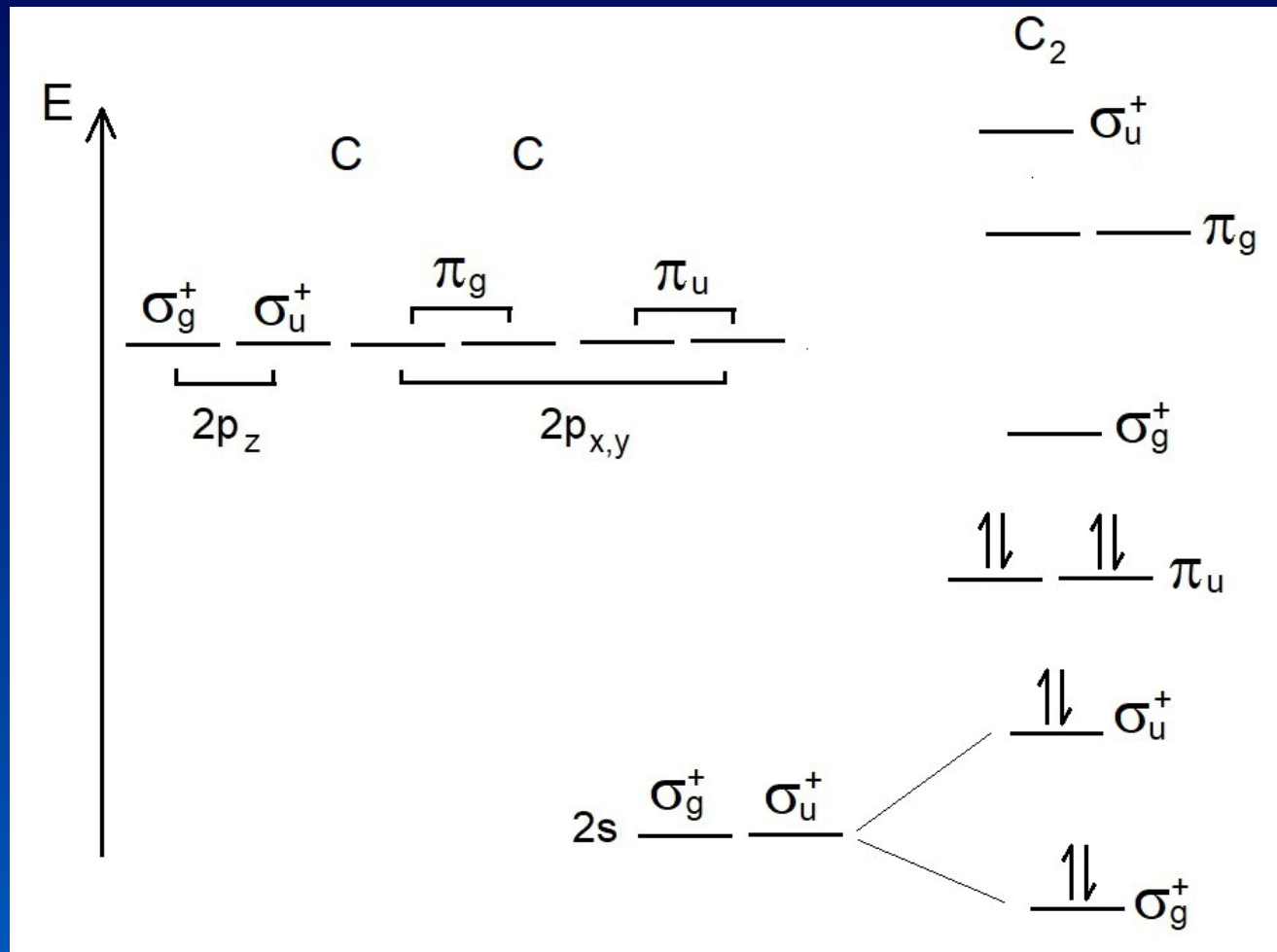


Termos espectroscópicos para moléculas

dicarbono - C₂

01/11/2023

$C_2 - D_{\infty h}$

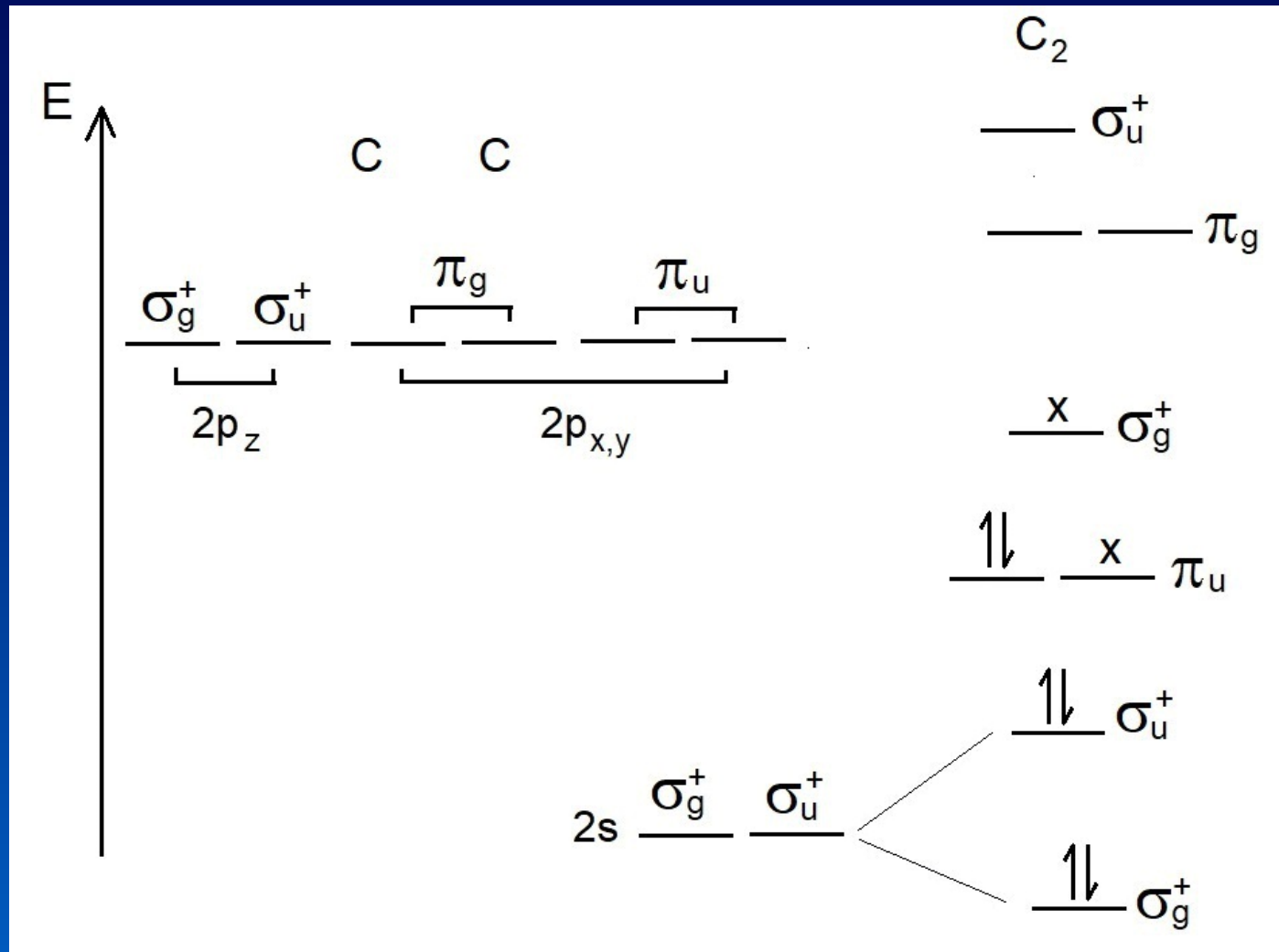


$D_{\infty h}$

$D_{\infty h}$	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	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 $\varphi = 90^{\circ}$ $\cos\varphi = 0$ $\cos 2\varphi = -1$

