



Aplicação de simetria para a visualização dos orbitais moleculares de moléculas pequenas e compostos de coordenação

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Aula 6



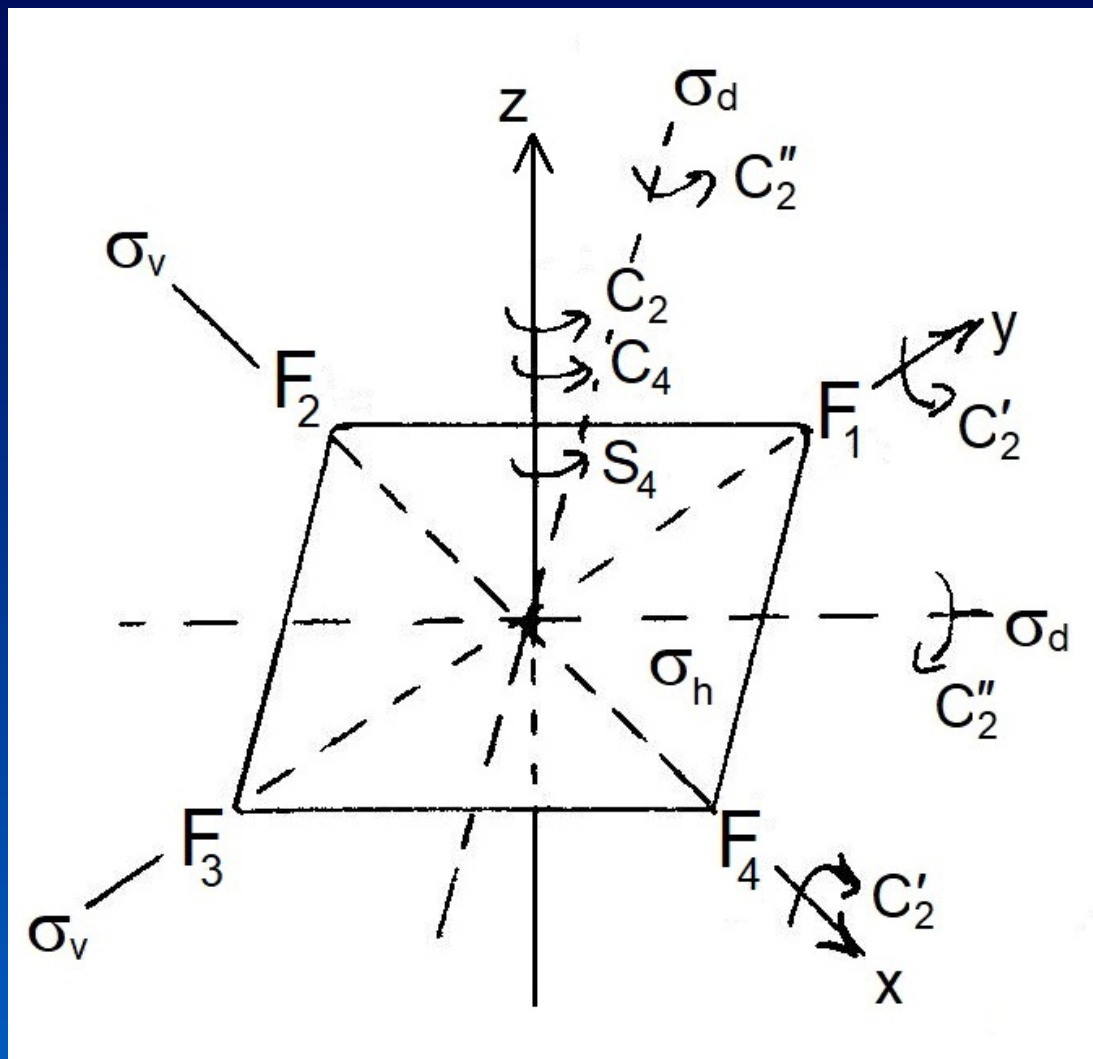
Sociedade Brasileira de Química

11 a 15 de março de 2024

$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

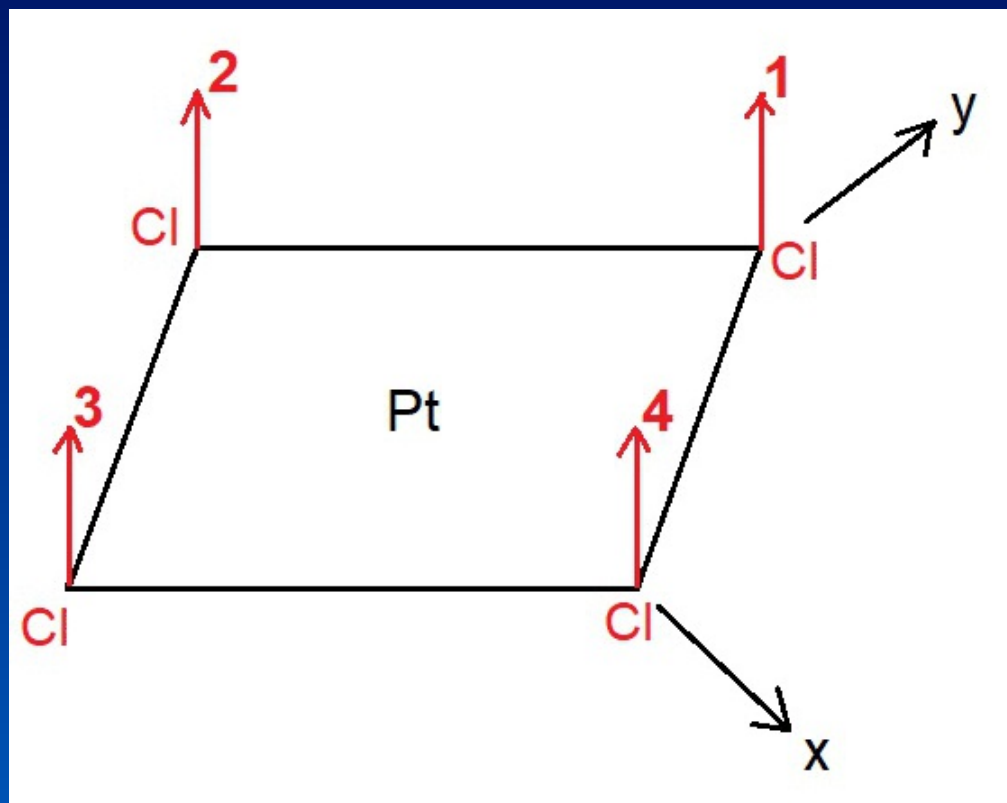
D_{4h}	E	2C_4	C_2	$2\text{C}_2'$	$2\text{C}_2''$	i	2S_4	σ_h	$2\sigma_v$	$2\sigma_d$
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1
B_{1g}	1	-1	1	1	-1	1	-1	1	1	-1
B_{2g}	1	-1	1	-1	1	1	-1	1	-1	1
E_g	2	0	-2	0	0	2	0	-2	0	0
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1
B_{1u}	1	-1	1	1	-1	-1	1	-1	-1	1
B_{2u}	1	-1	1	-1	1	-1	1	-1	1	-1
E_u	2	0	-2	0	0	-2	0	2	0	0

$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$



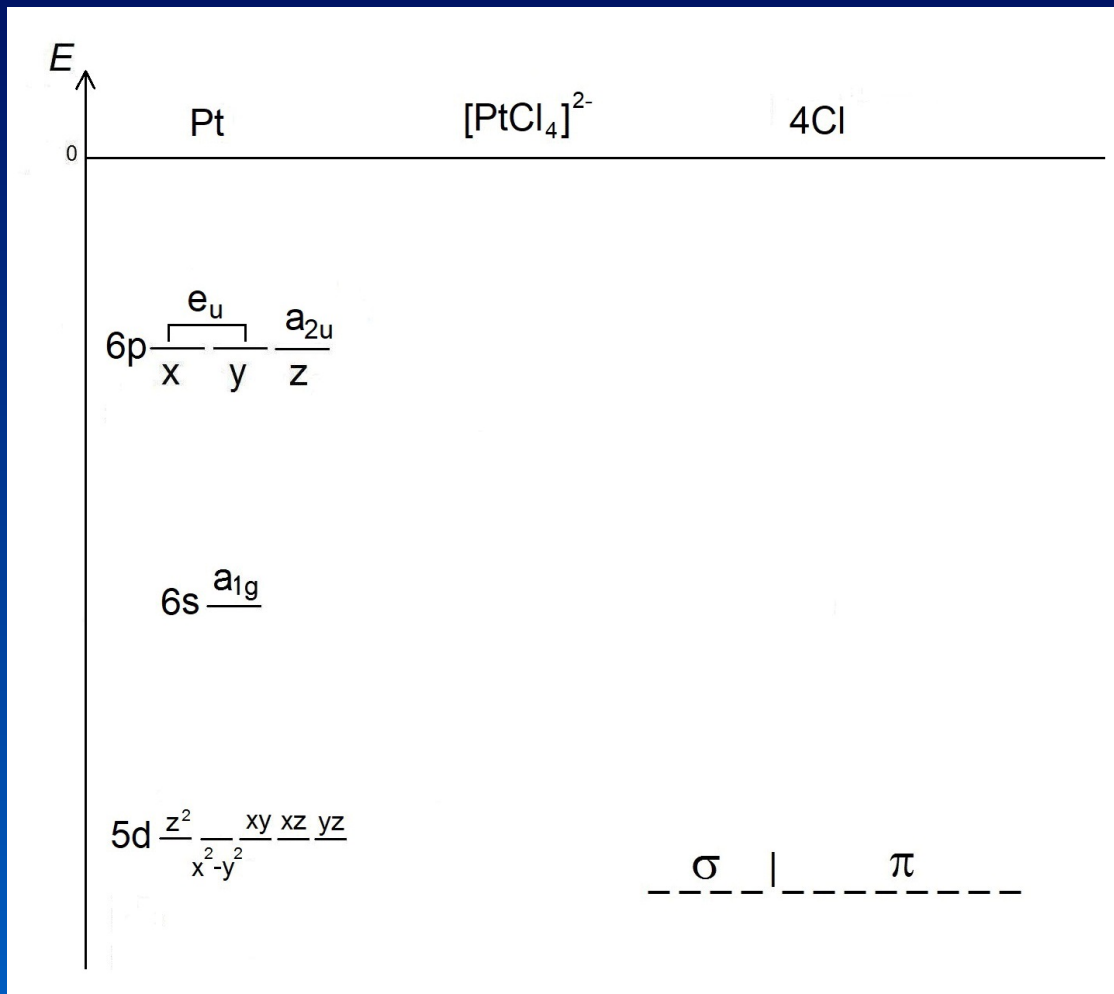


Sistema π



$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

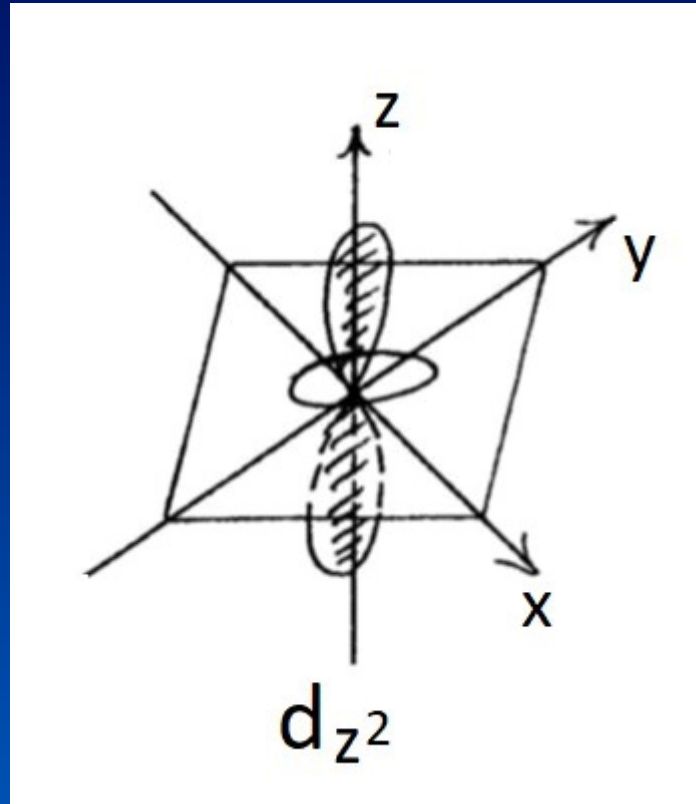
Construindo o diagrama de energia dos orbitais moleculares



Aproveitando os resultados do metano plano, D_{4h}

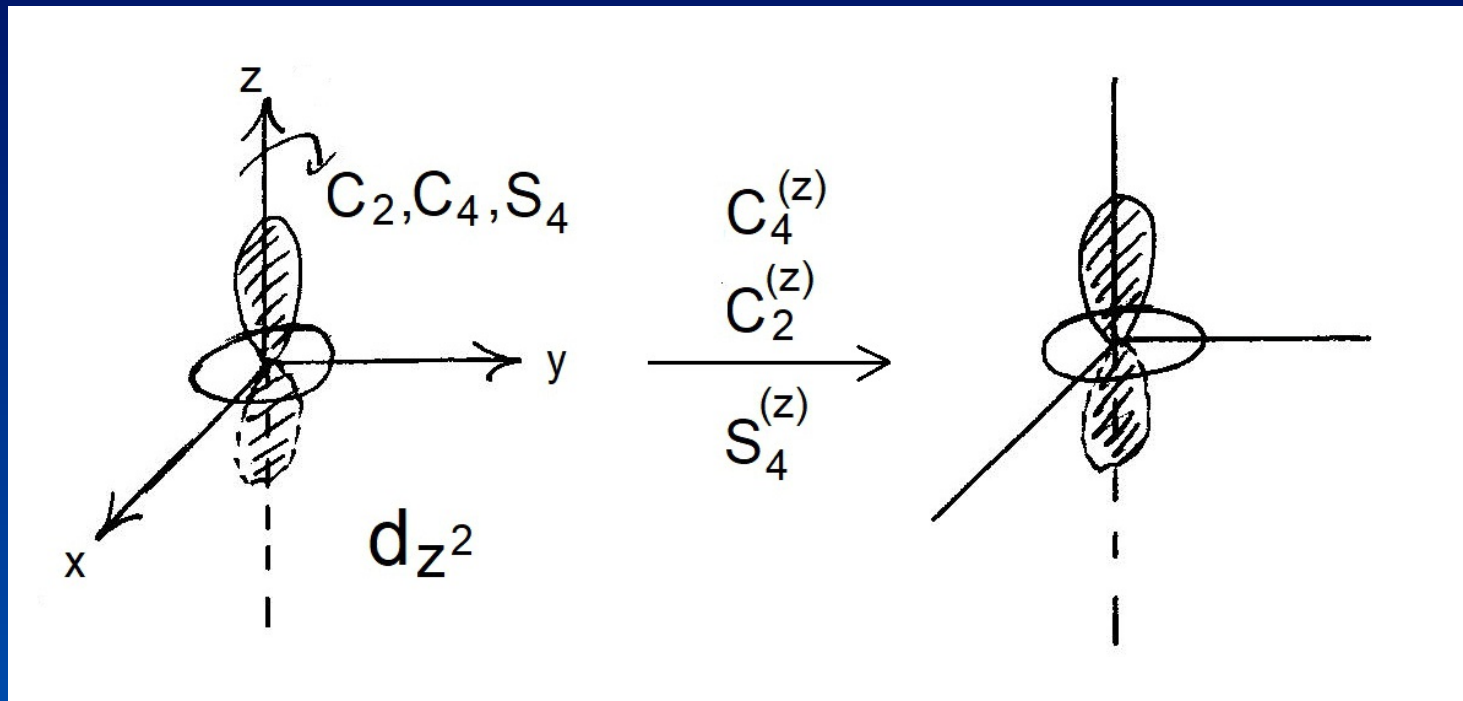
$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Classificando o orbital $5d(z^2)$ do Pt



$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Classificando o orbital $5d(z^2)$ do Pt



Classificando os orbitais $6p_x$ e $6p_y$ do Pt - INSEPARÁVEIS

D_{4h}	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1
B_{1g}	1	-1	1	1	-1	1	-1	1	1	-1
B_{2g}	1	-1	1	-1	1	1	-1	1	-1	1
E_g	2	0	-2	0	0	2	0	-2	0	0
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1
B_{1u}	1	-1	1	1	-1	-1	1	-1	-1	1
B_{2u}	1	-1	1	-1	1	-1	1	-1	1	-1
E_u	2	0	-2	0	0	-2	0	2	0	0

