MÉTODO DO OPERADOR PROJEÇÃO

Simetria Octaédrica

Resultado das 48 operações de simetria aplicadas sobre um orbital σ:

$E\ \sigma_y = \sigma_y$

$^{xyz}C_3\ \sigma_y = \sigma_x$

$^{xyz}C_3^{\ 2}\ \sigma_y = \sigma_z$

$^{x(-y)z}C_3\ \sigma_y = \sigma_{-z}$

$^{x(-y)z}C_3^{\ 2}\ \sigma_y = \sigma_{-x}$

$^{(-x)(-y)z}C_3\ \sigma_y = \sigma_x$

$^{(-x)(-y)z}C_3^{\ 2}\ \sigma_y = \sigma_{-z}$

$^{(-x)yz}C_3\ \sigma_y = \sigma_z$

$^{(-x)yz}C_3^{\ 2}\ \sigma_y = \sigma_{-x}$

$^{xy}C_2^{\ \perp z}\ \sigma_y = \sigma_x$

$^{x(-y)}C_2^{\ \perp z}\ \sigma_y = \sigma_{-x}$

$^{yz}C_2^{\ \perp x}\ \sigma_y = \sigma_z$

$^{(-y)z}C_2^{\ \perp x}\ \sigma_y = \sigma_{-z}$

$^{xz}C_2^{\ \perp y}\ \sigma_y = \sigma_{-y}$

$^{(-x)z}C_2^{\ \perp y}\ \sigma_y = \sigma_{-y}$

$^{z}C_4\ \sigma_y = \sigma_x$

$^{z}C_4^{\ 3}\ \sigma_y = \sigma_{-x}$

$^{x}C_4\ \sigma_y = \sigma_{-z}$

$^{x}C_4^{\ 3}\ \sigma_y = \sigma_z$

$^{y}C_4\ \sigma_y = \sigma_y$

$^{y}C_4^{\ 3}\ \sigma_y = \sigma_y$

$^{z}C_2(=C_4^{\ 2})\ \sigma_y = \sigma_{-y}$

$^{x}C_2(=C_4^{\ 2})\ \sigma_y = \sigma_{-y}$

$^{y}C_2(=C_4^{\ 2})\ \sigma_y = \sigma_y$

$i\ \sigma_y = \sigma_{-y}$

$^{z}S_4\ \sigma_y = \sigma_x$

$^{z}S_4^{\ 3}\ \sigma_y = \sigma_{-x}$

$^{x}S_4\ \sigma_y = \sigma_{-z}$

$^{x}S_4^{\ 3}\ \sigma_y = \sigma_z$

$^{y}S_4\ \sigma_y = \sigma_{-y}$

$^{y}S_4^{\ 3}\ \sigma_y = \sigma_{-y}$

$^{xyz}S_6\ \sigma_y = \sigma_{-z}$

$^{xyz}S_6^{\ 5}\ \sigma_y = \sigma_{-x}$

$^{x(-y)z}S_6\ \sigma_y = \sigma_x$

$^{x(-y)z}S_6^{\ 5}\ \sigma_y = \sigma_z$

$^{(-x)(-y)z}S_6\ \sigma_y = \sigma_z$

$^{(-x)(-y)z}S_6^{\ 5}\ \sigma_y = \sigma_{-x}$

$^{(-x)yz}S_6\ \sigma_y = \sigma_x$

$^{(-x)yz}S_6^{\ 5}\ \sigma_y = \sigma_{-z}$

$^{\perp z}\sigma_h\ \sigma_y = \sigma_y$

$^{\perp y}\sigma_h\ \sigma_y = \sigma_{-y}$

$^{\perp x}\sigma_h\ \sigma_y = \sigma_y$

$^{z}\sigma_d^{\ \perp xy}\ \sigma_y = \sigma_x$

$^{z}\sigma_d^{\ \perp x(-y)}\ \sigma_y = \sigma_{-x}$

$^{x}\sigma_d^{\ \perp yz}\ \sigma_y = \sigma_z$

$^{x}\sigma_d^{\ \perp (-y)z}\ \sigma_y = \sigma_{-z}$

$^{y}\sigma_d^{\ \perp xz}\ \sigma_y = \sigma_y$

$^{y}\sigma_d^{\ \perp (-x)z}\ \sigma_y = \sigma_y$

Simetria Octaédrica

Resultado das 48 operações de simetria aplicadas sobre um orbital π:

E	$\pi_y^{//z}$	$=$	$\pi_y^{//z}$
${}^{xyz}C_3$	$\pi_y^{//z}$	$=$	$\pi_z^{//x}$
${}^{xyz}C_3^2$	$\pi_y^{//z}$	$=$	$\pi_x^{//y}$
${}^{x(-y)z}C_3$	$\pi_y^{//z}$	$=$	$-\pi_{-x}^{//y}$
${}^{x(-y)z}C_3^2$	$\pi_y^{//z}$	$=$	$\pi_{-z}^{//x}$
${}^{(-x)(-y)z}C_3$	$\pi_y^{//z}$	$=$	$-\pi_{-z}^{//x}$
${}^{(-x)(-y)z}C_3^2$	$\pi_y^{//z}$	$=$	$-\pi_x^{//y}$
${}^{(-x)yz}C_3$	$\pi_y^{//z}$	$=$	$\pi_{-x}^{//y}$
${}^{(-x)yz}C_3^2$	$\pi_y^{//z}$	$=$	$-\pi_z^{//x}$
${}^{xy}C_2^{\perp z}$	$\pi_y^{//z}$	$=$	$-\pi_x^{//z}$
${}^{x(-y)}C_2^{\perp z}$	$\pi_y^{//z}$	$=$	$-\pi_{-x}^{//z}$
${}^{yz}C_2^{\perp x}$	$\pi_y^{//z}$	$=$	$\pi_z^{//y}$
${}^{(-y)z}C_2^{\perp x}$	$\pi_y^{//z}$	$=$	$-\pi_{-z}^{//y}$
${}^{xz}C_2^{\perp y}$	$\pi_y^{//z}$	$=$	$\pi_{-y}^{//x}$
${}^{(-x)z}C_2^{\perp y}$	$\pi_y^{//z}$	$=$	$-\pi_{-y}^{//x}$
${}^{z}C_4$	$\pi_y^{//z}$	$=$	$\pi_{-x}^{//z}$
${}^{z}C_4^3$	$\pi_y^{//z}$	$=$	$\pi_x^{//z}$
${}^{x}C_4$	$\pi_y^{//z}$	$=$	$-\pi_z^{//y}$
${}^{x}C_4^3$	$\pi_y^{//z}$	$=$	$\pi_{-z}^{//y}$
${}^{y}C_4$	$\pi_y^{//z}$	$=$	$\pi_y^{//x}$
${}^{y}C_4^3$	$\pi_y^{//z}$	$=$	$-\pi_y^{//x}$
${}^{z}C_2\,(=C_4^2)$	$\pi_y^{//z}$	$=$	$\pi_{-y}^{//z}$
${}^{x}C_2\,(=C_4^2)$	$\pi_y^{//z}$	$=$	$-\pi_{-y}^{//z}$
${}^{y}C_2\,(=C_4^2)$	$\pi_y^{//z}$	$=$	$-\pi_y^{//z}$
i	$\pi_y^{//z}$	$=$	$-\pi_{-y}^{//z}$
${}^{z}S_4$	$\pi_y^{//z}$	$=$	$-\pi_{-x}^{//z}$
${}^{z}S_4^3$	$\pi_y^{//z}$	$=$	$-\pi_x^{//z}$
${}^{x}S_4$	$\pi_y^{//z}$	$=$	$-\pi_z^{//y}$
${}^{x}S_4^3$	$\pi_y^{//z}$	$=$	$\pi_{-z}^{//y}$
${}^{y}S_4$	$\pi_y^{//z}$	$=$	$\pi_{-y}^{//x}$
${}^{y}S_4^3$	$\pi_y^{//z}$	$=$	$-\pi_{-y}^{//x}$
${}^{xyz}S_6$	$\pi_y^{//z}$	$=$	$-\pi_{-x}^{//y}$
${}^{xyz}S_6^5$	$\pi_y^{//z}$	$=$	$-\pi_{-z}^{//x}$
${}^{x(-y)z}S_6$	$\pi_y^{//z}$	$=$	$-\pi_z^{//x}$
${}^{x(-y)z}S_6^5$	$\pi_y^{//z}$	$=$	$\pi_x^{//y}$
${}^{(-x)(-y)z}S_6$	$\pi_y^{//z}$	$=$	$\pi_{-x}^{//y}$
${}^{(-x)(-y)z}S_6^5$	$\pi_y^{//z}$	$=$	$\pi_z^{//x}$
${}^{(-x)yz}S_6$	$\pi_y^{//z}$	$=$	$\pi_{-z}^{//x}$
${}^{(-x)yz}S_6^5$	$\pi_y^{//z}$	$=$	$-\pi_x^{//y}$
${}^{\perp z}\sigma_h$	$\pi_y^{//z}$	$=$	$-\pi_y^{//z}$
${}^{\perp y}\sigma_h$	$\pi_y^{//z}$	$=$	$\pi_{-y}^{//z}$
${}^{\perp x}\sigma_h$	$\pi_y^{//z}$	$=$	$\pi_y^{//z}$
${}^{z}\sigma_d^{\perp xy}$	$\pi_y^{//z}$	$=$	$\pi_x^{//z}$
${}^{z}\sigma_d^{\perp x(-y)}$	$\pi_y^{//z}$	$=$	$\pi_{-x}^{//z}$
${}^{x}\sigma_d^{\perp yz}$	$\pi_y^{//z}$	$=$	$\pi_z^{//y}$
${}^{x}\sigma_d^{\perp (-y)z}$	$\pi_y^{//z}$	$=$	$-\pi_{-z}^{//y}$
${}^{y}\sigma_d^{\perp xz}$	$\pi_y^{//z}$	$=$	$\pi_y^{//x}$
${}^{y}\sigma_d^{\perp (-x)z}$	$\pi_y^{//z}$	$=$	$-\pi_y^{//x}$