$C_2 - D_{\infty h}$ (primeiro estado excitado)



$D_{\infty h}$

$D_{\infty h}$	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

$\Sigma_{g}^{+} \otimes \Pi_{u}$	2	0	0	-2	0	0 = Π_{u}
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$C_2 - D_{\infty h}$

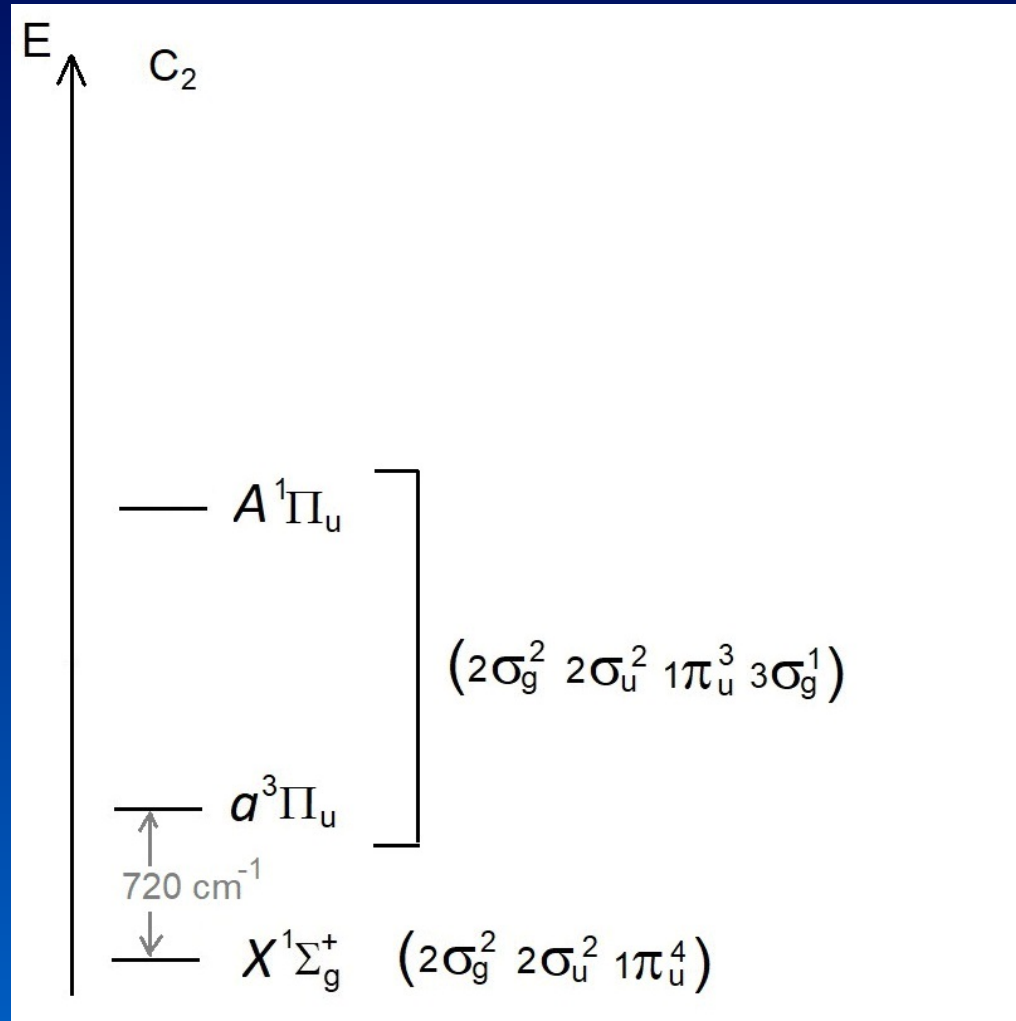
Determinando os singletos e tripletos

Nesse caso, como os elétrons não estão em orbitais degenerados, podemos ter as possibilidades singlete e tripleto.