$5d_{z^2}$

1

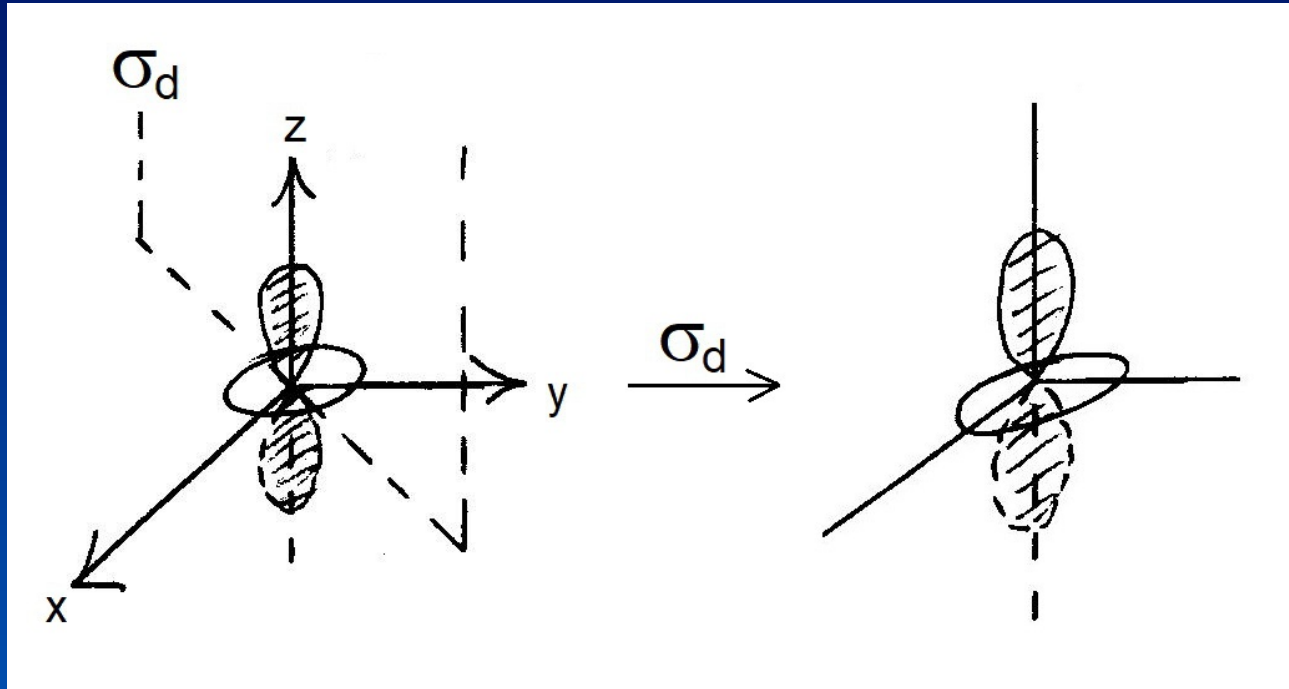
1

1

1

$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Classificando o orbital $5d(z^2)$ do Pt



Classificando os orbitais $6p_x$ e $6p_y$ do Pt - INSEPARÁVEIS

D_{4h}	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1
B_{1g}	1	-1	1	1	-1	1	-1	1	1	-1
B_{2g}	1	-1	1	-1	1	1	-1	1	-1	1
E_g	2	0	-2	0	0	2	0	-2	0	0
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1
B_{1u}	1	-1	1	1	-1	-1	1	-1	-1	1
B_{2u}	1	-1	1	-1	1	-1	1	-1	1	-1
E_u	2	0	-2	0	0	-2	0	2	0	0

$5d_{z^2}$	1	1	1				1			1
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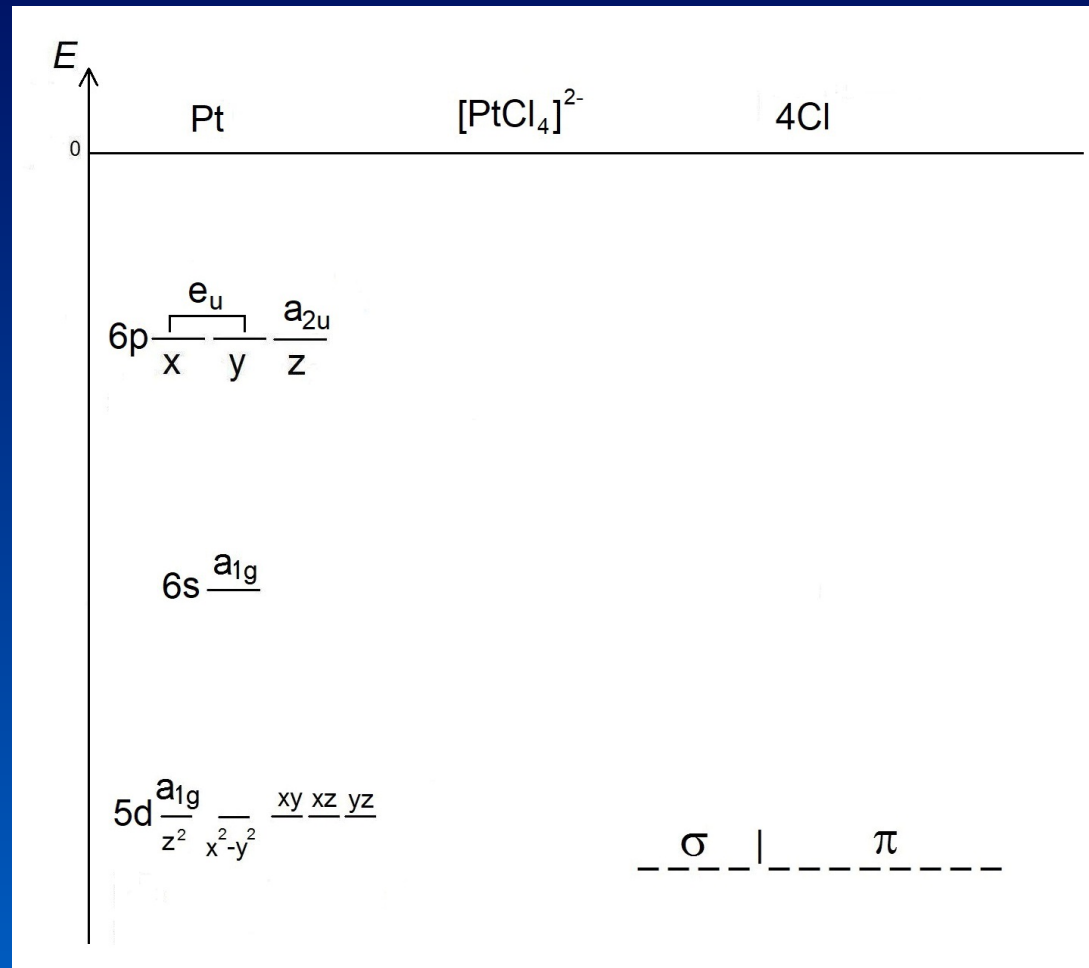
Classificando os orbitais $6p_x$ e $6p_y$ do Pt - INSEPARÁVEIS

D_{4h}	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1
B_{1g}	1	-1	1	1	-1	1	-1	1	1	-1
B_{2g}	1	-1	1	-1	1	1	-1	1	-1	1
E_g	2	0	-2	0	0	2	0	-2	0	0
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1
B_{1u}	1	-1	1	1	-1	-1	1	-1	-1	1
B_{2u}	1	-1	1	-1	1	-1	1	-1	1	-1
E_u	2	0	-2	0	0	-2	0	2	0	0

$5d_{z^2}$	1	1	1	1	1	1	1	1	1	1	A_{1g}
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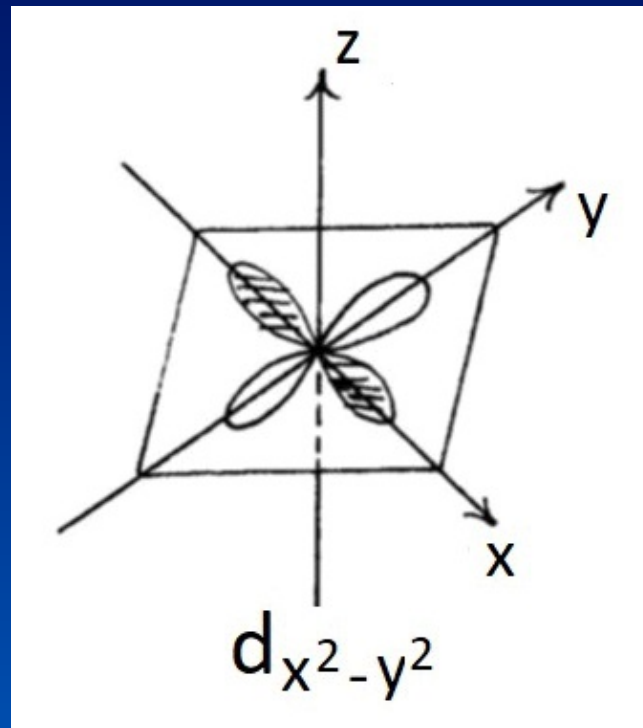
$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Construindo o diagrama de energia dos orbitais moleculares



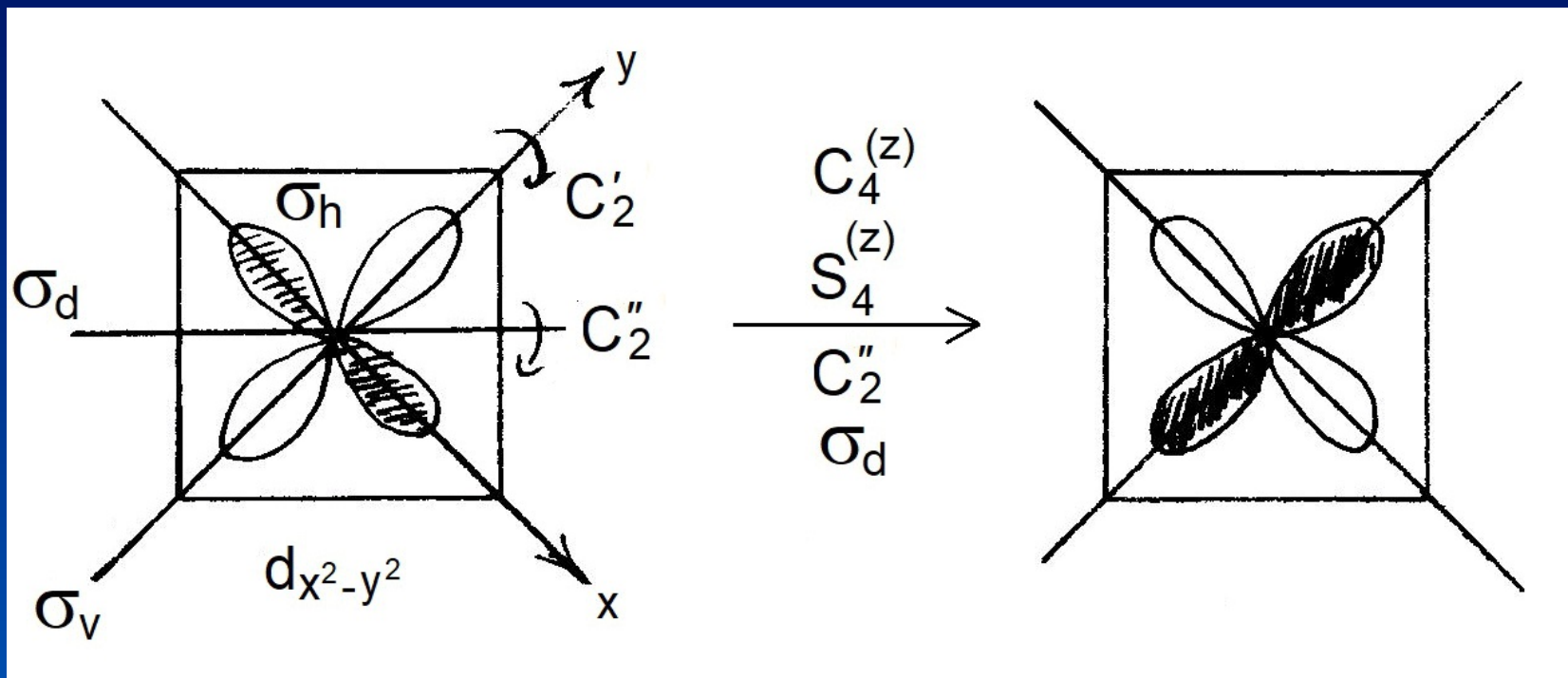
$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Classificando o orbital $5d(x^2-y^2)$ do Pt



$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Classificando o orbital $5d(x^2-y^2)$ do Pt



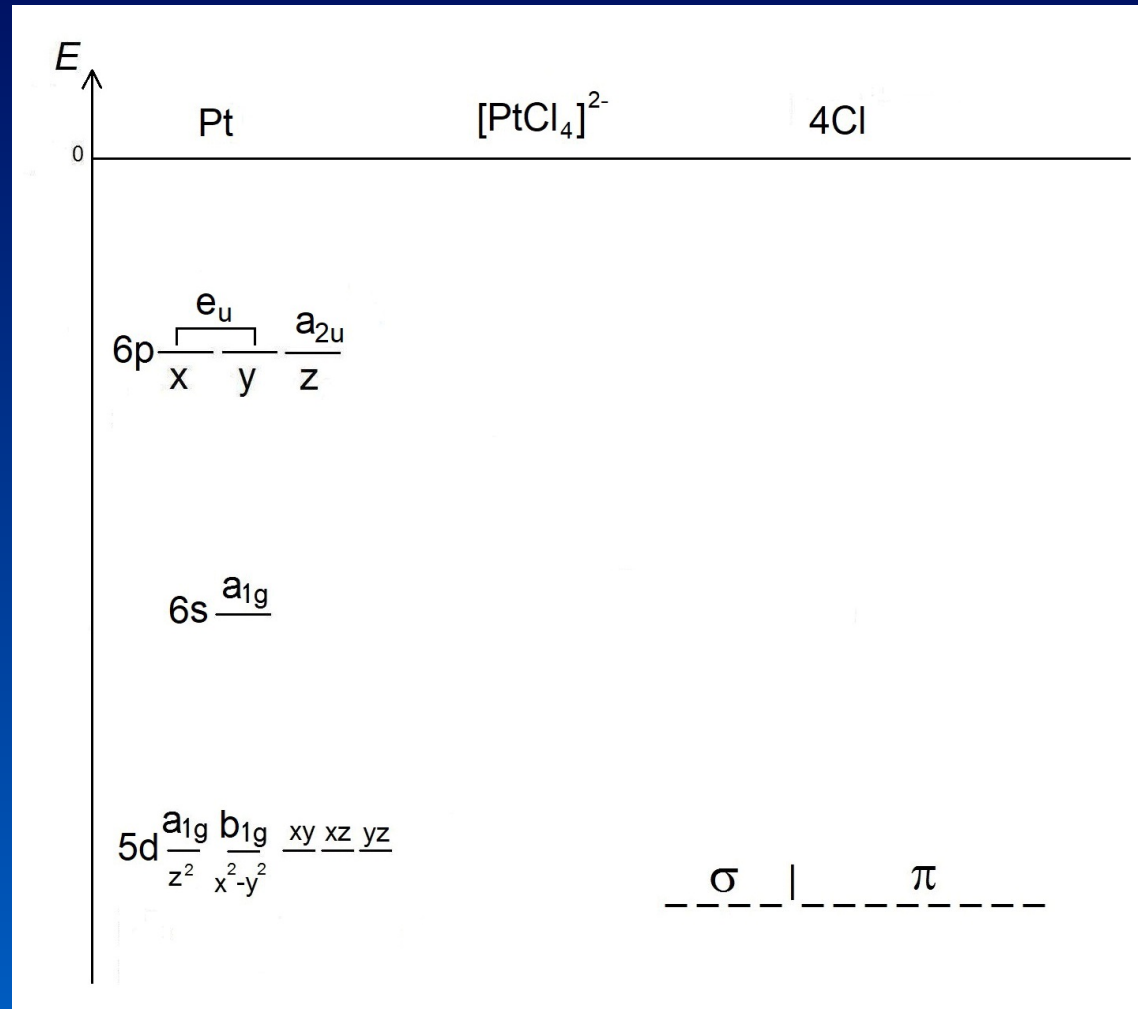
Classificando os orbitais $6p_x$ e $6p_y$ do Pt - INSEPARÁVEIS

D_{4h}	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1
B_{1g}	1	-1	1	1	-1	1	-1	1	1	-1
B_{2g}	1	-1	1	-1	1	1	-1	1	-1	1
E_g	2	0	-2	0	0	2	0	-2	0	0
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1
B_{1u}	1	-1	1	1	-1	-1	1	-1	-1	1
B_{2u}	1	-1	1	-1	1	-1	1	-1	1	-1
E_u	2	0	-2	0	0	-2	0	2	0	0

$5d_{x^2-y^2}$ 1 -1 -1 -1 -1 B_{1g}

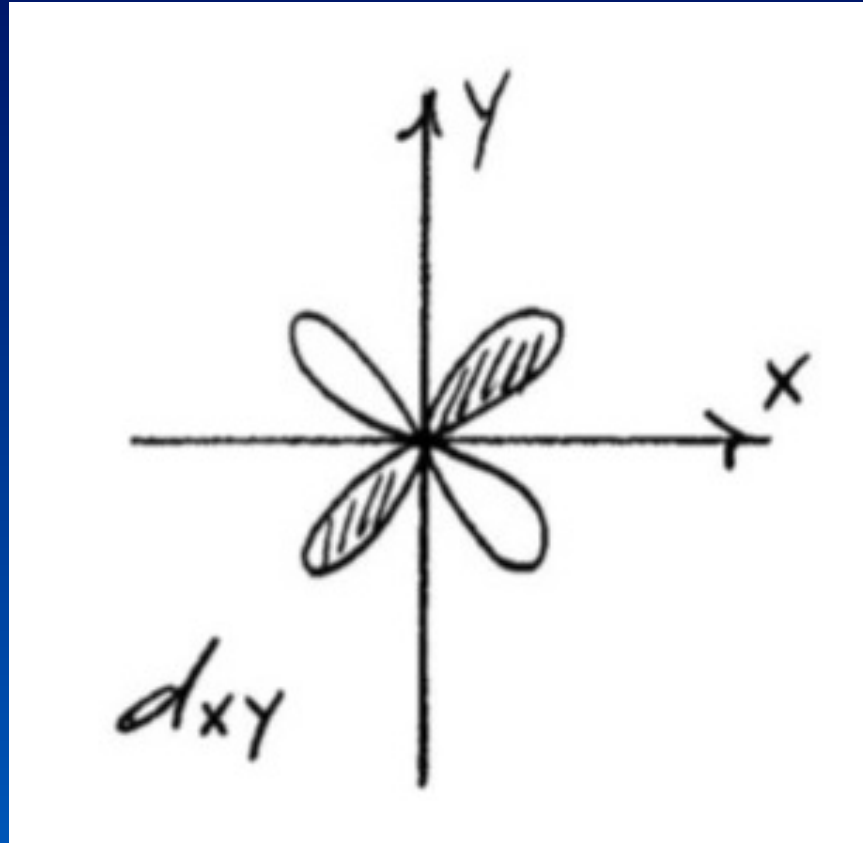
$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Construindo o diagrama de energia dos orbitais moleculares



