Química cuántica I: orbitales hidrogenoides

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Las funciones de onda de átomos hidrogenoides son de la forma

$$\psi(r,\theta,\phi) = R_{nl}(r)\, Y_l^m(\theta,\phi)$$

donde

$$n = 1,2,3\ldots \qquad l = 0,1,2,\ldots,n-1 \qquad m = 0,\pm1,\pm2,\ldots,\pm l$$

Algunas funciones radiales:

$$R_{10} = 2(Z/a_0)^{3/2}\, e^{-\sigma} \qquad R_{30} = \frac{2(Z/a_0)^{3/2}}{9\sqrt{3}}\,(3 - 2\sigma + 2\sigma^2/9)\, e^{-\sigma/3}$$

$$R_{20} = \frac{(Z/a_0)^{3/2}}{2\sqrt{2}}\,(2-\sigma)\, e^{-\sigma/2} \qquad R_{31} = \frac{4(Z/a_0)^{3/2}}{27\sqrt{6}}\,(2-\sigma/3)\,\sigma\, e^{-\sigma/3}$$

$$R_{21} = \frac{(Z/a_0)^{3/2}}{2\sqrt{6}}\,\sigma\, e^{-\sigma/2} \qquad R_{32} = \frac{4(Z/a_0)^{3/2}}{81\sqrt{30}}\,\sigma^2\, e^{-\sigma/3}$$

donde

$$a_0 = \frac{\hbar^2}{m_e e^2} = 0.52918\text{Å} \qquad \sigma = \frac{Zr}{a_0}\,.$$

a_0 se llama el radio de Bohr.

Algunos armónicos esféricos son:

$$Y_0^0 = \left(\frac{1}{4\pi}\right)^{1/2} \qquad Y_2^0 = \left(\frac{5}{16\pi}\right)^{1/2}(3\cos^2\theta - 1)$$

$$Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2}\cos\theta \qquad Y_2^{\pm1} = \left(\frac{15}{8\pi}\right)^{1/2}\operatorname{sen}\theta\cos\theta\, e^{\pm i\phi}$$

$$Y_1^{\pm1} = \left(\frac{3}{8\pi}\right)^{1/2}\operatorname{sen}\theta\, e^{\pm i\phi} \qquad Y_2^{\pm2} = \left(\frac{15}{32\pi}\right)^{1/2}\operatorname{sen}^2\theta\, e^{\pm 2i\phi}$$

Además

$$\int_0^\infty [R_{nl}(r)]^2 r^2 dr = 1$$

$$\int_0^{2\pi}\int_0^{\pi} [Y_l^m(\theta,\phi)]^2 \operatorname{sen}\theta d\theta d\phi = 1$$

Los orbitales hidrogenoides son ortonormales:

$$\int_0^\infty\int_0^{2\pi}\int_0^{\pi} \psi_{nlm}(r,\theta,\phi)^*\, \psi_{n'l'm'}(r,\theta,\phi)\, r^2 \operatorname{sen}\theta\, d\theta\, d\phi\, dr = \delta_{n,n'}\delta_{l,l'}\delta_{m,m'}$$

Tabla 1. Orbitales hidrogenoides para $n = 1, 2, 3$. Además, $\sigma = Zr/a_0$, donde Z y a_0 son el número atómico y el radio de Bohr, respectivamente.

n	l	m	
1	0	0	$\psi_{100} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-\sigma}$
2	0	0	$\psi_{200} = \frac{1}{\sqrt{32\pi}}\left(\frac{Z}{a_0}\right)^{3/2} (2-\sigma)e^{-\sigma/2}$
	1	0	$\psi_{210} = \frac{1}{\sqrt{32\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2}\cos\theta$
	1	±1	$\psi_{21\pm1} = \frac{1}{\sqrt{64\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2}\operatorname{sen}\theta e^{\pm i\phi}$
3	0	0	$\psi_{300} = \frac{1}{81\sqrt{3\pi}}\left(\frac{Z}{a_0}\right)^{3/2} (27-18\sigma+2\sigma^2)e^{-\sigma/3}$
	1	0	$\psi_{310} = \frac{\sqrt{2}}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} (6\sigma-\sigma^2)e^{-\sigma/3}\cos\theta$
	1	±1	$\psi_{31\pm1} = \frac{1}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} (6\sigma-\sigma^2)e^{-\sigma/3}\operatorname{sen}\theta e^{\pm i\phi}$
	2	0	$\psi_{320} = \frac{1}{81\sqrt{6\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/3}(3\cos^2\theta-1)$
	2	±1	$\psi_{32\pm1} = \frac{1}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/3}\operatorname{sen}\theta\cos\theta e^{\pm i\phi}$
	2	±2	$\psi_{32\pm2} = \frac{1}{162\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/3}\operatorname{sen}^2\theta e^{\pm 2i\phi}$

Tabla 2. Orbitales hidrogenoides reales para $n = 1, 2, 3$.

n	l	m	
1	0	0	$\psi_{1s} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-\sigma}$
2	0	0	$\psi_{2s} = \frac{1}{\sqrt{32\pi}}\left(\frac{Z}{a_0}\right)^{3/2} (2-\sigma)e^{-\sigma/2}$
	1	0	$\psi_{2p_z} = \frac{1}{\sqrt{32\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2}\cos\theta$
	1	±1	$\psi_{2p_x} = \frac{1}{\sqrt{32\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2}\operatorname{sen}\theta\cos\phi$
			$\psi_{2p_y} = \frac{1}{\sqrt{32\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2}\operatorname{sen}\theta\sin\phi$
3	0	0	$\psi_{3s} = \frac{1}{81\sqrt{3\pi}}\left(\frac{Z}{a_0}\right)^{3/2} (27-18\sigma+2\sigma^2)e^{-\sigma/3}$
	1	0	$\psi_{3p_z} = \frac{\sqrt{2}}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} (6\sigma-\sigma^2)e^{-\sigma/3}\cos\theta$
	1	±1	$\psi_{3p_x} = \frac{\sqrt{2}}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} (6\sigma-\sigma^2)e^{-\sigma/3}\operatorname{sen}\theta\cos\phi$
			$\psi_{3p_y} = \frac{\sqrt{2}}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} (6\sigma-\sigma^2)e^{-\sigma/3}\operatorname{sen}\theta\operatorname{sen}\phi$
	2	0	$\psi_{3d_{z^2}} = \frac{1}{81\sqrt{6\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/3}(3\cos^2\theta-1)$
	2	±1	$\psi_{3d_{xz}} = \frac{\sqrt{2}}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/3}\operatorname{sen}\theta\cos\theta\cos\phi$
			$\psi_{3d_{yz}} = \frac{\sqrt{2}}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/3}\operatorname{sen}\theta\cos\theta\operatorname{sen}\phi$
	2	±2	$\psi_{3d_{x^2-y^2}} = \frac{1}{81\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/3}\operatorname{sen}^2\theta\cos 2\phi$
			$\psi_{3d_{xy}} = \frac{1}{81\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/3}\operatorname{sen}^2\theta\operatorname{sen} 2\phi$