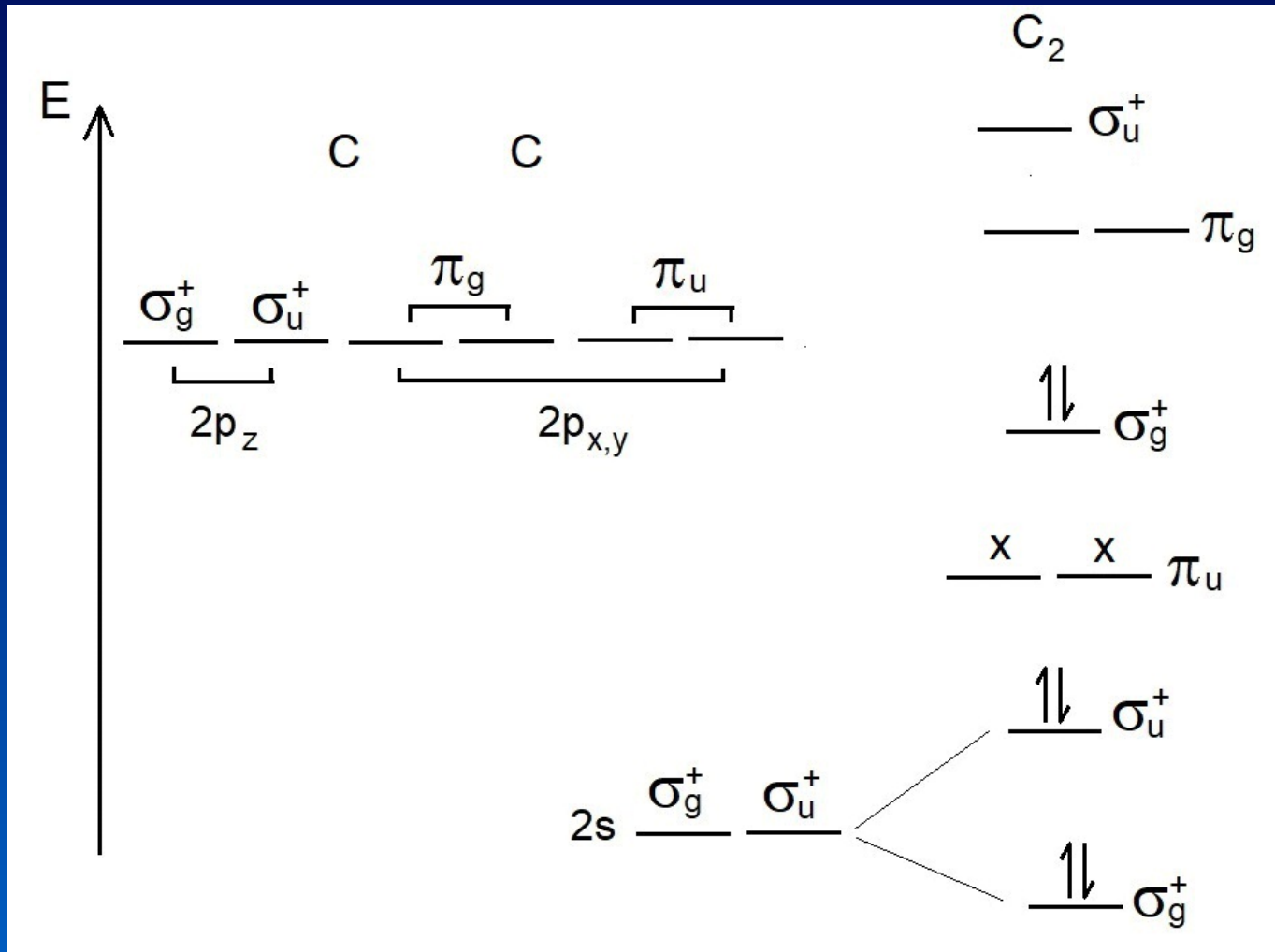
$C_2 - D_{\infty h}$

Níveis de energia do primeiro estado excitado da molécula



$C_2 - D_{\infty h}$

Excitando 2 elétrons



$D_{\infty h}$

$D_{\infty h}$	E	$2C_{\infty}^{\phi}$	$\infty\sigma_v$	i	$2S_{\infty}^{\phi}$	∞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
$\Pi_u \otimes \Pi_u$	4	0	0	4	0	0
					$\Sigma_g^+ \oplus \Sigma_g^- \oplus \Delta_g$	