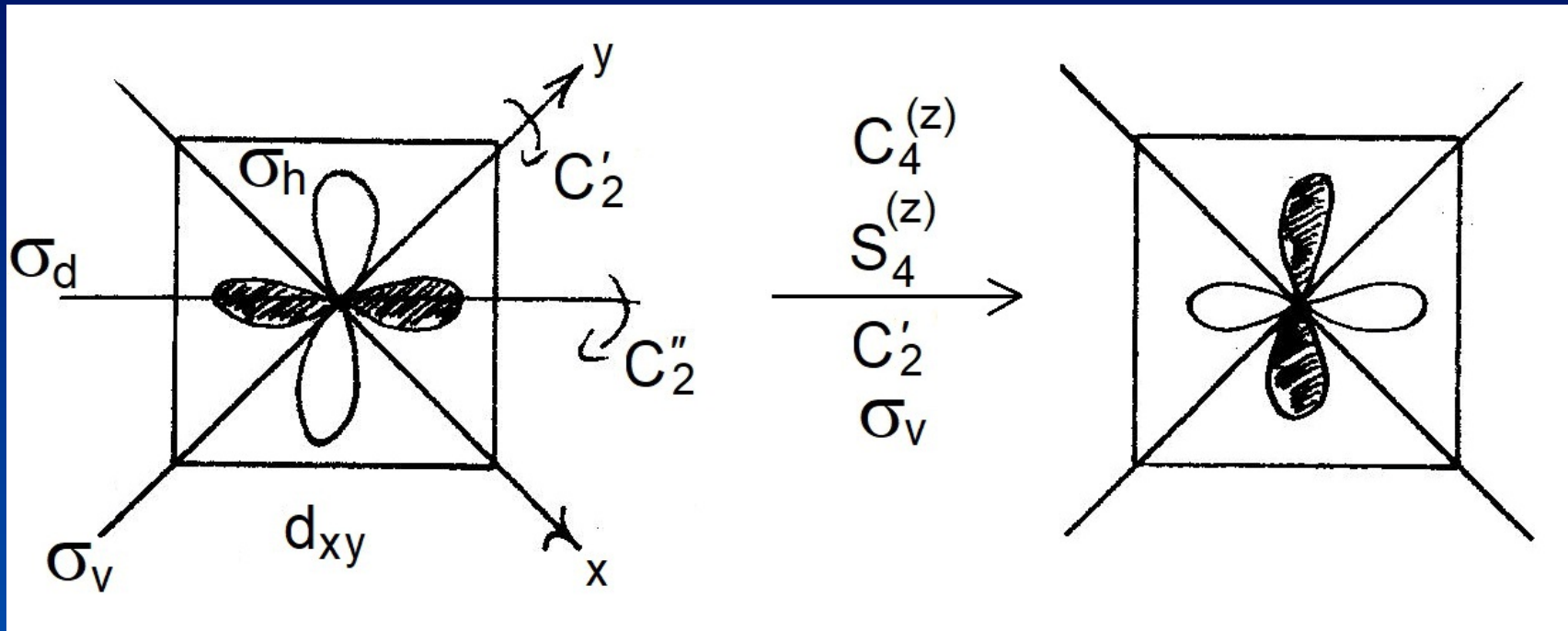


Classificando o orbital 5d(xy) do Pt



$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Classificando o orbital $5d_{xy}$ do Pt



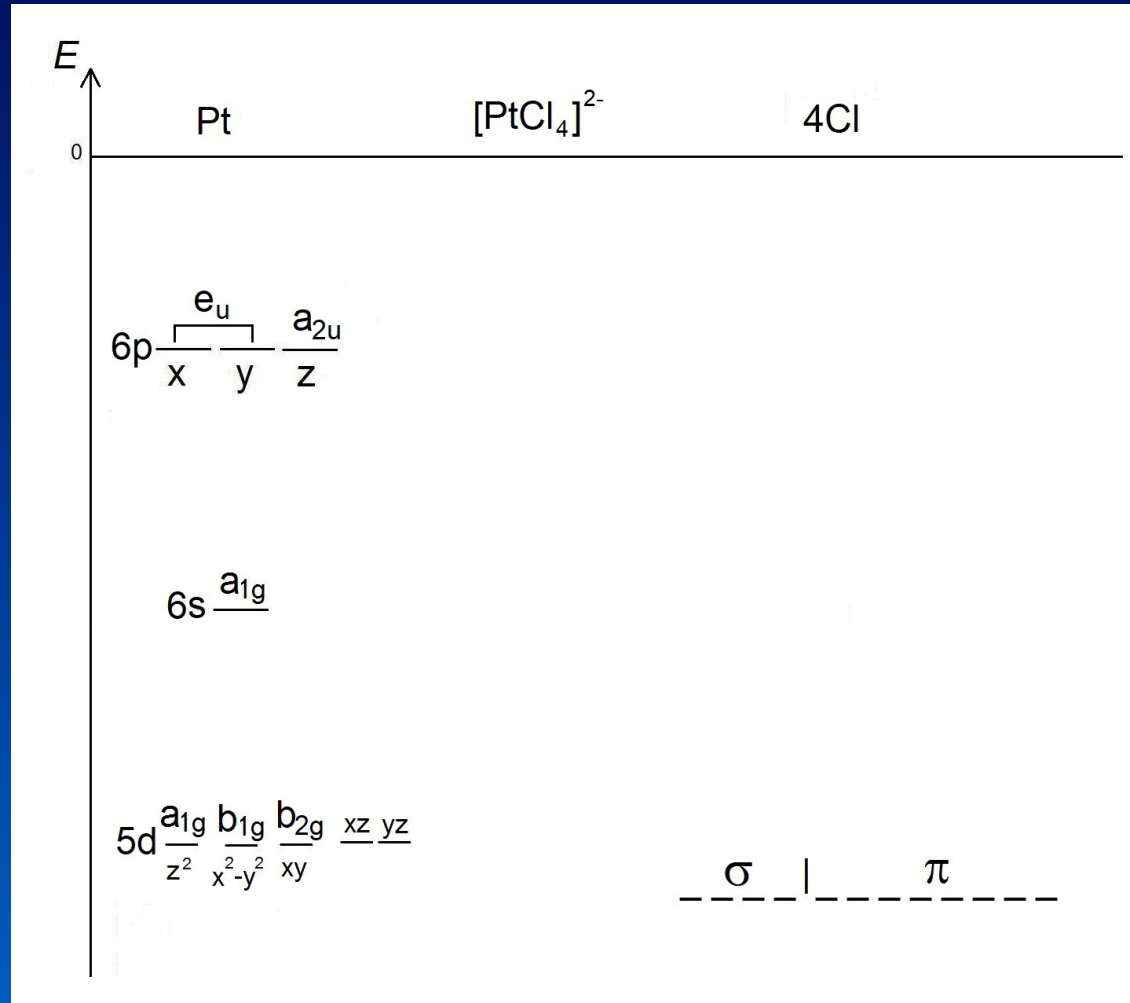
Classificando os orbitais $5d_{xy}$ do Pt

D_{4h}	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1
B_{1g}	1	-1	1	1	-1	1	-1	1	1	-1
B_{2g}	1	-1	1	-1	1	1	-1	1	-1	1
E_g	2	0	-2	0	0	2	0	-2	0	0
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1
B_{1u}	1	-1	1	1	-1	-1	1	-1	-1	1
B_{2u}	1	-1	1	-1	1	-1	1	-1	1	-1
E_u	2	0	-2	0	0	-2	0	2	0	0

$5d_{xy}$	1	-1		-1			-1		-1		B_{2g}
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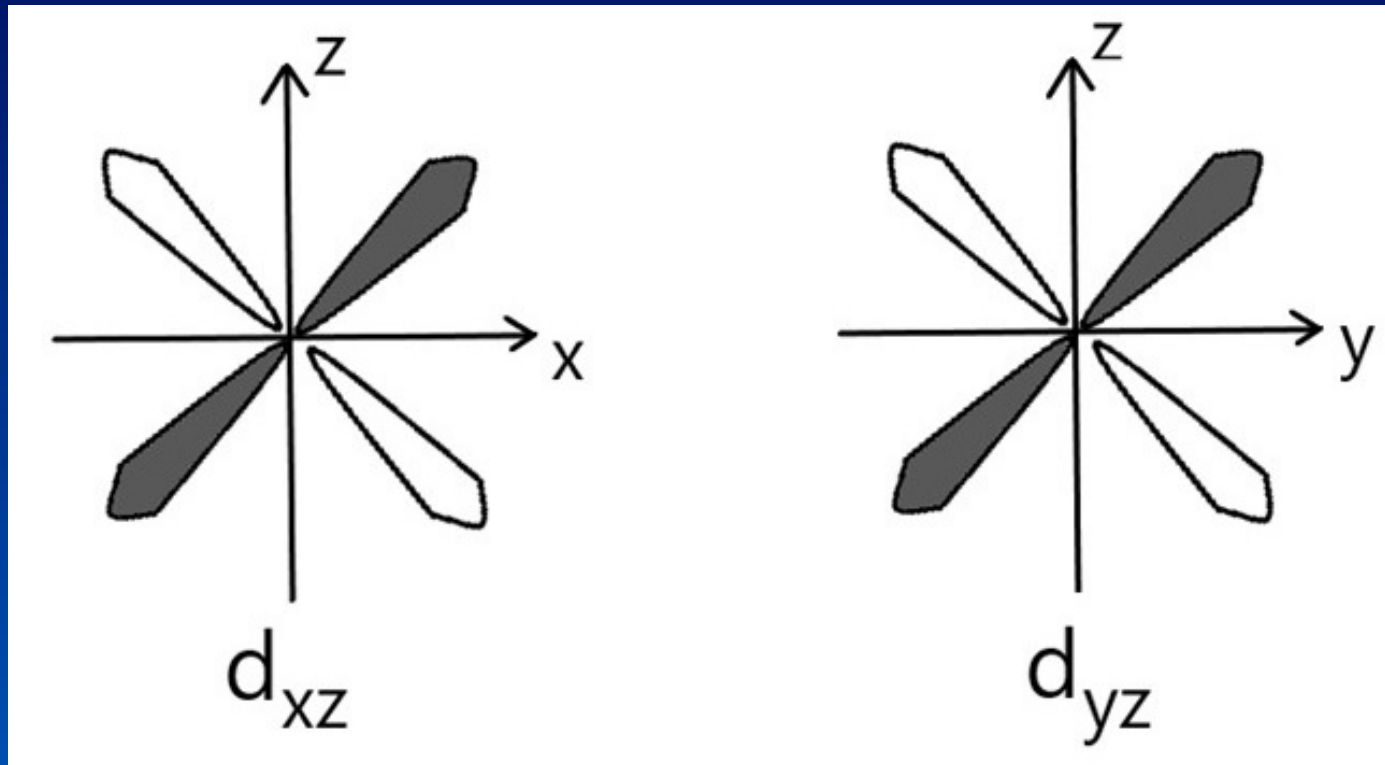
$[\text{PtCl}_4]^{2-} - D_{4h}$

Construindo o diagrama de energia dos orbitais moleculares



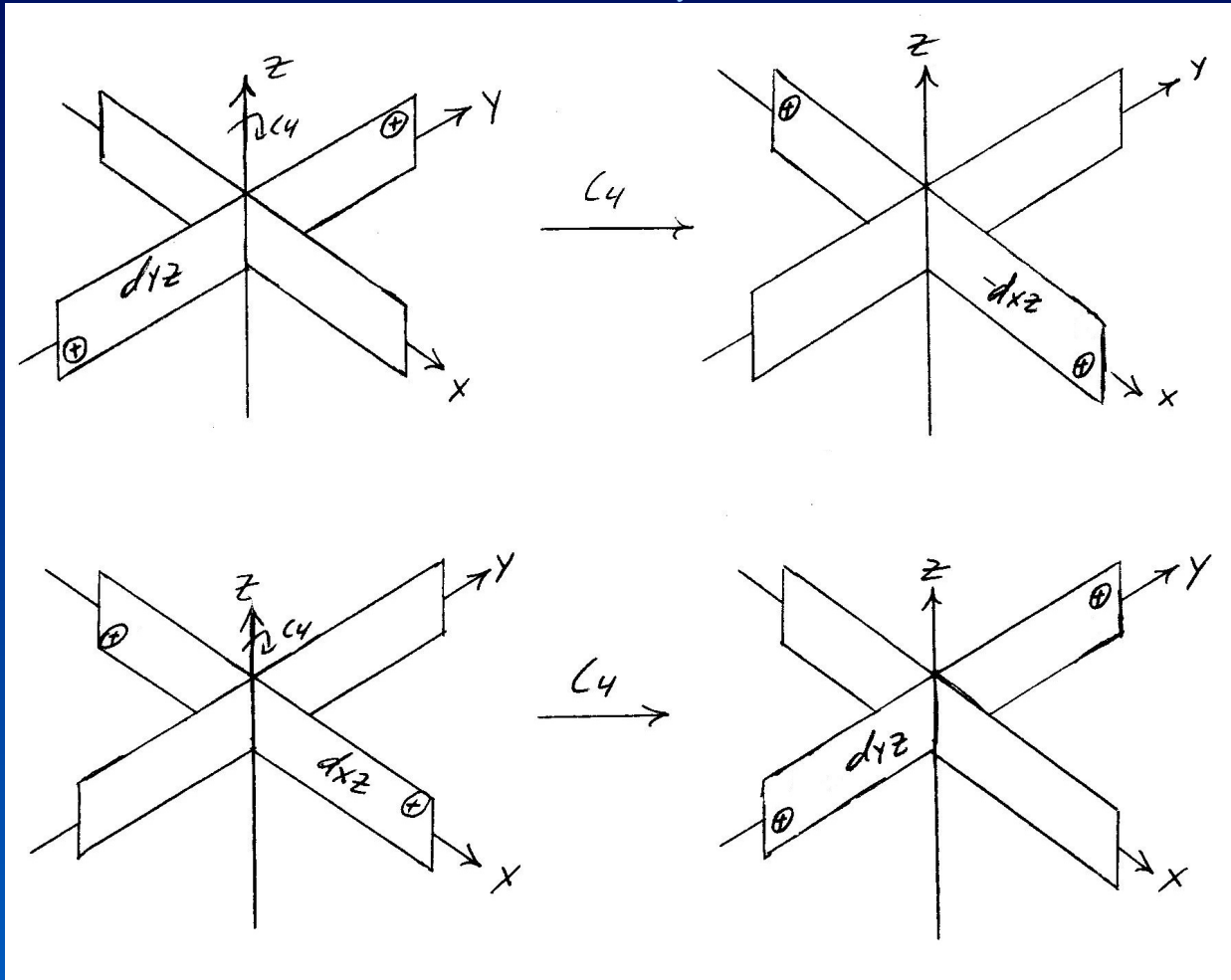
$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Classificando os orbitais $5d_{xz}$ e $5d_{yz}$ do Pt -INSEPARÁVEIS



$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Classificando os orbitais $5d_{xz}$ e $5d_{yz}$ do Pt -INSEPARÁVEIS



$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Classificando os orbitais $5d_{xz}$ e $5d_{yz}$ do Pt -INSEPARÁVEIS

$$\begin{array}{cc} & \begin{array}{cc} d_{xz} & d_{yz} \end{array} \\ \begin{array}{c} d_{xz} \\ d_{yz} \end{array} & \begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \end{array} \xrightarrow{C_4} \begin{array}{cc} & \begin{array}{cc} d_{xz} & d_{yz} \end{array} \\ \begin{array}{c} d_{xz} \\ d_{yz} \end{array} & \begin{array}{cc} 0 & 1 \\ -1 & 0 \end{array} \end{array} \quad \chi = 0$$

