σ_a also apply to a mixture of isotopes. Hence, if c_l denotes the mole fraction of isotopes of type l, so that

$$\sum_l c_l = 1, \tag{4.4.4.10}$$

then, for an isotopic mixture,

$$b_c = \sum_l c_l\, b_{cl}, \tag{4.4.4.11}$$

$$\sigma_s = \sum_l c_l\, \sigma_{sl}, \tag{4.4.4.12}$$

and

$$\sigma_a = \sum_l c_l\, \sigma_{al}. \tag{4.4.4.13}$$

The bound coherent scattering cross section of the mixture is given, as before, by

$$\sigma_c = 4\pi|b_c|^2, \tag{4.4.4.14}$$

while the bound incoherent scattering cross section is defined as

$$\sigma_i = \sigma_s - \sigma_c. \tag{4.4.4.15}$$

Hence, it follows that

$$\sigma_i \equiv 4\pi|b_i|^2 = \sigma_i(\text{spin}) + \sigma_i(\text{isotope}), \tag{4.4.4.16}$$

in which the contribution from spin incoherence is given by

$$\sigma_i(\text{spin}) = \sum_l c_l\sigma_{il} = 4\pi \sum_l c_l|b_{il}|^2, \tag{4.4.4.17}$$

and that from isotope incoherence is given by

$$\sigma_i(\text{isotope}) = 4\pi \sum_{l<l'} c_l c_{l'}|b_{cl} - b_{cl'}|^2. \tag{4.4.4.18}$$

Note that for a mixture of isotopes only the magnitude of b_i is defined by (4.4.4.16), and its sign is arbitrary. However, for the individual isotopes, both the magnitude and sign (or complex phase) of b_i are defined in (4.4.4.2).

4.4.4.4. *Correction for electromagnetic interactions*

The effective bound coherent scattering length that describes the interaction of a neutron with an atom includes additional contributions from electromagnetic interactions (Bacon, 1975; Sears, 1986*a*, 1996). For a neutral atom with atomic number Z, this quantity is of the form

$$b_c(q) = b_c(0) - b_e[Z - f(q)], \tag{4.4.4.19}$$

where q is the wavevector transfer in the collision, $b_c(0)$ and b_e are constants, and $f(q)$ is the atomic scattering factor (Section 6.1.1). The latter quantity is the Fourier transform of the electron number density and is normalized such that $f(0) = Z$.

The main contribution to $b_c(0)$ is from the nuclear interaction between the neutron and the nucleus but there is also a small electrostatic contribution ($\leq$0.5%) arising from the neutron electric polarizability. The coefficient b_e is called the neutron–electron scattering length and has the value $-1.32\ (4) \times 10^{-3}$ fm (Koester, Waschkowksi & Meier, 1988). This quantity is due mainly to the Foldy interaction with a small additional contribution (~10%) from the intrinsic charge distribution of the neutron.

The correction of the bound coherent scattering length for electromagnetic interactions requires a knowledge of the atomic scattering factor $f(q)$. Tables 6.1.1.1 and 6.1.1.3 provide accurate values of $f(q)$ obtained from relativistic Hartree–Fock calculations for all the atoms and chemically important ions in the Periodic Table. Alternatively, since the correction is small (~1%), one can often use the approximate analytical expression (Sears, 1986*a*, 1996)

$$f(q) = \frac{Z}{\sqrt{1 + 3(q/q_0)^2}} \tag{4.4.4.20}$$

with $q_0 = \gamma Z^{1/3}$. The value $\gamma = 1.90 \pm 0.07$ Å^{-1} provides a good fit to the Hartree–Fock results in Table 6.1.1.1 for $Z \geq 20$.

4.4.4.5. *Measurement of scattering lengths*

The development of modern neutron-optical techniques during the past 25 years has produced a dramatic increase in the accuracy with which scattering lengths can be measured (Koester, 1977; Klein & Werner, 1983; Werner & Klein, 1986; Sears, 1989; Koester, Rauch & Seymann, 1991). The measurements employ a number of effects – mirror reflection, prism refraction, gravity refractometry, Christiansen filter, and interferometry – all of which are based on the fact that the neutron index of refraction, n, is uniquely determined by $b_c(0)$ through the relation

$$n^2 = 1 - \frac{4\pi}{k^2}\,\rho\, b_c(0), \tag{4.4.4.21}$$

in which ρ is the number of atoms per unit volume. Apart from a small ($\leq$0.01%) local-field correction (Sears, 1985, 1989), this expression is exact.