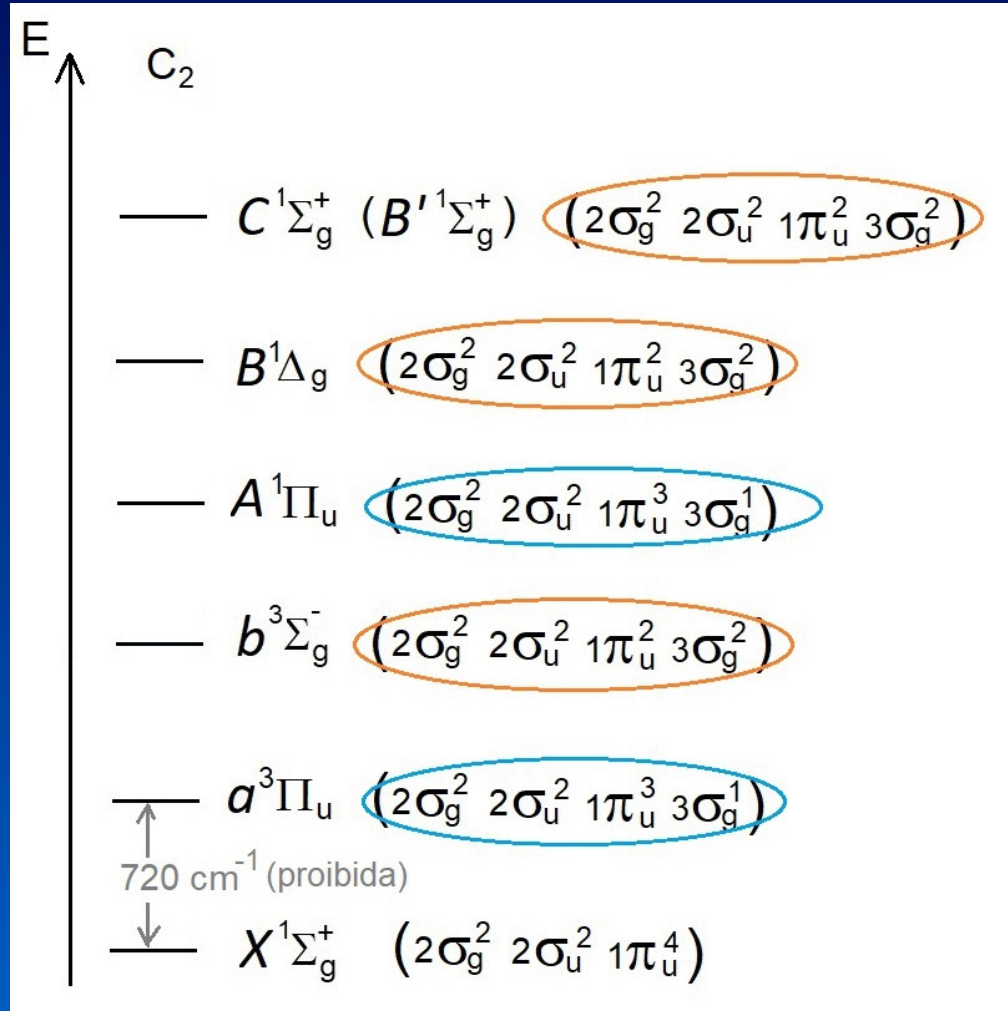
$C_2 - D_{\infty h}$

As multiplicidades de spin serão as mesmas para a configuração eletrônica mais estável do O_2