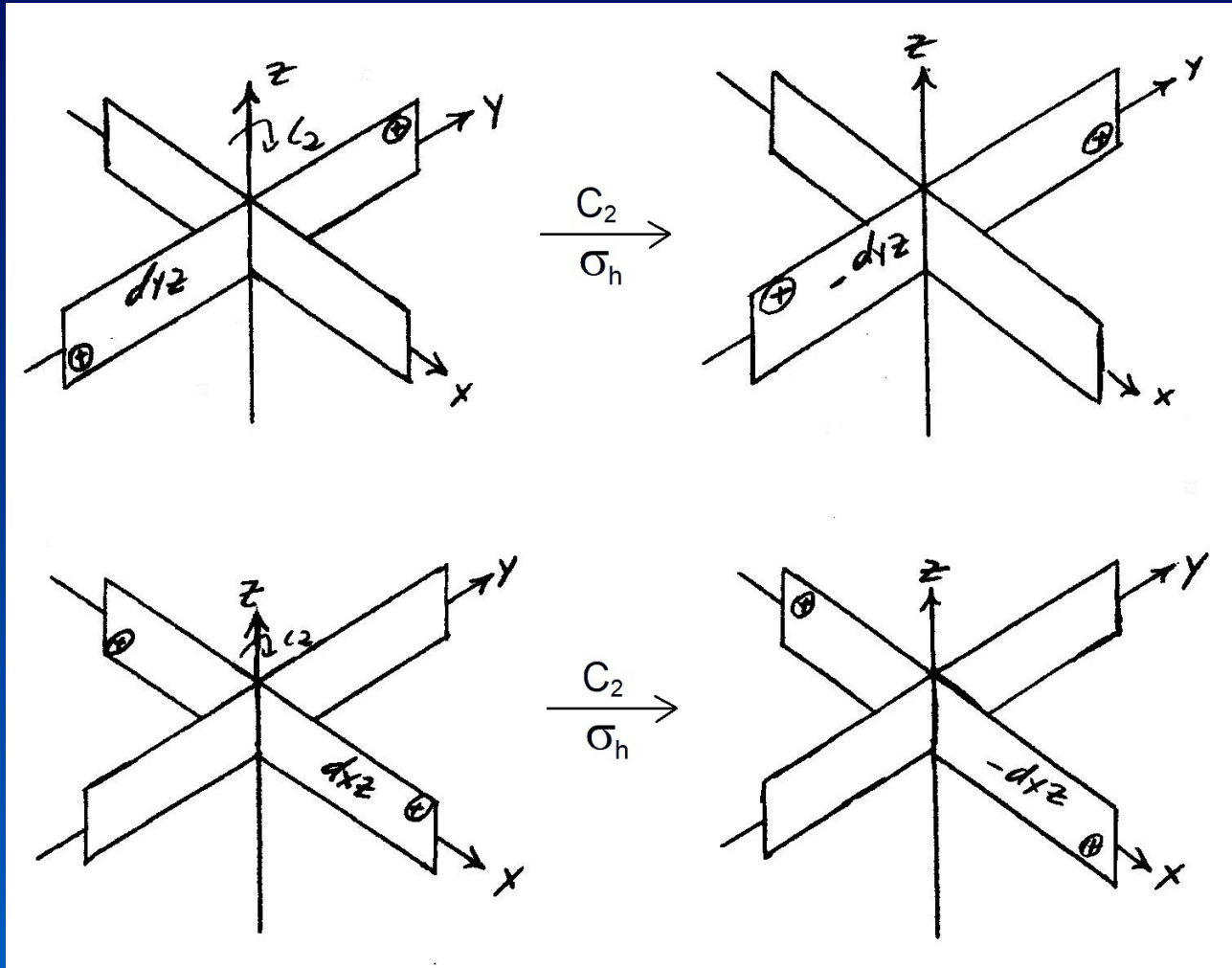
Classificando os orbitais $5d_{xz}$ e $5d_{yz}$ do Pt - INSEPARÁVEIS

D_{4h}	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1
B_{1g}	1	-1	1	1	-1	1	-1	1	1	-1
B_{2g}	1	-1	1	-1	1	1	-1	1	-1	1
E_g	2	0	-2	0	0	2	0	-2	0	0
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1
B_{1u}	1	-1	1	1	-1	-1	1	-1	-1	1
B_{2u}	1	-1	1	-1	1	-1	1	-1	1	-1
E_u	2	0	-2	0	0	-2	0	2	0	0

$5d_{xz,yz}$ 2 0

$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Classificando os orbitais $5d_{xz}$ e $5d_{yz}$ do Pt -INSEPARÁVEIS



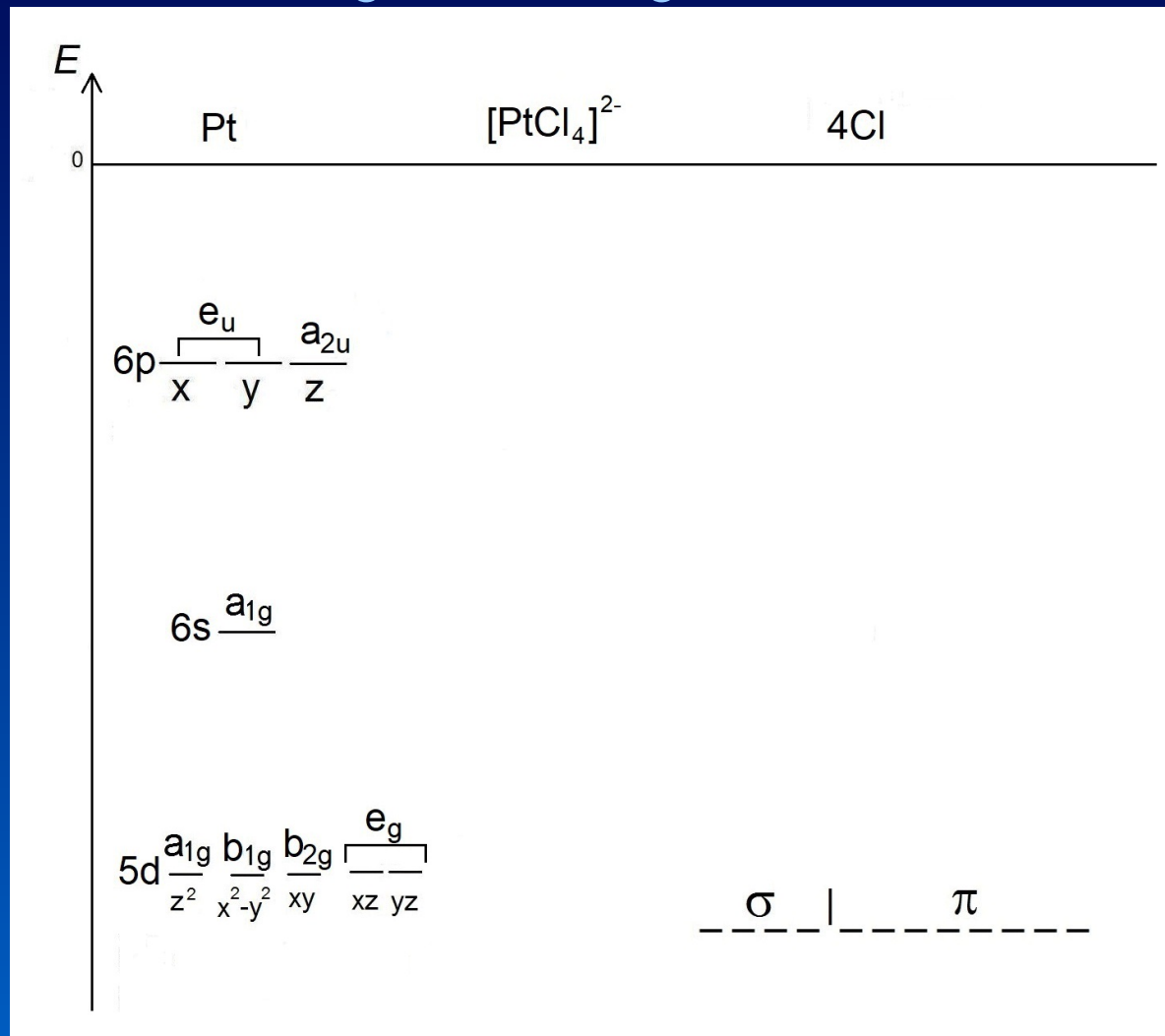
$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Classificando os orbitais $5d_{xz}$ e $5d_{yz}$ do Pt -INSEPARÁVEIS

$$\begin{array}{cc} & \begin{array}{cc} d_{xz} & d_{yz} \end{array} \\ \begin{array}{c} d_{xz} \\ d_{yz} \end{array} & \begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \end{array} \begin{array}{c} C_2 \\ \rightarrow \\ \sigma_h \end{array} \begin{array}{cc} & \begin{array}{cc} d_{xz} & d_{yz} \end{array} \\ \begin{array}{c} d_{xz} \\ d_{yz} \end{array} & \begin{array}{cc} -1 & 0 \\ 0 & -1 \end{array} \end{array} \chi = -2$$

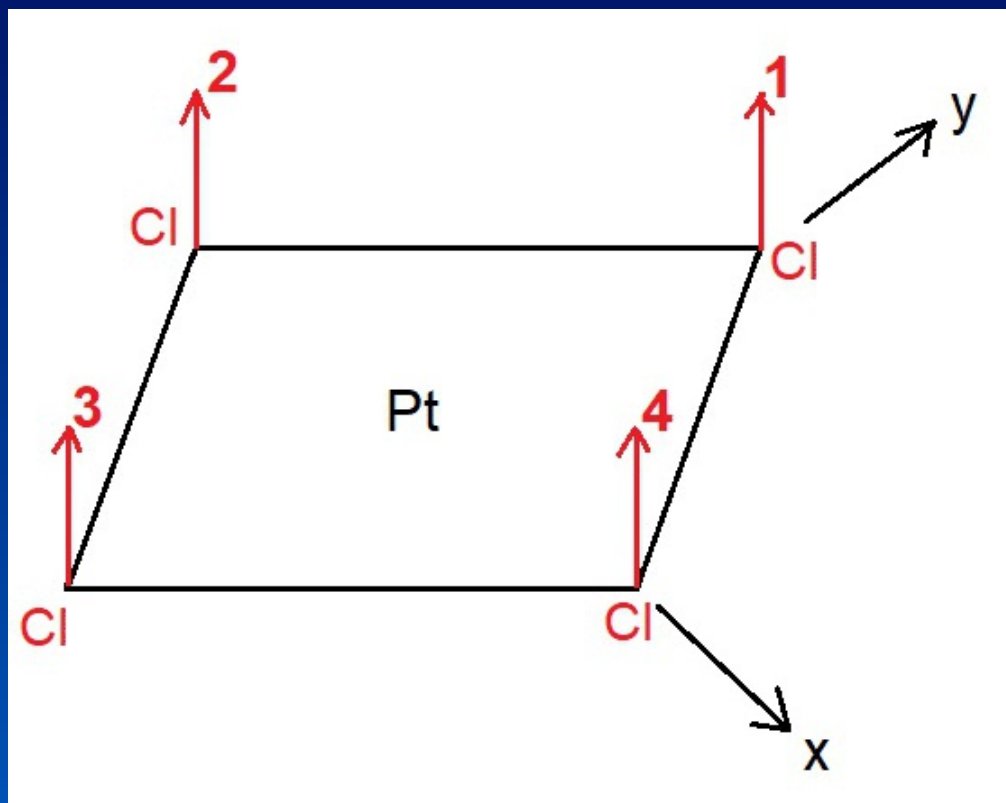
$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Construindo o diagrama de energia dos orbitais moleculares





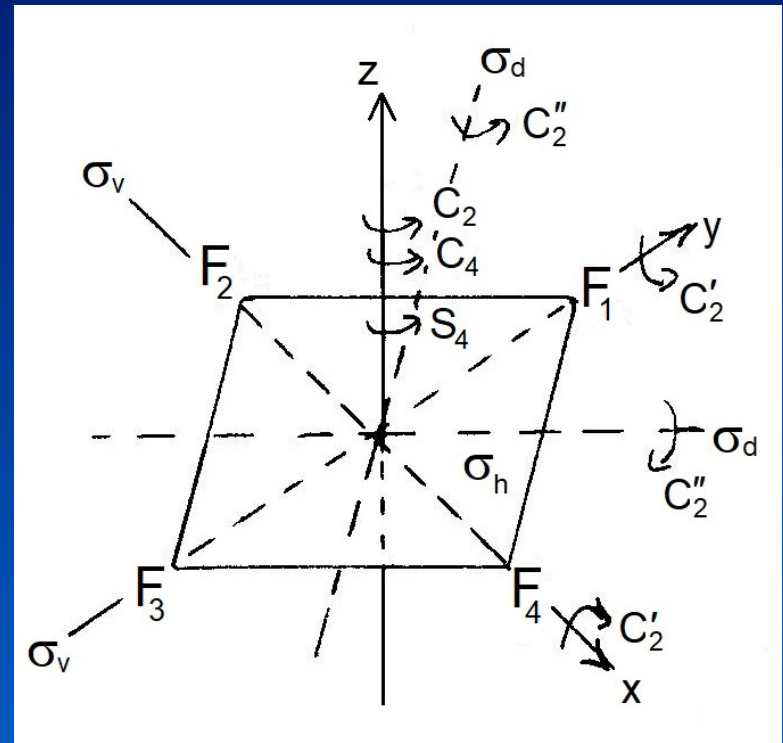
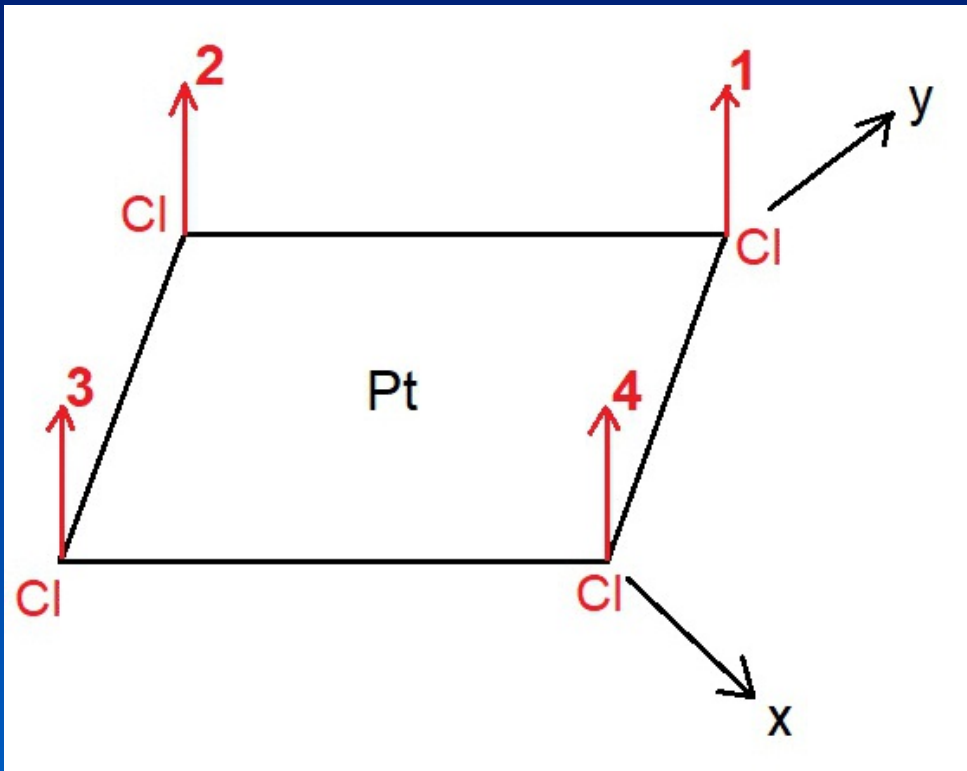
Sistema π



Classificando os orbitais $3p_z$ dos Cl - INSEPARÁVEIS

D_{4h} E $2C_4$ C_2 $2C_2'$ $2C_2''$ i $2S_4$ σ_h $2\sigma_v$ $2\sigma_d$

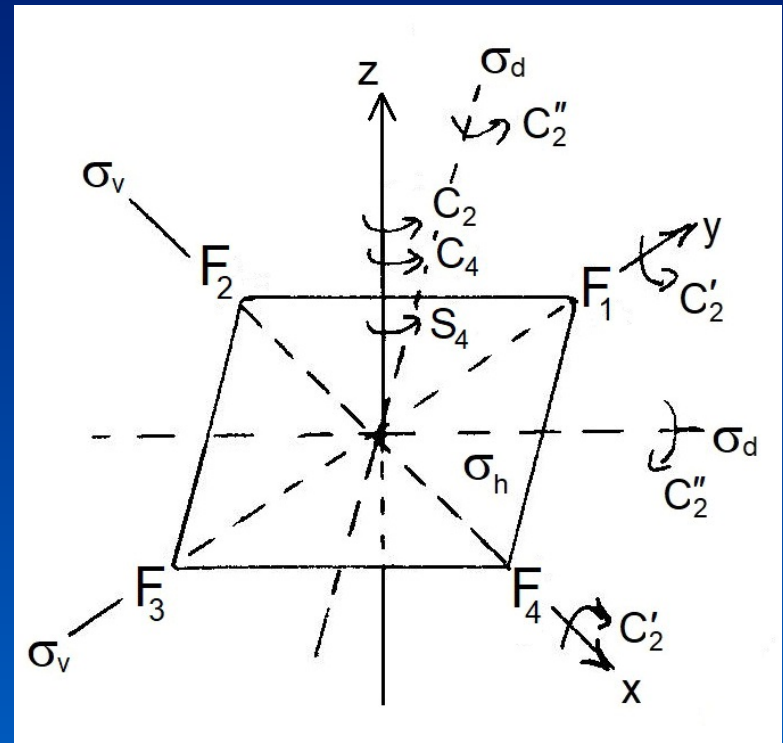
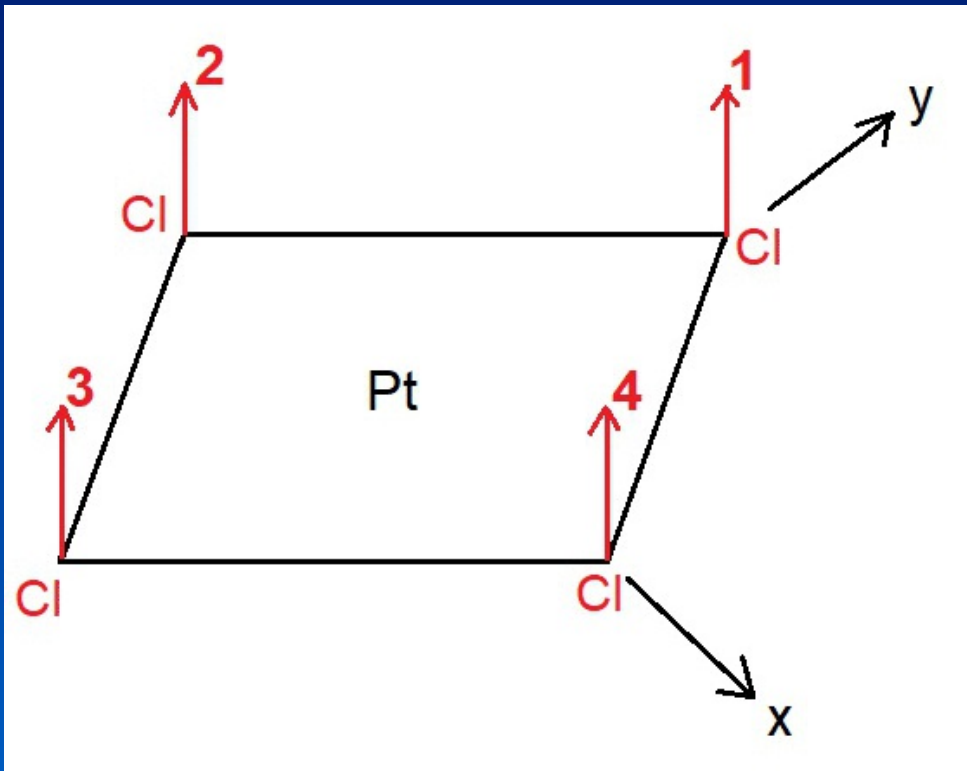
Cl(p_z) 4