In methods based on diffraction, such as Bragg reflection by powders or dynamical diffraction by perfect crystals, the measured quantity is the unit-cell structure factor $|F_{hkl}|$. This quantity depends on $b_c(q)$ in which q is equal to the magnitude of the reciprocal-lattice vector corresponding to the relevant Bragg planes, *i.e.*

$$q = 2k \sin\theta_{hkl}, \tag{4.4.4.22}$$

where θ_{hkl} is the Bragg angle. In dynamical diffraction measurements, it is usual for the authors to correct their results for electromagnetic interactions so that the published quantity is again $b_c(0)$. In the past, this correction has not usually been made for the scattering lengths obtained from Bragg reflection by powders. However, these latter measurements are accurate only to ±2 or 3% so that the correction is then relatively unimportant.

The essential point is that all the bound coherent scattering lengths in Table 4.4.4.1 with the experimental uncertainties less than 1% represent $b_c(0)$ and should therefore be corrected for electromagnetic interactions before being used in the interpretation of neutron diffraction experiments. Failure to make this correction will introduce systematic errors of 0.5 to 2% in the unit-cell structure factors at large q, and corresponding errors of 1 to 4% in the calculated intensities.

Expression (4.4.4.21) assumed that the neutrons and/or the nuclei are unpolarized. If the neutrons and the nuclei are both polarized then $b_c(0)$ is replaced by $\langle b(0)\rangle$, which depends on both the coherent and incoherent scattering lengths. If the coherent scattering length is known, neutron-optical experiments with polarized neutrons and nuclei can then be used to determine the incoherent scattering length (Glättli & Goldman, 1987).

4.4.4.6. *Compilation of scattering lengths and cross sections*

The bound scattering lengths and cross sections of almost all the elements in the Periodic Table, as well as those of the individual isotopes, are listed in Table 4.4.4.1. As in earlier versions of this table (Sears, 1984, 1986*b*, 1992*a*,*b*), our primary aim, has been to take the best current values of the bound coherent and incoherent neutron scattering lengths and to

Table 4.4.5.1. *$\langle j_0 \rangle$ form factors for 3d transition elements and their ions*

