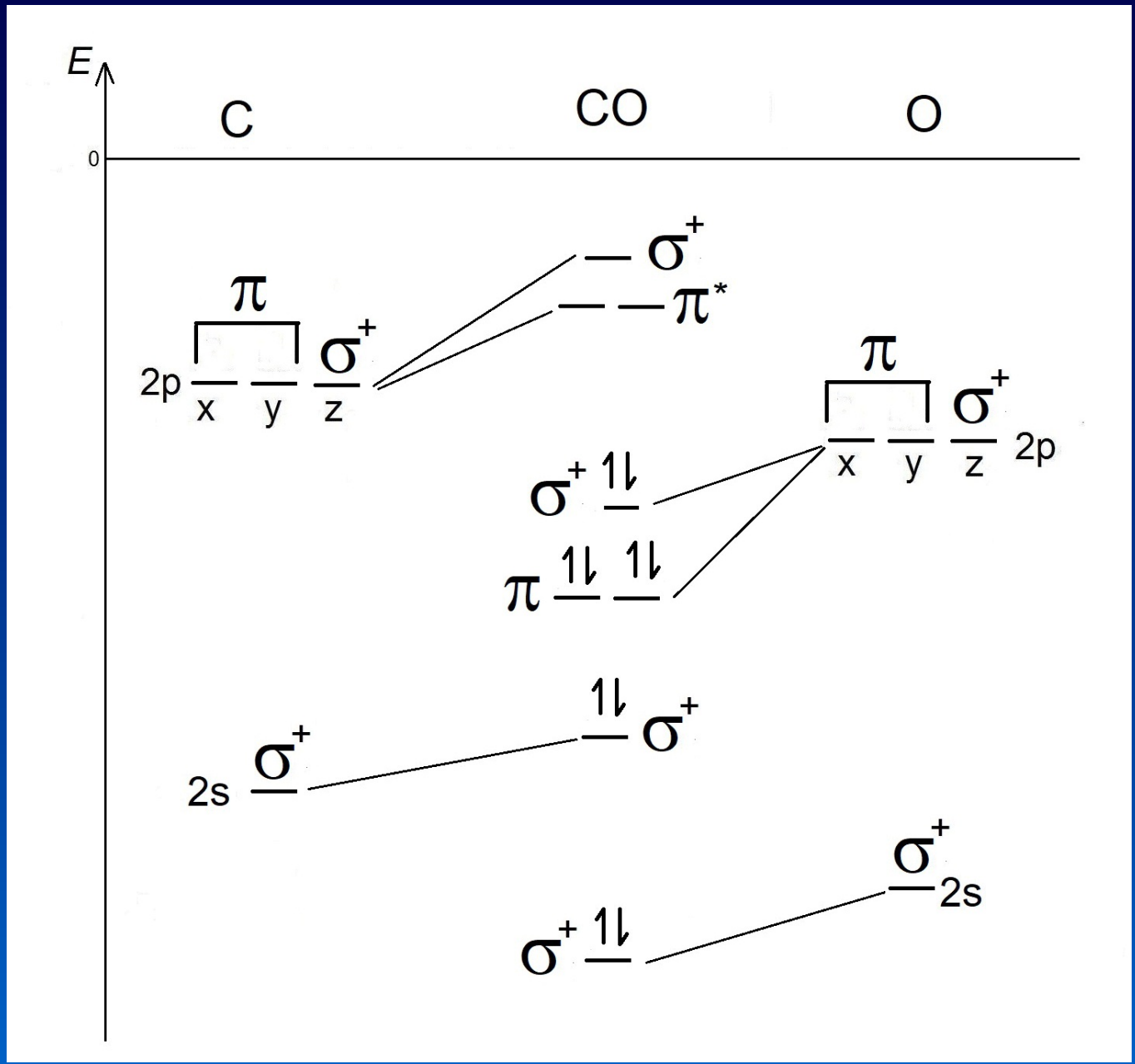
CO - $C_{\infty v}$

Orbitais do carbono $2p_x$ e $2p_y$ -inseparáveis
Orbitais do carbono ou do oxigênio
$2p_x$ e $2p_y$ - inseparáveis ($\varphi = 45°$)

$C_{\infty v}$	E	$2C_\infty^{\varphi}$	$\infty\sigma_v$	
Σ^+	1	1	1	
Σ^-	1	1	-1	
Π	2	$\sqrt{2}$	0	
Δ	2	0	0	
Φ	2	$-\sqrt{2}$	0	
$(p_x,p_y)_C$	2	$\sqrt{2}$	0	Π
$(p_x,p_y)_O$	2	$\sqrt{2}$	0	Π

$CO - C_{\infty v}$




E
C
CO
O
0
σ+
π*
π
2p
x
y
z
σ+
π
σ+
2p
x
y
z
σ+ 1↓
π 1↓ 1↓
1↓
σ+
2s
σ+
σ+
2s
σ+ 1↓

Espectros de fotoelétron - CO

Weller, M.; Overton, T.; Rourke, J.; Armstrong, F. Inorganic Chemistry, 6a ed., Oxford University Press, 2014. pg. 63.

Diatômicas homonucleares - $D_{\infty h}$

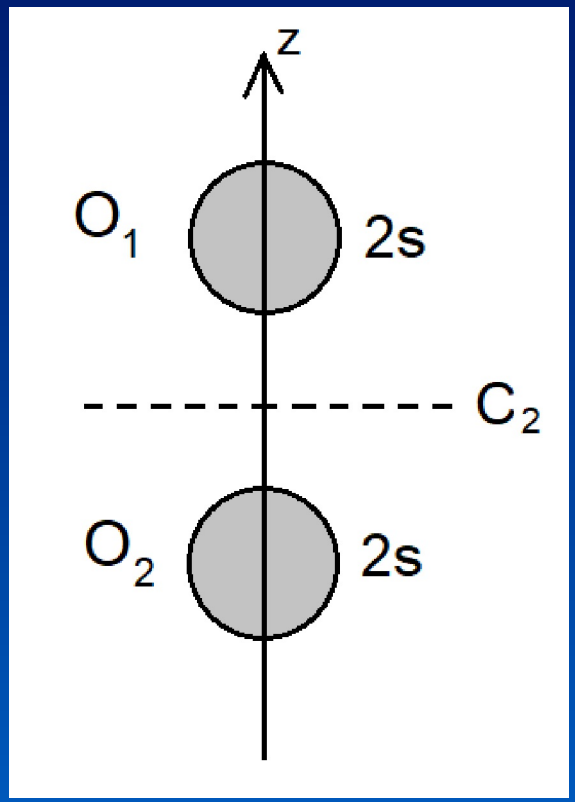
$D_{\infty h}$

$D_{\infty h}$	E	$2C_\infty^{\varphi}$	$\infty\sigma_v$	i	$2S_\infty^{\varphi}$	∞C_2
Σ_g^+	1	1	1	1	1	1
Σ_g^-	1	1	-1	1	1	-1
Π_g	2	$2\cos\varphi$	0	2	$-2\cos\varphi$	0
Δ_g	2	$2\cos2\varphi$	0	2	$2\cos2\varphi$	0
Σ_u^+	1	1	1	-1	-1	-1
Σ_u^-	1	1	-1	-1	-1	1
Π_u	2	$2\cos\varphi$	0	-2	$2\cos\varphi$	0
Δ_u	2	$2\cos2\varphi$	0	-2	$-2\cos2\varphi$	0

Dioxigênio - O_2

O_2 - $D_{\infty h}$

Orbitais 2s - inseparáveis



O_2 - $D_{\infty h}$

Orbitais 2s - inseparáveis

	$2s(O_1)$	$2s(O_2)$
$2s(O_1)$	1	0
$2s(O_2)$	0	1

$E, C_\infty \rightarrow \sigma_v$

	$2s(O_1)$	$2s(O_2)$
$2s(O_1)$	1	0
$2s(O_2)$	0	1

$\chi = 2$

Dioxigênio - O_2 - $D_{\infty h}$

$D_{\infty h}$	E	$2C_\infty^{\varphi}$	$\infty\sigma_v$	i	$2S_\infty^{\varphi}$	∞C_2
Σ_g^+	1	1	1	1	1	1
Σ_g^-	1	1	-1	1	1	-1
Π_g	2	$2\cos\varphi$	0	2	$-2\cos\varphi$	0
Δ_g	2	$2\cos2\varphi$	0	2	$2\cos2\varphi$	0
Σ_u^+	1	1	1	-1	-1	-1
Σ_u^-	1	1	-1	-1	-1	1
Π_u	2	$2\cos\varphi$	0	-2	$2\cos\varphi$	0
Δ_u	2	$2\cos2\varphi$	0	-2	$-2\cos2\varphi$	0
$2s(O_1,O_2)$	2	2	2			

O_2 - $D_{\infty h}$

Orbitais 2s - inseparáveis

	$2s(O_1)$	$2s(O_2)$
$2s(O_1)$	1	0
$2s(O_2)$	0	1

i, C_2 $\rightarrow$ S_∞

	$2s(O_1)$	$2s(O_2)$
$2s(O_1)$	0	1
$2s(O_2)$	1	0

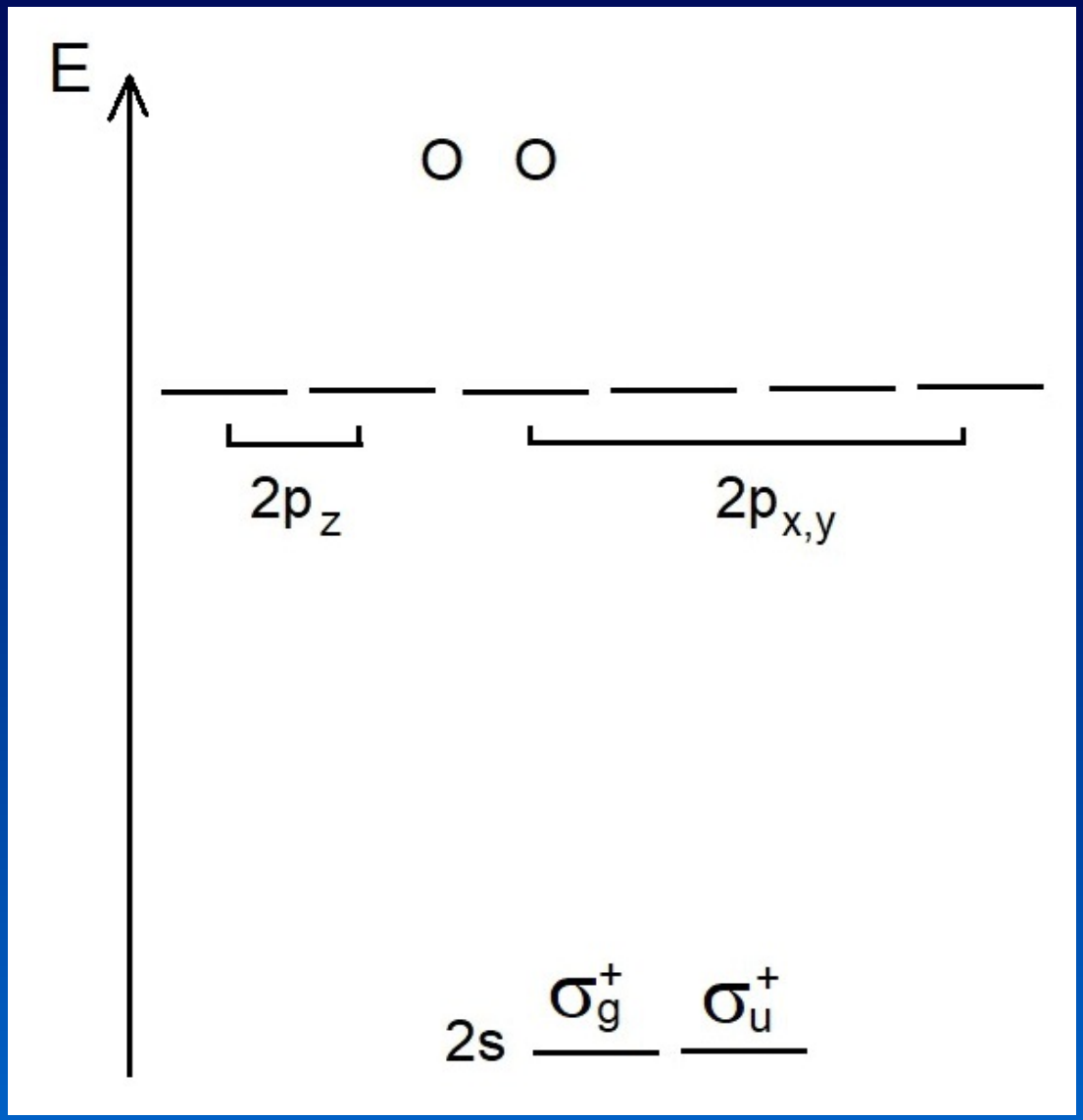
$\chi = 0$

Dioxigênio - O_2 - $D_{\infty h}$

$D_{\infty h}$	E	$2C_\infty^{\varphi}$	$\infty\sigma_v$	i	$2S_\infty^{\varphi}$	∞C_2
Σ_g^+	1	1	1	1	1	1
Σ_g^-	1	1	-1	1	1	-1
Π_g	2	$2\cos\varphi$	0	2	$-2\cos\varphi$	0
Δ_g	2	$2\cos2\varphi$	0	2	$2\cos2\varphi$	0
Σ_u^+	1	1	1	-1	-1	-1
Σ_u^-	1	1	-1	-1	-1	1
Π_u	2	$2\cos\varphi$	0	-2	$2\cos\varphi$	0
Δ_u	2	$2\cos2\varphi$	0	-2	$-2\cos2\varphi$	0
$2s(O_1,O_2)$	2	2	2	0	0	0

