ORBITAIS ATÔMICOS

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$$\psi_{n,l,m_l}(r,\theta,\varphi) = R_{n,l}(r)\ \Theta_{l,m_l}(\theta)\ \Phi_{m_l}(\varphi) = R(r)Y^l_{m_l}(\theta,\varphi)$$

$$\Gamma = \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} \quad \sigma = \frac{Zr}{a_0} \quad \rho = \frac{2Z}{na_0}$$

$$\sigma = \frac{n\rho r}{2}; \quad \rho r = \frac{2\sigma}{n}; \quad \frac{\rho r}{2} = \frac{\sigma}{n}; \quad \rho = \frac{2\sigma}{nr}; \quad \rho^2 r^2 = \frac{4\sigma^2}{n^2}$$

$$\hbar = \frac{h}{2\pi}$$

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2} = \frac{\varepsilon_0 h^2}{me^2\pi} = 0,529\ \text{Å} = 0,529\times 10^{-10}\ m$$

Harmônicos esféricos $Y^l_{m_l}(\theta,\varphi) = \Theta_{l,m_l}(\theta)\ \Phi_{m_l}(\varphi)$

$x = r \operatorname{sen}\theta \cos\varphi$ $\qquad$ $\operatorname{sen}\theta\cos\varphi = x/r$

$y = r \operatorname{sen}\theta \operatorname{sen}\varphi$ $\qquad$ $\operatorname{sen}\theta\operatorname{sen}\varphi = y/r$

$z = r\cos\theta$ $\qquad$ $\cos\theta = z/r$

$$r^2 = x^2 + y^2 + z^2$$

$$d\tau = r^2 \operatorname{sen}\theta\, dr\, d\theta\, d\varphi$$

$$0 \le \theta \le \pi$$

$$0 \le \varphi \le 2\pi$$

Números complexos

$z = x + iy = r(\cos\theta + i \operatorname{sen}\theta)$

$e^z = e^{x + iy} = e^x e^{iy}$

$e^{iy} = \cos y + i \operatorname{sen} y$

$e^{-iy} = \cos y - i \operatorname{sen} y$

$e^{-iy} + e^{iy} = \cos y - i \operatorname{sen} y + \cos y + i \operatorname{sen} y = 2\cos y$

$e^{-iy} - e^{iy} = \cos y - i \operatorname{sen} y - \cos y - i \operatorname{sen} y = -2i \operatorname{sen} y$

Orbitais s

A parte angular é a mesma para todos os orbitais s, correspondendo a $l = 0$ e $m_l = 0$.

$$\Theta_{0,0} = \frac{1}{\sqrt{2}} \qquad \Phi_0 = \frac{1}{\sqrt{2\pi}} \qquad Y_0^0 = \Theta_{0,0}\Phi_0 = \frac{1}{2\sqrt{\pi}}$$

Orbital 1s ($n = 1$, $l = 0$, $m_l = 0$)

$$R_{1,0} = 2\,\Gamma\, e^{-\frac{Zr}{a_0}} = 2\,\Gamma\, e^{-\sigma} = 2\,\Gamma\, e^{-\frac{\rho r}{2}}$$

$$\psi_{1s} = \psi_{1,0,0} = R_{1,0}\,\Theta_{0,0}\,\Phi_0 = R_{1,0}\,Y_0^0$$

$$\psi_{1s} = \frac{1}{\sqrt{\pi}}\,\Gamma\, e^{-\frac{Zr}{a_0}} = \frac{1}{\sqrt{\pi}}\,\Gamma\, e^{-\sigma} = \frac{1}{\sqrt{\pi}}\,\Gamma\, e^{-\frac{\rho r}{2}}$$

Orbital 2s ($n = 2$, $l = 0$, $m_l = 0$)

$$R_{2,0} = \frac{1}{2\sqrt{2}}\,\Gamma\left(2-\frac{Zr}{a_0}\right) e^{-\frac{Zr}{2a_0}} = \frac{1}{2\sqrt{2}}\,\Gamma(2-\sigma)\, e^{-\frac{\sigma}{2}} = \frac{1}{2\sqrt{2}}\,\Gamma(2-\rho r)\, e^{-\frac{\rho r}{2}}$$

$$\psi_{2s} = \psi_{2,0,0} = R_{2,0}\,\Theta_{0,0}\,\Phi_0 = R_{2,0}\,Y_0^0$$

$$\psi_{2s} = \frac{1}{4\sqrt{2\pi}}\,\Gamma\left(2-\frac{Zr}{a_0}\right) e^{-\frac{Zr}{2a_0}} = \frac{1}{4\sqrt{2\pi}}\,\Gamma(2-\sigma)\, e^{-\frac{\sigma}{2}} = \frac{1}{4\sqrt{2\pi}}\,\Gamma(2-\rho r)\, e^{-\frac{\rho r}{2}}$$