Classificando os orbitais $3p_z$ dos Cl - INSEPARÁVEIS

D_{4h} E $2C_4$ C_2 $2C_2'$ $2C_2''$ i $2S_4$ σ_h $2\sigma_v$ $2\sigma_d$

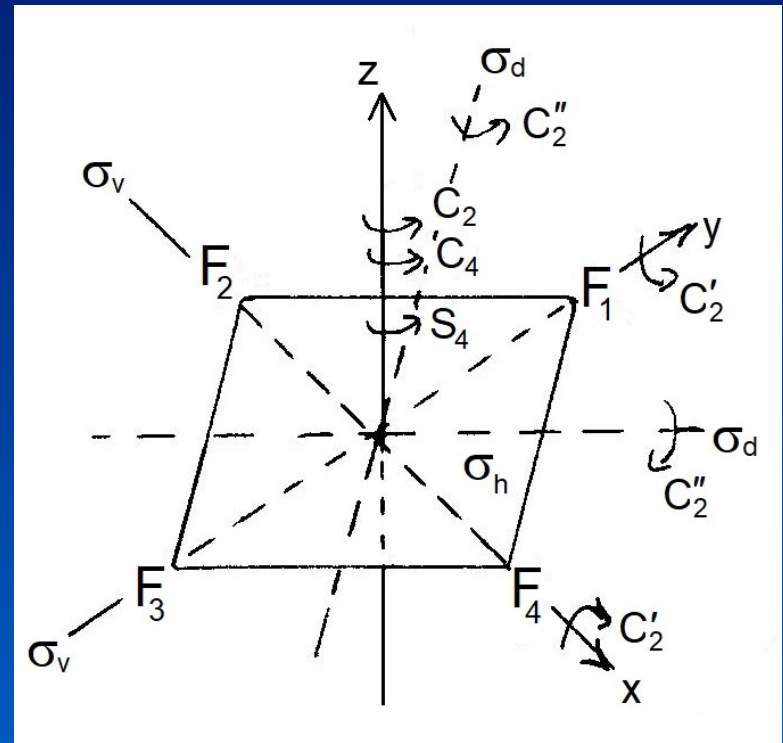
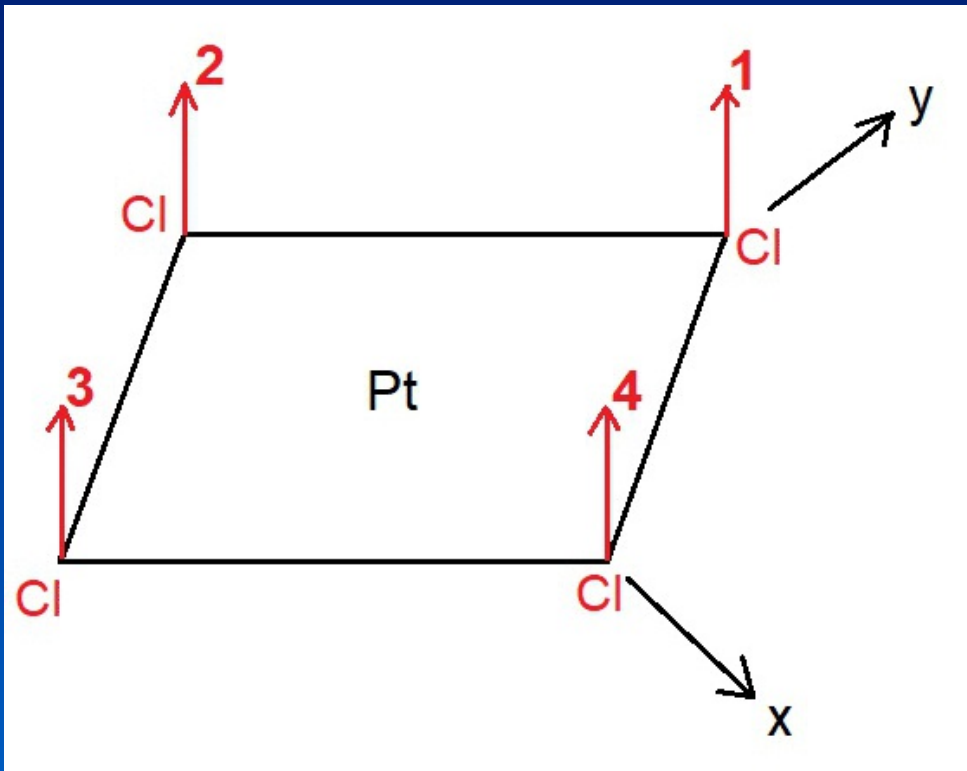
Cl(p_z) 4 0 0 ? 0



Classificando os orbitais $3p_z$ dos Cl - INSEPARÁVEIS

D_{4h} E $2C_4$ C_2 $2C_2'$ $2C_2''$ i $2S_4$ σ_h $2\sigma_v$ $2\sigma_d$

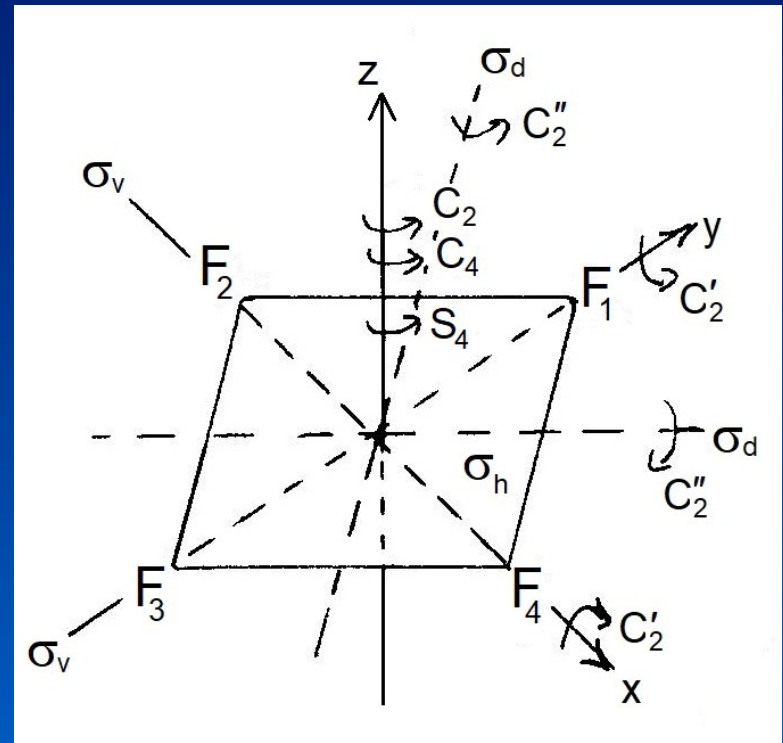
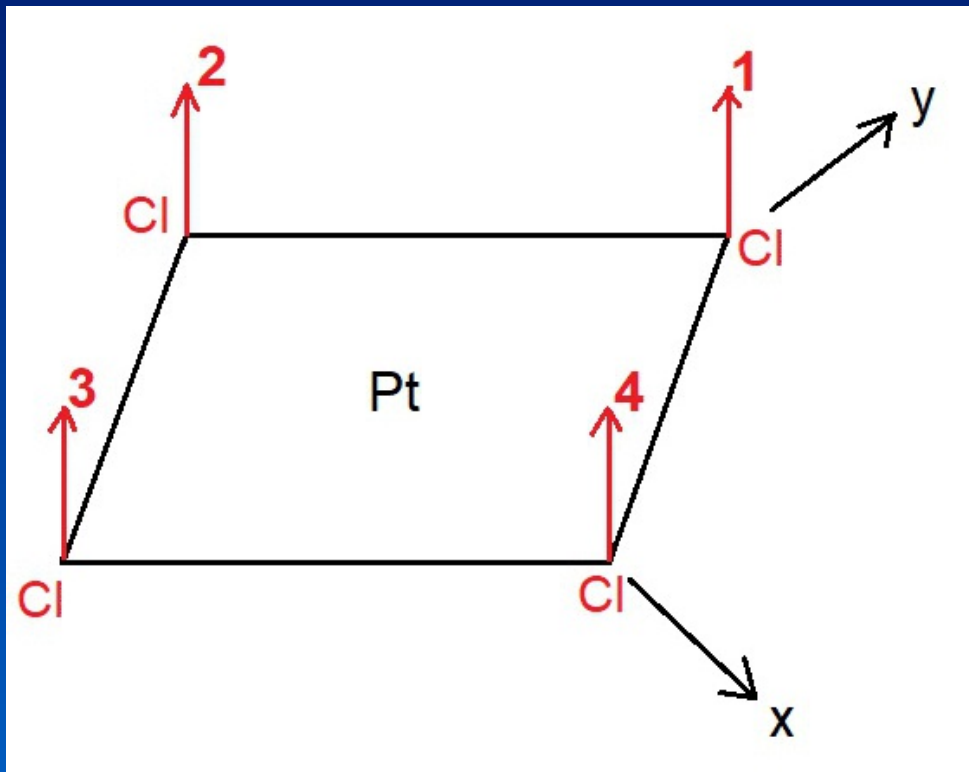
Cl(p_z) 4 0 0 ? 0 0 ?



Classificando os orbitais $3p_z$ dos Cl - INSEPARÁVEIS

D_{4h} E $2C_4$ C_2 $2C_2'$ $2C_2''$ i $2S_4$ σ_h $2\sigma_v$ $2\sigma_d$

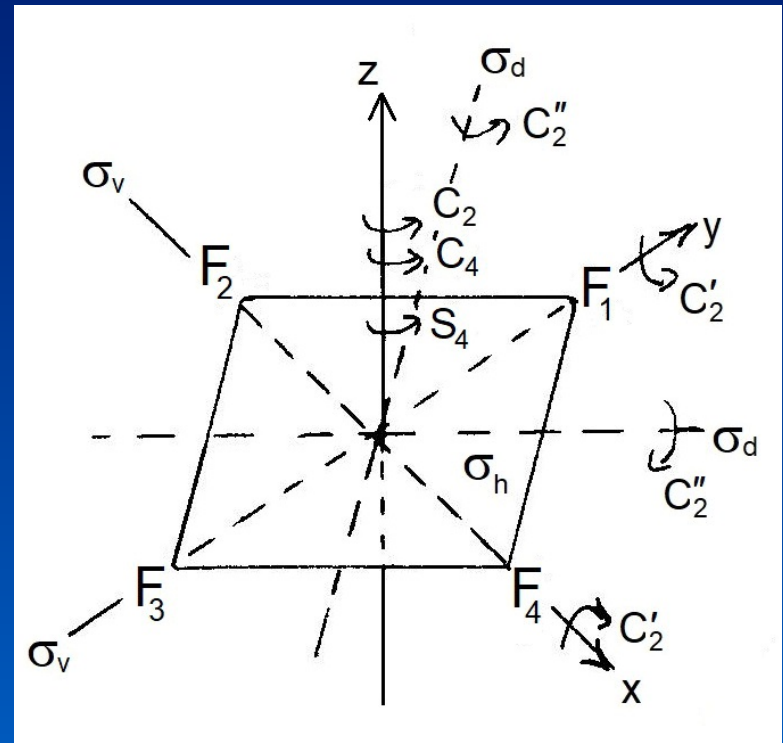
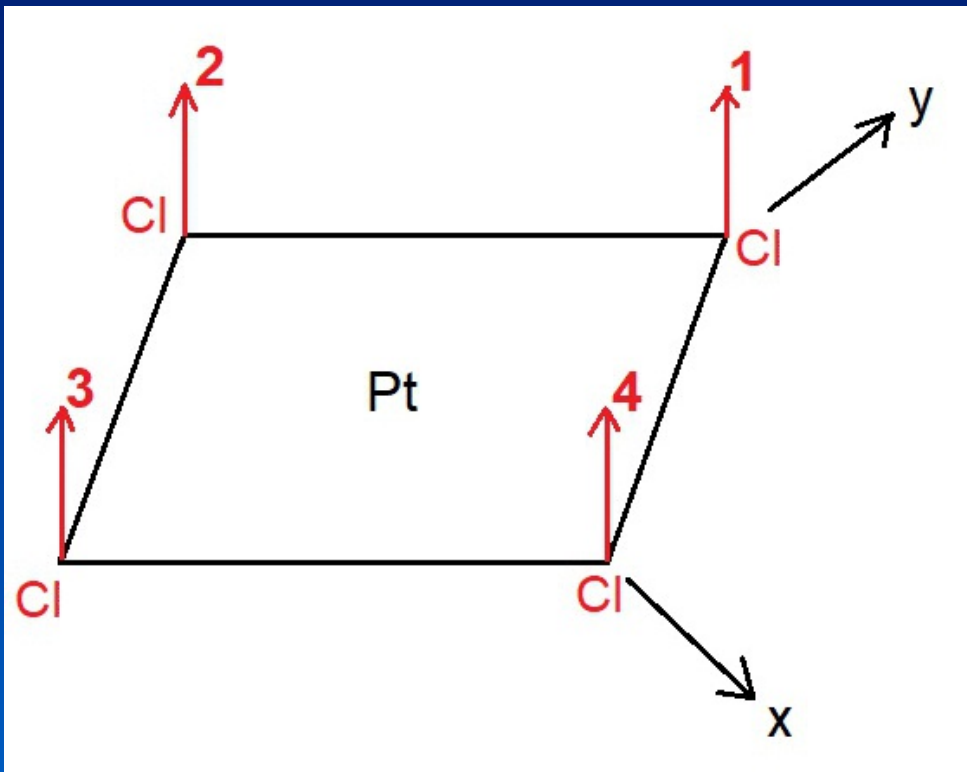
Cl(p_z) 4 0 0 ? 0 0 0 0



Classificando os orbitais $3p_z$ dos Cl - INSEPARÁVEIS

D_{4h} E $2C_4$ C_2 $2C_2'$ $2C_2''$ i $2S_4$ σ_h $2\sigma_v$ $2\sigma_d$

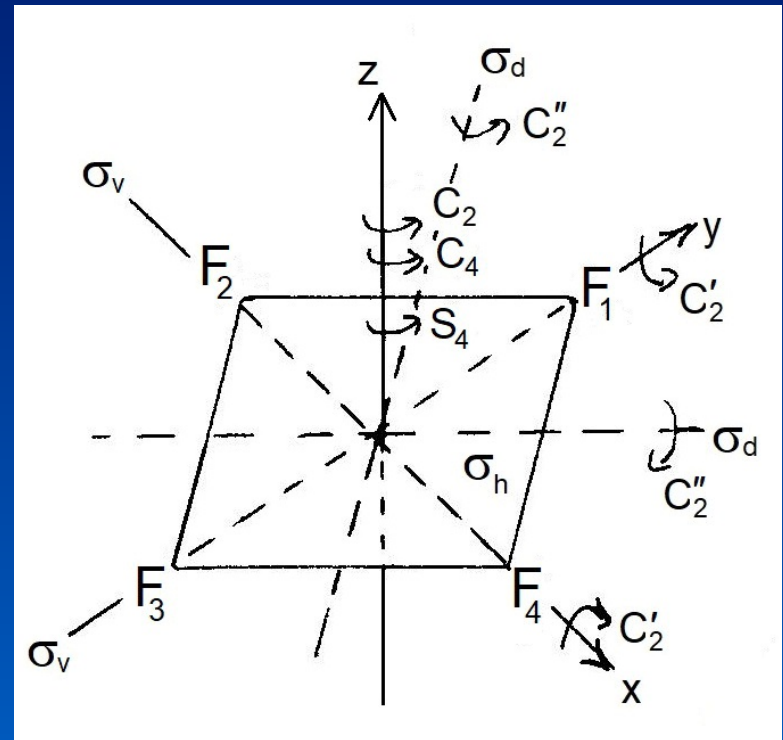
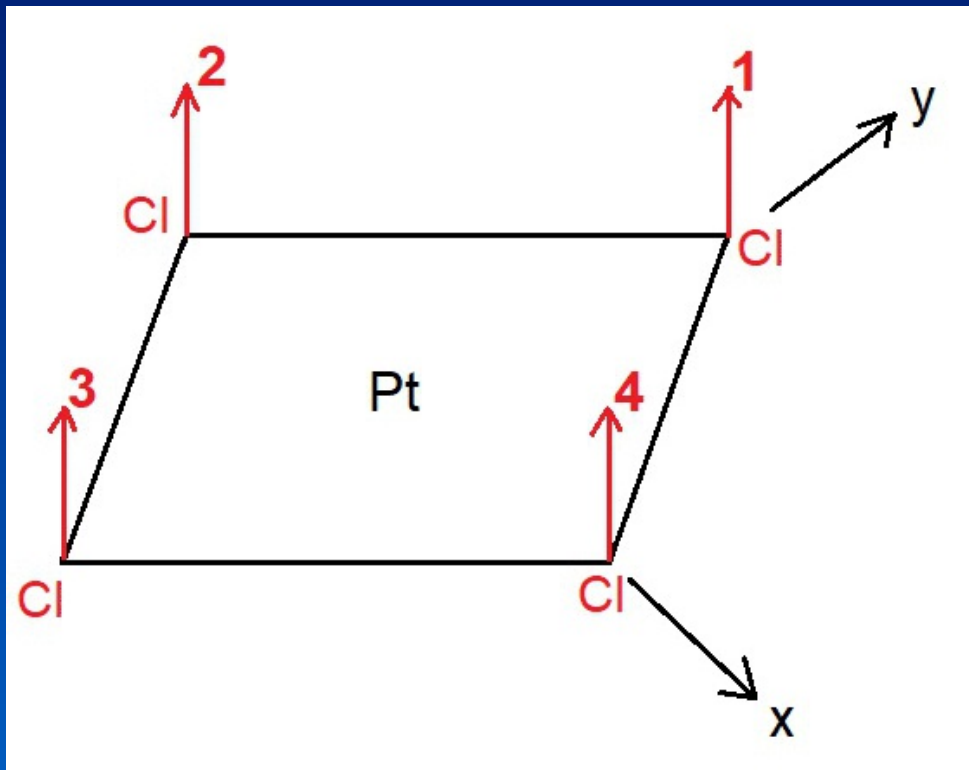
Cl(p_z) 4 0 0 -2 0 0 0 ? 0