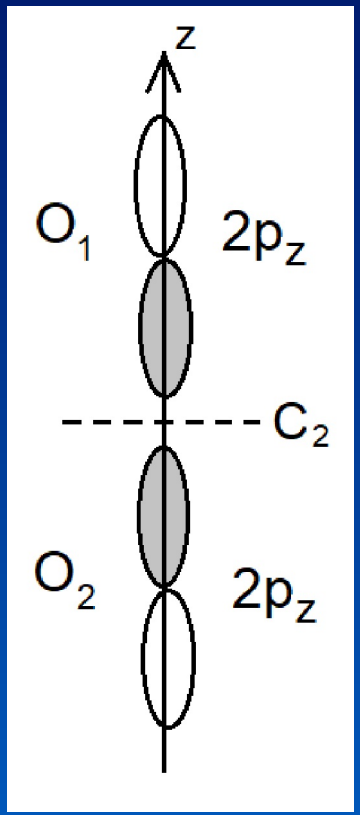
$$\Sigma_g^+ \oplus \Sigma_u^+$$

O_2 - $D_{\infty h}$



O_2 - $D_{\infty h}$

Orbitais $2p_z$ - inseparáveis



O_2 - $D_{\infty h}$

Orbitais $2p_z$ - INSEPARÁVEIS

	$2p_z(O_1)$	$2p_z(O_2)$
$2p_z(O_1)$	1	0
$2p_z(O_2)$	0	1

$E, C_\infty \rightarrow \sigma_v$

	$2p_z(O_1)$	$2p_z(O_2)$
$2p_z(O_1)$	1	0
$2p_z(O_2)$	0	1

$\chi = 2$

Dioxigênio - O_2 - $D_{\infty h}$

$D_{\infty h}$	E	$2C_\infty^{\varphi}$	$\infty\sigma_v$	i	$2S_\infty^{\varphi}$	∞C_2
Σ_g^+	1	1	1	1	1	1
Σ_g^-	1	1	-1	1	1	-1
Π_g	2	$2\cos\varphi$	0	2	$-2\cos\varphi$	0
Δ_g	2	$2\cos2\varphi$	0	2	$2\cos2\varphi$	0
Σ_u^+	1	1	1	-1	-1	-1
Σ_u^-	1	1	-1	-1	-1	1
Π_u	2	$2\cos\varphi$	0	-2	$2\cos\varphi$	0
Δ_u	2	$2\cos2\varphi$	0	-2	$-2\cos2\varphi$	0
$2p_z(O_1,O_2)$	2	2	2			

O_2 - $D_{\infty h}$

Orbitais $2p_z$ - INSEPARÁVEIS

	$2p_z(O_1)$	$2p_z(O_2)$
$2p_z(O_1)$	1	0
$2p_z(O_2)$	0	1

i, C_2 $\rightarrow$ S_∞

	$2p_z(O_1)$	$2p_z(O_2)$
$2p_z(O_1)$	0	1
$2p_z(O_2)$	1	0

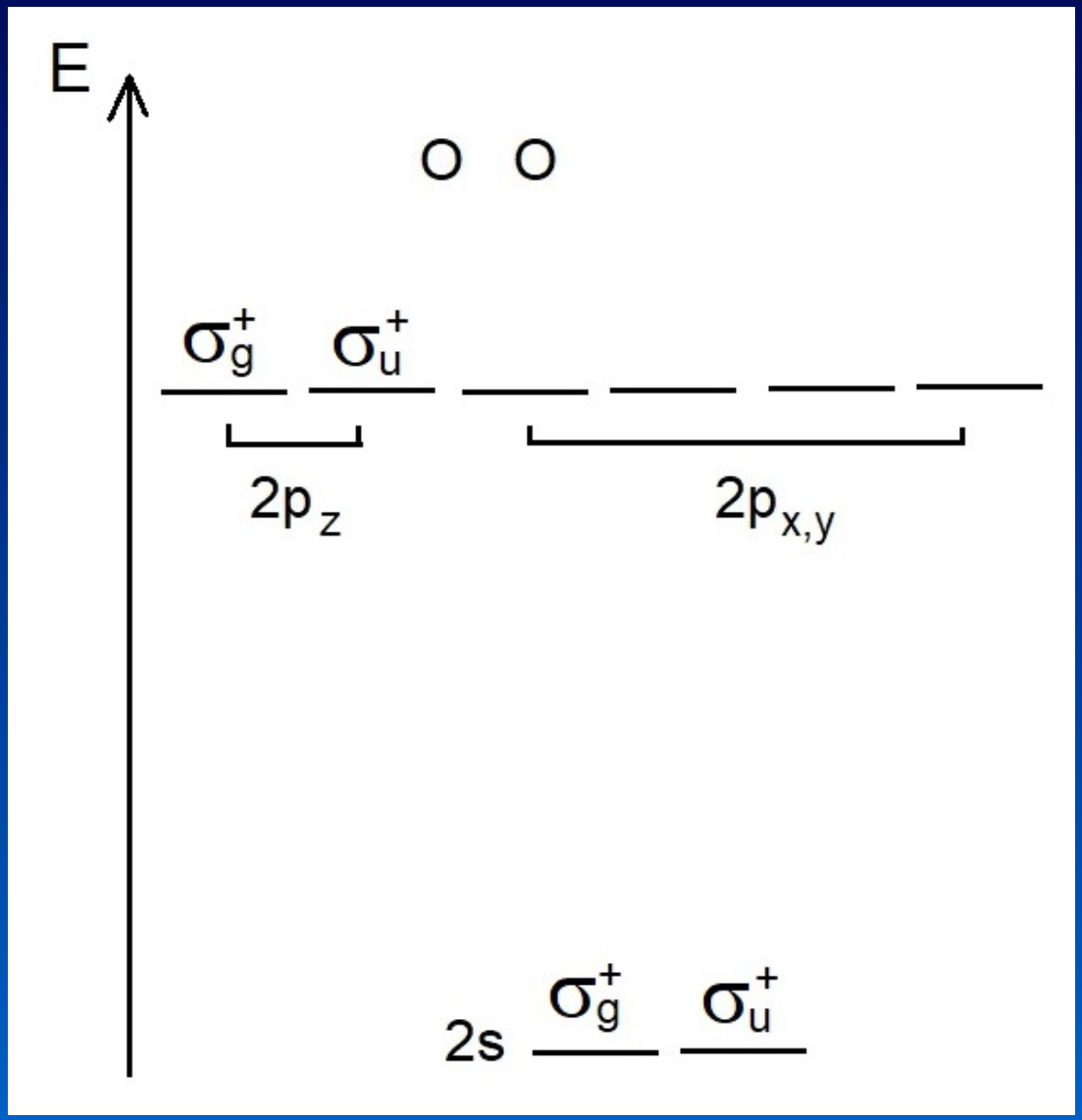
$\chi = 0$

Dioxigênio - O_2 - $D_{\infty h}$

$D_{\infty h}$	E	$2C_\infty^{\varphi}$	$\infty\sigma_v$	i	$2S_\infty^{\varphi}$	∞C_2
Σ_g^+	1	1	1	1	1	1
Σ_g^-	1	1	-1	1	1	-1
Π_g	2	$2\cos\varphi$	0	2	$-2\cos\varphi$	0
Δ_g	2	$2\cos2\varphi$	0	2	$2\cos2\varphi$	0
Σ_u^+	1	1	1	-1	-1	-1
Σ_u^-	1	1	-1	-1	-1	1
Π_u	2	$2\cos\varphi$	0	-2	$2\cos\varphi$	0
Δ_u	2	$2\cos2\varphi$	0	-2	$-2\cos2\varphi$	0
$2p_z(O_1,O_2)$	2	2	2	0	0	0

