

# The Complete Hydrogen Orbitals (Atkins)

## 1s Orbital

$$\psi(1s) = R_{10} Y_{00} \quad \text{--- (1)}$$

$$\psi(2s) = R_{20} Y_{00} \quad \text{--- (2)}$$

$$\psi(2p_z) = R_{21} Y_{10} \quad \text{--- (3)}$$

$$\psi(2p_x) = R_{21} Y_{11} \quad \text{--- (4)}$$

$$\psi(2p_y) = R_{21} Y_{1-1} \quad \text{--- (5)}$$

Where  $R_{nl}$  are the radial functions and where  $Y_{lm}$  are the spherical harmonics.

## The Spherical Harmonics $(r, \theta, \phi)$

$$Y(0,0) = \frac{1}{2\pi^{1/2}} \quad \text{--- (6)}$$

$$Y(1,0) = \frac{1}{2} \left(\frac{3}{\pi}\right)^{1/2} \cos\theta \quad \text{--- (7)}$$

$$Y(1,1) = -\frac{1}{2} \left(\frac{3}{2\pi}\right)^{1/2} \sin\theta e^{i\phi} \quad \text{--- (8)}$$

$$Y(1,-1) = \frac{1}{2} \left(\frac{3}{2\pi}\right)^{1/2} \sin\theta e^{-i\phi} \quad \text{--- (9)}$$

## The Radial Functions

$n$	$l$	$R_{nl}(r)$
1	0 (1s)	$2(1/a)^{3/2} \exp(-r/a)$
2	0 (2s)	$(1/a)^{3/2} (1/(2\sqrt{5})) (2-r/a) \exp(-r/(2a))$
	1 (2p)	$(1/a)^{3/2} (1/(2\sqrt{6})) \frac{r}{a} \exp(-r/(2a))$

2)

So:

$$\psi(1s) = \frac{1}{2\pi^{1/2}} \cdot 2 \left(\frac{1}{a}\right)^{3/2} \exp(-r/a) \quad - (10)$$

$$\psi(2s) = \frac{1}{2\pi^{1/2}} \cdot \frac{1}{2\sqrt{5}} \cdot \left(2 - \frac{r}{a}\right) \exp(-r/(2a)) \quad - (11)$$

$$\psi(2p_z) = \frac{1}{2} \left(\frac{3}{\pi}\right)^{1/2} \cos\theta \cdot \left(\frac{1}{a}\right)^{3/2} \left(\frac{1}{2\sqrt{6}}\right) \frac{r}{a} \exp(-r/(2a)) \quad - (12)$$

$$\psi(2p_x) = -\frac{1}{2} \left(\frac{3}{2\pi}\right)^{1/2} \sin\theta e^{i\phi} \cdot \left(\frac{1}{a}\right)^{3/2} \left(\frac{1}{2\sqrt{6}}\right) \frac{r}{a} \exp(-r/(2a)) \quad - (13)$$

$$\psi(2p_y) = \frac{1}{2} \left(\frac{3}{2\pi}\right)^{1/2} \sin\theta e^{-i\phi} \cdot \left(\frac{1}{a}\right)^{3/2} \left(\frac{1}{2\sqrt{6}}\right) \frac{r}{a} \exp(-r/(2a)) \quad - (14)$$