0rbital 3s (n = 3, l = 0, m_l = 0)

$$R_{3,0} = \frac{2}{81\sqrt{3}}\,\Gamma\left(27 - 18\frac{Zr}{a_0} + 2\left(\frac{Zr}{a_0}\right)^2\right)e^{-\frac{\sigma}{3}}$$

$$R_{3,0} = \frac{2}{81\sqrt{3}}\,\Gamma(27 - 18\sigma + 2\sigma^2)\,e^{-\frac{\sigma}{3}} = \frac{1}{9\sqrt{3}}\,\Gamma(6 - 6\rho r + \rho^2 r^2)\,e^{-\frac{\rho r}{2}}$$

$$\psi_{3s} = \psi_{3,0,0} = R_{3,0}\,\Theta_{0,0}\,\Phi_0 = R_{3,0}\,Y_0^0$$

$$\psi_{3s} = \frac{1}{81\sqrt{3\pi}}\,\Gamma\left(27 - 18\frac{Zr}{a_0} + 2\left(\frac{Zr}{a_0}\right)^2\right)e^{-\frac{Zr}{3a_0}}$$

$$\psi_{3s} = \frac{1}{81\sqrt{3\pi}}\,\Gamma(27 - 18\sigma + 2\sigma^2)\,e^{-\frac{\sigma}{3}}$$

$$\psi_{3s} = \frac{1}{18\sqrt{3\pi}}\,\Gamma(6 - 6\rho r + \rho^2 r^2)\,e^{-\frac{\rho r}{2}}$$

Orbitais p_z

A parte angular é a mesma para todos os orbitais p_z, correspondendo a l = 1 e m_l = 0.

$$\Theta_{1,0} = \frac{\sqrt{6}}{2}\cos\theta \qquad \Phi_0 = \frac{1}{\sqrt{2\pi}} \qquad Y_0^1 = \Theta_{1,0}\Phi_0 = \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta$$

Parte angular em coordenadas cartesianas:

$$\Theta_{1,0} = \frac{\sqrt{6}}{2}\frac{z}{r} \qquad \Phi_0 = \frac{1}{\sqrt{2\pi}} \qquad Y_0^1 = \Theta_{1,0}\Phi_0 = \frac{1}{2}\sqrt{\frac{3}{\pi}}\frac{z}{r}$$

Orbital $2p_z$ (*n* = 2, *l* = 1, m_l = 0)

$$R_{2,1} = \frac{1}{2\sqrt{6}}\Gamma\sigma e^{-\frac{\sigma}{2}} \qquad \Theta_{1,0} = \frac{\sqrt{6}}{2}\cos\theta \qquad \Phi_0 = \frac{1}{\sqrt{2\pi}}$$

$$\psi_{2p_z} = \psi_{2,1,0} = \frac{1}{4\sqrt{2\pi}}\Gamma\sigma e^{-\frac{\sigma}{2}}\cos\theta$$

Em coordenadas cartesianas

$$\psi_{2p_z} = \psi_{2,1,0} = \frac{1}{4\sqrt{2\pi}}\Gamma\sigma e^{-\frac{\sigma}{2}}\frac{z}{r}$$

Orbital $3p_z$ (*n* = 3, *l* = 1, m_l = 0)

$$R_{3,1} = \frac{2\sqrt{2}}{81\sqrt{3}}\Gamma(6-\sigma)\sigma e^{-\frac{\sigma}{3}} \qquad \Theta_{1,0} = \frac{\sqrt{6}}{2}\cos\theta \qquad \Phi_0 = \frac{1}{\sqrt{2\pi}}$$

$$\psi_{3p_z} = \psi_{3,1,0} = \frac{\sqrt{2}}{81\sqrt{\pi}}\Gamma(6-\sigma)\sigma e^{-\frac{\sigma}{3}}\cos\theta$$

