

TABLE 6-5
The Complete Hydrogenlike Atomic Wave Functions for $n = 1, 2$, and 3 . The Quantity Z Is the Atomic Number of the Nucleus, and $\sigma = Zr/a_0$, Where a_0 is the Bohr Radius.

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

TABLE 6-6

The Complete Hydrogenlike Atomic Wave Functions Expressed as Real Functions for $n = 1, 2$, and 3. The Quantity Z Is the Atomic Number of the Nucleus and $\sigma = Zr/a_0$, Where a_0 Is the Bohr Radius.

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|------------------------------------|--|
| $n = 1, \quad l = 0, \quad m = 0;$ | $\psi_{1s} = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} e^{-\sigma}$ |
| $n = 2, \quad l = 0, \quad m = 0;$ | $\psi_{2s} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} (2 - \sigma) e^{-\sigma/2}$ |
| $l = 1, \quad m = 0;$ | $\psi_{2p_z} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma e^{-\sigma/2} \cos \theta$ |
| $l = 1, \quad m = \pm 1;$ | $\psi_{2p_x} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma e^{-\sigma/2} \sin \theta \cos \phi$ |
| | $\psi_{2p_y} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma e^{-\sigma/2} \sin \theta \sin \phi$ |
| $n = 3, \quad l = 0, \quad m = 0;$ | $\psi_{3s} = \frac{1}{81\sqrt{3\pi}} \left(\frac{Z}{a_0} \right)^{3/2} (27 - 18\sigma + 2\sigma^2) e^{-\sigma/3}$ |
| $l = 1, \quad m = 0;$ | $\psi_{3p_z} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma (6 - \sigma) e^{-\sigma/3} \cos \theta$ |
| $l = 1, \quad m = \pm 1;$ | $\psi_{3p_x} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma (6 - \sigma) e^{-\sigma/3} \sin \theta \cos \phi$ |
| | $\psi_{3p_y} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma (6 - \sigma) e^{-\sigma/3} \sin \theta \sin \phi$ |
| $l = 2, \quad m = 0;$ | $\psi_{3d_{z^2}} = \frac{1}{81\sqrt{6\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma^2 e^{-\sigma/3} (3 \cos^2 \theta - 1)$ |
| $l = 2, \quad m = \pm 1;$ | $\psi_{3d_{xz}} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma^2 e^{-\sigma/3} \sin \theta \cos \theta \cos \phi$ |
| | $\psi_{3d_{yz}} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma^2 e^{-\sigma/3} \sin \theta \cos \theta \sin \phi$ |
| $l = 2, \quad m = \pm 2;$ | $\psi_{3d_{x^2-y^2}} = \frac{1}{81\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma^2 e^{-\sigma/3} \sin^2 \theta \cos 2\phi$ |
| | $\psi_{3d_{xy}} = \frac{1}{81\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma^2 e^{-\sigma/3} \sin^2 \theta \sin 2\phi$ |