Atom or ion	*A*	*a*	*B*	*b*	*C*	*c*	*D*	*e*
Sc	0.2512	90.030	0.3290	39.402	0.4235	14.322	−0.0043	0.2029
Sc^{+}	0.4889	51.160	0.5203	14.076	−0.0286	0.179	0.0185	0.1217
Sc^{2+}	0.5048	31.403	0.5186	10.990	−0.0241	1.183	0.0000	0.0578
Ti	0.4657	33.590	0.5490	9.879	−0.0291	0.323	0.0123	0.1088
Ti^{+}	0.5093	36.703	0.5032	10.371	−0.0263	0.311	0.0116	0.1125
Ti^{2+}	0.5091	24.976	0.5162	8.757	−0.0281	0.916	0.0015	0.0589
Ti^{3+}	0.3571	22.841	0.6688	8.931	−0.0354	0.483	0.0099	0.0575
V	0.4086	28.811	0.6077	8.544	−0.0295	0.277	0.0123	0.0970
V^{+}	0.4444	32.648	0.5683	9.097	−0.2285	0.022	0.2150	0.1111
V^{2+}	0.4085	23.853	0.6091	8.246	−0.1676	0.041	0.1496	0.0593
V^{3+}	0.3598	19.336	0.6632	7.617	−0.3064	0.030	0.2835	0.0515
V^{4+}	0.3106	16.816	0.7198	7.049	−0.0521	0.302	0.0221	0.0433
Cr	0.1135	45.199	0.3481	19.493	0.5477	7.354	−0.0092	0.1975
Cr^{+}	−0.0977	0.047	0.4544	26.005	0.5579	7.489	0.0831	0.1114
Cr^{2+}	1.2024	−0.005	0.4158	20.548	0.6032	6.956	−1.2218	0.0572
Cr^{3+}	−0.3094	0.027	0.3680	17.035	0.6559	6.524	0.2856	0.0436
Cr^{4+}	−0.2320	0.043	0.3101	14.952	0.7182	6.173	0.2042	0.0419
Mn	0.2438	24.963	0.1472	15.673	0.6189	6.540	−0.0105	0.1748
Mn^{+}	−0.0138	0.421	0.4231	24.668	0.5905	6.655	−0.0010	0.1242
Mn^{2+}	0.4220	17.684	0.5948	6.0050	0.0043	−0.609	−0.0219	0.0589
Mn^{3+}	0.4198	14.283	0.6054	5.469	0.9241	−0.009	−0.9498	0.0392
Mn^{4+}	0.3760	12.566	0.6602	5.133	−0.0372	0.563	0.0011	0.0393
Fe	0.0706	35.008	0.3589	15.358	0.5819	5.561	−0.0114	0.1398
Fe^{+}	0.1251	34.963	0.3629	15.514	0.5223	5.591	−0.0105	0.1301
Fe^{2+}	0.0263	34.960	0.3668	15.943	0.6188	5.594	−0.0119	0.1437
Fe^{3+}	0.3972	13.244	0.6295	4.903	−0.0314	0.350	0.0044	0.0441
Fe^{4+}	0.3782	11.380	0.6556	4.592	−0.0346	0.483	0.0005	0.0362
Co	0.4139	16.162	0.6013	4.780	−0.1518	0.021	0.1345	0.1033
Co^{+}	0.0990	33.125	0.3645	15.177	0.5470	5.008	−0.0109	0.0983
Co^{2+}	0.4332	14.355	0.5857	4.608	−0.0382	0.134	0.0179	0.0711
Co^{3+}	0.3902	12.508	0.6324	4.457	−0.1500	0.034	0.1272	0.0515
Co^{4+}	0.3515	10.778	0.6778	4.234	−0.0389	0.241	0.0098	0.0390
Ni	−0.0172	35.739	0.3174	14.269	0.7136	4.566	−0.0143	0.1072
Ni^{+}	0.0705	35.856	0.3984	13.804	0.5427	4.397	−0.0118	0.0738
Ni^{2+}	0.0163	35.883	0.3916	13.223	0.6052	4.339	−0.0133	0.0817
Ni^{3+}	0.0012	35.000	0.3468	11.987	0.6667	4.252	−0.0148	0.0883
Ni^{4+}	−0.0090	35.861	0.2776	11.790	0.7474	4.201	−0.0163	0.0966
Cu	0.0909	34.984	0.4088	11.443	0.5128	3.825	−0.0124	0.0513
Cu^{+}	0.0749	34.966	0.4147	11.764	0.5238	3.850	−0.0127	0.0591
Cu^{2+}	0.0232	34.969	0.4023	11.564	0.5882	3.843	−0.0137	0.0532
Cu^{3+}	0.0031	34.907	0.3582	10.914	0.6531	3.828	−0.0147	0.0665
Cu^{4+}	−0.0132	30.682	0.2801	11.163	0.7490	3.817	−0.0165	0.0767

compute from them a consistent set of bound scattering cross sections. In the present version, we have used the values of the coherent and incoherent scattering lengths recommended by Koester, Rauch & Seymann (1991), supplemented with a few more recently measured values, and have computed from them the corresponding scattering cross sections. The trailing digits in parentheses give the standard errors calculated from the errors in the input data using the statistical theory of error propagation (Young, 1962). The imaginary parts of the scattering lengths, which are appreciable only for strongly absorbing nuclides, were calculated from the measured absorption cross sections (Mughabghab, Divadeenam & Holden, 1981; Mughabghab, 1984) and are listed beneath the real parts of Table 4.4.4.1.

In a few cases, where the scattering lengths have not yet been measured directly, the available scattering cross-section data (Mughabghab, Divadeenam & Holden, 1981; Mughabghab, 1984) were used to obtain the scattering lengths. Equations (4.4.4.11), (4.4.4.12), and (4.4.4.13) were used, where necessary, to fill gaps in Table 4.4.4.1. For some elements, these relations indicated inconsistencies in the data. In such cases, appropriate adjustments in the values of some of the quantities were made. In almost all cases, such adjustments were comparable with the stated errors. Finally, for some elements, it was necessary to estimate arbitrarily the scattering lengths of one or two isotopes in order to be able to complete the table. Such estimates are indicated by the letter '*E*' and were usually made only for isotopes of low natural abundance where the estimated values have only a marginal effect on the final results. Apart from the inclusion of new data for Ti and Mn, the values listed in Table 4.4.4.1 are the same as in Sears (1992*b*).

4.4.5. Magnetic form factors (By P. J. Brown)

The form factors used in the calculations of the cross sections for magnetic scattering of neutrons are defined in Subsection 6.1.2.3 as

$$\langle j_l(k) \rangle = \int_0^\infty U^2(r) j_l(kr) 4\pi r^2 \, \mathrm{d}r, \qquad (4.4.5.1)$$