Em coordenadas cartesianas

$$\psi_{3p_z} = \psi_{3,1,0} = \frac{\sqrt{2}}{81\sqrt{\pi}}\Gamma(6-\sigma)\sigma e^{-\frac{\sigma}{3}}\frac{z}{r}$$

Orbitais p com $m_l \neq 0$ (orbitais 2p complexos)

PARTE ANGULAR

***l* = 1, *m*$_l$ = 1**

$$\Theta_{1,1} = -\frac{\sqrt{3}}{2}\ \mathrm{sen}\,\theta \qquad \Phi_1 = \frac{1}{\sqrt{2\pi}}\, e^{i\varphi}$$

$$Y_1^1 = \Theta_{1,1}\Phi_1 = -\sqrt{\frac{3}{8\pi}}\ sen\theta\ e^{i\varphi} = -\sqrt{\frac{3}{8\pi}}\ (sen\theta\cos\varphi + i sen\theta\ sen\varphi)$$

$$Y_1^1 = -\sqrt{\frac{3}{8\pi}}\left(\frac{x + iy}{r}\right)$$

***l* = 1, *m*$_l$ = -1**

$$\Theta_{1,-1} = \frac{\sqrt{3}}{2}\ \mathrm{sen}\,\theta \qquad \Phi_{-1} = \frac{1}{\sqrt{2\pi}}\, e^{-i\varphi}$$

$$Y_{-1}^1 = \Theta_{1,-1}\Phi_{-1} = \sqrt{\frac{3}{8\pi}}\ \mathrm{sen}\theta\ e^{-i\varphi} = \sqrt{\frac{3}{8\pi}}\ (\mathrm{sen}\theta\cos\varphi - i\mathrm{sen}\theta\ \mathrm{sen}\varphi)$$

$$Y_{-1}^1 = \sqrt{\frac{3}{8\pi}}\left(\frac{x - iy}{r}\right)$$

Os harmônicos esféricos para $m_l \neq 0$ podem ser combinados, obtendo-se as funções reais, P_x e P_y.

$$P_x = \frac{1}{\sqrt{2}}(Y_{-1}^1 - Y_1^1) = \sqrt{\frac{3}{4\pi}}\frac{x}{r} = \sqrt{\frac{3}{4\pi}}\ \mathrm{sen}\,\theta\ \cos\varphi$$

$$P_y = \frac{i}{\sqrt{2}}(Y_{-1}^1 + Y_1^1) = \sqrt{\frac{3}{4\pi}}\frac{y}{r} = \sqrt{\frac{3}{4\pi}}\ \mathrm{sen}\,\theta\ \mathrm{sen}\varphi$$

Orbitais $2p_x$ e $2p_y$

$$R_{2,1} = \frac{1}{2\sqrt{6}}\,\Gamma\,\sigma\,e^{-\frac{\sigma}{2}}$$

$$\psi_{2p_x} = R_{2,1}P_x = \frac{1}{4\sqrt{2\pi}}\,\Gamma\,\sigma\,e^{-\frac{\sigma}{2}}\,\frac{x}{r} = \frac{1}{4\sqrt{2\pi}}\,\Gamma\,\sigma\,e^{-\frac{\sigma}{2}}\,\mathrm{sen}\theta\,\cos\varphi$$

$$\psi_{2p_y} = R_{2,1}P_y = \frac{1}{4\sqrt{2\pi}}\,\Gamma\,\sigma\,e^{-\frac{\sigma}{2}}\,\frac{y}{r} = \frac{1}{4\sqrt{2\pi}}\,\Gamma\,\sigma\,e^{-\frac{\sigma}{2}}\,\mathrm{sen}\theta\,\mathrm{sen}\varphi$$

Orbitais $3p_x$ e $3p_y$

$$R_{3,1} = \frac{2\sqrt{2}}{81\sqrt{3}}\,\Gamma\,(6 - \sigma)\,\sigma\,e^{-\frac{\sigma}{3}}$$

$$\psi_{3p_x} = R_{3,1}P_x = \frac{\sqrt{2}}{81\sqrt{\pi}}\,\Gamma\,\sigma\,e^{-\frac{\sigma}{2}}\,\frac{x}{r} = \frac{\sqrt{2}}{81\sqrt{\pi}}\,\Gamma\,\sigma\,e^{-\frac{\sigma}{2}}\,\mathrm{sen}\theta\,\cos\varphi$$

$$\psi_{3p_y} = R_{3,1}P_y = \frac{\sqrt{2}}{81\sqrt{\pi}}\,\Gamma\,\sigma\,e^{-\frac{\sigma}{2}}\,\frac{y}{r} = \frac{\sqrt{2}}{81\sqrt{\pi}}\,\Gamma\,\sigma\,e^{-\frac{\sigma}{2}}\,\mathrm{sen}\theta\,\mathrm{sen}\varphi$$