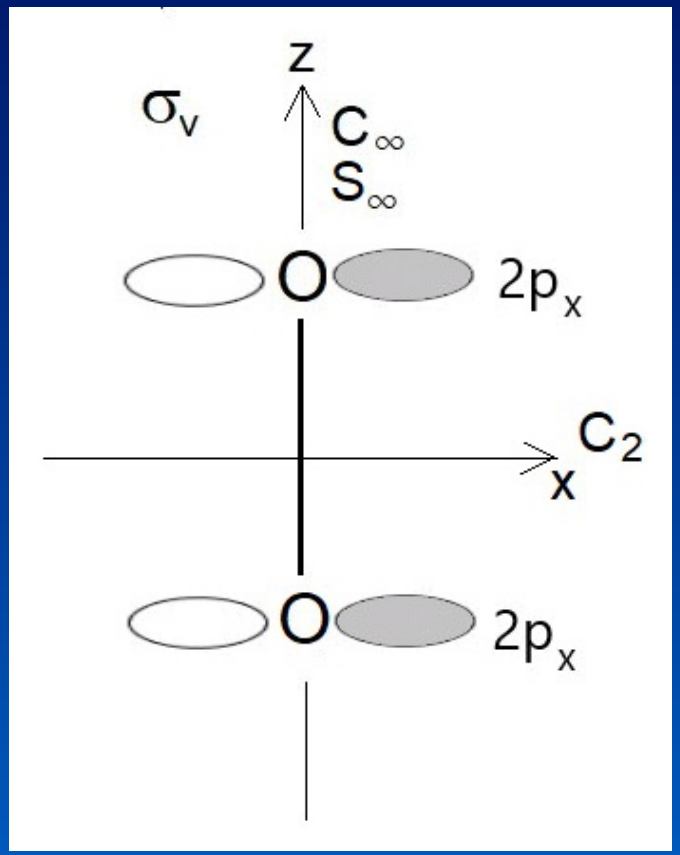
$$\Sigma_g^+ \oplus \Sigma_u^+$$

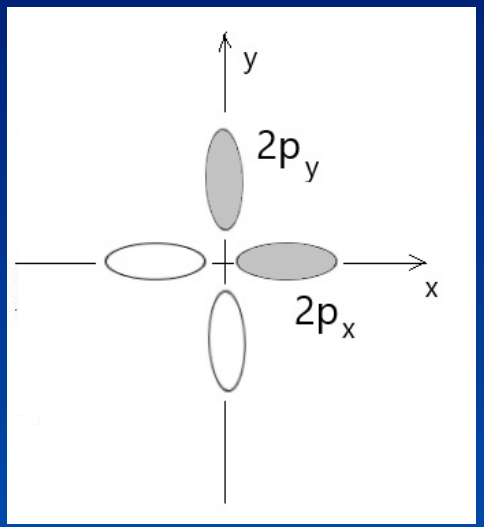
O_2 - $D_{\infty h}$



Orbitais $2p_x$ e $2p_y$ dos dois oxigênios -inseparáveis

O_2 - $D_{\infty h}$





Escolhendo $\varphi = 90°$

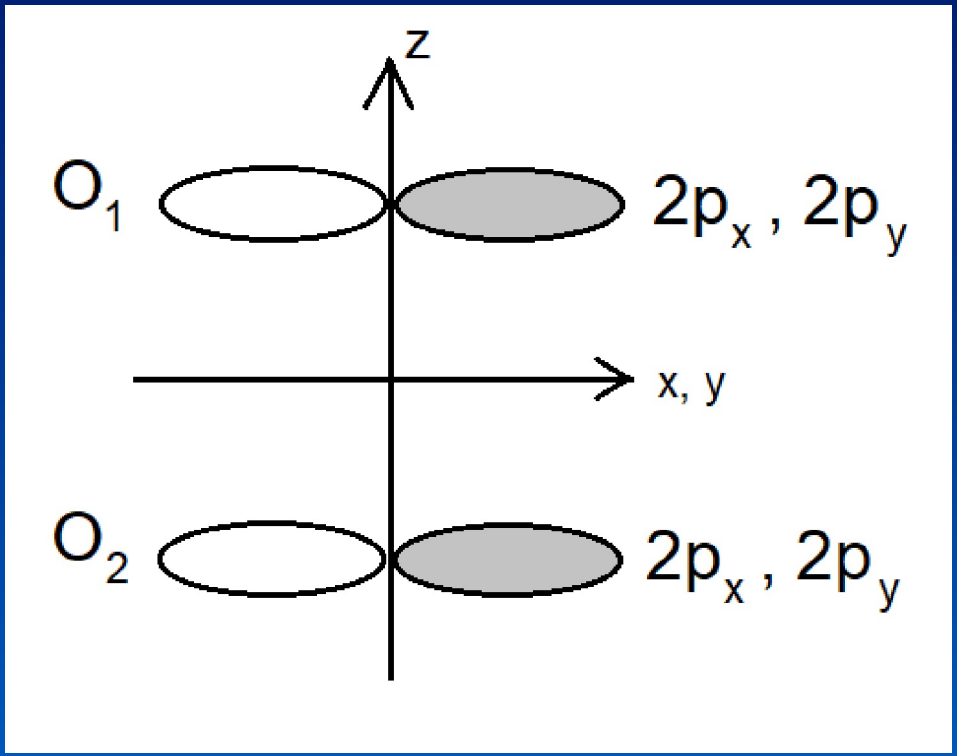
$C_\infty{}^{\varphi} = C_4$

$p_x \rightarrow p_y$

$p_y \rightarrow -p_x$

O_2 - $D_{\infty h}$

Orbitais $2p_x$ e $2p_y$ dos dois oxigênios, inseparáveis



$D_{\infty h}$

$D_{\infty h}$	E	$2C_\infty^{\varphi}$	$\infty\sigma_v$	i	$2S_\infty^{\varphi}$	∞C_2
Σ_g^+	1	1	1	1	1	1
Σ_g^-	1	1	-1	1	1	-1
Π_g	2	$2\cos\varphi$	0	2	$-2\cos\varphi$	0
Δ_g	2	$2\cos2\varphi$	0	2	$2\cos2\varphi$	0
Σ_u^+	1	1	1	-1	-1	-1
Σ_u^-	1	1	-1	-1	-1	1
Π_u	2	$2\cos\varphi$	0	-2	$2\cos\varphi$	0
Δ_u	2	$2\cos2\varphi$	0	-2	$-2\cos2\varphi$	0

Escolhendo $\varphi = 90°$ $\cos\varphi = 0$ $\cos2\varphi = -1$

$D_{\infty h}$

$D_{\infty h}$	E	$2C_{\infty}^{\varphi}$	$\infty\sigma_v$	i	$2S_{\infty}^{\varphi}$	∞C_2
Σ_g^+	1	1	1	1	1	1
Σ_g^-	1	1	-1	1	1	-1
Π_g	2	0	0	2	0	0
Δ_g	2	-2	0	2	-2	0
Σ_u^+	1	1	1	-1	-1	-1
Σ_u^-	1	1	-1	-1	-1	1
Π_u	2	0	0	-2	0	0
Δ_u	2	-2	0	-2	2	0

Escolhendo $\varphi = 90°$ $\cos\varphi = 0$ $\cos 2\varphi = -1$

O_2 - $D_{\infty h}$

Orbitais $2p_x$ e $2p_y$ dos dois oxigênios - INSEPARÁVEIS

	$2p_x^1$	$2p_y^1$	$2p_x^2$	$2p_y^2$
$2p_x^1$	1	0	0	0
$2p_y^1$	0	1	0	0
$2p_x^2$	0	0	1	0
$2p_y^2$	0	0	0	1

$\chi = 4$

$C_\infty^{\varphi = 90°} \rightarrow$

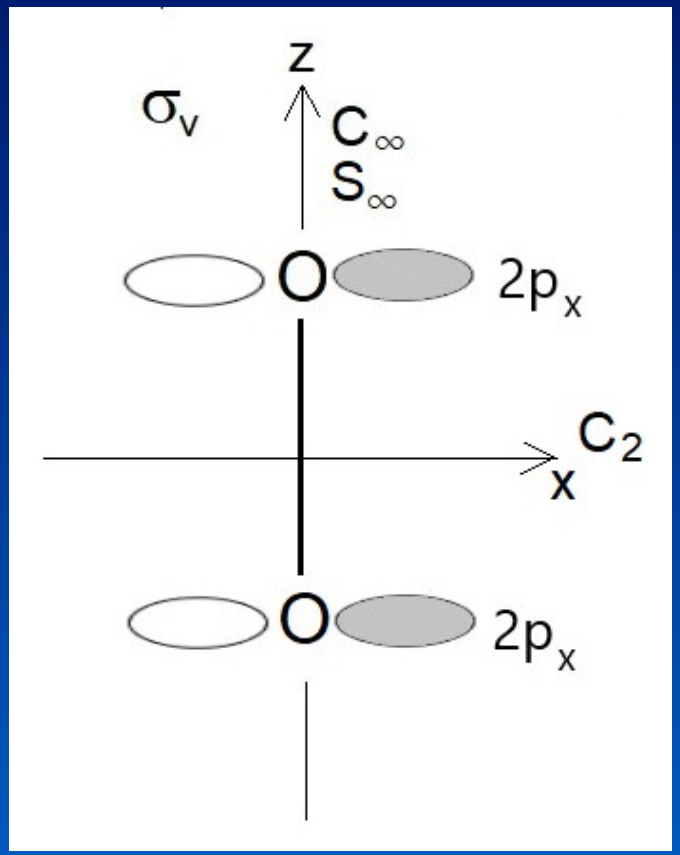
	$2p_x^1$	$2p_y^1$	$2p_x^2$	$2p_y^2$
$2p_x^1$	0	1	0	0
$2p_y^1$	-1	0	0	0
$2p_x^2$	0	0	0	1
$2p_y^2$	0	0	-1	0

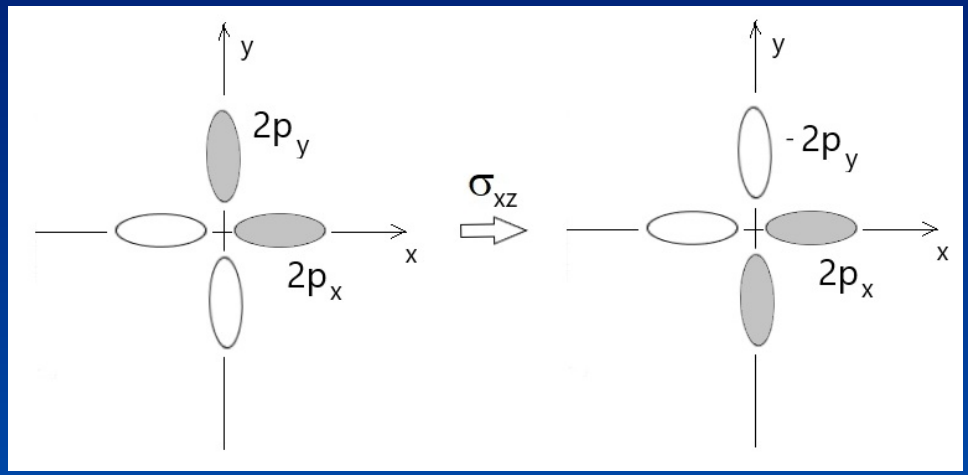
$\chi = 0$

Dioxigênio - O_2 - $D_{\infty h}$

$D_{\infty h}$	E	$2C_\infty^{\varphi}$	$\infty\sigma_v$	i	$2S_\infty^{\varphi}$	∞C_2
Σ_g^+	1	1	1	1	1	1
Σ_g^-	1	1	-1	1	1	-1
Π_g	2	0	0	2	0	0
Δ_g	2	-2	0	2	-2	0
Σ_u^+	1	1	1	-1	-1	-1
Σ_u^-	1	1	-1	-1	-1	1
Π_u	2	0	0	-2	0	0
Δ_u	2	-2	0	-2	2	0
$2p_{x,y}(O_1,O_2)$	4	0				

Orbitais $2p_x$ e $2p_y$ dos dois oxigênios -inseparáveis O_2 - $D_{\infty h}$





O_2 - $D_{\infty h}$

Orbitais $2p_x$ e $2p_y$ dos dois oxigênios - INSEPARÁVEIS

	$2p_x^1$	$2p_y^1$	$2p_x^2$	$2p_y^2$
$2p_x^1$	1	0	0	0
$2p_y^1$	0	1	0	0
$2p_x^2$	0	0	1	0
$2p_y^2$	0	0	0	1

$\chi = 4$

$\sigma_v^{(xz)}$ $\rightarrow$

	$2p_x^1$	$2p_y^1$	$2p_x^2$	$2p_y^2$
$2p_x^1$	1	0	0	0
$2p_y^1$	0	-1	0	0
$2p_x^2$	0	0	1	0
$2p_y^2$	0	0	0	-1

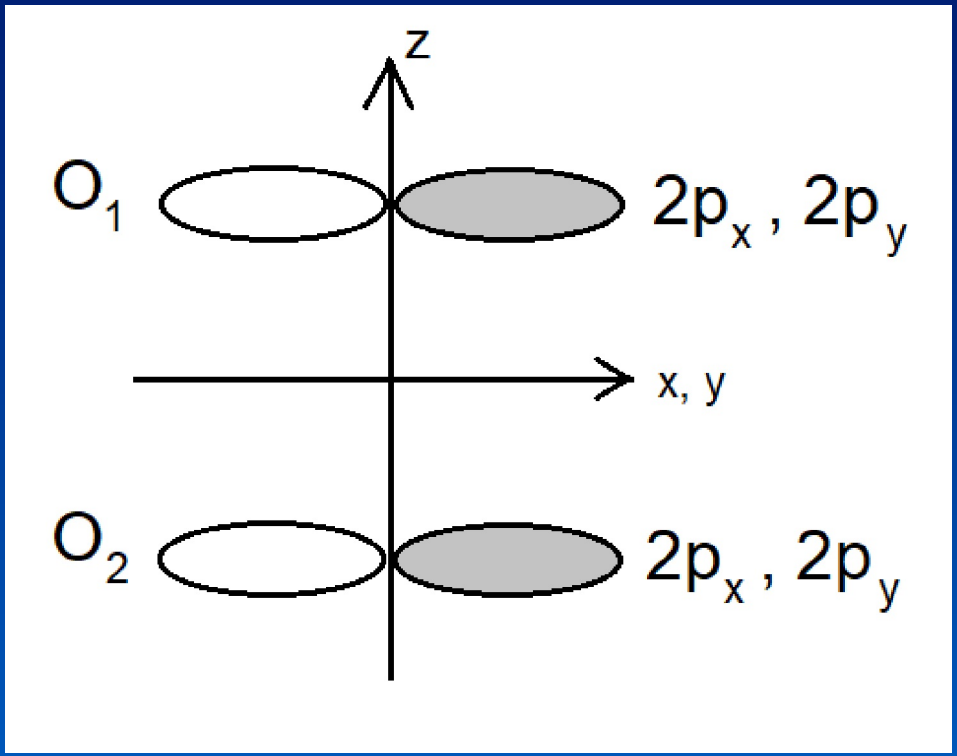
$\chi = 0$

Dioxigênio - O_2 - $D_{\infty h}$

$D_{\infty h}$	E	$2C_\infty^{\varphi}$	$\infty\sigma_v$	i	$2S_\infty^{\varphi}$	∞C_2
Σ_g^+	1	1	1	1	1	1
Σ_g^-	1	1	-1	1	1	-1
Π_g	2	0	0	2	0	0
Δ_g	2	-2	0	2	-2	0
Σ_u^+	1	1	1	-1	-1	-1
Σ_u^-	1	1	-1	-1	-1	1
Π_u	2	0	0	-2	0	0
Δ_u	2	-2	0	-2	2	0
$2p_{x,y}(O_1,O_2)$	4	0	0			

O_2 - $D_{\infty h}$

Orbitais $2p_x$ e $2p_y$ dos dois oxigênios, inseparáveis



O_2 - $D_{\infty h}$

Orbitais $2p_x$ e $2p_y$ dos dois oxigênios - INSEPARÁVEIS

	$2p_x^1$	$2p_y^1$	$2p_x^2$	$2p_y^2$
$2p_x^1$	1	0	0	0
$2p_y^1$	0	1	0	0
$2p_x^2$	0	0	1	0
$2p_y^2$	0	0	0	1

