Appendix III: Atomic orbitals

The angular functions presented in Table 1 are derived from the wavefunctions for one-electron systems, *e.g.* the hydrogen atom. However, they can be

Table 1 The normalized atomic orbitals.

ℓ	m	symbol[a]	normalizing factor	angular function
0	0	s	$\frac{1}{2}\sqrt{\frac{1}{\pi}}$	
1	0	p_z	$\frac{1}{2}\sqrt{\frac{3}{\pi}}$	$\cos\theta$
	±1	p_x	$\frac{1}{2}\sqrt{\frac{3}{\pi}}$	$\sin\theta\cos\varphi$
		p_y	$\frac{1}{2}\sqrt{\frac{3}{\pi}}$	$\sin\theta\sin\varphi$
2	0	d_{z^2}	$\frac{1}{4}\sqrt{\frac{5}{\pi}}$	$3\cos^2\theta - 1$
	±1	d_{xz}	$\frac{1}{2}\sqrt{\frac{15}{\pi}}$	$\sin\theta\cos\theta\cos\varphi$
		d_{yz}	$\frac{1}{2}\sqrt{\frac{15}{\pi}}$	$\sin\theta\cos\theta\sin\varphi$
	±2	$d_{x^2-y^2}$	$\frac{1}{4}\sqrt{\frac{15}{\pi}}$	$\sin^2\theta\cos 2\varphi$
		d_{xy}	$\frac{1}{4}\sqrt{\frac{15}{\pi}}$	$\sin^2\theta\cos 2\varphi$
3	0	f_{z^3}	$\frac{1}{4}\sqrt{\frac{7}{\pi}}$	$5\cos^3\theta - 3\cos\theta$
	±1	f_{xz^2}	$\frac{1}{8}\sqrt{\frac{42}{\pi}}$	$\sin\theta(5\cos^2\theta - 1)\cos\varphi$
		f_{yz^2}	$\frac{1}{8}\sqrt{\frac{42}{\pi}}$	$\sin\theta(5\cos^2\theta - 1)\sin\varphi$
	±2	$f_{z(x^2-y^2)}$	$\frac{1}{4}\sqrt{\frac{105}{\pi}}$	$\sin^2\theta\cos\theta\cos 2\varphi$
		f_{zxy}	$\frac{1}{4}\sqrt{\frac{105}{\pi}}$	$\sin^2\theta\cos\theta\sin 2\varphi$
	±3	$f_{x(x^2-3y^2)}$	$\frac{1}{8}\sqrt{\frac{70}{\pi}}$	$\sin^3\theta\cos 3\varphi$
		$f_{y(3x^2-y^2)}$	$\frac{1}{8}\sqrt{\frac{70}{\pi}}$	$\sin^3\theta\sin 3\varphi$

[a]Note that d_{z^2} is the short notation for $d_{2z^2-x^2-y^2}$, as it appears in the cubic point groups (Appendix VII). Similarly, f_{z^3}, f_{xz^2} and f_{yz^2} are the abbreviated symbols for $f_{z(5z^2-3r^2)}$, $f_{x(5z^2-r^2)}$ and $f_{y(5z^2-r^2)}$, respectively, where $r^2 = x^2 + y^2 + z^2$.

applied as "atomic orbitals" to polyelectron systems, as the appropriate wavefunctions are written as products of those for hydrogen. Although the radial part of the functions is modified by the effect of electron–electron interaction,

