

Appendix IV: Radial Wavefunctions for Hydrogenlike Species

The normalized radial wavefunctions for hydrogenlike atoms can be expressed by

$$R_{n,\ell}(\rho) = -\sqrt{\frac{4(n-\ell-1)!}{n^4[(n+\ell)!]^3}} \left(\frac{Z}{a_0}\right)^{3/2} \left(\frac{2\rho}{n}\right)^\ell e^{-\rho/n} \mathcal{L}_{n-1}^{2\ell+1}(2\rho/n), \quad (1)$$

with $\rho = Zr/a_0$, where r is the radial distance, Z is the atomic number and a_0 is the radius of the first Bohr orbit. The associated Laguerre polynomials, $\mathcal{L}_{n-1}^{2\ell+1}(2\rho/n)$, were introduced in Section 3.4.3. Here they have been multiplied by $(2\rho/n)^\ell e^{-\rho/n}$, which is the appropriate integrating factor. The radial functions $R_{n,\ell}(\rho)$ are given in Table 1 for the first three “shells” of hydrogenlike species.

Table 1 Some of the normalized radial wavefunctions for hydrogenlike species.

n	ℓ	symbol	normalizing factor	radial function
1	0	1s	$2(Z/a_0)^{3/2}$	$e^{-\rho}$
2	0	2s	$\frac{1}{2\sqrt{2}}(Z/a_0)^{3/2}$	$(2-\rho)e^{-\rho/2}$
	1	2p	$\frac{1}{2\sqrt{6}}(Z/a_0)^{3/2}$	$\rho e^{-\rho/2}$
3	0	3s	$\frac{2}{81\sqrt{3}}(Z/a_0)^{3/2}$	$(27-18\rho+2\rho^2)e^{-\rho/3}$
	1	3p	$\frac{4}{81\sqrt{6}}(Z/a_0)^{3/2}$	$\rho(6-\rho)e^{-\rho/3}$
	2	3d	$\frac{4}{81\sqrt{30}}(Z/a_0)^{3/2}$	$\rho^2 e^{-\rho/3}$