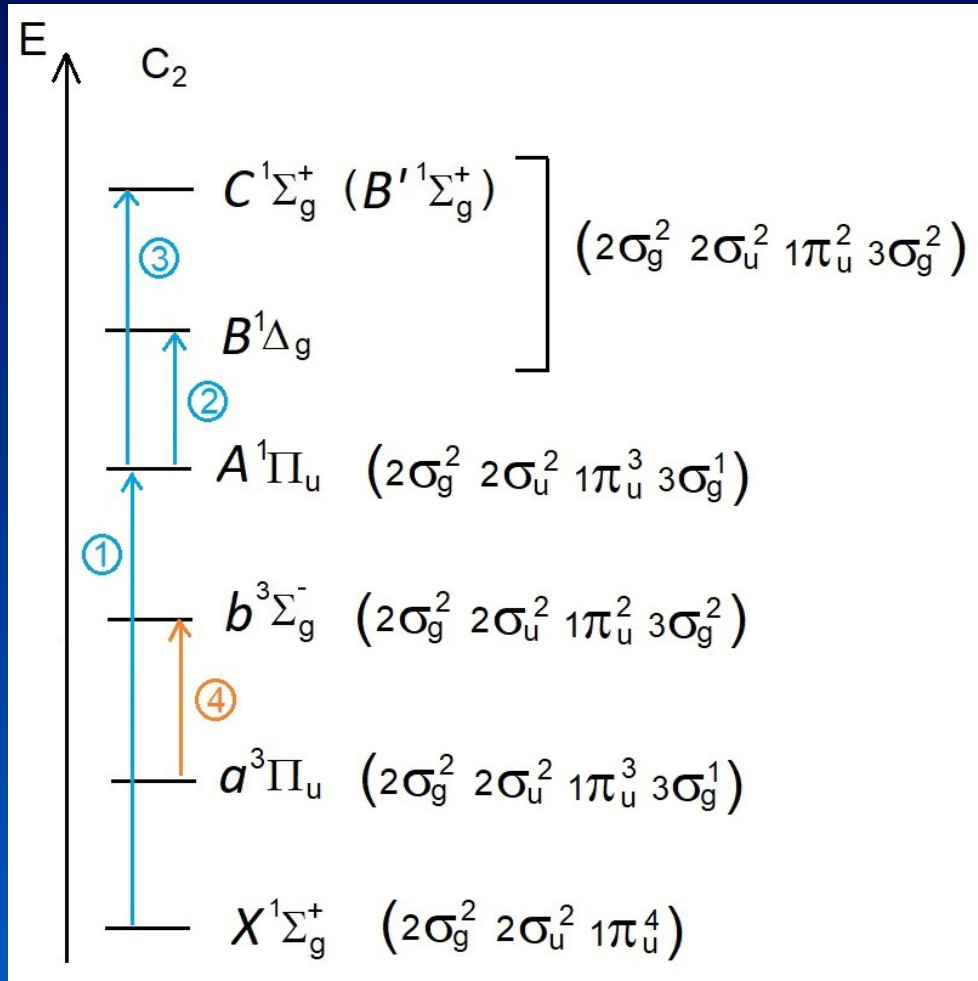
$C_2 - D_{\infty h}$

Níveis de energia da molécula



$C_2 - D_{\infty h}$

Transições permitidas



① 8.268 cm^{-1} (Phillips)