$\chi = 4$

i $\rightarrow$

	$2p_x^1$	$2p_y^1$	$2p_x^2$	$2p_y^2$
$2p_x^1$	0	0	-1	0
$2p_y^1$	0	0	0	-1
$2p_x^2$	-1	0	0	0
$2p_y^2$	0	-1	0	0

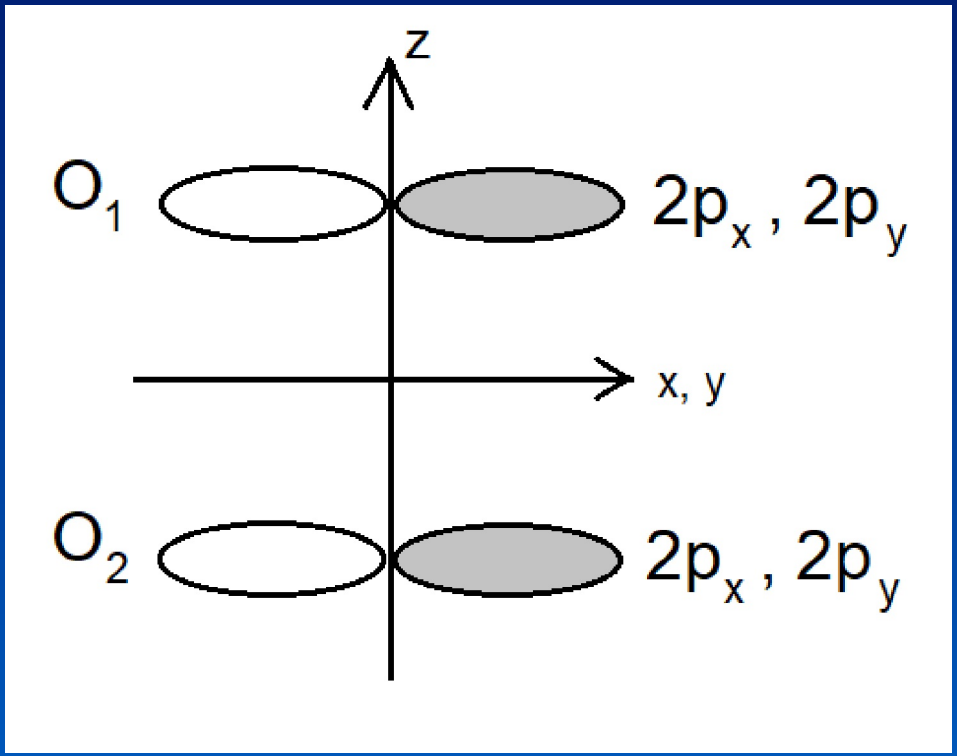
$\chi = 0$

Dioxigênio - O_2 - $D_{\infty h}$

$D_{\infty h}$	E	$2C_\infty^{\varphi}$	$\infty\sigma_v$	i	$2S_\infty^{\varphi}$	∞C_2
Σ_g^+	1	1	1	1	1	1
Σ_g^-	1	1	-1	1	1	-1
Π_g	2	0	0	2	0	0
Δ_g	2	-2	0	2	-2	0
Σ_u^+	1	1	1	-1	-1	-1
Σ_u^-	1	1	-1	-1	-1	1
Π_u	2	0	0	-2	0	0
Δ_u	2	-2	0	-2	2	0
$2p_{x,y}(O_1,O_2)$	4	0	0	0		

O_2 - $D_{\infty h}$

Orbitais $2p_x$ e $2p_y$ dos dois oxigênios, inseparáveis



O_2 - $D_{\infty h}$

Orbitais $2p_x$ e $2p_y$ dos dois oxigênios - INSEPARÁVEIS

	$2p_x^1$	$2p_y^1$	$2p_x^2$	$2p_y^2$
$2p_x^1$	1	0	0	0
$2p_y^1$	0	1	0	0
$2p_x^2$	0	0	1	0
$2p_y^2$	0	0	0	1

$\chi = 4$

$S_\infty^{\varphi = 90°}$ $\rightarrow$

	$2p_x^1$	$2p_y^1$	$2p_x^2$	$2p_y^2$
$2p_x^1$	0	0	0	1
$2p_y^1$	0	0	-1	0
$2p_x^2$	0	1	0	0
$2p_y^2$	-1	0	0	0

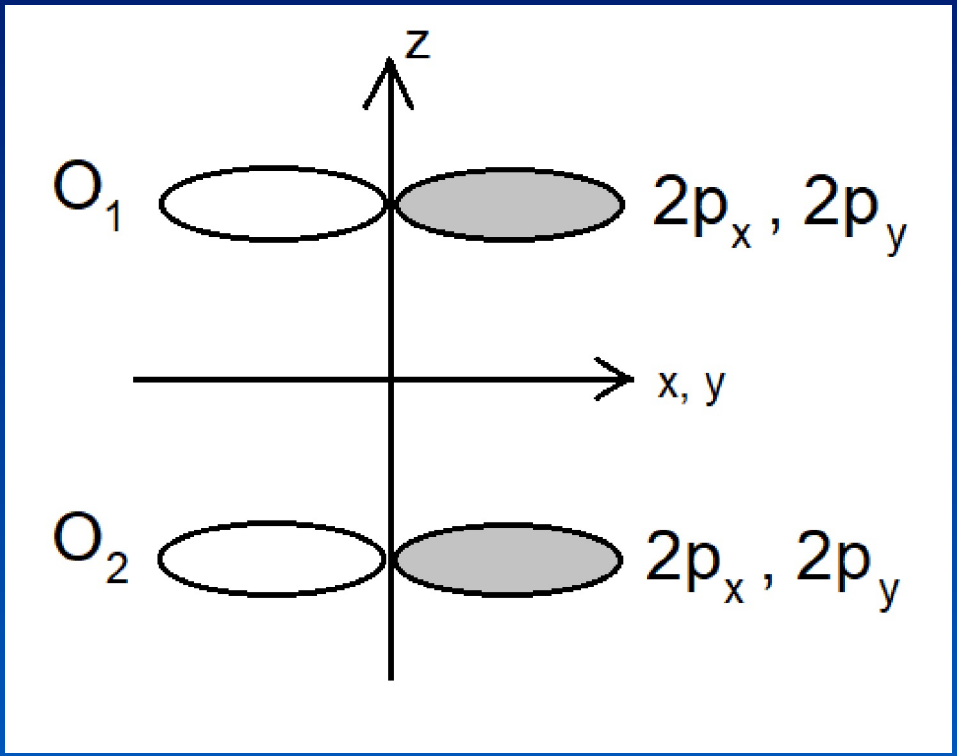
$\chi = 0$

Dioxigênio - O_2 - $D_{\infty h}$

$D_{\infty h}$	E	$2C_\infty^{\varphi}$	$\infty\sigma_v$	i	$2S_\infty^{\varphi}$	∞C_2
Σ_g^+	1	1	1	1	1	1
Σ_g^-	1	1	-1	1	1	-1
Π_g	2	0	0	2	0	0
Δ_g	2	-2	0	2	-2	0
Σ_u^+	1	1	1	-1	-1	-1
Σ_u^-	1	1	-1	-1	-1	1
Π_u	2	0	0	-2	0	0
Δ_u	2	-2	0	-2	2	0
$2p_{x,y}(O_1,O_2)$	4	0	0	0	0	

O_2 - $D_{\infty h}$

Orbitais $2p_x$ e $2p_y$ dos dois oxigênios, inseparáveis



O_2 - $D_{\infty h}$

Orbitais $2p_x$ e $2p_y$ dos dois oxigênios - INSEPARÁVEIS

	$2p_x^1$	$2p_y^1$	$2p_x^2$	$2p_y^2$
$2p_x^1$	1	0	0	0
$2p_y^1$	0	1	0	0
$2p_x^2$	0	0	1	0
$2p_y^2$	0	0	0	1

$\chi = 4$

$C_2^x \rightarrow$

	$2p_x^1$	$2p_y^1$	$2p_x^2$	$2p_y^2$
$2p_x^1$	0	0	1	0
$2p_y^1$	0	0	0	-1
$2p_x^2$	1	0	0	0
$2p_y^2$	0	-1	0	0

