

Funciones de onda del átomo de hidrógeno

$$\Psi_{n,l,m}(r, \theta, \phi) = R_{n,l}(r)\Theta_{l,m}(\theta)\Phi_m(\phi)$$

$$\Psi_{n,l,m}(r, \theta, \phi) = R_{n,l}(r)Y_{l,m}(\theta, \phi)$$

Tabla 1: Funciones radiales del átomo de hidrógeno

n	l	$R_{n,l}(r)$
1	0	$2 \left(\frac{Z}{a_0} \right)^{3/2} e^{-Zr/a_0}$
2	0	$\frac{1}{2\sqrt{2}} \left(\frac{Z}{a_0} \right)^{3/2} \left(2 - \frac{Zr}{a_0} \right) e^{-Zr/2a_0}$
2	1	$\frac{1}{2\sqrt{6}} \left(\frac{Z}{a_0} \right)^{3/2} \left(\frac{Zr}{a_0} \right) e^{-Zr/2a_0}$
3	0	$\frac{2}{81\sqrt{3}} \left(\frac{Z}{a_0} \right)^{3/2} \left[2 \left(\frac{Zr}{a_0} \right)^2 - 18 \left(\frac{Zr}{a_0} \right) + 27 \right] e^{-Zr/3a_0}$
3	1	$\frac{2\sqrt{2}}{81\sqrt{3}} \left(\frac{Z}{a_0} \right)^{3/2} \left[6 - \left(\frac{Zr}{a_0} \right) \right] \left(\frac{Zr}{a_0} \right) e^{-Zr/3a_0}$
3	2	$\frac{2\sqrt{2}}{81\sqrt{15}} \left(\frac{Z}{a_0} \right)^{3/2} \left(\frac{Zr}{a_0} \right)^2 e^{-Zr/3a_0}$

Tabla 2: Funciones angulares del átomo de hidrógeno

l	m	$Y_{l,m}(\theta, \phi) = \Theta_{l,m}(\theta) \Phi_{l,m}(\phi)$
0	0	$(1/4\pi)^{1/2}$
1	0	$(3/4\pi)^{1/2} \cos \theta$
1	1	$(3/8\pi)^{1/2} \sin \theta e^{i\phi}$
1	-1	$(3/8\pi)^{1/2} \sin \theta e^{-i\phi}$
2	0	$(5/16\pi)^{1/2} (3 \cos^2 \theta - 1)$
2	1	$(15/8\pi)^{1/2} \sin \theta \cos \theta e^{i\phi}$
2	-1	$(15/8\pi)^{1/2} \sin \theta \cos \theta e^{-i\phi}$
2	2	$(15/32\pi)^{1/2} \sin^2 \theta e^{2i\phi}$
2	-2	$(15/32\pi)^{1/2} \sin^2 \theta e^{-2i\phi}$

Tabla 3: Funciones de onda hidrogenoides reales

$\Psi_{n,l,m}(r, \theta, \phi) = R_{n,l}(r)Y_{l,m}(\theta, \phi)$
$1s = \frac{1}{\pi^{1/2}} \left(\frac{Z}{a_0} \right)^{3/2} e^{-Zr/a_0}$
$2s = \frac{1}{4(2\pi)^{1/2}} \left(\frac{Z}{a_0} \right)^{3/2} \left(2 - \frac{Zr}{a_0} \right) e^{-Zr/2a_0}$
$2p_z = \frac{1}{4(2\pi)^{1/2}} \left(\frac{Z}{a_0} \right)^{5/2} r e^{-Zr/2a_0} \cos \theta$
$2p_x = \frac{1}{4(2\pi)^{1/2}} \left(\frac{Z}{a_0} \right)^{5/2} r e^{-Zr/2a_0} \sin \theta \cos \phi$
$2p_y = \frac{1}{4(2\pi)^{1/2}} \left(\frac{Z}{a_0} \right)^{5/2} r e^{-Zr/2a_0} \sin \theta \sin \phi$
$3s = \frac{1}{81(3\pi)^{1/2}} \left(\frac{Z}{a_0} \right)^{3/2} \left(27 - 18 \frac{Zr}{a_0} + 2 \frac{Z^2 r^2}{a_0^2} \right) e^{-Zr/a_0}$
$3p_z = \frac{2^{1/2}}{81\pi^{1/2}} \left(\frac{Z}{a_0} \right)^{5/2} \left(6 - \frac{Zr}{a_0} \right) r e^{-Zr/3a_0} \cos \theta$
$3p_x = \frac{2^{1/2}}{81\pi^{1/2}} \left(\frac{Z}{a_0} \right)^{5/2} \left(6 - \frac{Zr}{a_0} \right) r e^{-Zr/3a_0} \sin \theta \cos \phi$
$3p_y = \frac{2^{1/2}}{81\pi^{1/2}} \left(\frac{Z}{a_0} \right)^{5/2} \left(6 - \frac{Zr}{a_0} \right) r e^{-Zr/3a_0} \sin \theta \sin \phi$
$3d_{z^2} = \frac{1}{81(6\pi)^{1/2}} \left(\frac{Z}{a_0} \right)^{7/2} r^2 e^{-Zr/3a_0} (3 \cos^2 \theta - 1)$
$3d_{xz} = \frac{2^{1/2}}{81\pi^{1/2}} \left(\frac{Z}{a_0} \right)^{7/2} r^2 e^{-Zr/3a_0} \sin \theta \cos \theta \cos \phi$
$3d_{yz} = \frac{2^{1/2}}{81\pi^{1/2}} \left(\frac{Z}{a_0} \right)^{7/2} r^2 e^{-Zr/3a_0} \sin \theta \cos \theta \sin \phi$
$3d_{x^2-y^2} = \frac{1}{81(2\pi)^{1/2}} \left(\frac{Z}{a_0} \right)^{7/2} r^2 e^{-Zr/3a_0} \sin^2 \theta \cos 2\phi$
$3d_{xy} = \frac{1}{81(2\pi)^{1/2}} \left(\frac{Z}{a_0} \right)^{7/2} r^2 e^{-Zr/3a_0} \sin^2 \theta \sin 2\phi$