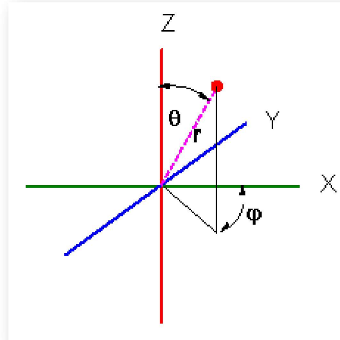
The Hydrogen Atomic Orbitals: the Mathematics

The wavefunction is dependent on the three quantum numbers *n*, *l*, and *m* as well as the location of the electron (which in polar coordinates depends on the distance from the nucleus r, and θ the angle to the Z-axis and ϕ the angle from the X-axis (see the figure to the right)). In general the following equation can be used to determine the functions for any atomic orbital.



$$\Psi_{n,l,m,r,\theta,\phi} = \sqrt{\frac{(n-l-1)!}{n((n+l)!^3)}}\left(\frac{1}{na_0}\right)^{\frac{3}{2}+l} r^l e^{\left(\frac{-r}{na_0}\right)}(n+l)!\left(\sum_{i=0}^{n-l-1}\frac{(-1)^i(n+l)!\left(\frac{2r}{na_0}\right)^i}{(n-l-1-i)!(2l+1+i)!i!}\right)\cdot$$

$$\sqrt{(2l+1)(l-|m|)!(l+|m|)!}\,\sin(\theta)^{|m|}\left(\sum_{i=0}^{l-|m|}\frac{(l!)^2(\cos(\theta)-1)^{l-|m|-i}(\cos(\theta)+1)^i}{(l-1)!i!(l-|m|-i)!(|m|+i)!}\right)e^{Im\phi}\frac{1}{\sqrt{\pi}l!}$$

$$a_0 = \frac{\varepsilon_0 h^2}{\pi m_e e^2} = \text{bohr radius} = 0.5292\ \text{Å}$$

the function $e^{Im\varphi}$ will become a function of sin(|*m*|*φ*) when *m* is negative or cos(|*m*|*φ*) when *m* is positive

Although the equations looking very intimidating, when you remember that there are limited allowed values for n, l and m the equations simplify considerably. The allowed values are:

- n = 0, 1, 2, ...
- l = 0, 1, 2, ... (n-1)
- m = -l ... 0 ... l

When these allowed combinations are substituted into the equation above the Hydrogenic Wavefunction (shown below) result. Note the Wavefunction will be composed of two parts, the first dependent on e^r which is the radial part of the wavefunction. The second depends on the sin and/or cos of θ and ϕ, and is the azimuthal part of the wavefunction.

Orbital	**The Hydrogenic Wavefunctions ($\Psi_{n,l,m}$)**	**Number of Nodes**		
		Spherical	**Planar**	**Conical**
1s	$\Psi_{1,0,0} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}} e^{\frac{-Zr}{a_0}}$	0	0	0
2s	$\Psi_{2,0,0} = \frac{1}{\sqrt{32\pi}}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\left(2-\frac{Zr}{a_0}\right) e^{\frac{-Zr}{2a_0}}$	1	0	0
$2p_y$	$\Psi_{2,1,-1} = \frac{1}{\sqrt{32\pi}}\left(\frac{Z}{a_0}\right)^{\frac{5}{2}} r e^{\frac{-Zr}{2a_0}}\sin(\theta)\sin(\phi)$	0	1	0
$2p_z$	$\Psi_{2,1,0} = \frac{1}{\sqrt{32\pi}}\left(\frac{Z}{a_0}\right)^{\frac{5}{2}} r e^{\frac{-Zr}{2a_0}}\cos(\theta)$	0	1	0
$2p_x$	$\Psi_{2,1,1} = \frac{1}{\sqrt{32\pi}}\left(\frac{Z}{a_0}\right)^{\frac{5}{2}} r e^{\frac{-Zr}{2a_0}}\sin(\theta)\cos(\phi)$	0	1	0
3s	$\Psi_{3,0,0} = \frac{1}{81\sqrt{3\pi}}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\left(27-18\frac{Zr}{a_0}+2\left(\frac{Zr}{a_0}\right)^2\right) e^{\frac{-Zr}{3a_0}}$	2	0	0