Orbitais d (m_l = 0)

A parte angular é a mesma para todos os orbitais d(z^2), na verdade, d($2z^2 - x^2 - y^2$), correspondendo a l = 2 e m_l = 0.

$$\Theta_{2,0} = \frac{1}{2}\sqrt{\frac{5}{2}}\,(3\cos^2\theta - 1) \qquad \Phi_0 = \frac{1}{\sqrt{2\pi}}$$

$$Y_0^2 = \Theta_{2,0}\Phi_0 = \frac{1}{4}\sqrt{\frac{5}{\pi}}(3\cos^2\theta - 1) = \frac{1}{4}\sqrt{\frac{5}{\pi}}\,\frac{(2z^2 - x^2 - y^2)}{r^2}$$

Orbital 3d(z^2) (n = 3, l = 2, m_l = 0)

$$R_{3,2} = \frac{2\sqrt{2}}{81\sqrt{15}}\Gamma\left(\frac{Z}{a_0}\right)^2 r^2 e^{-\frac{Zr}{3a_0}} = \frac{2\sqrt{2}}{81\sqrt{15}}\Gamma\sigma^2 e^{-\frac{\sigma}{3}} = \frac{1}{9\sqrt{30}}\Gamma\rho^2 r^2 e^{-\frac{\rho r}{2}}$$

$$\psi_{3d_{z^2}} = \psi_{3,2,0} = R_{3,2}\Theta_{2,0}\Phi_0 = R_{3,2}Y_0^2$$

$$\psi_{3d_{z^2}} = \frac{1}{81\sqrt{6\pi}}\,\frac{Z}{a_0}\Gamma^2 r^2 e^{-\frac{Zr}{3a_0}}(3\cos^2\theta - 1)$$

$$\psi_{3d_{z^2}} = \frac{1}{81\sqrt{6\pi}}\,\Gamma\sigma^2 e^{-\frac{\sigma}{3}}(3\cos^2\theta - 1)$$

$$\psi_{3d_{z^2}} = \frac{1}{36\sqrt{3\pi}}\,\Gamma\rho^2 r^2\, e^{-\frac{\rho r}{2}}(3\cos^2\theta - 1)$$

Em coordenadas cartesianas

$$\psi_{3d_{z^2}} = \frac{1}{81\sqrt{6\pi}}\,\frac{Z}{a_0}\Gamma^2 r^2 e^{-\frac{Zr}{3a_0}}\left(\frac{2z^2 - x^2 - y^2}{r^2}\right)$$

$$\psi_{3d_{z^2}} = \frac{1}{81\sqrt{6\pi}}\,\Gamma\sigma^2 e^{-\frac{\sigma}{3}}\left(\frac{2z^2 - x^2 - y^2}{r^2}\right)$$

$$\psi_{3d_{z^2}} = \frac{1}{36\sqrt{3\pi}}\,\Gamma\rho^2 r^2\, e^{-\frac{\rho r}{2}}\left(\frac{2z^2 - x^2 - y^2}{r^2}\right)$$

Orbital 4d(z²) (n = 4, l = 2, m_l = 0)

$$R_{4,2} = \frac{1}{384\sqrt{5}} \Gamma\left(6 - \frac{\sigma}{2}\right) \sigma^2 e^{-\frac{\sigma}{4}} \qquad \Theta_{2,0} = \frac{1}{2}\sqrt{\frac{5}{2}}\,(3\cos^2\theta - 1) \qquad \Phi_0 = \frac{1}{\sqrt{2\pi}}$$

$$\psi_{3d_{z^2}} = \psi_{3,2,0} = \frac{1}{81\sqrt{6\pi}}\,\Gamma(6 - \sigma)\sigma\, e^{-\frac{\sigma}{3}}\,(3\cos^2\theta - 1)$$