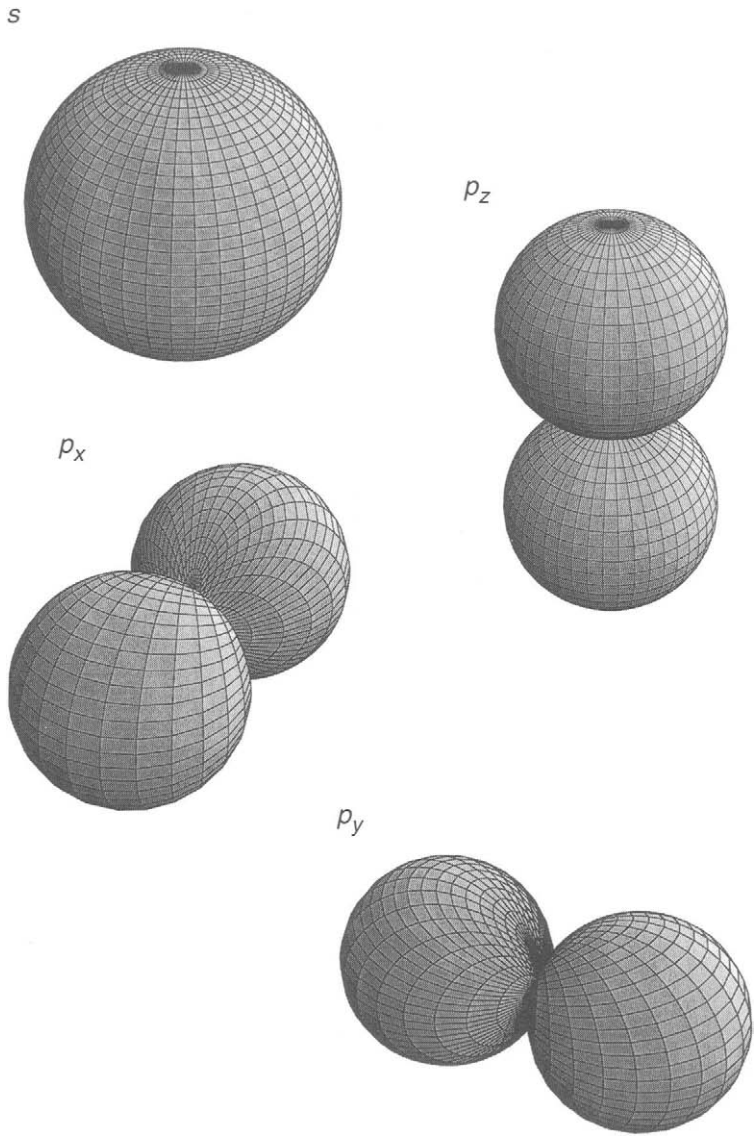

Fig. 1 Some of the atomic orbitals.

the angular parts retain their symmetry. In effect, the functions given here can be employed to describe the basic symmetry of polyelectronic atoms and ions.

Three-dimensional representations of the angular dependence of some of the atomic orbitals are shown in Fig. 1. The coordinate axes and angles are defined in Fig. 6-5.

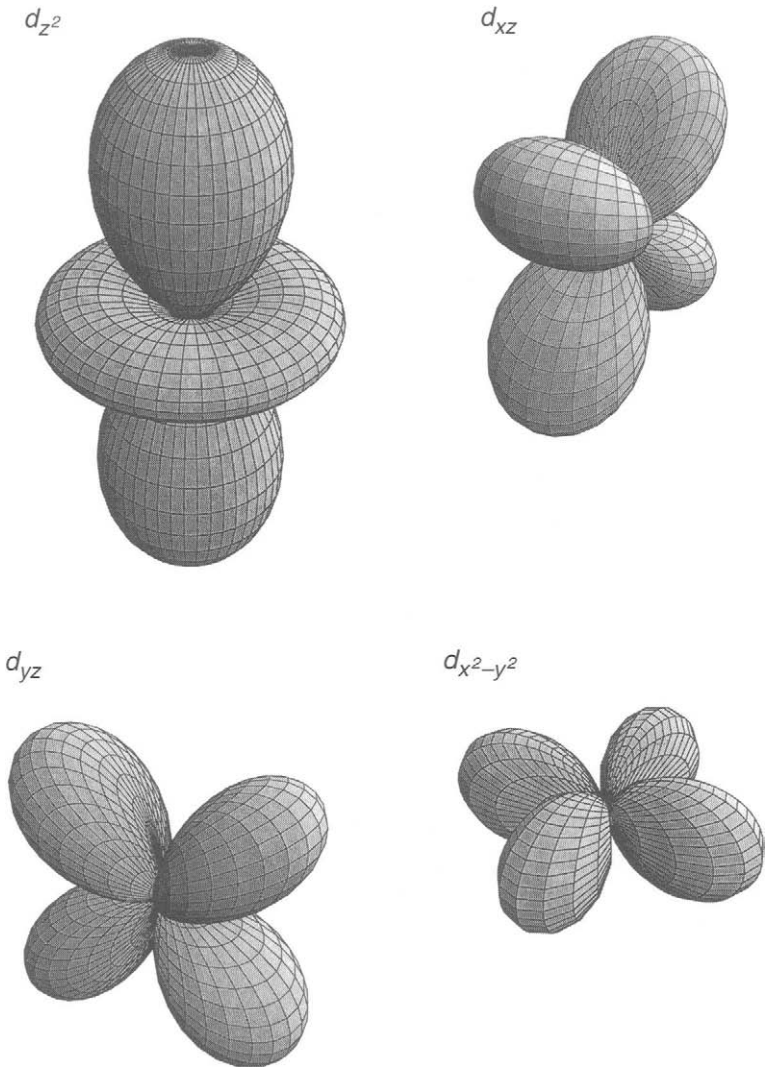

Fig. 1 (*continued*).