Classificando os orbitais $3p_z$ dos Cl - INSEPARÁVEIS

D_{4h} E $2C_4$ C_2 $2C_2'$ $2C_2''$ i $2S_4$ σ_h $2\sigma_v$ $2\sigma_d$

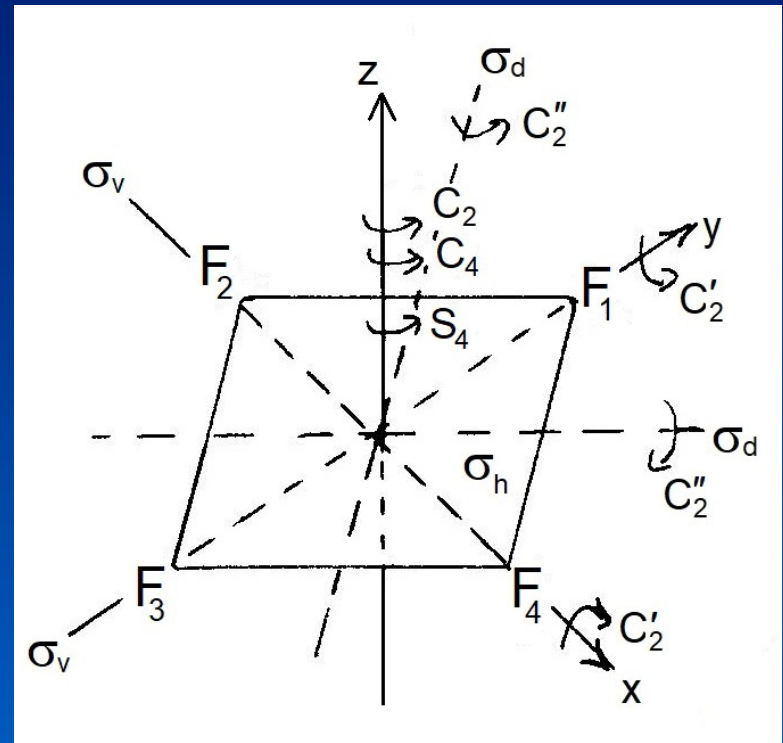
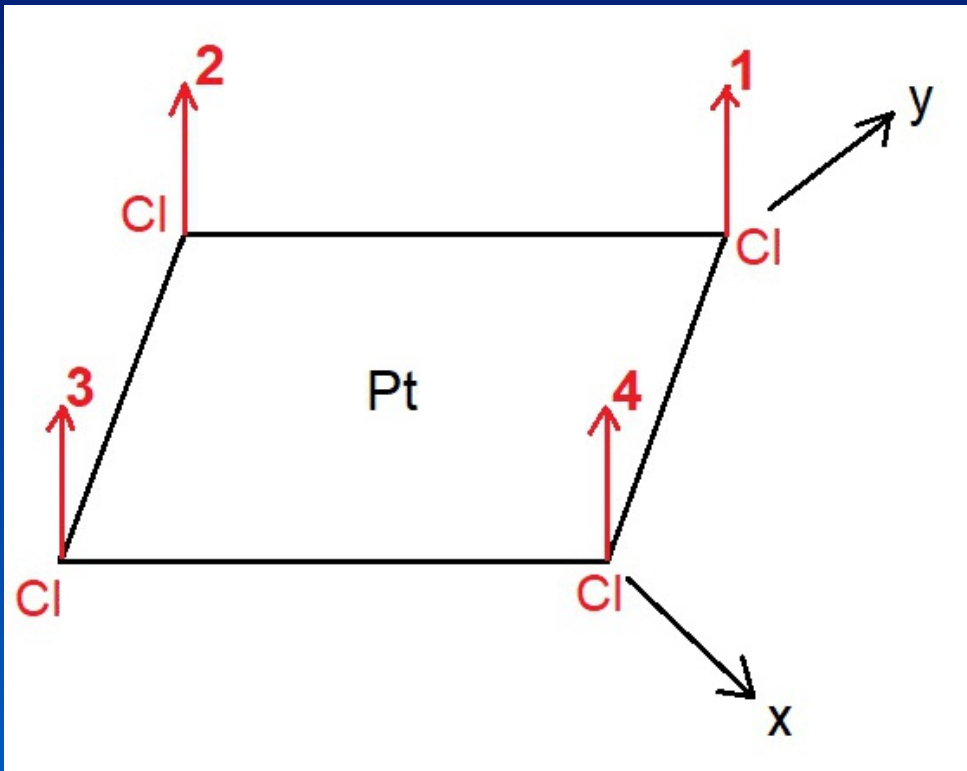
Cl(p_z) 4 0 0 -2 0 0 0 -4 ? 0



Classificando os orbitais $3p_z$ dos Cl - INSEPARÁVEIS

D_{4h} E $2C_4$ C_2 $2C_2'$ $2C_2''$ i $2S_4$ σ_h $2\sigma_v$ $2\sigma_d$

Cl(p_z) 4 0 0 -2 0 0 0 -4 2 0

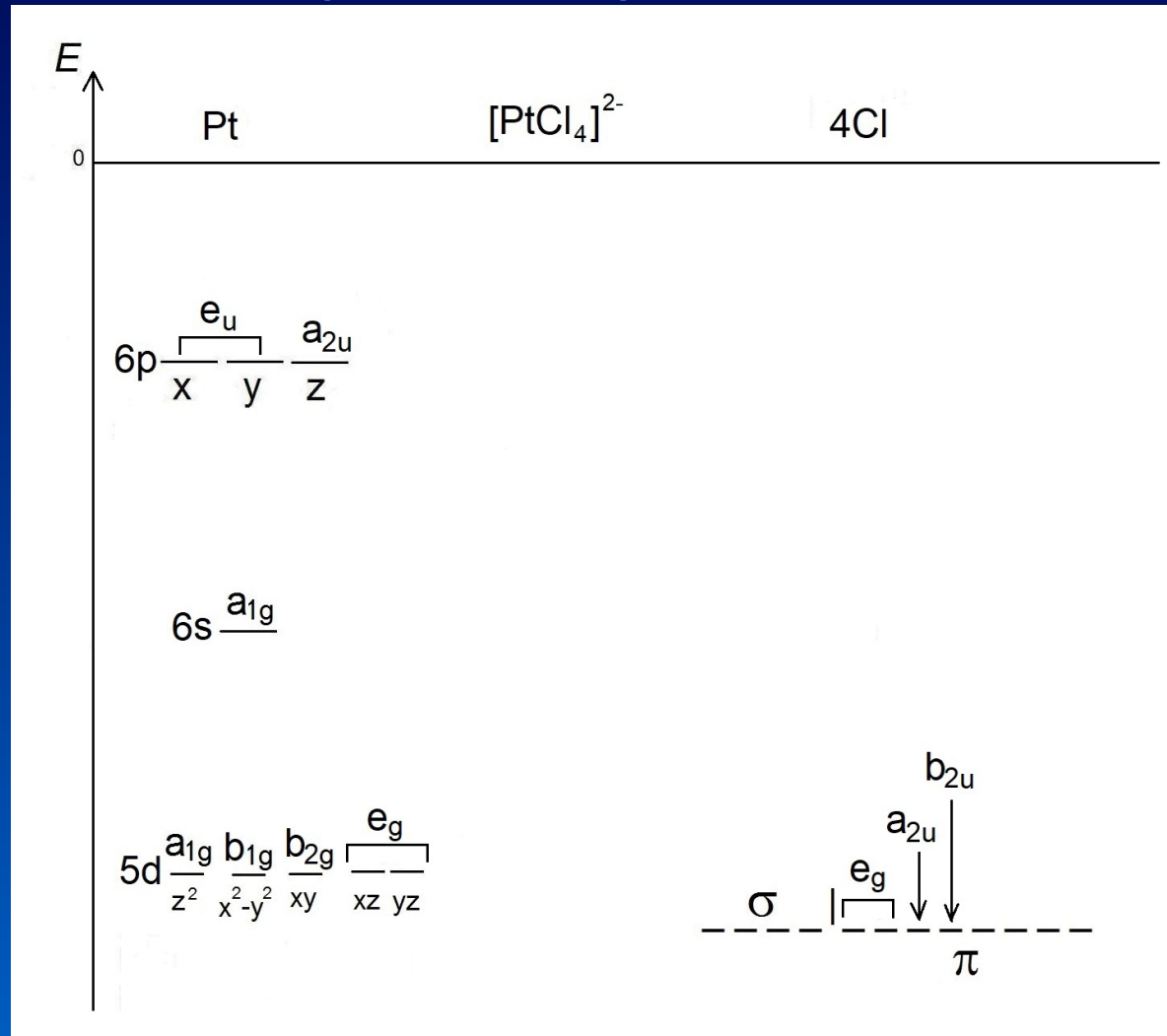


Classificando os orbitais $3p_z$ dos Cl - INSEPARÁVEIS

	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$
D_{4h}	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$
E_g	2	0	-2	0	0	2	0	-2	0	0
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1
B_{2u}	1	-1	1	-1	1	-1	1	-1	1	-1
<hr/>										
Cl(p_z)	4	0	0	-2	0	0	0	-4	2	0
									$E_g + A_{2u} + B_{2u}$	

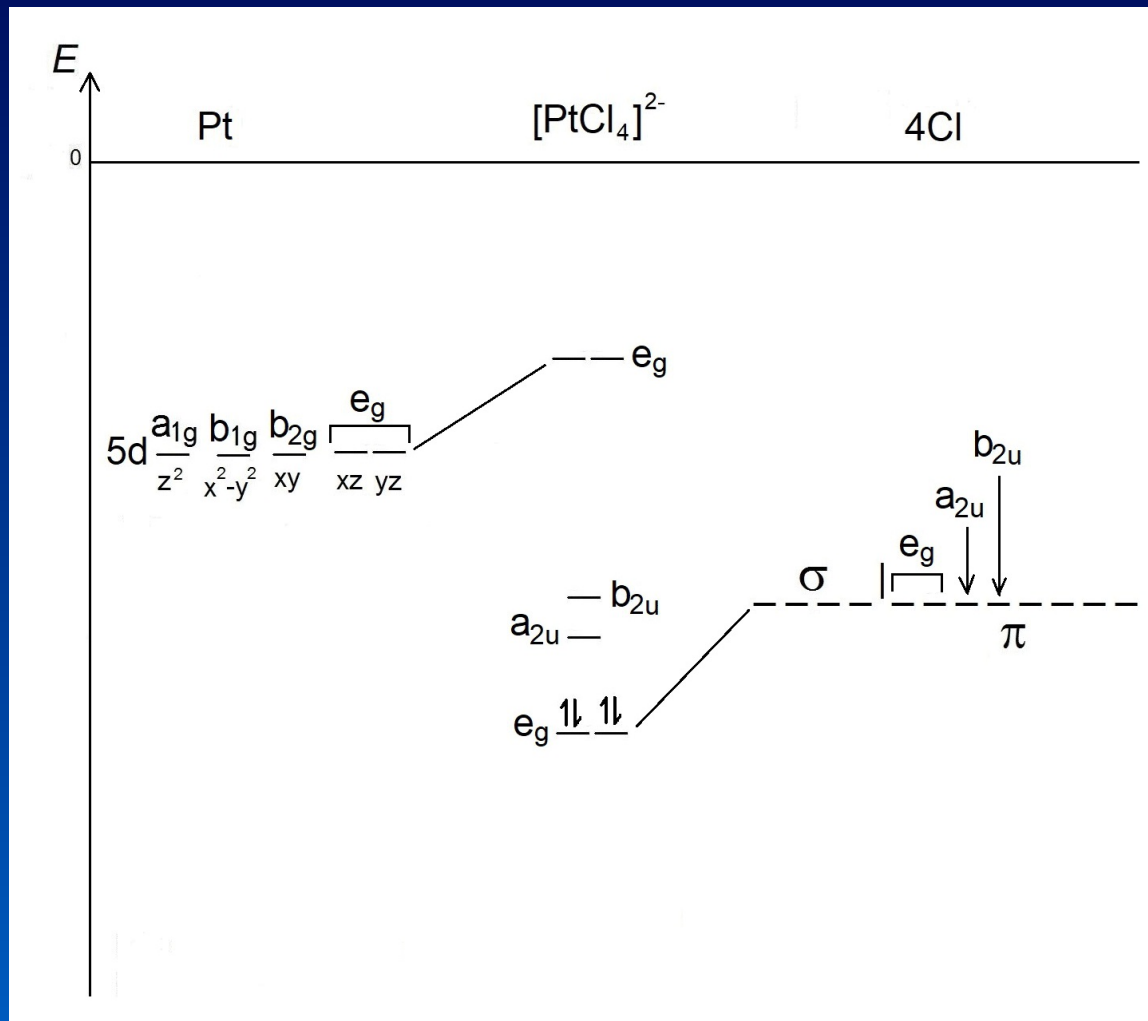
$[\text{PtCl}_4]^{2-} - D_{4h}$

Construindo o diagrama de energia dos orbitais moleculares



$[\text{PtCl}_4]^{2-} - D_{4h}$

Construindo o diagrama de energia dos orbitais moleculares



Desenhando os orbitais moleculares

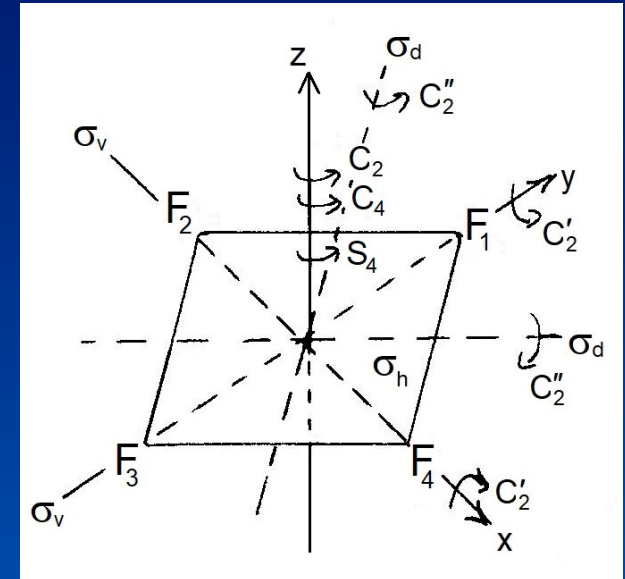
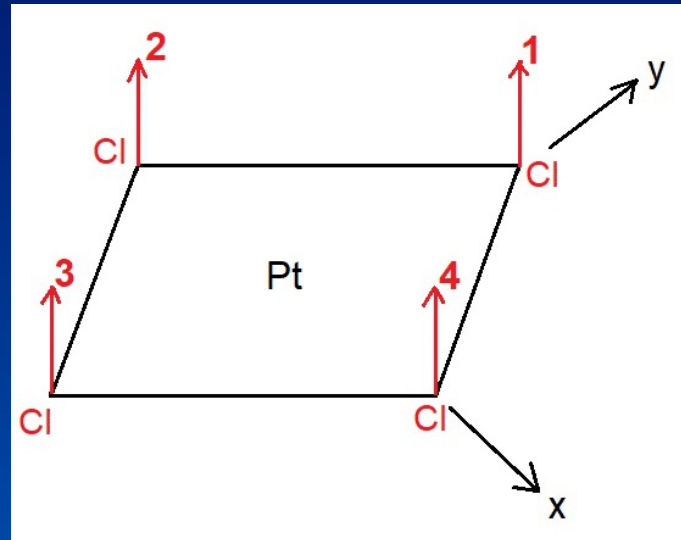
Método do Operador Projeção

$$\hat{P}(\varphi_i) = \sum_R \chi_R \hat{R}(\varphi_i)$$

$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Aplicando o Método do Operador Projeção aos orbitais πE_g