Matrizes para a Repres. Irred. E_g
do grupo O_h

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

$$C_3 = \begin{bmatrix} -½ & \\ & -½ \end{bmatrix}$$

$$^{xy}C_2^{\perp z} = {}^{x(-y)}C_2^{\perp z} = \begin{bmatrix} 1 & \\ & -1 \end{bmatrix}$$

$$^{xz}C_2^{\perp y} = {}^{x(-z)}C_2^{\perp y} = {}^{yz}C_2^{\perp x} = {}^{y(-z)}C_2^{\perp x} = \begin{bmatrix} -½ & \\ & ½ \end{bmatrix}$$

$$^{z}C_4 = {}^{z}C_4^3 = \begin{bmatrix} 1 & \\ & -1 \end{bmatrix}$$

$$^{x}C_4 = {}^{x}C_4^3 = {}^{y}C_4 = {}^{y}C_4^3 = \begin{bmatrix} -½ & \\ & ½ \end{bmatrix}$$

$$^{z}C_2(=C_4^2) = {}^{x}C_2(=C_4^2) = {}^{y}C_2(=C_4^2) = \begin{bmatrix} 1 & \\ & 1 \end{bmatrix}$$

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

$$^{z}S_4 = {}^{z}S_4^3 = \begin{bmatrix} 1 & \\ & -1 \end{bmatrix}$$

$$^{x}S_4 = {}^{x}S_4^3 = {}^{y}S_4 = {}^{y}S_4^3 = \begin{bmatrix} -½ & \\ & ½ \end{bmatrix}$$

$$S_6 = \begin{bmatrix} -½ & \\ & -½ \end{bmatrix}$$

$$^{\perp z}\sigma_h = {}^{\perp y}\sigma_h = {}^{\perp x}\sigma_h = \begin{bmatrix} 1 & \\ & 1 \end{bmatrix}$$

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

$$^{x}\sigma_d^{\perp yz} = {}^{x}\sigma_d^{\perp(-y)z} = {}^{y}\sigma_d^{\perp xz} = {}^{y}\sigma_d^{\perp(-x)z} = \begin{bmatrix} -½ & \\ & ½ \end{bmatrix}$$