Em coordenadas cartesianas

$$R_{42} = \frac{1}{384\sqrt{5}}\left[\frac{Z}{a_0}\right]^{\frac{3}{2}}\left(6 - \frac{\sigma}{2}\right) \sigma^2 e^{-\frac{\sigma}{4}} \qquad Y_0^2 = \Theta\Phi = \frac{1}{4}\sqrt{\frac{5}{\pi}}\,\frac{(2z^2 - x^2 - y^2)}{r^2}$$

Orbitais d com $m_l \neq \pm 1$ (orbitais d complexos)

$n = 3$, $l = 2$, $m_l = 1$

$$R_{32} = \frac{1}{81\sqrt{15}}\left[\frac{2Z}{a_0}\right]^{\frac{3}{2}} \sigma^2 e^{-\frac{\sigma}{3}}$$

$$\Theta = \frac{\sqrt{15}}{2}\cos\theta \, \mathrm{sen}\,\theta \qquad \Phi = \frac{1}{\sqrt{2\pi}} e^{i\varphi}$$

$$Y_1^2 = \sqrt{\frac{15}{8\pi}} \cos\theta \, sen\theta \; e^{i\varphi} = \sqrt{\frac{15}{8\pi}} \left(\cos\theta \, sen\theta \cos\varphi + i\cos\theta \, sen\theta \, sen\varphi\right)$$

$$Y_1^2 = \sqrt{\frac{15}{8\pi}} \, \frac{z(x + iy)}{r^2}$$

n = 3, $l = 2$, $m_l = -1$

$$R_{32} = \frac{1}{81\sqrt{15}}\left[\frac{2Z}{a_0}\right]^{\frac{3}{2}} \sigma^2 e^{-\frac{\sigma}{3}}$$

$$\Theta = \frac{\sqrt{15}}{2}\cos\theta \, \mathrm{sen}\,\theta \qquad \Phi = \frac{1}{\sqrt{2\pi}} e^{-i\varphi}$$

$$Y_{-1}^2 = \sqrt{\frac{15}{8\pi}} \cos\theta \, sen\theta \; e^{i\varphi} = \sqrt{\frac{15}{8\pi}} \left(\cos\theta \, sen\theta \cos\varphi - i\cos\theta \, sen\theta \, sen\varphi\right)$$

$$Y_{-1}^2 = \sqrt{\frac{15}{8\pi}} \, \frac{z(x - iy)}{r^2}$$

Funções reais dos orbitais *d* em coordenadas polares

para m_l = 1 e -1

A parte radial é a mesma para todos os orbitais 3*d*.

$$R_{32} = \frac{1}{81\sqrt{15}}\left[\frac{2Z}{a_0}\right]^{\frac{3}{2}} \sigma^2 e^{-\frac{\sigma}{3}}$$

$$\frac{1}{\sqrt{2}}(Y_{-1}^2 + Y_1^2) = \frac{1}{2}\sqrt{\frac{15}{\pi}}\cos\theta \ \mathrm{sen}\theta \ \cos\varphi$$

$$\frac{i}{\sqrt{2}}(Y_{-1}^2 - Y_1^2) = \frac{1}{2}\sqrt{\frac{15}{\pi}}\cos\theta \ \mathrm{sen}\theta \ \mathrm{sen}\varphi$$

Funções reais dos orbitais *d* em coordenadas cartesianas

para m_l = 1 e -1

A parte radial é a mesma para todos os orbitais 3*d*.

$$R_{32} = \frac{1}{81\sqrt{15}}\left[\frac{2Z}{a_0}\right]^{\frac{3}{2}} \sigma^2 e^{-\frac{\sigma}{3}}$$

$$\frac{1}{\sqrt{2}}(Y_{-1}^2 + Y_1^2) = \frac{1}{2}\sqrt{\frac{15}{\pi}}\ \frac{xz}{r^2}$$

$$\frac{i}{\sqrt{2}}(Y_{-1}^2 - Y_1^2) = \frac{1}{2}\sqrt{\frac{15}{\pi}}\ \frac{yz}{r^2}$$

Orbitais d com $m_l \neq \pm 2$ (orbitais d complexos)