② 3.590 cm^{-1}

③ 6.928 cm^{-1}

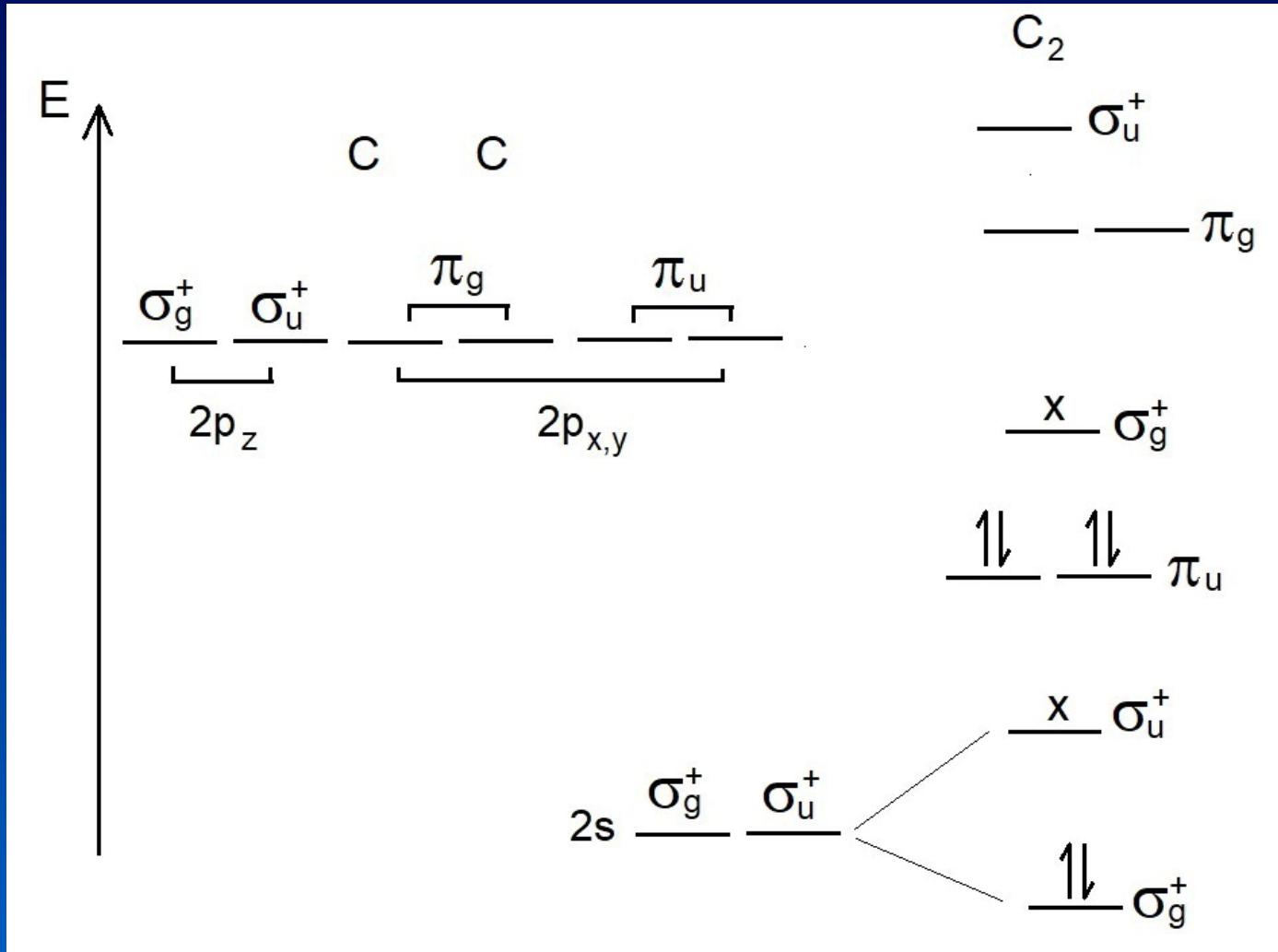
④ 5.632 cm^{-1} (Ballik-Ramsay)

Como a região do visível vai de 12.500 a 25.000 cm^{-1} , todas as bandas estão no infravermelho.

- 1) Douay, Nietmann, Bernath, *J. Mol. Spect.* 131, 261 (1988).
- 2) Bernath, *Spectra of Atoms and Molecules*, 3a ed., Oxford University Press, 2016. pg 346.