Matrizes para a Repres. Irred. T_{1u}
do grupo O_h

Base utilizada: p_x, p_y, p_z

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

$$C_3 = \begin{bmatrix} 0 & & \\ & 0 & \\ & & 0 \end{bmatrix}$$

$$^{xy}C_2^{\perp z} = {}^{x(-y)}C_2^{\perp z} = \begin{bmatrix} 0 & & \\ & 0 & \\ & & -1 \end{bmatrix}$$

$$^{yz}C_2^{\perp x} = {}^{(-y)z}C_2^{\perp x} = \begin{bmatrix} -1 & & \\ & 0 & \\ & & 0 \end{bmatrix}$$

$$^{xz}C_2^{\perp y} = {}^{(-x)z}C_2^{\perp y} = \begin{bmatrix} 0 & & \\ & -1 & \\ & & 0 \end{bmatrix}$$

$$^{z}C_4 = {}^{z}C_4^3 = \begin{bmatrix} 0 & & \\ & 0 & \\ & & 1 \end{bmatrix}$$

$$^{x}C_4 = {}^{x}C_4^3 = \begin{bmatrix} 1 & & \\ & 0 & \\ & & 0 \end{bmatrix}$$

$$^{y}C_4 = {}^{y}C_4^3 = \begin{bmatrix} 0 & & \\ & 1 & \\ & & 0 \end{bmatrix}$$

$$^{z}C_2(=C_4^2) = \begin{bmatrix} -1 & & \\ & -1 & \\ & & 1 \end{bmatrix}$$

$$^{x}C_2(=C_4^2) = \begin{bmatrix} 1 & & \\ & -1 & \\ & & -1 \end{bmatrix}$$

$$^{y}C_2(=C_4^2) = \begin{bmatrix} -1 & & \\ & 1 & \\ & & -1 \end{bmatrix}$$

$$i = \begin{bmatrix} -1 & & \\ & -1 & \\ & & -1 \end{bmatrix}$$

$$^{z}S_4 = {}^{z}S_4^3 = \begin{bmatrix} 0 & & \\ & 0 & \\ & & -1 \end{bmatrix}$$

$$^{x}S_4 = {}^{x}S_4^3 = \begin{bmatrix} -1 & & \\ & 0 & \\ & & 0 \end{bmatrix}$$

$$^{y}S_4 = {}^{y}S_4^3 = \begin{bmatrix} 0 & & \\ & -1 & \\ & & 0 \end{bmatrix}$$

$$S_6 = \begin{bmatrix} 0 & & \\ & 0 & \\ & & 0 \end{bmatrix}$$

Matrizes para a Repres. Irred. T_{1u}
do grupo O_h (continuação)

$$^{\perp z}\sigma_h = \begin{bmatrix} 1 & & \\ & 1 & \\ & & -1 \end{bmatrix}$$

$$^{\perp y}\sigma_h = \begin{bmatrix} 1 & & \\ & -1 & \\ & & 1 \end{bmatrix}$$

$$^{\perp x}\sigma_h = \begin{bmatrix} -1 & & \\ & 1 & \\ & & 1 \end{bmatrix}$$

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

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

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

Matrizes para a Repres. Irred. T_{2g} do grupo O_h (base utilizada: orbitais d_{xy} d_{xz}, d_{yz})

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

$$^{xyz}C_3 = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$$

$$^{xyz}C_3^2 = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

$$^{x(-y)z}C_3 = \begin{bmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{bmatrix}$$

$$^{x(-y)z}C_3^2 = \begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{bmatrix}$$

$$^{(-x)(-y)z}C_3 = \begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{bmatrix}$$

$$^{(-x)(-y)z}C_3^2 = \begin{bmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

$$^{(-x)yz}C_3 = \begin{bmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{bmatrix}$$

$$^{(-x)yz}C_3^2 = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{bmatrix}$$

$$^{xy}C_2^{\perp z} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix}$$

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

$$^{yz}C_2^{\perp x} = \begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

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

$$^{xz}C_2^{\perp y} = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix}$$

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

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

$$^{z}C_4^3 = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}$$

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

Matrizes para a Repres. Irred. T_{2g}
do grupo O_h (continuação)

$$^{y}C_4^3 = \begin{bmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$

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

$$^{x}C_4^3 = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$^{z}C_2\,(=C_4^2) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$^{y}C_2\,(=C_4^2) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$^{x}C_2\,(=C_4^2) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

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

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

$$^{z}S_4^3 = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}$$

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

$$^{y}S_4^3 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{bmatrix}$$

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

$$^{x}S_4^3 = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$^{xyz}S_6 = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

$$^{xyz}S_6^5 = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$$

$$^{x(-y)z}S_6 = \begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{bmatrix}$$

$$^{x(-y)z}S_6^5 = \begin{bmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{bmatrix}$$

$$^{(-x)(-y)z}S_6 = \begin{bmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