$n = 3, l = 2, m_l = 2$

$$R = \frac{1}{81\sqrt{15}}\left[\frac{2Z}{a_0}\right]^{\frac{3}{2}} \sigma^2 e^{-\frac{\sigma}{3}} \qquad \Theta = \frac{\sqrt{15}}{4} sen^2\theta \qquad \Phi = \frac{1}{\sqrt{2\pi}} e^{i2\varphi}$$

$$Y_2^2 = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\, sen^2\theta\; e^{i2\varphi} = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\, sen^2\theta\,(\cos 2\varphi + i\, sen 2\varphi)$$

$$Y_2^2 = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\, sen^2\theta(\cos^2\varphi - sen^2\varphi + i2sen\,\varphi\cos\varphi)$$

$$Y_1^2 = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\, \frac{(x + iy)^2}{r^2}$$

$n = 3, l = 2, m_l = -2$

$$R = \frac{1}{81\sqrt{15}}\left[\frac{2Z}{a_0}\right]^{\frac{3}{2}} \sigma^2 e^{-\frac{\sigma}{3}} \qquad \Theta = \frac{\sqrt{15}}{4} sen^2\theta \qquad \Phi = \frac{1}{\sqrt{2\pi}} e^{-i2\varphi}$$

$$Y_{-2}^2 = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\, sen^2\theta\; e^{-i2\varphi} = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\, sen^2\theta\,(\cos 2\varphi - i\, sen 2\varphi)$$

$$Y_{-2}^2 = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\, sen^2\theta(\cos^2\varphi - sen^2\varphi - i2sen\,\varphi\cos\varphi)$$

$$Y_{-2}^2 = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\, \frac{(x - iy)^2}{r^2}$$

Funções reais dos orbitais *d* em coordenadas polares

para m_l = 2 e -2

A parte radial é a mesma para todos os orbitais 3*d*.

$$R_{32} = \frac{1}{81\sqrt{15}}\left[\frac{2Z}{a_0}\right]^{\frac{3}{2}} \sigma^2 e^{-\frac{\sigma}{3}}$$

$$\frac{1}{\sqrt{2}}(Y_{-2}^2 + Y_2^2) = \frac{1}{4}\sqrt{\frac{15}{\pi}}\,\mathrm{sen}^2\theta\,(\cos^2\varphi - \mathrm{sen}^2\varphi) = \frac{1}{4}\sqrt{\frac{15}{\pi}}\,\mathrm{sen}^2\theta\,\cos 2\varphi$$

$$\frac{i}{\sqrt{2}}(Y_{-2}^2 - Y_2^2) = \frac{i}{4}\sqrt{\frac{15}{\pi}}\,\mathrm{sen}^2\theta\,(-i2\,\mathrm{sen}\varphi\cos\varphi) = \frac{1}{4}\sqrt{\frac{15}{\pi}}\,\mathrm{sen}^2\theta\,\mathrm{sen}2\varphi$$

Funções reais dos orbitais *d* em coordenadas cartesianas

para m_l = 2 e -2

A parte radial é a mesma para todos os orbitais 3*d*.

$$R_{32} = \frac{1}{81\sqrt{15}}\left[\frac{2Z}{a_0}\right]^{\frac{3}{2}} \sigma^2 e^{-\frac{\sigma}{3}}$$

$$\frac{1}{\sqrt{2}}(Y_{-2}^2 + Y_2^2) = \frac{1}{4}\sqrt{\frac{15}{\pi}}\,\frac{x^2 - Y^2}{r^2}$$

$$\frac{i}{\sqrt{2}}(Y_{-2}^2 - Y_2^2) = \frac{1}{2}\sqrt{\frac{15}{\pi}}\,\frac{xy}{r^2}$$

Orbitais f

Orbital 4f(z^3) (n = 4, l = 3, m_l = 0)

Na verdade, 4f($z(2z^2 - 3x^2 - 3y^2)$)

pois ($5\cos^3\theta - 3\cos\theta$) = $z(5z^2 - 3r^2)/r^3 = z(2z^2 - 3x^2 - 3y^2)/r^3$

$$R_{43} = \frac{1}{768\sqrt{35}}\left[\frac{Z}{a_0}\right]^{\frac{3}{2}} \sigma^3 e^{-\frac{\sigma}{4}}$$

$$\Theta = \frac{3\sqrt{14}}{4}\left(\frac{5}{3}\cos^3\theta - \cos\theta\right) \qquad \Phi = \frac{1}{\sqrt{2\pi}}$$

Parte angular em coordenadas cartesianas

$$Y_0^3 = \Theta\Phi = \frac{1}{4}\sqrt{\frac{7}{\pi}}\,\frac{z(2z^2 - 3x^2 - 3y^2)}{r^3}$$

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