$3p_y$	$\Psi_{3,1,-1} = \frac{1}{81}\sqrt{\frac{2}{\pi}}\left(\frac{Z}{a_0}\right)^{\frac{5}{2}}\left(6-\frac{Zr}{a_0}\right)re^{\frac{-Zr}{3a_0}}\sin(\theta)\sin(\phi)$	1	1	0
$3p_z$	$\Psi_{3,1,0} = \frac{1}{81}\sqrt{\frac{2}{\pi}}\left(\frac{Z}{a_0}\right)^{\frac{5}{2}}\left(6-\frac{Zr}{a_0}\right)re^{\frac{-Zr}{3a_0}}\cos(\theta)$	1	1	0
$3p_x$	$\Psi_{3,1,1} = \frac{1}{81}\sqrt{\frac{2}{\pi}}\left(\frac{Z}{a_0}\right)^{\frac{5}{2}}\left(6-\frac{Zr}{a_0}\right)re^{\frac{-Zr}{3a_0}}\sin(\theta)\cos(\phi)$	1	1	0
$3d_{xy}$	$\Psi_{3,2,-2} = \frac{1}{81\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{\frac{7}{2}}r^2e^{\frac{-Zr}{3a_0}}\sin^2(\theta)\sin(2\phi)$	0	2	0
$3d_{yz}$	$\Psi_{3,2,-1} = \frac{\sqrt{2}}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{\frac{7}{2}}r^2e^{\frac{-Zr}{3a_0}}\sin(\theta)\cos(\theta)\sin(\phi)$	0	2	0
$3d_{z^2}$	$\Psi_{3,2,0} = \frac{1}{81\sqrt{6\pi}}\left(\frac{Z}{a_0}\right)^{\frac{7}{2}}r^2e^{\frac{-Zr}{3a_0}}\left(3\cos^2(\theta)-1\right)$	0	0	2
$3d_{xz}$	$\Psi_{3,2,1} = \frac{\sqrt{2}}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{\frac{7}{2}}r^2e^{\frac{-Zr}{3a_0}}\sin(\theta)\cos(\theta)\cos(\phi)$	0	2	0
$3d_{x^2-y^2}$	$\Psi_{3,2,2} = \frac{1}{81\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{\frac{7}{2}}r^2e^{\frac{-Zr}{3a_0}}\sin^2(\theta)\cos(2\phi)$	0	2	0
$4s$	$\Psi_{4,0,0} = \frac{1}{1536\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\left(192-144\frac{Zr}{a_0}+24\left(\frac{Zr}{a_0}\right)^2-\left(\frac{Zr}{a_0}\right)^3\right)e^{\frac{-Zr}{4a_0}}$	3	0	0
$4p_y$	$\Psi_{4,1,-1} = \frac{1}{512\sqrt{5\pi}}\left(\frac{Z}{a_0}\right)^{\frac{5}{2}}\left(80-20\frac{Zr}{a_0}+\left(\frac{Zr}{a_0}\right)^2\right)re^{\frac{-Zr}{4a_0}}\sin(\theta)\sin(\phi)$	2	1	0
$4p_z$	$\Psi_{4,1,0} = \frac{1}{512\sqrt{5\pi}}\left(\frac{Z}{a_0}\right)^{\frac{5}{2}}\left(80-20\frac{Zr}{a_0}+\left(\frac{Zr}{a_0}\right)^2\right)re^{\frac{-Zr}{4a_0}}\cos(\theta)$	2	1	0
$4p_x$	$\Psi_{4,1,1} = \frac{1}{512\sqrt{5\pi}}\left(\frac{Z}{a_0}\right)^{\frac{5}{2}}\left(80-20\frac{Zr}{a_0}+\left(\frac{Zr}{a_0}\right)^2\right)re^{\frac{-Zr}{4a_0}}\sin(\theta)\cos(\phi)$	2	1	0