Matrizes para a Repres. Irred. T_{2g}

do grupo O_h (continuação)

$$^{(-x)(-y)z}S_6^5 = \begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{bmatrix}$$

$$^{(-x)yz}S_6 = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{bmatrix}$$

$$^{(-x)yz}S_6^5 = \begin{bmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{bmatrix}$$

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

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

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

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

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

$$^{y}\sigma_d^{\perp xz} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$

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

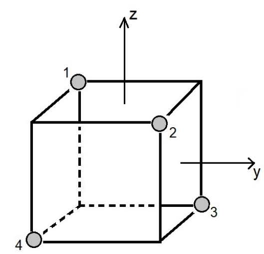
$$^{x}\sigma_d^{\perp yz} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

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

MÉTODO DO OPERADOR PROJEÇÃO

Simetria Tetraédrica

Resultado das 24 operações de simetria aplicadas sobre um orbital σ:



$E\ \sigma_1 = \sigma_1$

${}^{(1)}C_3\ \sigma_1 = \sigma_1$

${}^{(1)}C_3^{\,2}\ \sigma_1 = \sigma_1$

${}^{(2)}C_3\ \sigma_1 = \sigma_4$

${}^{(2)}C_3^{\,2}\ \sigma_1 = \sigma_3$

${}^{(3)}C_3\ \sigma_1 = \sigma_2$

${}^{(3)}C_3^{\,2}\ \sigma_1 = \sigma_4$

${}^{(4)}C_3\ \sigma_1 = \sigma_3$

${}^{(4)}C_3^{\,2}\ \sigma_1 = \sigma_2$

${}^{x}C_2\ \sigma_1 = \sigma_3$

${}^{y}C_2\ \sigma_1 = \sigma_4$

${}^{z}C_2\ \sigma_1 = \sigma_2$

${}^{x}S_4\ \sigma_1 = \sigma_4$

${}^{x}S_4^{\,3}\ \sigma_1 = \sigma_2$

${}^{y}S_4\ \sigma_1 = \sigma_2$

${}^{y}S_4^{\,3}\ \sigma_1 = \sigma_3$

${}^{z}S_4\ \sigma_1 = \sigma_4$

${}^{z}S_4^{\,3}\ \sigma_1 = \sigma_3$

${}^{z12}\sigma_d\ \sigma_1 = \sigma_1$

${}^{z34}\sigma_d\ \sigma_1 = \sigma_2$

${}^{x23}\sigma_d\ \sigma_1 = \sigma_4$

${}^{x14}\sigma_d\ \sigma_1 = \sigma_1$

${}^{y24}\sigma_d\ \sigma_1 = \sigma_3$

${}^{y13}\sigma_d\ \sigma_1 = \sigma_1$

Matrizes para a Repres. Irred. T_2 no grupo T_d. Base utilizada: orbitais d_{xy}, d_{xz}, d_{yz}

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

$$C_3 = \begin{bmatrix} 0 & & \\ & 0 & \\ & & 0 \end{bmatrix}$$

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

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

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

$$^{z}S_4 = {}^{z}S_4^3 = \begin{bmatrix} -1 & & \\ & 0 & \\ & & 0 \end{bmatrix}$$

$$^{y}S_4 = {}^{y}S_4^3 = \begin{bmatrix} 0 & & \\ & -1 & \\ & & 0 \end{bmatrix}$$

$$^{x}S_4 = {}^{x}S_4^3 = \begin{bmatrix} 0 & & \\ & 0 & \\ & & -1 \end{bmatrix}$$

$$^{x\text{-}24}\sigma_d = {}^{x\text{-}13}\sigma_d = \begin{bmatrix} 0 & & \\ & 0 & \\ & & 1 \end{bmatrix}$$

$$^{y\text{-}23}\sigma_d = {}^{y\text{-}14}\sigma_d = \begin{bmatrix} 0 & & \\ & 1 & \\ & & 0 \end{bmatrix}$$

$$^{z\text{-}12}\sigma_d = {}^{z\text{-}34}\sigma_d = \begin{bmatrix} 1 & & \\ & 0 & \\ & & 0 \end{bmatrix}$$