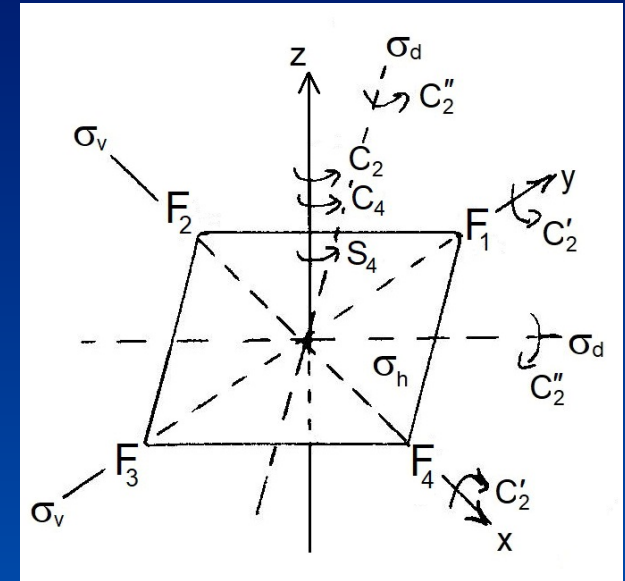
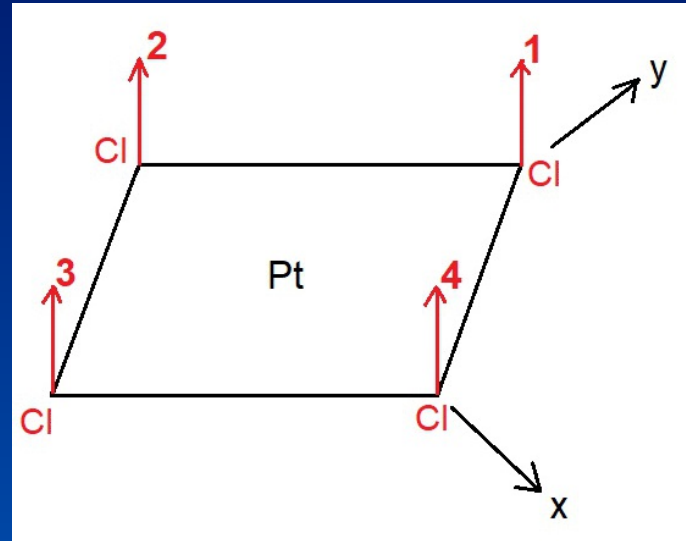
E	φ_1
C_4	φ_2
C_4^3	φ_4
C_2	φ_3
(x) C_2'	$-\varphi_3$
(y) C_2'	$-\varphi_1$
(xy) C_2''	$-\varphi_4$
(-xy) C_2''	$-\varphi_2$



$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Aplicando o Método do Operador Projeção aos orbitais πE_g

i	$-\varphi_3$
S_4	$-\varphi_2$
S_4^3	$-\varphi_4$
σ_h	$-\varphi_1$
(xz) σ_v	φ_3
(yz) σ_v	φ_1
(xy) σ_d	φ_4
$(-xy)$ σ_d	φ_2



$[\text{PtCl}_4]^{2-} - \text{D}_{4\text{h}}$

Aplicando o Método do Operador Projeção aos orbitais πE_g

		$E_g^{(11)}$
E	φ_1	1
C_4	φ_2	0
C_4^3	φ_4	0
C_2	φ_3	-1
$(x)C_2'$	$-\varphi_3$	-1
$(y)C_2'$	$-\varphi_1$	1
$(xy)C_2''$	$-\varphi_4$	0
$(-xy)C_2''$	$-\varphi_2$	0

$$E = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$C_4 = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

$$C_4^{-1} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

$$C_2 = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$^{(x)}C_2' = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$^{(y)}C_2' = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$^{(xy)}C_2'' = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}$$

$$^{(\bar{xy})}C_2'' = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\hat{P}_{E_g^{11}}(\varphi_1) = 0 \times \varphi_1 + 0 \times \varphi_2 + 0 \times \varphi_3 + 0 \times \varphi_4$$

$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Aplicando o Método do Operador Projeção aos orbitais πE_g

\dot{i}	$-\varphi_3$	1
S_4	$-\varphi_2$	0
S_4^3	$-\varphi_4$	0
σ_h	$-\varphi_1$	-1
$(xz)\sigma_v$	φ_3	1
$(yz)\sigma_v$	φ_1	-1
$(xy)\sigma_d$	φ_4	0
$(-xy)\sigma_d$	φ_2	0

$E_g^{(11)}$

$$\dot{i} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$S_4 = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

$$S_4^{-1} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

$$\sigma_h = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$(xz)\sigma_v = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$(yz)\sigma_v = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$((xy)z)\sigma_d = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$(\bar{x}y)z)\sigma_d = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}$$

$$\hat{P}_{E_g^{11}}(\varphi_1) = 0 \times \varphi_1 + 0 \times \varphi_2 + 0 \times \varphi_3 + 0 \times \varphi_4$$

$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Aplicando o Método do Operador Projeção aos orbitais πE_g

$$\hat{P}_{E_g}^{11}(\varphi_1) = 0$$

$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Aplicando o Método do Operador Projeção aos orbitais πE_g

	φ_1	φ_2	φ_3	φ_4	$E_g^{(12)}$
E					0
C_4					1
C_4^3					-1
C_2					0
$(x)C_2'$					0
$(y)C_2'$					0
$(xy)C_2''$					-1
$(-xy)C_2''$					1

$$E = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$C_4 = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

$$C_4^{-1} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

$$C_2 = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$^{(x)}C_2' = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$^{(y)}C_2' = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$^{(xy)}C_2'' = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}$$

$$^{(\bar{xy})}C_2'' = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\hat{P}_{E_g^{12}}(\varphi_1) = 0 \times \varphi_1 + 0 \times \varphi_2 + 0 \times \varphi_3 - 0 \times \varphi_4$$

$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Aplicando o Método do Operador Projeção aos orbitais πE_g

		$E_g^{(12)}$
\dot{i}	$-\varphi_3$	0
S_4	$-\varphi_2$	1
S_4^3	$-\varphi_4$	-1
σ_h	$-\varphi_1$	0
$(xz)\sigma_v$	φ_3	0
$(yz)\sigma_v$	φ_1	0
$(xy)\sigma_d$	φ_4	1
$(-xy)\sigma_d$	φ_2	-1

$$\dot{i} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$S_4 = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

$$S_4^{-1} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

$$\sigma_h = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}$$

$${}^{(xz)}\sigma_v = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$${}^{(yz)}\sigma_v = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$$

$${}^{((xy)z)}\sigma_d = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$${}^{(\bar{x}y)z}\sigma_d = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}$$

$$\hat{P}_{E_g^{12}}(\varphi_1) = 0 \times \varphi_1 - 2 \times \varphi_2 + 0 \times \varphi_3 + 2 \times \varphi_4$$

$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Aplicando o Método do Operador Projeção aos orbitais πE_g

$$\hat{P}_{E_g^{11}}(\varphi_1) = 0$$

$$\hat{P}_{E_g^{12}}(\varphi_1) = -\varphi_2 + \varphi_4$$

$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Aplicando o Método do Operador Projeção aos orbitais πE_g

		$E_g^{(21)}$
E	φ_1	0
C_4	φ_2	-1
C_4^3	φ_4	1
C_2	φ_3	0
$(x)C_2'$	$-\varphi_3$	0
$(y)C_2'$	$-\varphi_1$	0
$(xy)C_2''$	$-\varphi_4$	-1
$(-xy)C_2''$	$-\varphi_2$	1

$$E = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$C_4 = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

$$C_4^{-1} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

$$C_2 = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$^{(x)}C_2' = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$^{(y)}C_2' = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$^{(xy)}C_2'' = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}$$

$$^{(\bar{xy})}C_2'' = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\hat{P}_{E_g^{21}}(\varphi_1) = 0 \times \varphi_1 - 2 \times \varphi_2 + 0 \times \varphi_3 + 2 \times \varphi_4$$

$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Aplicando o Método do Operador Projeção aos orbitais πE_g

		$E_g^{(21)}$
\dot{i}	$-\varphi_3$	0
S_4	$-\varphi_2$	-1
S_4^3	$-\varphi_4$	1
σ_h	$-\varphi_1$	0
$(xz)\sigma_v$	φ_3	0
$(yz)\sigma_v$	φ_1	0
$(xy)\sigma_d$	φ_4	1
$(-xy)\sigma_d$	φ_2	-1

$$\dot{i} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$S_4 = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

$$S_4^{-1} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

$$\sigma_h = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}$$

$${}^{(xz)}\sigma_v = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$${}^{(yz)}\sigma_v = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$$

$${}^{((xy)z)}\sigma_d = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$${}^{(\bar{x}y)z}\sigma_d = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}$$

$$\hat{P}_{E_g^{21}}(\varphi_1) = 0 \times \varphi_1 - (2+0) \times \varphi_2 + 0 \times \varphi_3 + (2+0) \times \varphi_4$$

$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Aplicando o Método do Operador Projeção aos orbitais πE_g

$$\hat{P}_{E_g^{11}}(\varphi_1) = 0$$

$$\hat{P}_{E_g^{12}}(\varphi_1) = -\varphi_2 + \varphi_4$$

$$\hat{P}_{E_g^{21}}(\varphi_1) = -\varphi_2 + \varphi_4$$

$[\text{PtCl}_4]^{2-} - \text{D}_{4\text{h}}$

Aplicando o Método do Operador Projeção aos orbitais πE_g

		$E_g^{(22)}$
E	φ_1	1
C_4	φ_2	0
C_4^3	φ_4	0
C_2	φ_3	-1
$(x)C_2'$	$-\varphi_3$	1
$(y)C_2'$	$-\varphi_1$	-1
$(xy)C_2''$	$-\varphi_4$	0
$(-xy)C_2''$	$-\varphi_2$	0

$$E = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$C_4 = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

$$C_4^{-1} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

$$C_2 = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$^{(x)}C_2' = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$^{(y)}C_2' = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$^{(xy)}C_2'' = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}$$

$$^{(\bar{xy})}C_2'' = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\hat{P}_{E_g^{22}}(\varphi_1) = 2 \times \varphi_1 + 0 \times \varphi_2 - 2 \times \varphi_3 + 0 \times \varphi_4$$

$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Aplicando o Método do Operador Projeção aos orbitais πE_g

		$E_g^{(22)}$
\dot{i}	$-\varphi_3$	1
S_4	$-\varphi_2$	0
S_4^3	$-\varphi_4$	0
σ_h	$-\varphi_1$	-1
$(xz)\sigma_v$	φ_3	-1
$(yz)\sigma_v$	φ_1	1
$(xy)\sigma_d$	φ_4	0
$(-xy)\sigma_d$	φ_2	0

$$\dot{i} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$S_4 = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

$$S_4^{-1} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

$$\sigma_h = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$(xz)\sigma_v = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$(yz)\sigma_v = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$((xy)z)\sigma_d = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$(\bar{x}y)z)\sigma_d = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}$$

$$\hat{P}_{E_g^{22}}(\varphi_1) = (2+2)\times\varphi_1 - 0\times\varphi_2 - (2+2)\times\varphi_3 + 0\times\varphi_4$$

$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Aplicando o Método do Operador Projeção aos orbitais πE_g

$$\hat{P}_{E_g^{11}}(\varphi_1) = 0$$

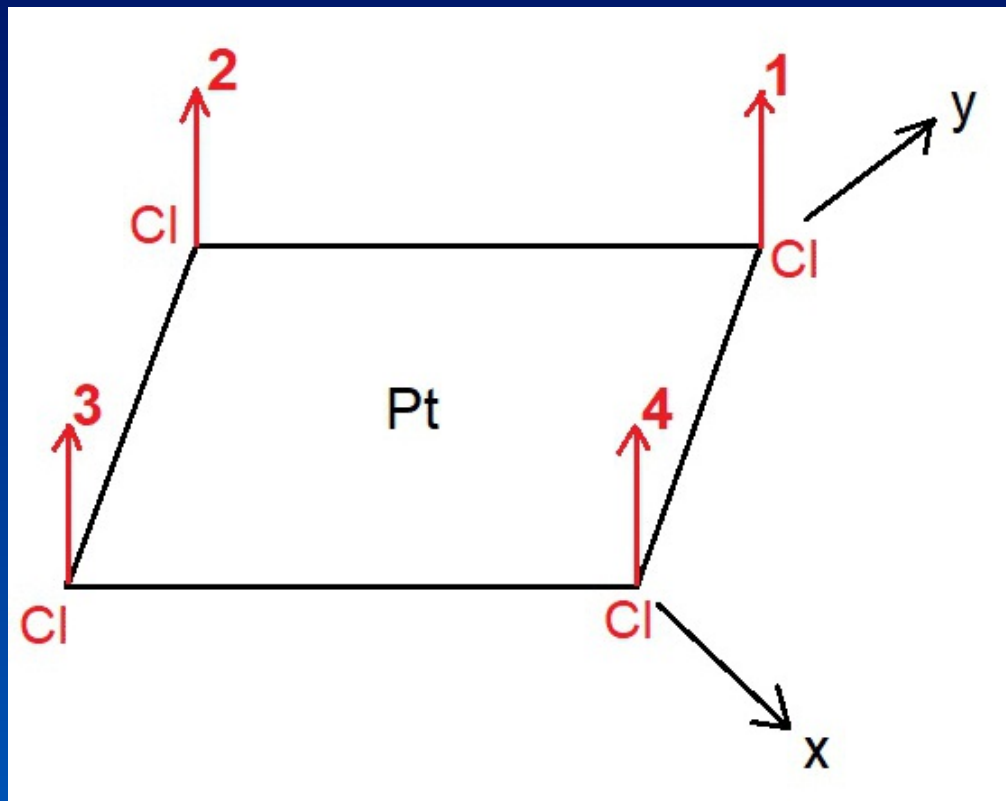
$$\hat{P}_{E_g^{12}}(\varphi_1) = -\varphi_2 + \varphi_4$$

$$\hat{P}_{E_g^{21}}(\varphi_1) = -\varphi_2 + \varphi_4$$

$$\hat{P}_{E_g^{22}}(\varphi_1) = \varphi_1 - \varphi_3$$

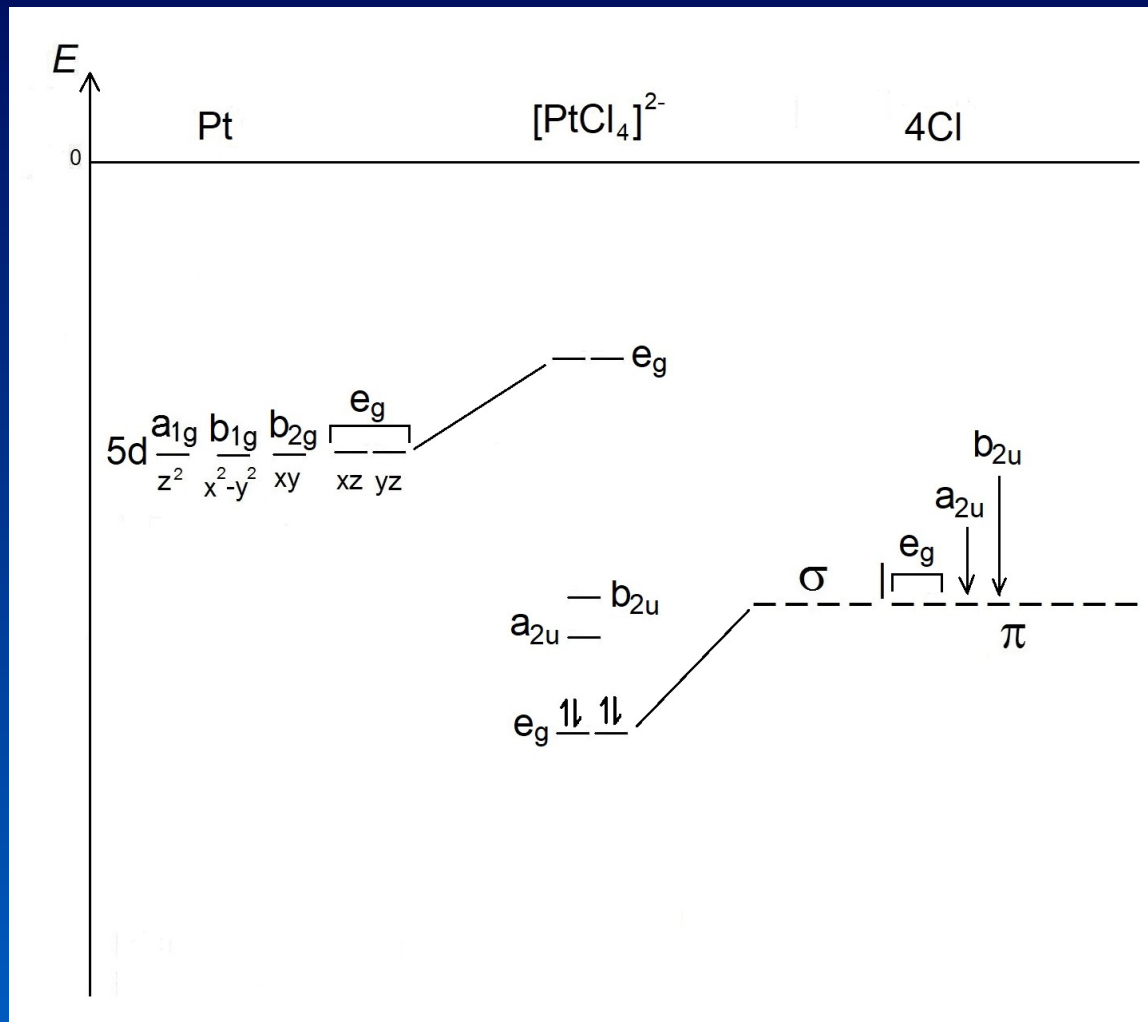


Sistema π



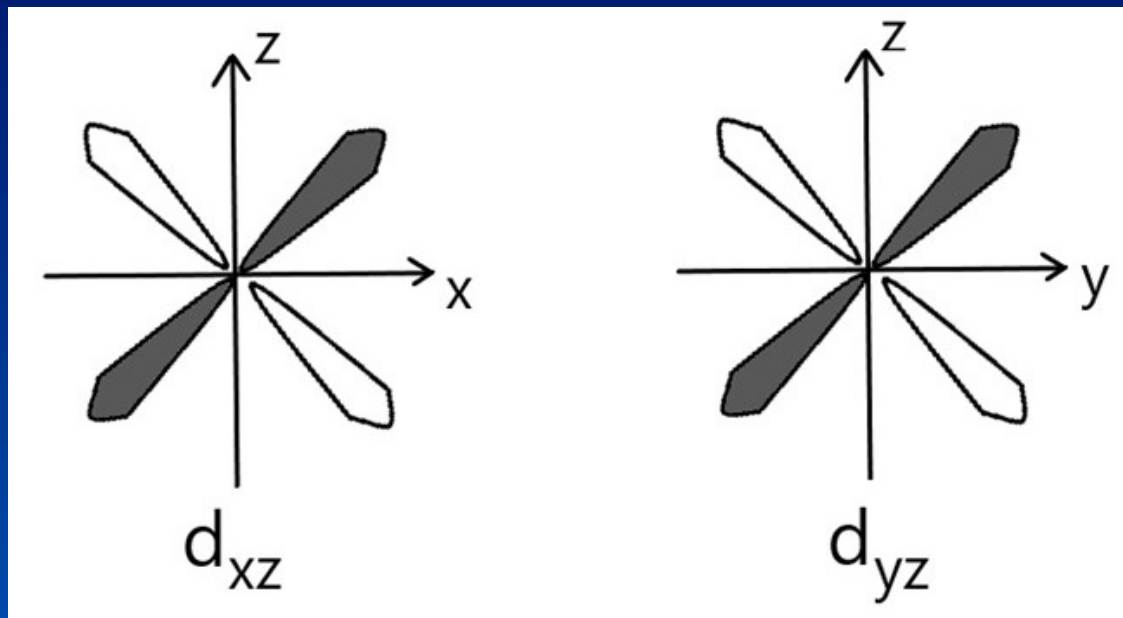
$[\text{PtCl}_4]^{2-} - D_{4h}$

Construindo o diagrama de energia dos orbitais moleculares



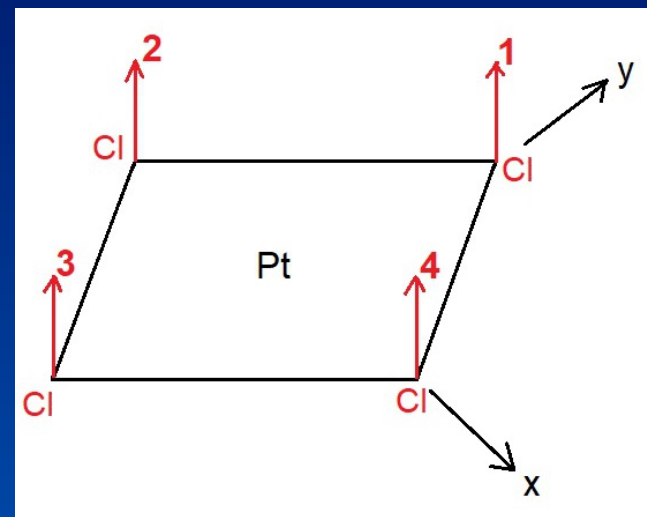
$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Sistema π