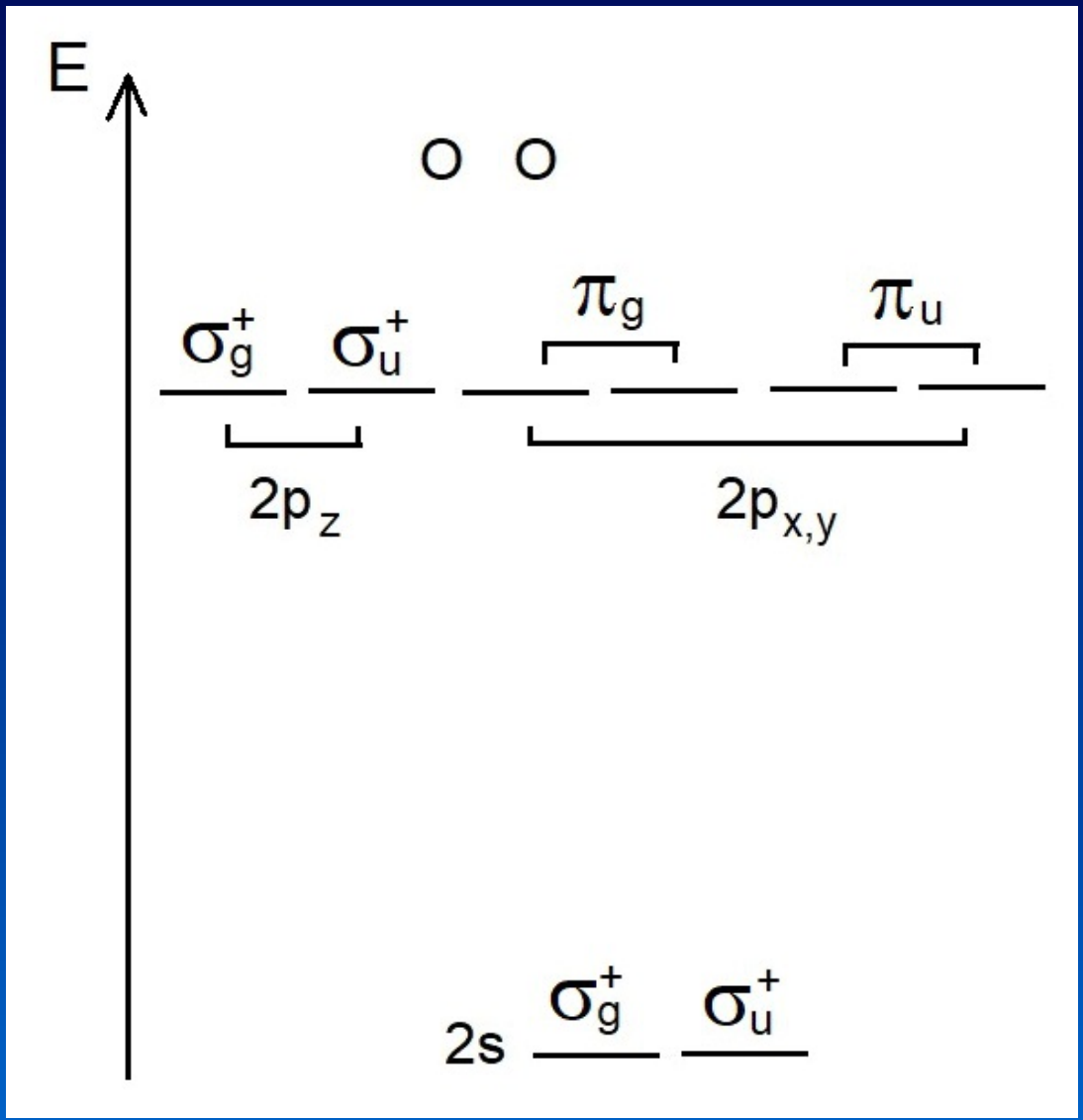
$\chi = 0$

Dioxigênio - O_2 - $D_{\infty h}$

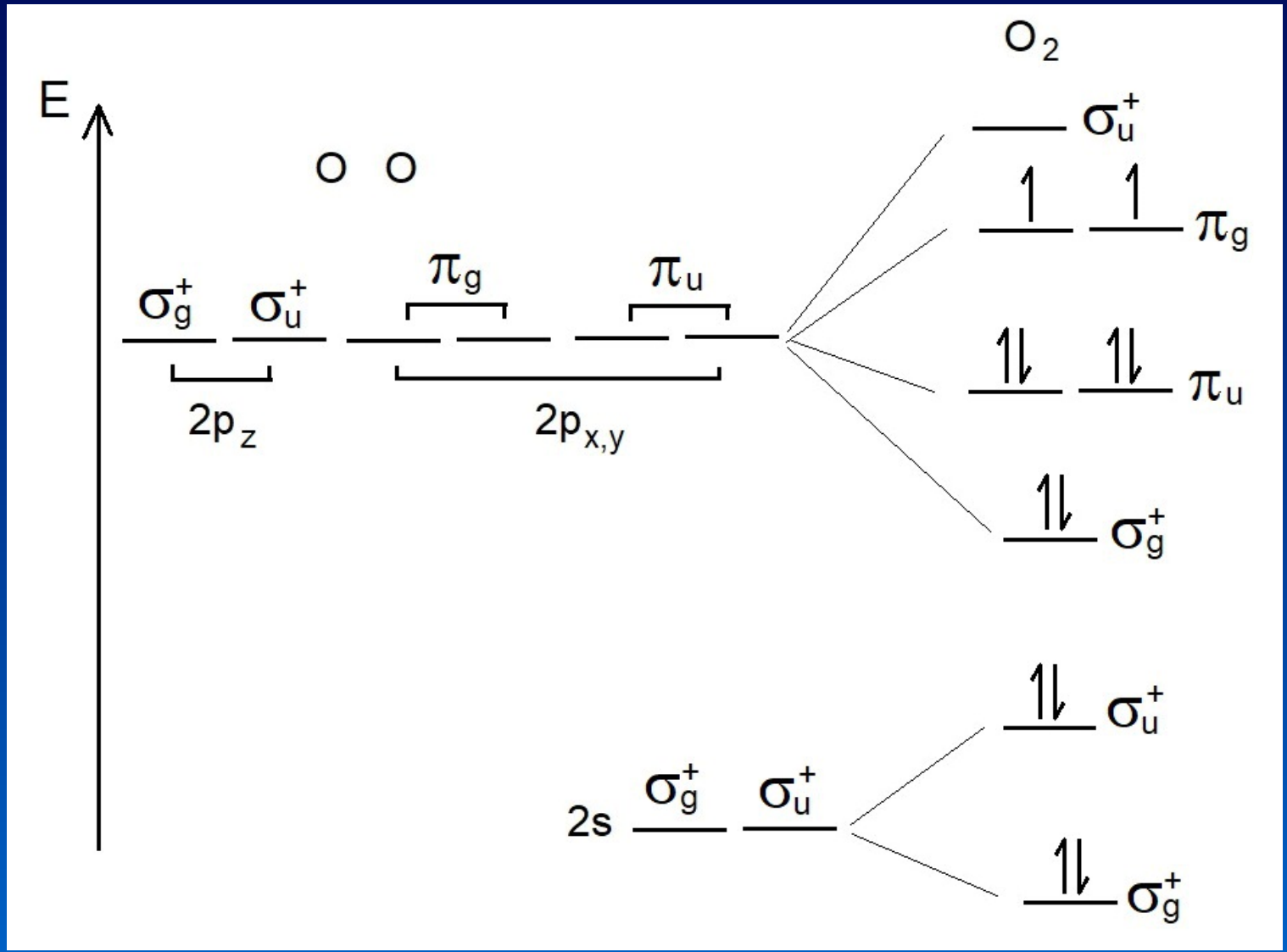
$D_{\infty h}$	E	$2C_\infty^\varphi$	$\infty\sigma_v$	i	$2S_\infty^\varphi$	∞C_2
Σ_g^+	1	1	1	1	1	1
Σ_g^-	1	1	-1	1	1	-1
Π_g	2	0	0	2	0	0
Δ_g	2	-2	0	2	-2	0
Σ_u^+	1	1	1	-1	-1	-1
Σ_u^-	1	1	-1	-1	-1	1
Π_u	2	0	0	-2	0	0
Δ_u	2	-2	0	-2	2	0
$2p_{x,y}(O_1,O_2)$	4	0	0	0	0	0

$\Pi_g \oplus \Pi_u$

O_2 - $D_{\infty h}$



O_2 - $D_{\infty h}$


E
O O
σ_g^+
σ_u^+
π_g
π_u
$2p_z$
$2p_{x,y}$
O_2
σ_u^+
π_g
π_u
σ_g^+
2s
σ_g^+
σ_u^+
σ_u^+
σ_g^+

Espectros de fotoelétron - O_2

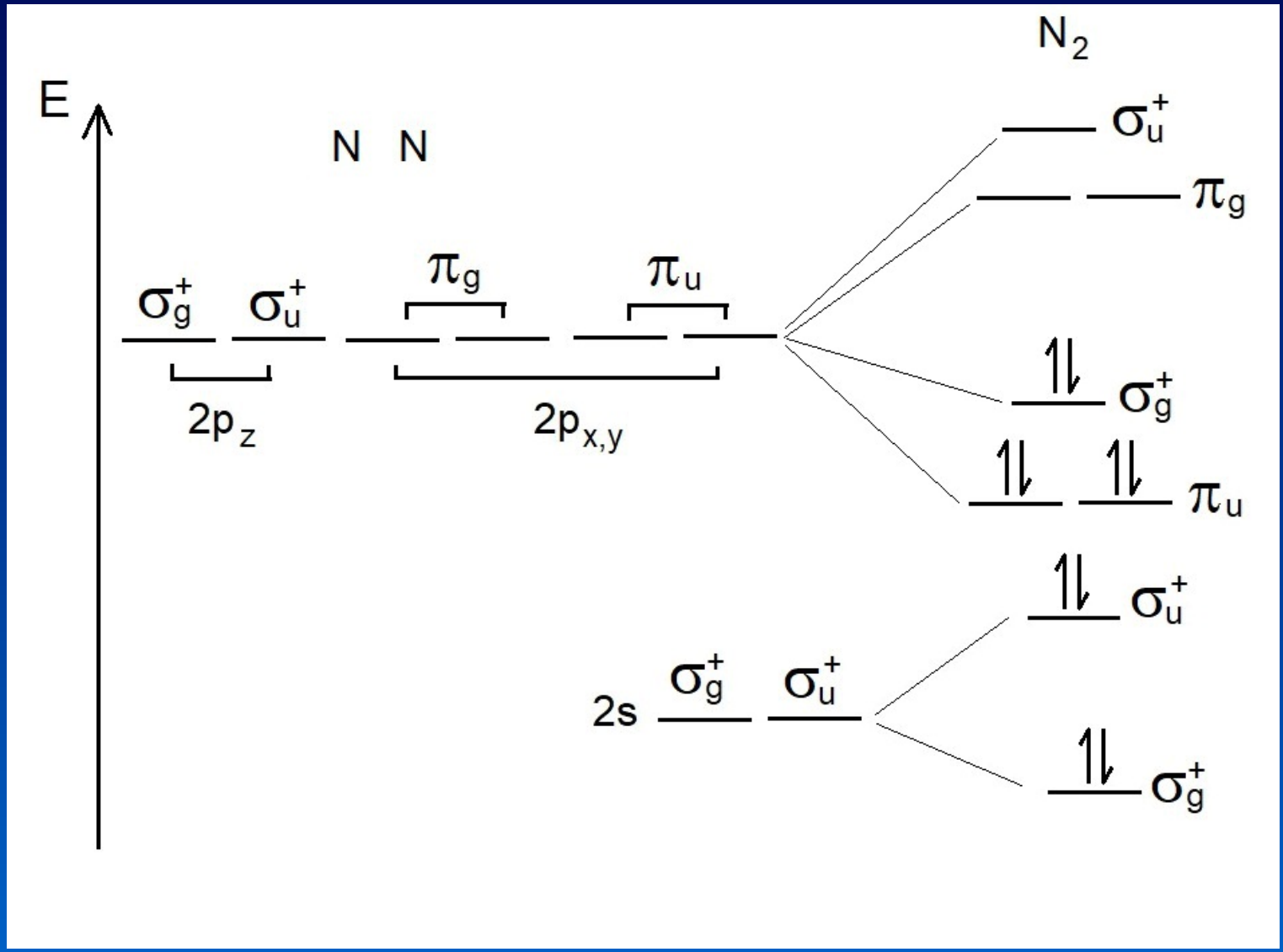
- Weller, M.; Overton, T.; Rourke, J.; Armstrong, F. *Inorganic Chemistry*, 6ª ed., Oxford University Press, 2014. pg. 256.

- Miessler, G. L.; Tarr, D. A. *Inorganic Chemistry*, Prentice-Hall, 1991. pg. 134 (reproduzindo espectro de Eland, J. H. *Photoelectron Spectroscopy*, Butterworths, 1974. pg. 11)

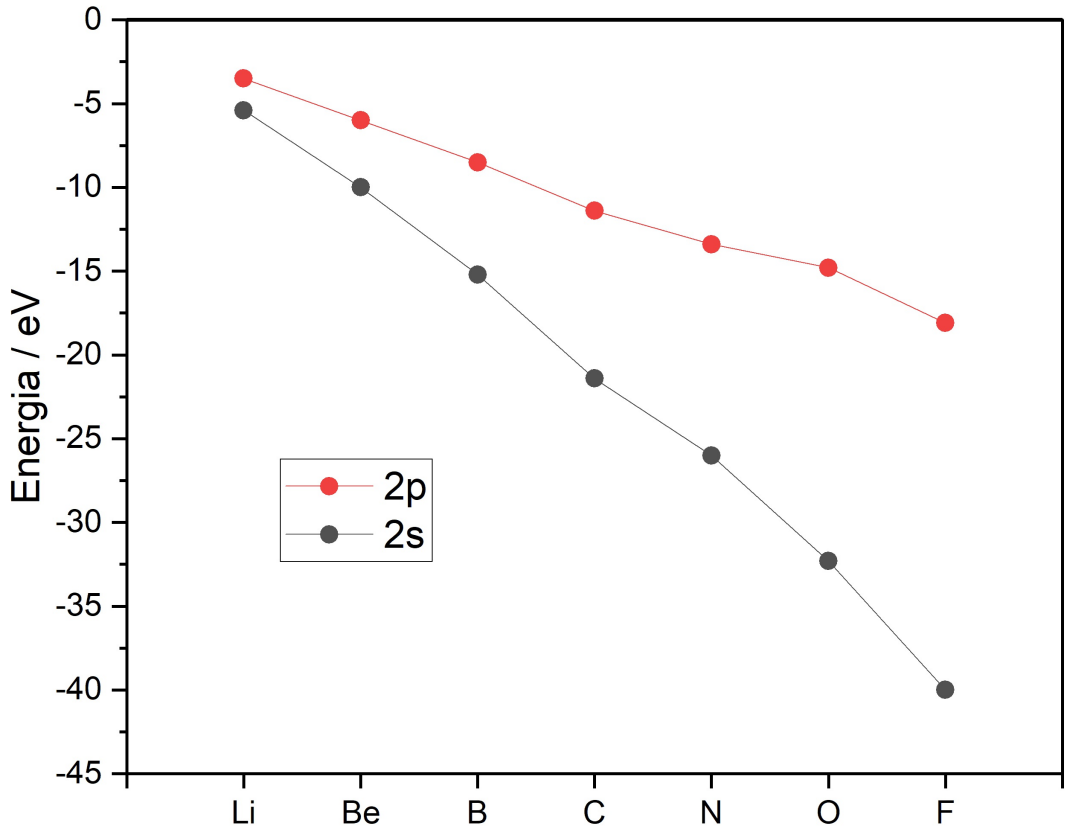
Espectro de fotoelétron - N_2

- Miessler, G. L.; Tarr, D. A. *Inorganic Chemistry*, Prentice-Hall, 1991. pg. 133 (reproduzindo espectro de Gardner, J. L.; Samson, J. A. R. *PJ. Chem. Phys.* *62*:1447 (1975)).