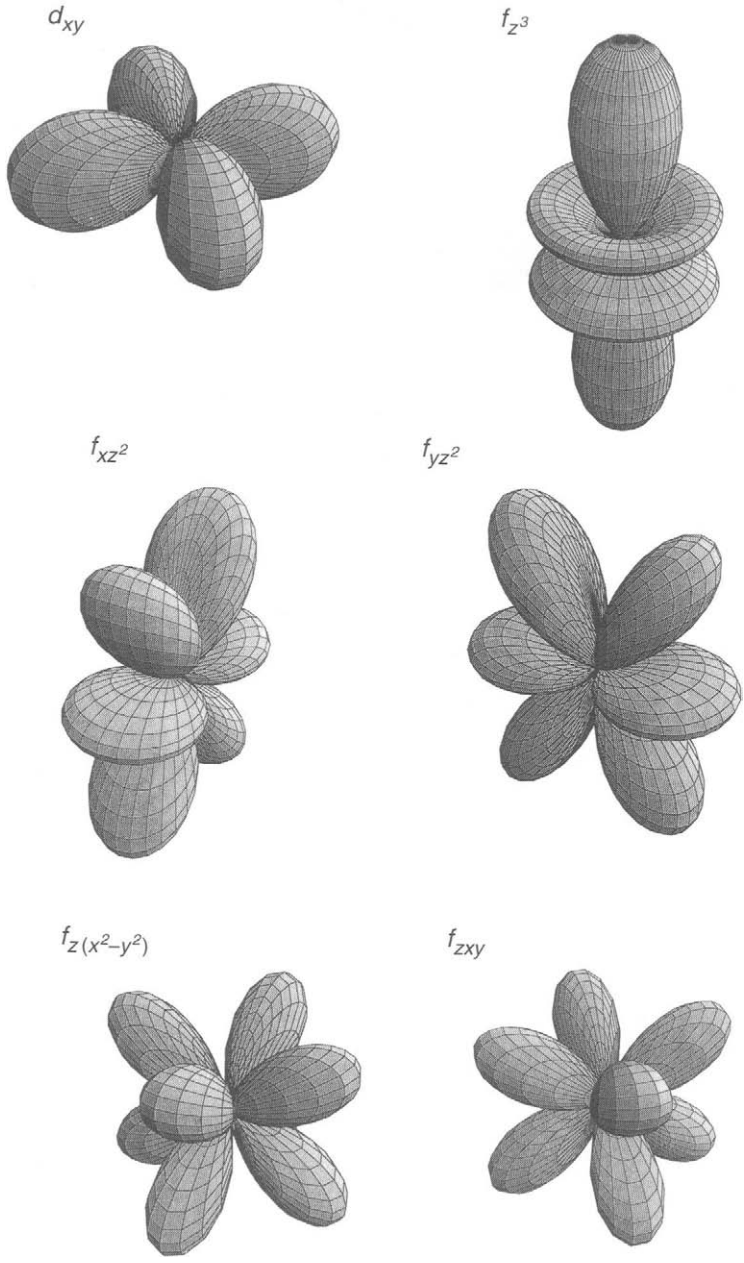

Fig. 1 (*continued*).

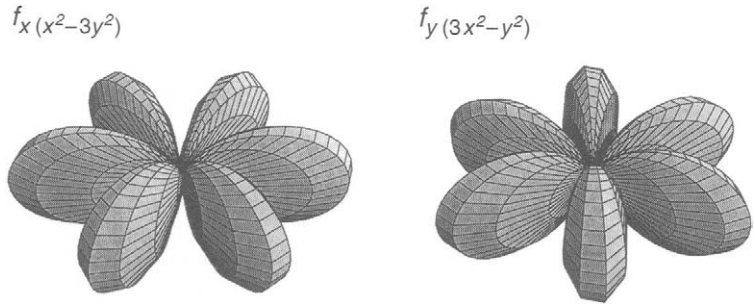

Fig. 1 (*continued*).