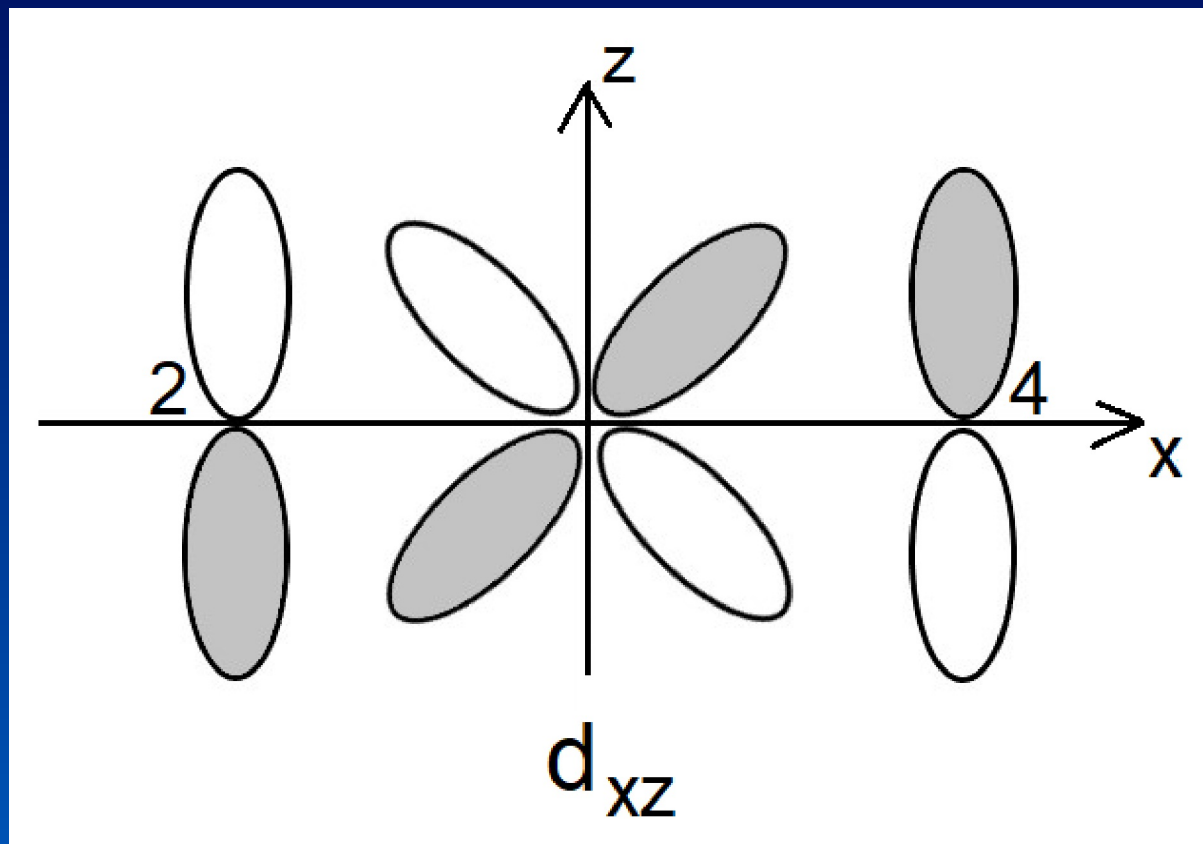
$$-\varphi_2 + \varphi_4$$

$$\varphi_1 - \varphi_3$$



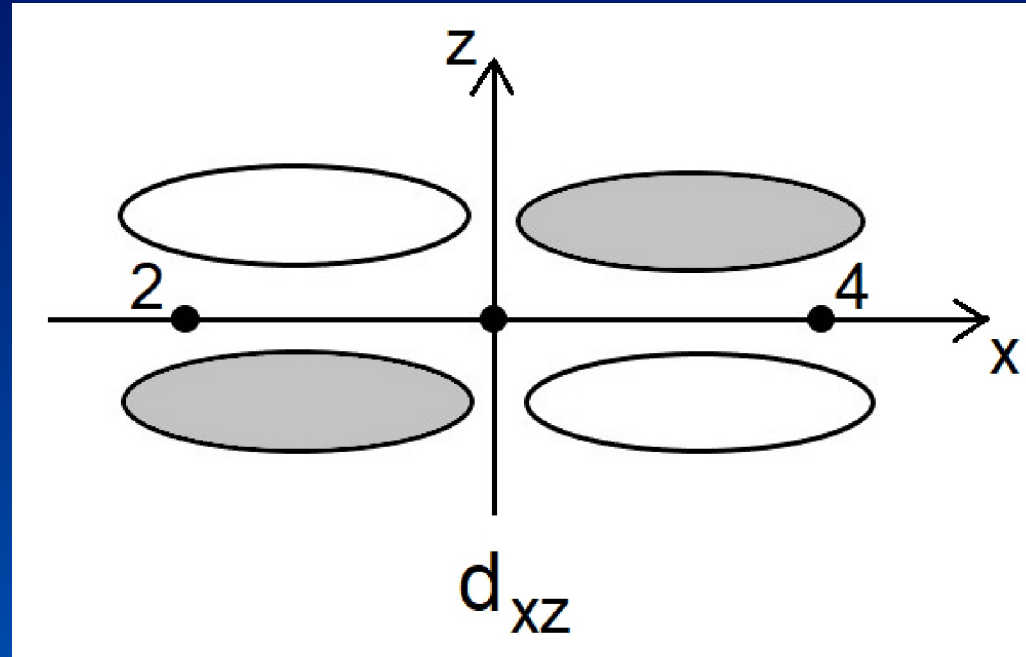
$[\text{PtCl}_4]^{2-} - \text{D}_{4h}$

Sistema π



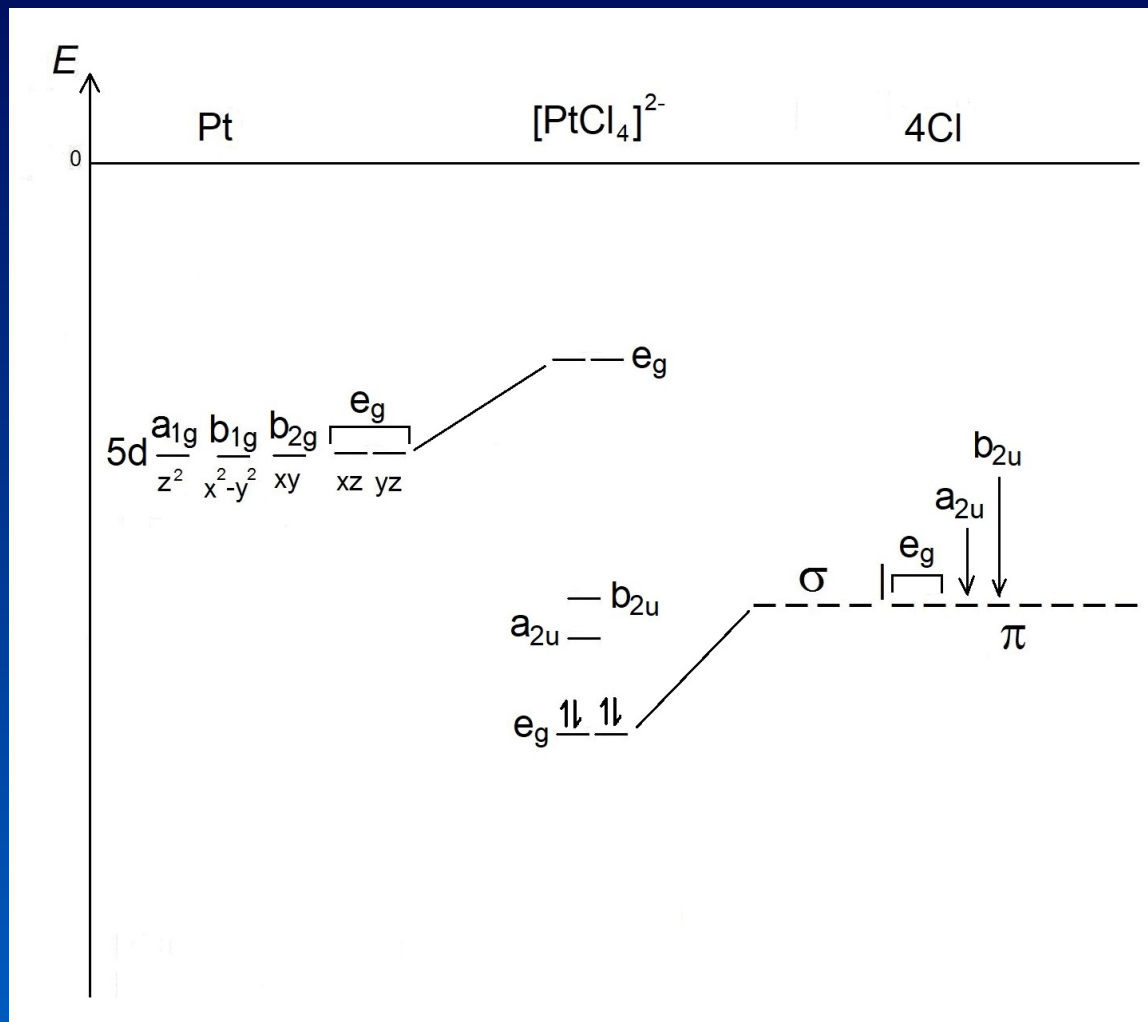


Sistema π



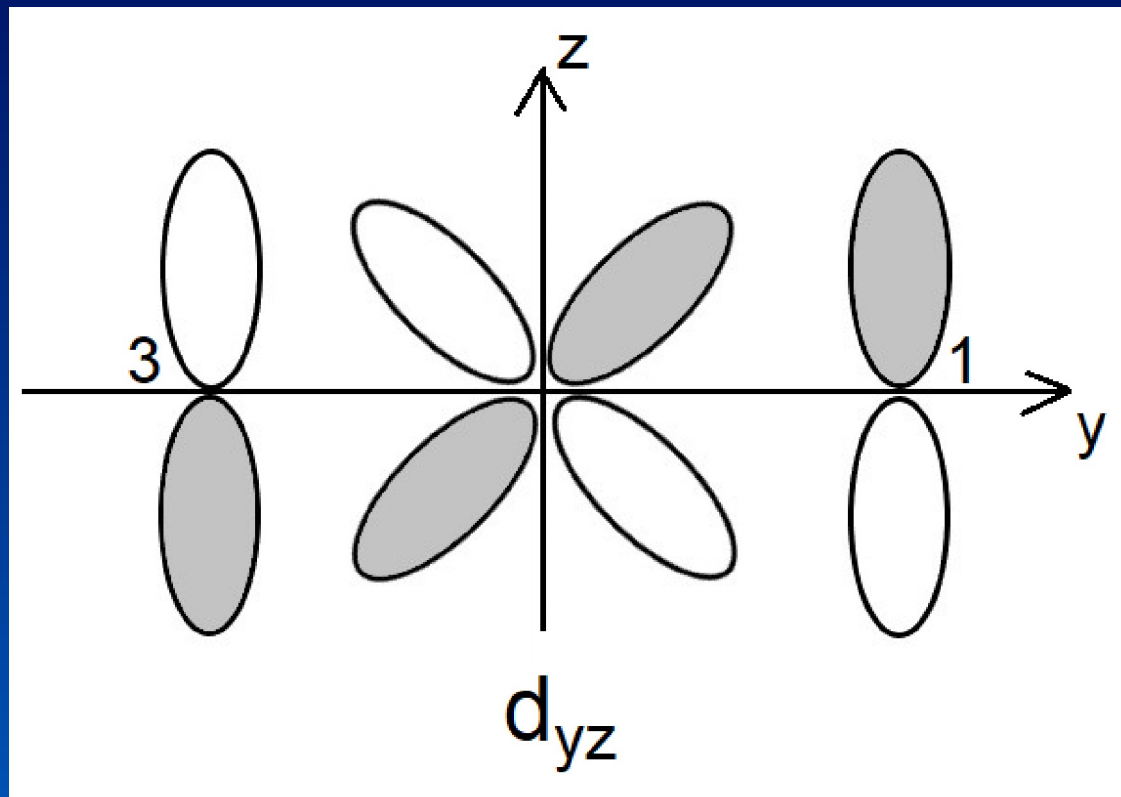
$[\text{PtCl}_4]^{2-} - D_{4h}$

Construindo o diagrama de energia dos orbitais moleculares



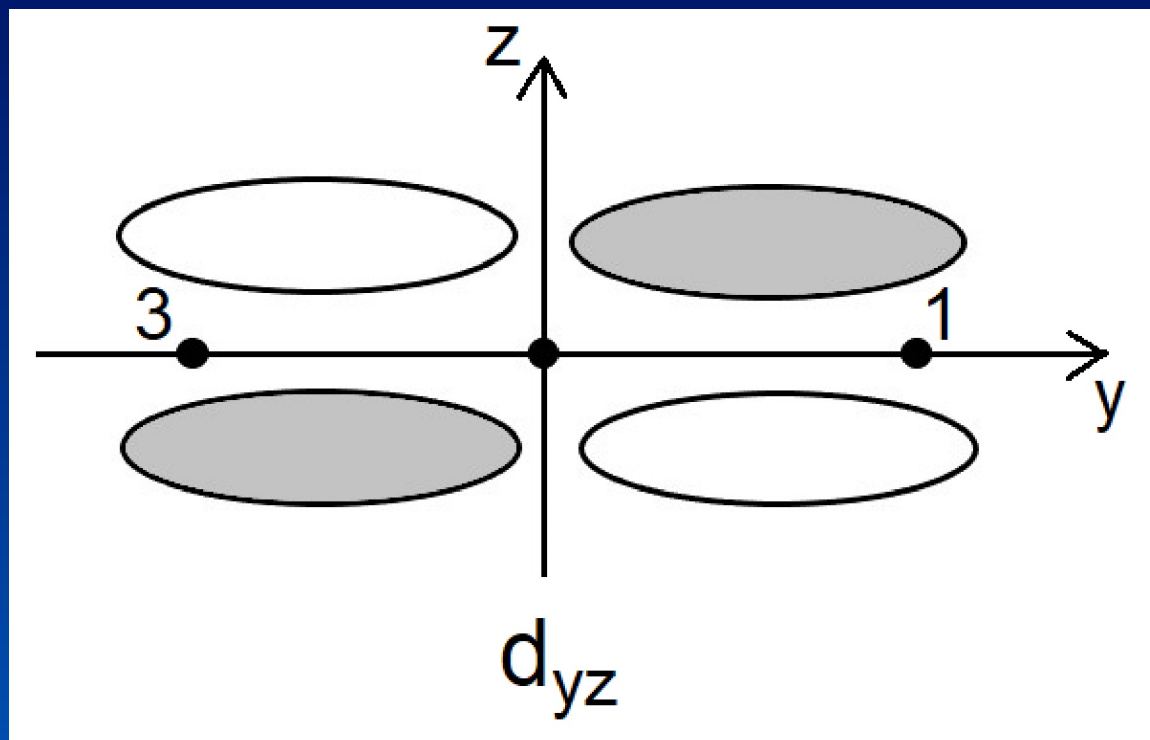


Sistema π





Sistema π



FIM DA AULA 6