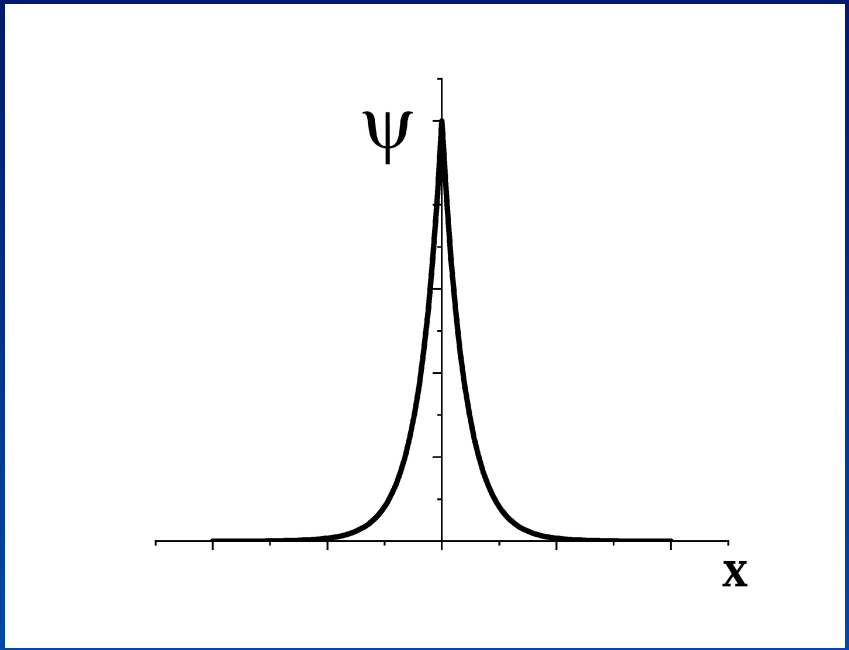
N_2 - $D_{\infty h}$


E
N N
N_2
σ_g^+
σ_u^+
π_g
π_u
$2p_z$
$2p_{x,y}$
2s
σ_g^+
σ_u^+
π_g
σ_u^+
σ_g^+
π_u
σ_u^+
σ_g^+

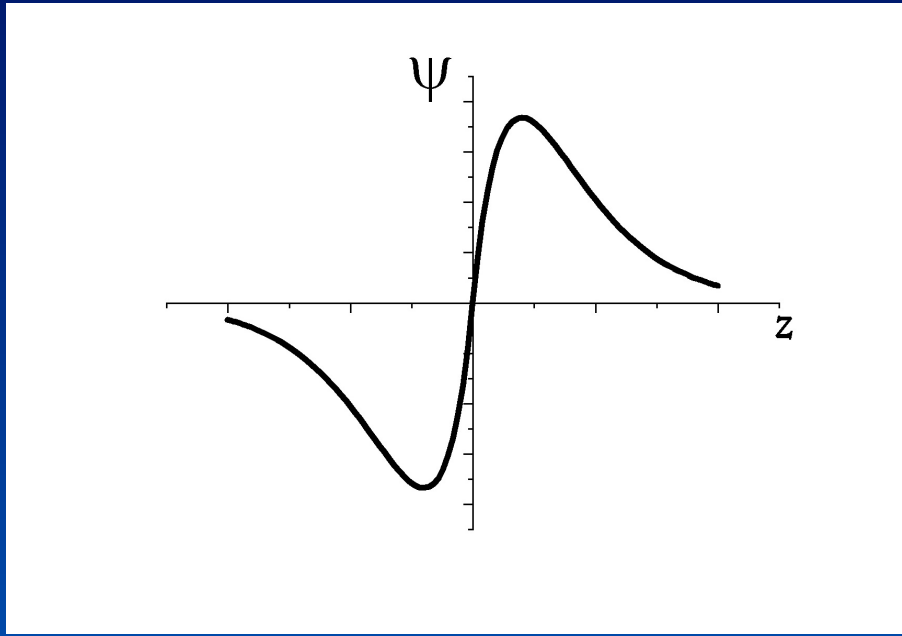
Energias dos orbitais atômicos



Funções de onda dos orbitais atômicos

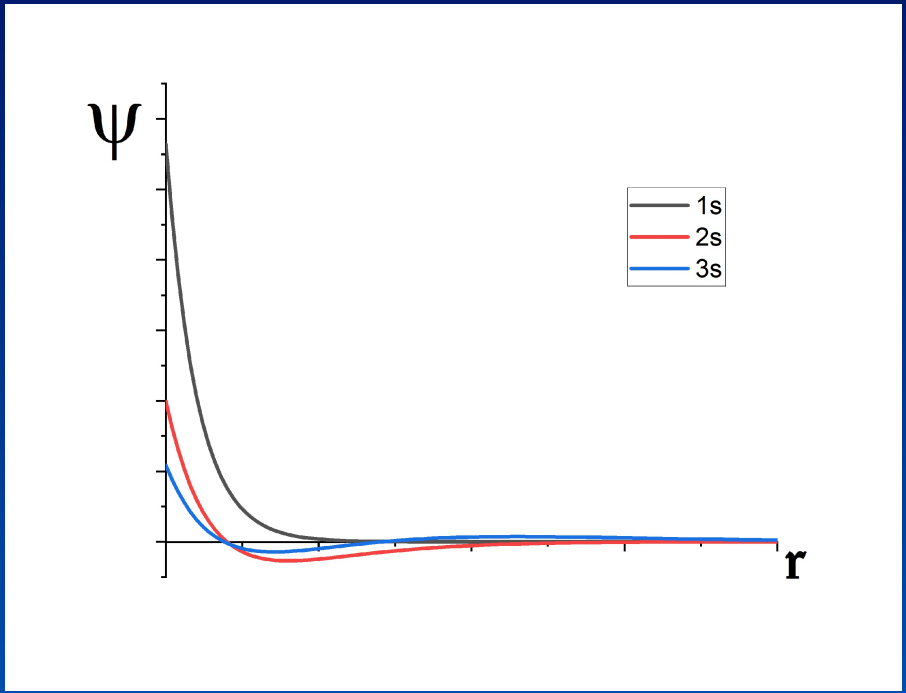


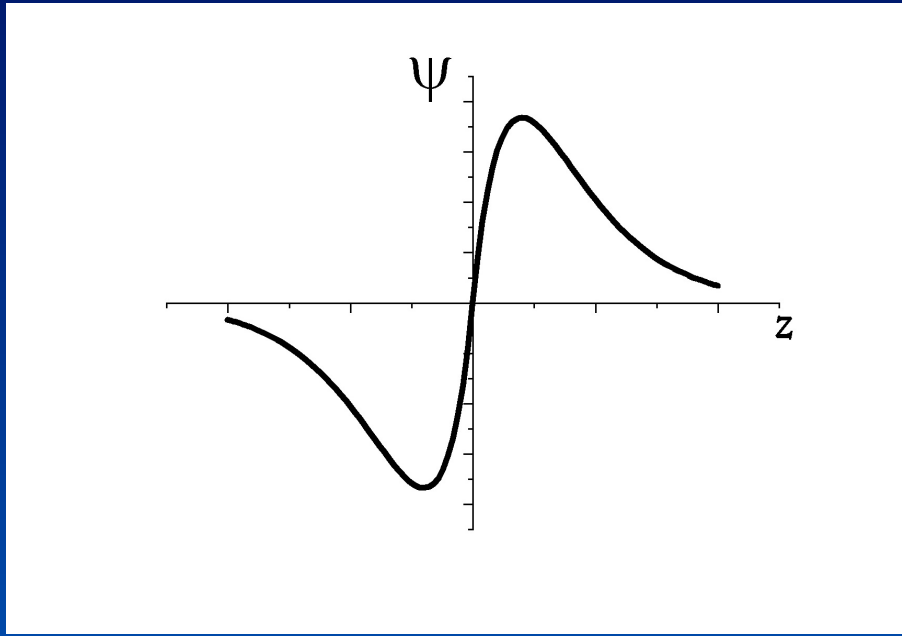
1s



2p

Funções de onda dos orbitais atômicos





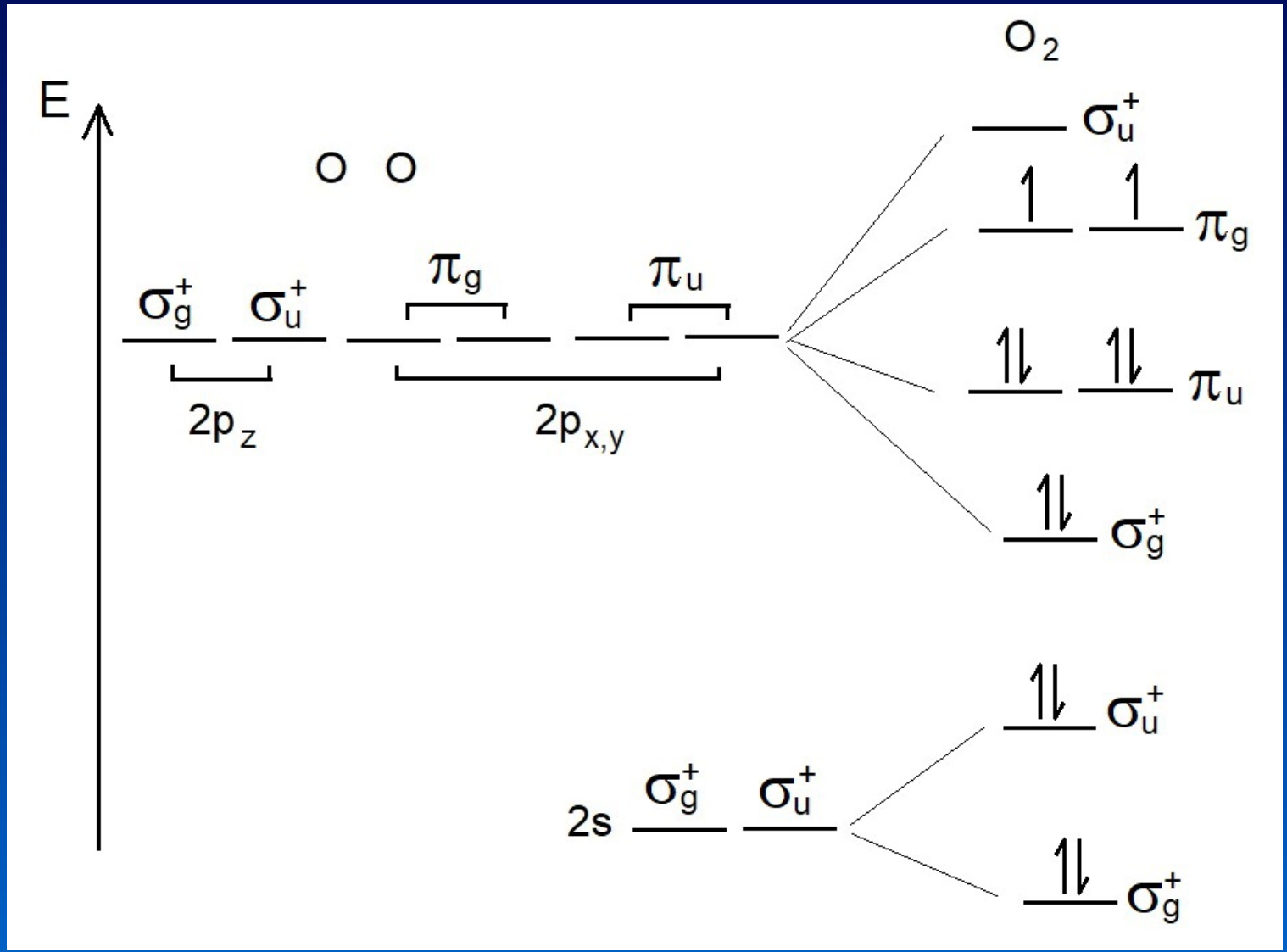
1s, 2s, 3s

2p

Desenhando os orbitais moleculares

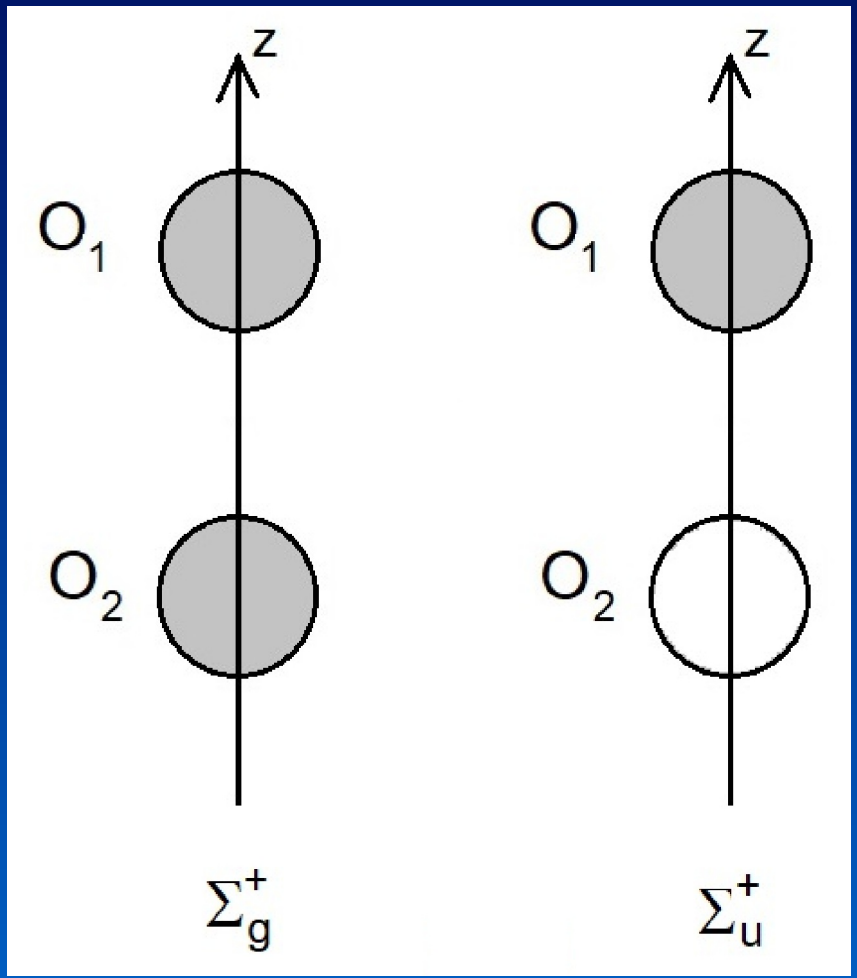
dioxigênio - O_2

O_2 - $D_{\infty h}$


E
O O
σ_g^+
σ_u^+
π_g
π_u
$2p_z$
$2p_{x,y}$
2s
σ_g^+
σ_u^+
O_2
σ_u^+
π_g
π_u
σ_g^+
σ_u^+
σ_g^+

