

the electron is 1s: 0.30 instead;  
 (c) from each electron from groups inside the one of interest: 1.00 if the one of interest is d or f; 0.85 from each electron in the next inner group if the electron of interest is s or p; 1.00 for all deeper electrons.

Typical (and improved) values of  $Z^*$  are given in Table 9.1.

**Example.** Find expressions for the Slater type  $2s$ -,  $2p_z$ -, and  $2p_x$ -orbitals of nitrogen.

• **Method.** In each case  $Z^* = Z - \sigma$  has the same value. Use  $Z = 7$  and calculate  $\sigma$  for the configuration  $1s^2 2s^2 2p^2$  using the rules expressed above. For the  $2p_z$ -orbital use  $Y_{10}$  from Table 4.1. For the  $2p_x$ -orbital, use the linear combinations  $(Y_{1-1} - Y_{11})/\sqrt{2}$  corresponding to  $p_x = (p_+ + p_-)\sqrt{2}$ . Normalize the orbitals to unity.

• **Answer.**  $\sigma = 4 \times 0.35 + 2 \times 0.85 = 3.10$ , and so  $Z^* = 3.90$ . Use  $Y_{00} = (1/4\pi)^{1/2}$ , so

Table 9.1. Values of  $Z^* = Z - \sigma$  for neutral ground-state atoms

	H							He
1s	1 (1.000)							1.70 (1.6875)
	Li	Be	B	C	N	O	F	Ne
1s	2.70 (2.6906)	3.70 (3.6848)	4.70 (4.6795)	5.70 (5.6727)	6.70 (6.6651)	7.70 (7.6579)	8.70 (8.6501)	9.70 (9.6421)
2s	1.30 (1.2792)	1.95 (1.9120)	2.60 (2.5762)	3.25 (3.2166)	3.90 (3.8474)	4.55 (4.4916)	5.20 (5.1276)	5.85 (5.7584)
2p			2.60 (2.4214)	3.25 (3.1358)	3.90 (3.8340)	4.55 (4.4532)	5.20 (5.1000)	5.85 (5.7584)
	Na	Mg	Al	Si	P	S	Cl	Ar
1s	10.70 (10.6259)	11.70 (11.6089)	12.70 (12.5910)	13.70 (13.5745)	14.70 (14.5578)	15.70 (15.5409)	16.70 (16.5239)	17.70 (17.5075)
2s	6.85 (6.5714)	7.85 (7.3920)	8.85 (8.2136)	9.85 (9.0200)	10.85 (9.8250)	11.85 (10.6288)	12.85 (11.4304)	13.85 (12.2304)
2p	6.85 (6.8018)	7.85 (7.8258)	8.85 (8.9634)	9.85 (9.9450)	10.85 (10.9612)	11.85 (11.9770)	12.85 (12.9932)	13.85 (14.0082)
3s	2.20 (2.5074)	2.85 (3.3075)	3.50 (4.1172)	4.15 (4.9032)	4.80 (5.6418)	5.45 (6.3669)	6.10 (7.0683)	6.75 (7.7568)
3p			3.50 (4.0656)	4.15 (4.2852)	4.80 (4.8864)	5.45 (5.4819)	6.10 (6.1161)	6.75 (6.7641)

Figures in normal type are values of  $Z^*$  obtained on the basis of the Slater rules. The figures in parentheses are improved values of  $Z^*$  suggested by Clementi and Raimondi; see *Further reading*, p. 247.