Matrizes para a Repres. Irred. T_1 no grupo T_d. base utilizada: orbitais $f(x(z^2-y^2))$, $f(y(z^2-x^2))$, $f(z(x^2-y^2))$

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

$$C_3 = \begin{bmatrix} 0 & & \\ & 0 & \\ & & 0 \end{bmatrix}$$

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

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

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

$$^{z}S_4 = {}^{z}S_4^3 = \begin{bmatrix} 0 & & \\ & 0 & \\ & & 1 \end{bmatrix}$$

$$^{y}S_4 = {}^{y}S_4^3 = \begin{bmatrix} 0 & & \\ & 1 & \\ & & 0 \end{bmatrix}$$

$$^{x}S_4 = {}^{x}S_4^3 = \begin{bmatrix} 1 & & \\ & 0 & \\ & & 0 \end{bmatrix}$$

$$^{z\text{-}12}\sigma_d = {}^{z\text{-}34}\sigma_d = \begin{bmatrix} 0 & & \\ & 0 & \\ & & -1 \end{bmatrix}$$

$$^{y13}\sigma_d = {}^{y24}\sigma_d = \begin{bmatrix} 0 & & \\ & -1 & \\ & & 0 \end{bmatrix}$$

$$^{x14}\sigma_d = {}^{x23}\sigma_d = \begin{bmatrix} -1 & & \\ & 0 & \\ & & 0 \end{bmatrix}$$

Grupo D_{3h}

Representação Irredutível E’

Base: orbitais p_x e p_y

Orientação: um dos planos verticais é o xz e os outros dois a 120° deste.

Rotações: sentido anti-horário, ou seja, sentido trigonométrico.

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

$$C_3 = S_3 = \begin{bmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{bmatrix}$$

$$C_3^2 = S_3^5 = \begin{bmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{bmatrix}$$

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

$$^{(\bar{x}y)}C_2 = {}^{(\bar{x}y)}\sigma_v = \begin{bmatrix} -1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & 1/2 \end{bmatrix}$$

$$^{(\overline{xy})}C_2 = {}^{(\overline{xy})}\sigma_v = \begin{bmatrix} -1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & 1/2 \end{bmatrix}$$

-Grupo D_{3h}

Representação Irredutível E″

Base: orbitais d_{xz} e d_{yz}

Orientação: um dos planos verticais é o xz e os outros dois a 120° deste.

Rotações: sentido anti-horário, ou seja, sentido trigonométrico.

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

$$C_3 = \begin{bmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{bmatrix}$$

$$C_3^2 = \begin{bmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{bmatrix}$$

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

$$^{(\bar{x}y)}C_2 = \begin{bmatrix} 1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{bmatrix}$$

$$^{(\overline{xy})}C_2 = \begin{bmatrix} 1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{bmatrix}$$

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

$$S_3 = \begin{bmatrix} 1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & 1/2 \end{bmatrix}$$

$$S_3^5 = \begin{bmatrix} 1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & 1/2 \end{bmatrix}$$

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

$$^{(\bar{x}y)}\sigma = \begin{bmatrix} -1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & 1/2 \end{bmatrix}$$

$$^{(\overline{xy})}\sigma = \begin{bmatrix} -1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & 1/2 \end{bmatrix}$$

Grupo C_{3v}

Representação Irredutível E

Base: orbitais p_x e p_y

Orientação: um dos planos verticais é o xz e os outros dois a 120° deste.

Rotações: sentido anti-horário, ou seja, sentido trigonométrico.

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

$$C_3 = \begin{bmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{bmatrix}$$

$$C_3^2 = \begin{bmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{bmatrix}$$

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

$$^{(\bar{x}y)}\sigma_v = \begin{bmatrix} -1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & 1/2 \end{bmatrix}$$

$$^{(\overline{xy})}\sigma_v = \begin{bmatrix} -1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & 1/2 \end{bmatrix}$$

Grupo D_{4h}

Representação Irredutível E_u

Base: orbitais p_x e p_y

Rotações: sentido anti-horário, ou seja, sentido trigonométrico.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Grupo D_{4h}

Representação Irredutível E_g

Base: orbitais d_{xz} e d_{yz}

Rotações: sentido anti-horário, ou seja, sentido trigonométrico.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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