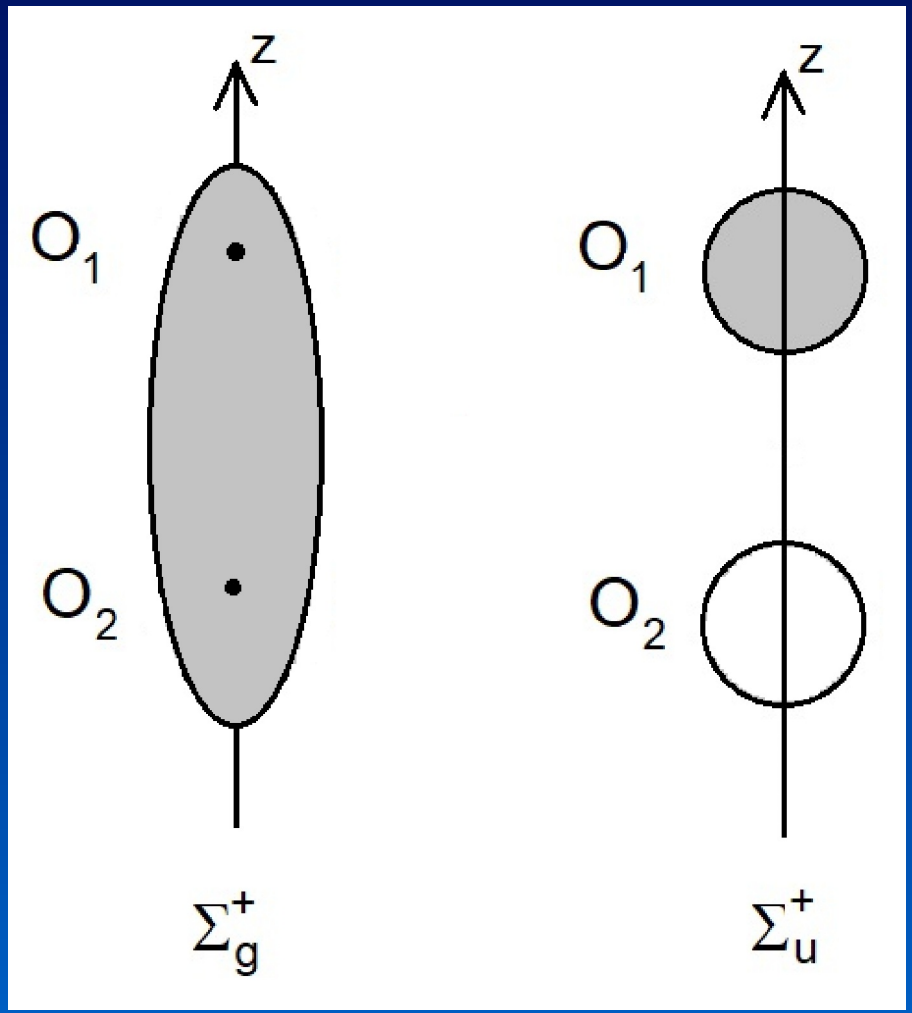
O_2 - $D_{\infty h}$

Os orbitais 2s podem formar uma combinação ligante e outra antiligante

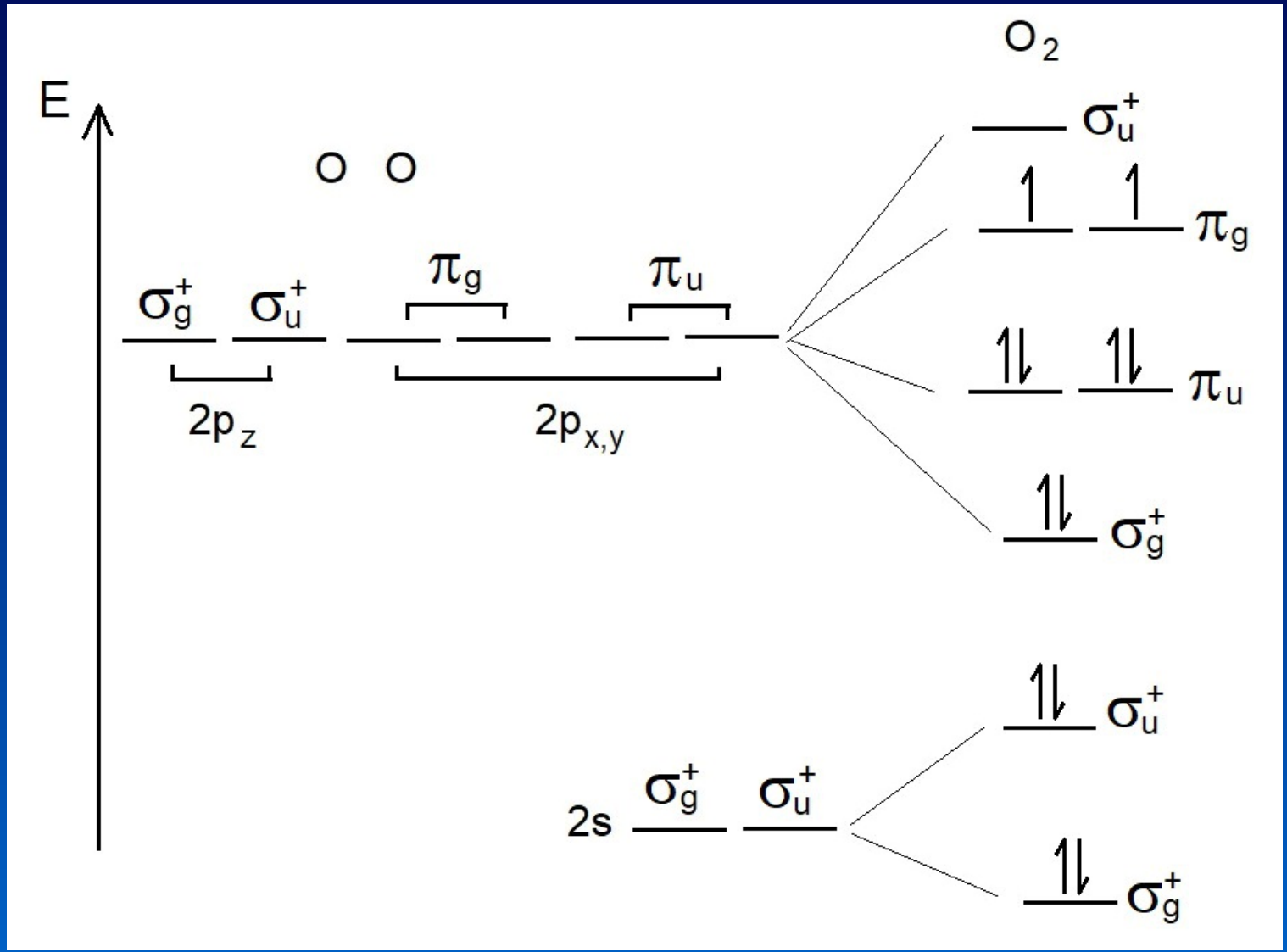


O_2 - $D_{\infty h}$

Os orbitais 2s podem formar uma combinação ligante e outra antiligante

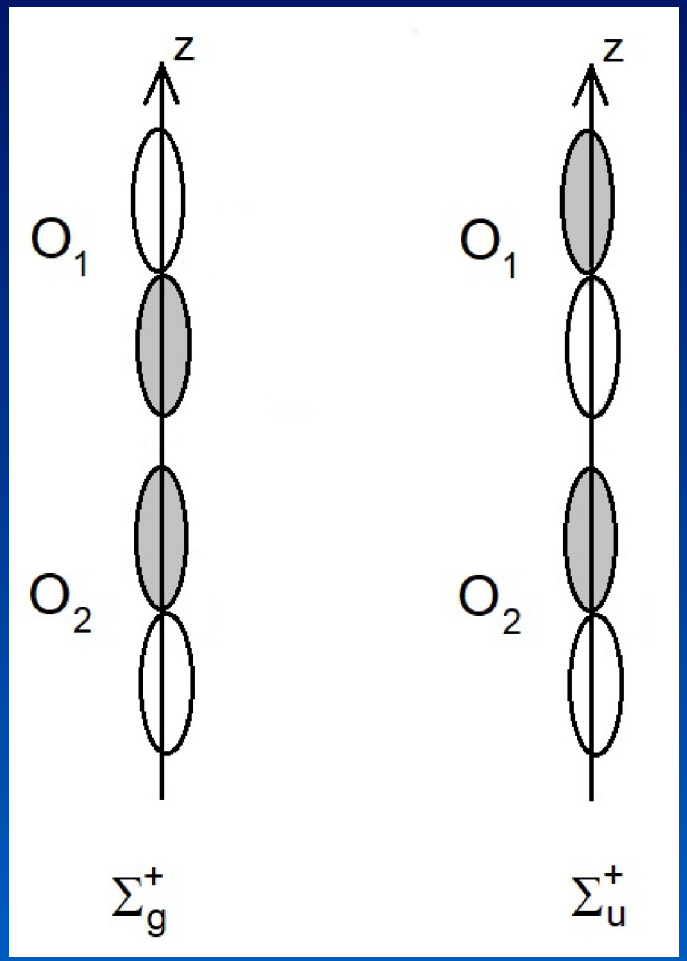


O_2 - $D_{\infty h}$


E
O O
σ_g^+
σ_u^+
π_g
π_u
$2p_z$
$2p_{x,y}$
2s
σ_g^+
σ_u^+
O_2
σ_u^+
π_g
π_u
σ_g^+
σ_u^+
σ_g^+

