

TABLE 2-3
Hydrogen Atom Wave Functions: Angular Functions

<i>l</i>	<i>m_l</i>	Angular factors		Real wave functions		
		Related to angular momentum	Functions of θ	In Polar coordinates	In Cartesian coordinates	Shapes
0(s)	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{2\sqrt{\pi}}$	$\frac{1}{2\sqrt{\pi}} \cos \theta$	 s
1(p)	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{6}}{2} \cos \theta$	$\frac{1}{2\sqrt{\pi}} \sqrt{\frac{3}{\pi}} \cos \theta$	$\frac{1}{2\sqrt{\pi}} \sqrt{\frac{3x}{\pi r}}$	 p _x
+1		$\frac{1}{\sqrt{2\pi}} e^{i\phi}$	$\frac{\sqrt{3}}{2} \sin \theta$	$\frac{1}{2\sqrt{\pi}} \sqrt{\frac{3}{\pi}} \sin \theta \cos \phi$	$\frac{1}{2\sqrt{\pi}} \sqrt{\frac{3y}{\pi r}}$	 p _y
-1		$\frac{1}{\sqrt{2\pi}} e^{-i\phi}$	$\frac{\sqrt{3}}{2} \sin \theta$	$\frac{1}{2\sqrt{\pi}} \sqrt{\frac{3}{\pi}} \sin \theta \sin \phi$	$\frac{1}{2\sqrt{\pi}} \sqrt{\frac{3z}{\pi r}}$	 p _z
2(d)	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{2} \sqrt{\frac{5}{2}} (3 \cos^2 \theta - 1)$	$\frac{1}{4} \sqrt{\frac{5}{\pi}} (3 \cos^2 \theta - 1)$	$\frac{1}{4} \sqrt{\frac{5}{\pi}} (2z^2 - x^2 - y^2)$	 d _{z^2}
+1		$\frac{1}{\sqrt{2\pi}} e^{i\phi}$	$\frac{\sqrt{15}}{2} \cos \theta \sin \theta$	$\frac{1}{2} \sqrt{\frac{15}{\pi}} \cos \theta \sin \theta \cos \phi$	$\frac{1}{2} \sqrt{\frac{15xz}{\pi r^2}}$	 d _{xy}
-1		$\frac{1}{\sqrt{2\pi}} e^{-i\phi}$	$\frac{\sqrt{15}}{2} \cos \theta \sin \theta$	$\frac{1}{2} \sqrt{\frac{15}{\pi}} \cos \theta \sin \theta \sin \phi$	$\frac{1}{2} \sqrt{\frac{15yz}{\pi r^2}}$	 d _{yz}
+2		$\frac{1}{\sqrt{2\pi}} e^{2i\phi}$	$\frac{\sqrt{15}}{4} \sin^2 \theta$	$\frac{1}{4} \sqrt{\frac{15}{\pi}} \sin^2 \theta \cos 2\phi$	$\frac{1}{4} \sqrt{\frac{15(x^2 - y^2)}{\pi r^2}}$	 d _{x^2-y^2}
-2		$\frac{1}{\sqrt{2\pi}} e^{-2i\phi}$	$\frac{\sqrt{15}}{4} \sin^2 \theta$	$\frac{1}{4} \sqrt{\frac{15}{\pi}} \sin^2 \theta \sin 2\phi$	$\frac{1}{4} \sqrt{\frac{15xy}{\pi r^2}}$	 d _{xy}

SOURCE: Adapted from G. M. Barrow, *Physical Chemistry*, 5th ed., McGraw-Hill, New York, 1988, p. 450, with permission.

NOTE: The relations $(e^{i\phi} - e^{-i\phi})/(2i) = \sin \phi$ and $(e^{i\phi} + e^{-i\phi})/2 = \cos \phi$ can be used to convert the exponential imaginary functions to real trigonometric functions, combining the two orbitals with $m_l = \pm 1$ to give two orbitals with $\sin \phi$ and $\cos \phi$. In a similar fashion, the orbitals with $m_l = \pm 2$ result in real functions with $\cos^2 \phi$ and $\sin^2 \phi$. These functions have then been converted to Cartesian form by using the functions $x = r \sin \theta \cos \phi$, $y = r \sin \theta \sin \phi$, and $z = r \cos \theta$.

TABLE 2-4
Hydrogen Atom Wave Functions: Radial Functions

<i>Orbital</i>	<i>n</i>	<i>l</i>	<i>R</i> (<i>r</i>)
1s	1	0	$R_{1s} = 2 \left[\frac{Z}{a_0} \right]^{3/2} e^{-\sigma}$
2s	2	0	$R_{2s} = \left[\frac{Z}{2a_0} \right]^{3/2} (2 - \sigma) e^{-\sigma/2}$
2p		1	$R_{2p} = \frac{1}{\sqrt{3}} \left[\frac{Z}{2a_0} \right]^{3/2} \sigma e^{-\sigma/2}$
3s	3	0	$R_{3s} = \frac{2}{27} \left[\frac{Z}{3a_0} \right]^{3/2} (27 - 18\sigma + 2\sigma^2) e^{-\sigma/3}$
3p		1	$R_{3p} = \frac{1}{81\sqrt{3}} \left[\frac{2Z}{a_0} \right]^{3/2} (6 - \sigma) \sigma e^{-\sigma/3}$
3d		2	$R_{3d} = \frac{1}{81\sqrt{15}} \left[\frac{2Z}{a_0} \right]^{3/2} \sigma^2 e^{-\sigma/3}$

The fourth quantum number explains several experimental observations. Two of these observations are that lines in alkali metal emission spectra are doubled, and that a