$C_2 - D_{\infty h}$

Excitando 1 elétron do penúltimo orbital ocupado



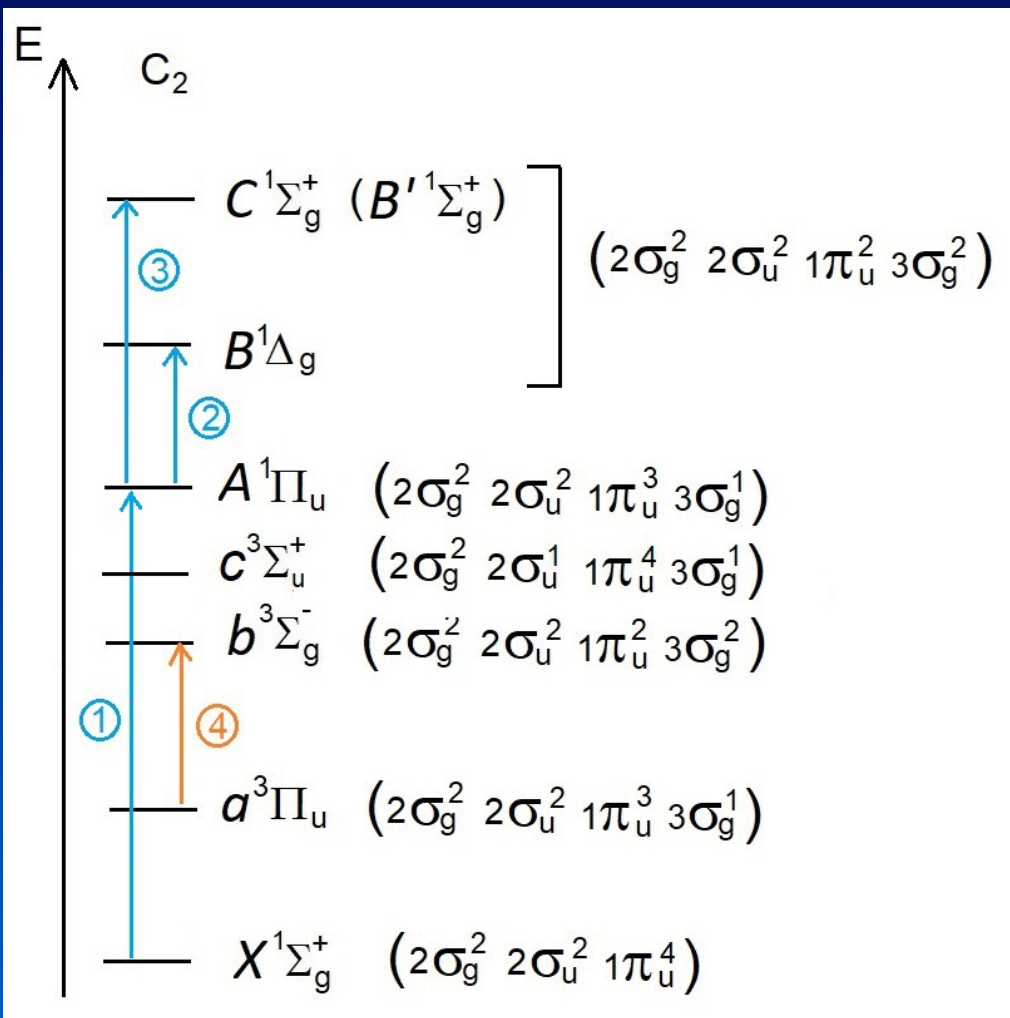
$D_{\infty h}$

$D_{\infty h}$	E	$2C_{\infty}^{\phi}$	$\infty\sigma_v$	i	$2S_{\infty}^{\phi}$	∞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

$\Sigma_{g}^{+} \otimes \Sigma_{u}^{+} = 1$	1	1	-1	-1	-1	$= \Sigma_{u}^{+}$
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$C_2 - D_{\infty h}$

Transições permitidas



① 8.268 cm^{-1} (Phillips)

② 3.590 cm^{-1}

③ 6.928 cm^{-1}

④ 5.632 cm^{-1} (Ballik-Ramsay)

Como a região do visível vai de 12.500 a 25.000 cm^{-1} , todas as bandas estão no infravermelho.

- 1) Douay, Nietmann, Bernath, *J. Mol. Spect.* 131, 261 (1988).
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