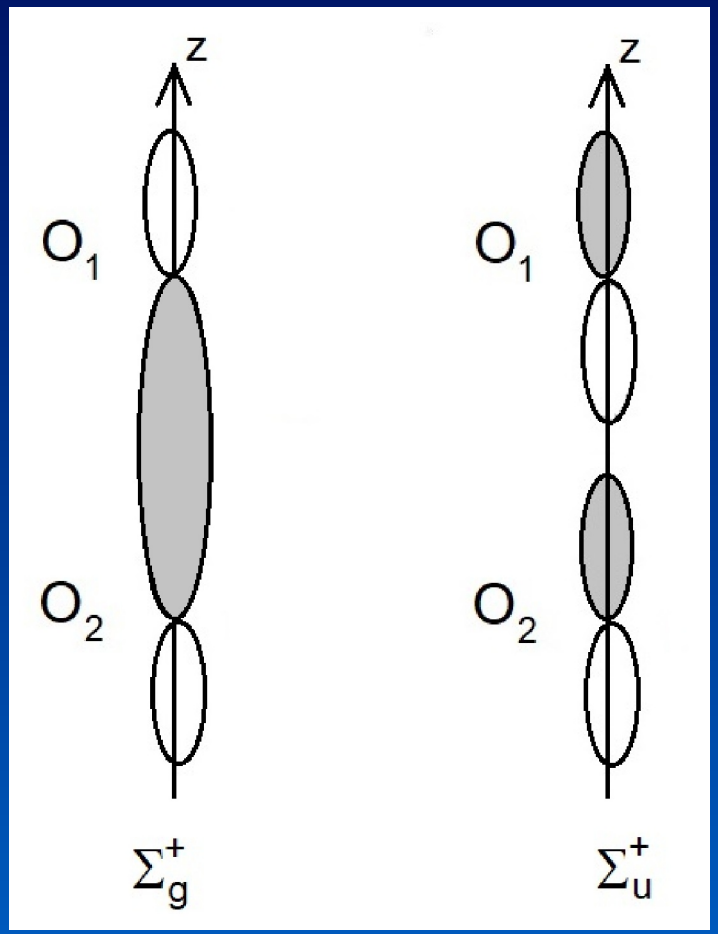
O_2 - $D_{\infty h}$

Os orbitais $2p_z$ também podem formar uma combinação σ ligante e antiligante

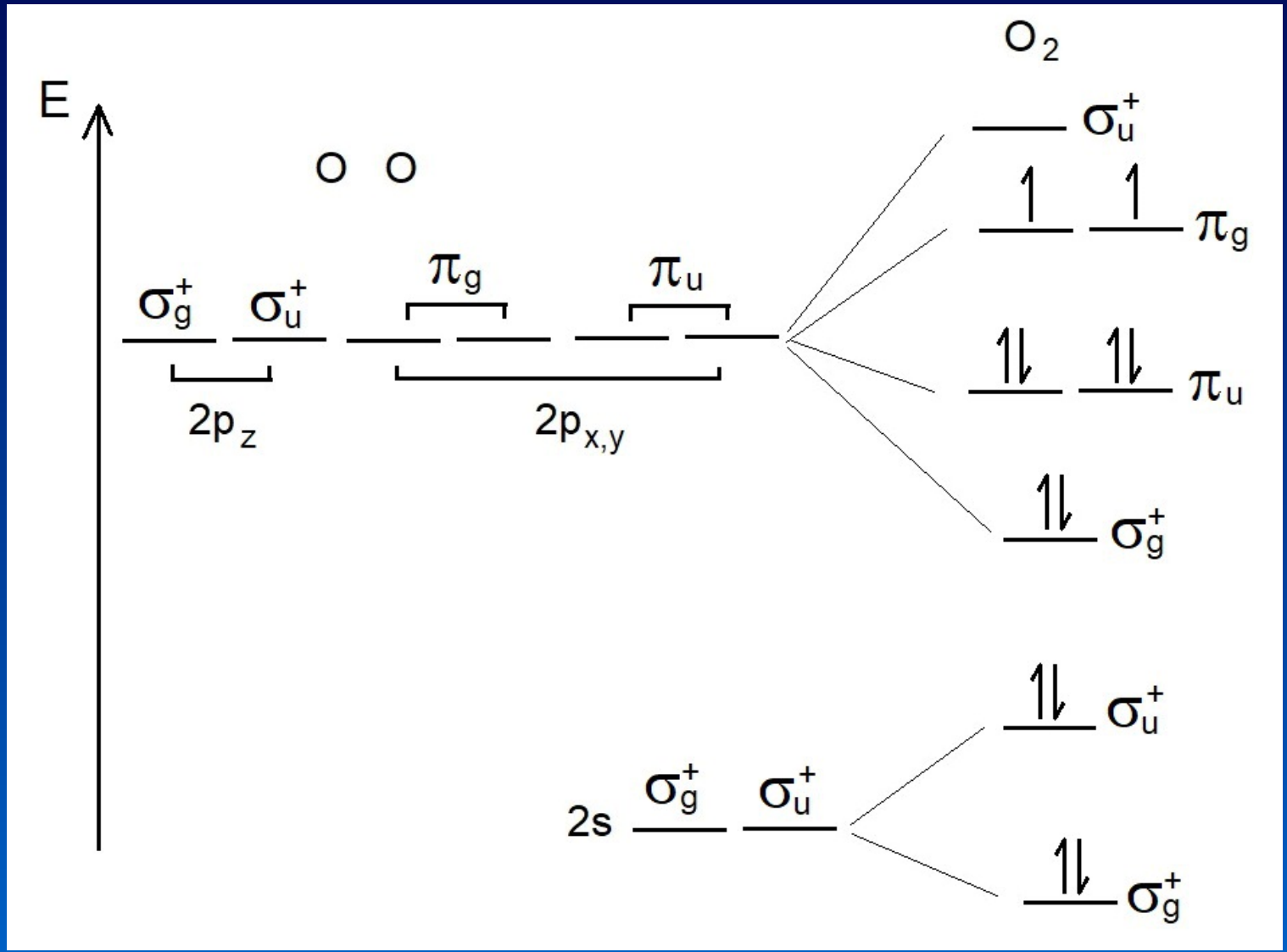


O_2 - $D_{\infty h}$

Os orbitais $2p_z$ também podem formar uma combinação σ ligante e antiligante

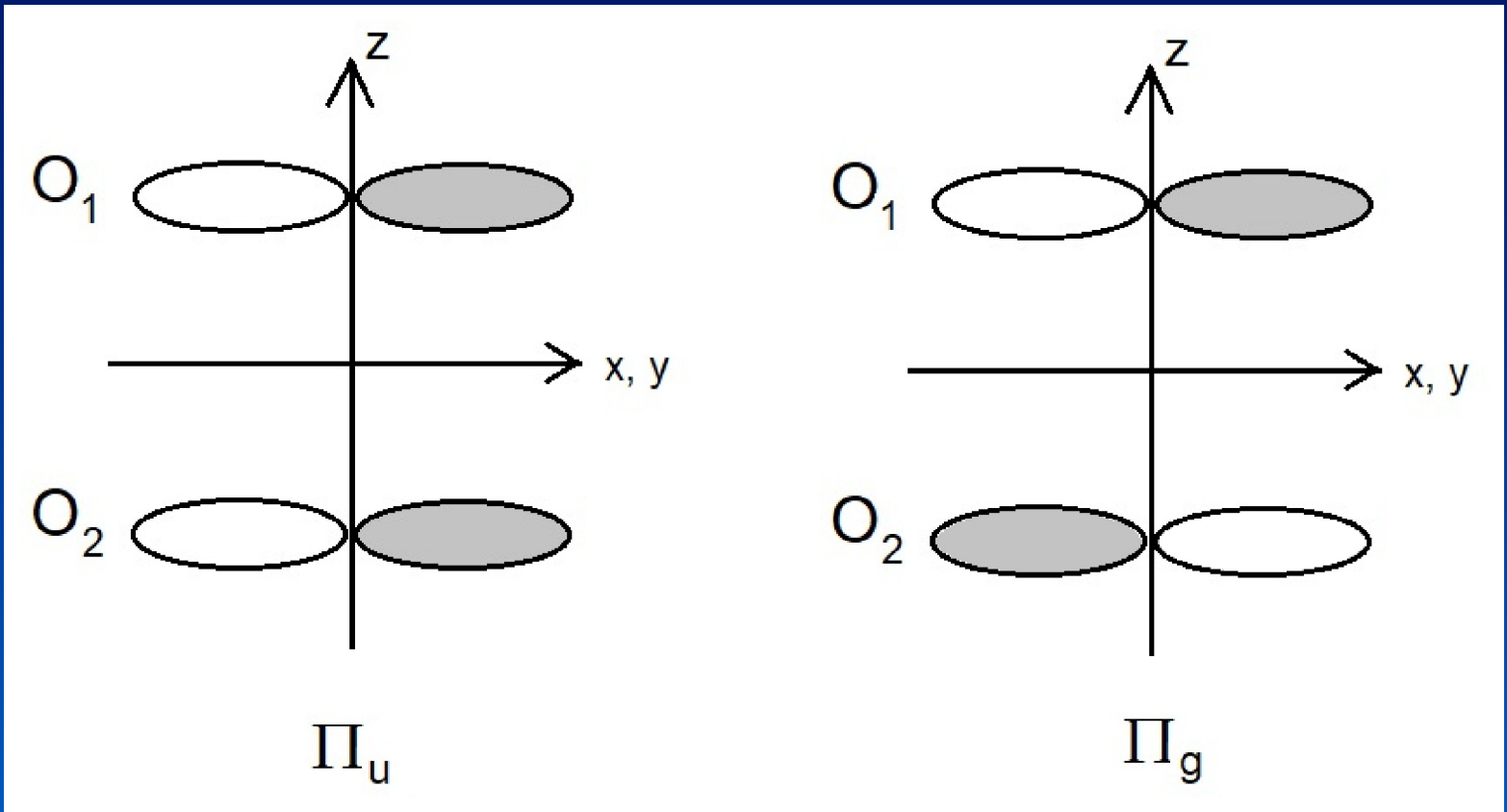


O_2 - $D_{\infty h}$


E
O O
σ_g^+
σ_u^+
π_g
π_u
$2p_z$
$2p_{x,y}$
2s
σ_g^+
σ_u^+
O_2
σ_u^+
π_g
π_u
σ_g^+
σ_u^+
σ_g^+

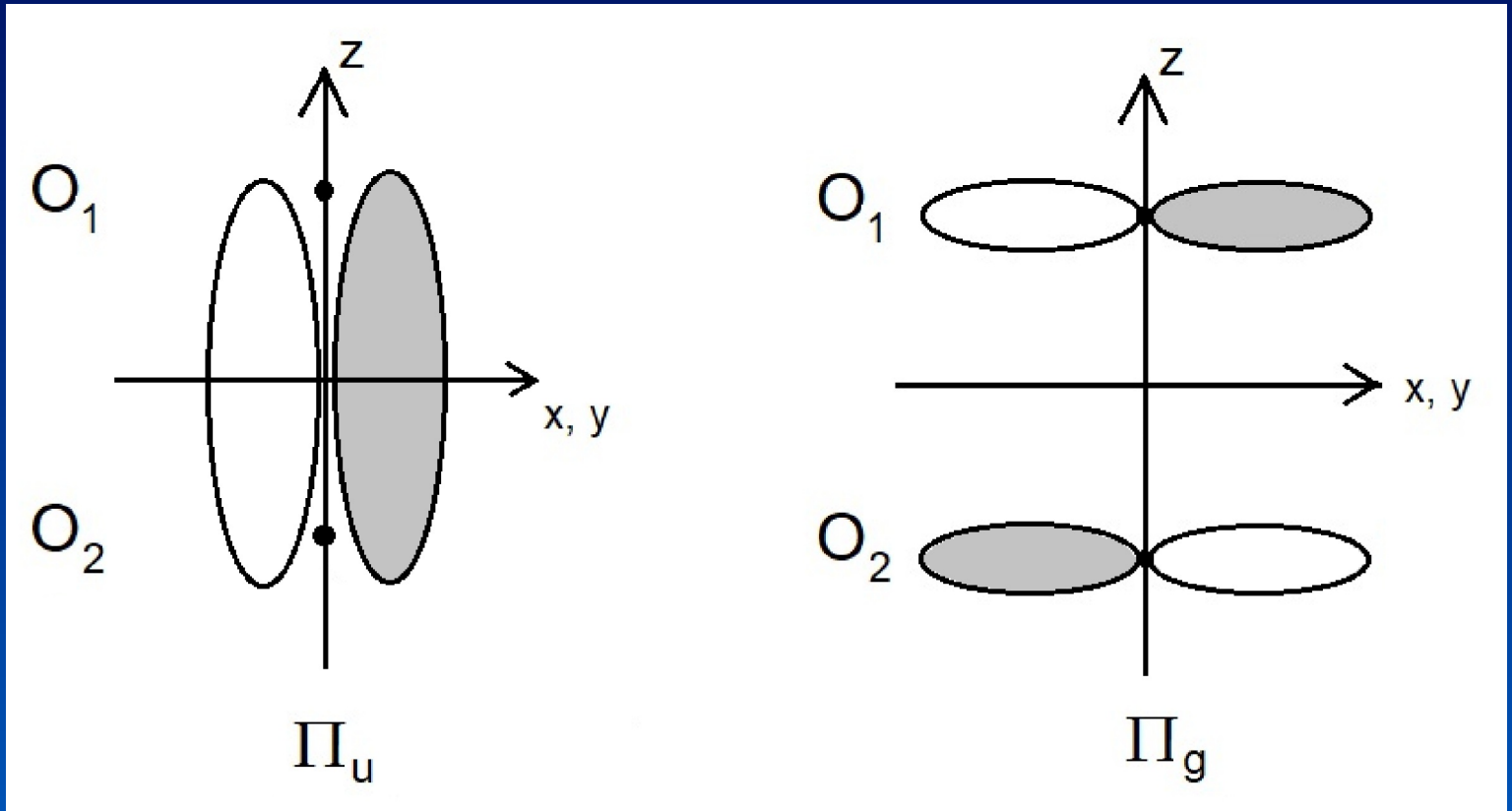
O_2 - $D_{\infty h}$

Os orbitais π (p_x,p_y) também formam combinações ligantes e antiligantes



O_2 - $D_{\infty h}$

Os orbitais π (p_x,p_y) também formam combinações ligantes e antiligantes



FIM