$4d_{xy}$	$\Psi_{4,2,-2} = \frac{\sqrt{3}}{1536\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{\frac{7}{2}}\left(12-\frac{Zr}{a_0}\right)r^2e^{\frac{-Zr}{4a_0}}\sin^2(\theta)\sin(2\phi)$	1	2	0
$4d_{yz}$	$\Psi_{4,2,-1} = \frac{\sqrt{3}}{3072\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{\frac{7}{2}}\left(12-\frac{Zr}{a_0}\right)r^2e^{\frac{-Zr}{4a_0}}\sin(\theta)\cos(\theta)\sin(\phi)$	1	2	0
$4d_{z^2}$	$\Psi_{4,2,0} = \frac{1}{3072\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{\frac{7}{2}}\left(12-\frac{Zr}{a_0}\right)r^2e^{\frac{-Zr}{4a_0}}3\cos^2(\theta)-1$	1	0	2
$4d_{xz}$	$\Psi_{4,2,1} = \frac{\sqrt{3}}{3072\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{\frac{7}{2}}\left(12-\frac{Zr}{a_0}\right)r^2e^{\frac{-Zr}{4a_0}}\sin(\theta)\cos(\theta)\cos(\phi)$	1	2	0
$4d_{x^2-y^2}$	$\Psi_{4,2,2} = \frac{\sqrt{3}}{1536\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{\frac{7}{2}}\left(12-\frac{Zr}{a_0}\right)r^2e^{\frac{-Zr}{4a_0}}\sin^2(\theta)\cos(2\phi)$	0	2	0
$4f_{y(3x^2-y^2)}$	$\Psi_{4,3,-3} = \frac{1}{3072\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{\frac{9}{2}}r^3e^{\frac{-Zr}{4a_0}}\sin^3(\theta)\sin(3\phi)$	0	3	0
$4f_{xyz}$	$\Psi_{4,3,-2} = \frac{\sqrt{3}}{3072\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{\frac{9}{2}}r^3e^{\frac{-Zr}{4a_0}}\sin^2(\theta)\cos(\theta)\sin(2\phi)$	0	3	0
$4f_{yz^2}$	$\Psi_{4,3,-1} = \frac{\sqrt{3}}{3072\sqrt{10\pi}}\left(\frac{Z}{a_0}\right)^{\frac{9}{2}}r^3e^{\frac{-Zr}{4a_0}}\sin(\theta)\left(5\cos^2(\theta)-1\right)\sin(\phi)$	0	3	0

$4f_{z^3}$	$\Psi_{4,3,0} = \frac{1}{3072\sqrt{5\pi}}\left(\frac{Z}{a_0}\right)^{\frac{9}{2}} r^3 e^{\frac{-Zr}{4a_0}}\left(5\cos^3(\theta) - 3\cos(\theta)\right)$	0	1	2
$4f_{xz^2}$	$\Psi_{4,3,1} = \frac{\sqrt{3}}{3072\sqrt{10\pi}}\left(\frac{Z}{a_0}\right)^{\frac{9}{2}} r^3 e^{\frac{-Zr}{4a_0}}\sin(\theta)\left(5\cos^2(\theta) - 1\right)\cos(\phi)$	0	3	0
$4f_{z(x^2-y^2)}$	$\Psi_{4,3,2} = \frac{\sqrt{3}}{3072\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{\frac{9}{2}} r^3 e^{\frac{-Zr}{4a_0}}\sin^2(\theta)\cos(\theta)\cos(2\phi)$	0	3	0
$4f_{x(x^2-3y^2)}$	$\Psi_{4,3,3} = \frac{1}{3072\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{\frac{9}{2}} r^3 e^{\frac{-Zr}{4a_0}}\sin^3(\theta)\cos(3\phi)$	0	3	0

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