$$I \propto \int \mathrm{d}^3k_i \int \mathrm{d}^3k_f P_i(\mathbf{k}_i) S(\mathbf{k}_i \rightarrow \mathbf{k}_f) P_f(\mathbf{k}_f), \qquad (4.4.3.1)$$

where $P_i(\mathbf{k}_i)$ is the probability that a neutron of wavevector $\mathbf{k}_i$ is incident on the sample, $P_f(\mathbf{k}_f)$ is the probability that a neutron of wavevector $\mathbf{k}_f$ is transmitted by the analyser system and $S(\mathbf{k}_i \rightarrow \mathbf{k}_f)$ is the probability that the sample scatters a neutron from $\mathbf{k}_i$ to $\mathbf{k}_f$. The fluctuation spectrum of the sample, $S(\mathbf{k}_i \rightarrow \mathbf{k}_f)$, does not depend separately on $\mathbf{k}_i$ and $\mathbf{k}_f$ but rather on the scattering vector $\mathbf{Q}$ and energy transfer $\hbar\omega$ defined by the conservation equations

$$\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f; \quad \hbar\omega = \frac{\hbar^2}{2m}(k_i^2 - k_f^2), \qquad (4.4.3.2)$$

where m is the neutron mass.

A number of methods of calculating the distribution functions $P_i(\mathbf{k}_i)$ and $P_f(\mathbf{k}_f)$ have been proposed. The method of independent distributions was used implicitly by Stedman (1968) and in more detail by Bjerrum Møller & Nielson (MN) (Nielsen & Bjerrum Møller, 1969; Bjerrum Møller & Nielsen, 1970) for three-axis spectrometers. Subsequently, the method has been extended to perfect-crystal monochromators (Pynn, Fujii & Shirane, 1983) and to time-of-flight spectrometers (Steinsvoll, 1973; Robinson, Pynn & Eckert, 1985). The method involves separating P_i and P_f into a product of independent distribution functions each of which can be convolved separately with the fluctuation spectrum $S(\mathbf{Q}, \omega)$ [*cf.* equation (4.4.3.1)]. Extremely simple results are obtained for the widths of scans through a phonon dispersion surface for spectrometers where the energy of scattered neutrons is analysed (Nielson & Bjerrum Møller, 1969). For diffractometers, the width of a scan through a Bragg peak may also be obtained (Pynn *et al.*, 1983), yielding a result equivalent to that given by Caglioti, Paoletti & Ricci (1960). In this case, however, the singular nature of the Bragg scattering process introduces a correlation between the distribution functions that contribute to P_i and P_f and the calculation is less transparent than it is for phonons.

A somewhat different approach, which does not explicitly separate the various contributions to the resolution, was proposed by Cooper & Nathans (CN) (Cooper & Nathans, 1967, 1968; Cooper, 1968). Minor errors were corrected by several authors (Werner & Pynn, 1971; Chesser & Axe, 1973). The CN method calculates the instrumental resolution function $R(\mathbf{Q} - \mathbf{Q}_0, \omega - \omega_0)$ as

$$R(\Delta\mathbf{Q}, \Delta\omega) = R_0 \exp -\tfrac{1}{2} \sum_{\alpha,\beta} M_{\alpha\beta} X_\alpha X_\beta, \qquad (4.4.3.3)$$

where X_1, X_2, and X_3 are the three components of $\Delta\mathbf{Q}$, $X_4 = \Delta\omega$, and $\mathbf{Q}_0$ and ω_0 are obtained from (4.4.3.2) by replacing $\mathbf{k}_i$ and $\mathbf{k}_f$ by $\mathbf{k}_I$ and $\mathbf{k}_F$, respectively. The matrix $\boldsymbol{M}$ is given in explicit form by several authors (Cooper & Nathans, 1967, 1968; Cooper, 1968; Werner & Pynn, 1971; Chesser & Axe, 1973) and the normalization R_0 has been discussed in detail by Dorner (1972). [A refutation (Tindle, 1984) of Dorner's work is incorrect.] Equation (4.4.3.3) implies that contours of constant transmission for the spectrometer [$R(\Delta\mathbf{Q}, \Delta\omega) = \text{constant}$] are ellipsoids in the four-dimensional $\mathbf{Q}$–ω space. Optimum resolution (focusing) is achieved by a scan that causes the resolution function to intersect the feature of interest in $S(\mathbf{Q}, \omega)$ (*e.g.* Bragg peak or phonon dispersion surface) for the minimum scan interval. The optimization of scans for a diffractometer has been considered by Werner (1971).

The MN and CN methods are equivalent. Using the MN formalism, it can be shown that

$$\boldsymbol{M} = (\boldsymbol{A})^{-1} \quad \text{with} \quad A_{\alpha\beta} = \sum_j \chi_{j\alpha}\chi_{j\beta}, \qquad (4.4.3.4)$$

where the $\chi_{j\alpha}$ are the components of the standard deviations of independent distributions (labelled by index j) defined by Bjerrum Møller & Nielsen (1970). In the limit $Q \rightarrow 0$, the matrices $\boldsymbol{M}$ and $\boldsymbol{A}$ are of rank three and other methods must be used to calculate the resolution ellipsoid (Mitchell, Cowley & Higgins, 1984). Nevertheless, the MN method may be used even in this case to calculate widths of scans.

To obtain the resolution function of a diffractometer (in which there is no analysis of scattered neutron energy) from the CN form for $\boldsymbol{M}$, it is sufficient to set to zero those contributions that arise from the mosaic of the analyser crystal. For elastic Bragg scattering, the problem is further simplified because X_4 [*cf.* equation (4.4.3.3)] is zero. The spectrometer resolution function is then an ellipsoid in $\mathbf{Q}$ space.

For the measurement of integrated intensities (of Bragg peaks for example), the normalization R_0 in (4.4.3.3) is required in order to obtain the Lorentz factor. The latter has been calculated for an arbitrary scan of a three-axis spectrometer (Pynn, 1975) and the results may be modified for a diffractometer as described in the preceding paragraph.

4.4.4. Scattering lengths for neutrons (By V. F. Sears)

The use of neutron diffraction for crystal-structure determinations requires a knowledge of the scattering lengths and the corresponding scattering and absorption cross sections of the elements and, in some cases, of individual isotopes. This information is needed to calculate unit-cell structure factors and to correct for effects such as absorption, self-shielding, extinction, thermal diffuse scattering, and detector efficiency (Bacon, 1975; Sears, 1989). Table 4.4.4.1 lists the best values of the neutron scattering lengths and cross sections that are available at the time of writing (January 1995). We begin by summarizing the basic relationships between the scattering lengths and cross sections of the elements and their isotopes that have been used in the compilation of this table. More background information can be found in, for example, the book by Sears (1989).

4.4.4.1. *Scattering lengths*

The scattering of a neutron by a single bound nucleus is described within the Born approximation by the Fermi pseudopotential,

$$V(\mathbf{r}) = \left(\frac{2\pi\hbar^2}{m}\right) b\delta(\mathbf{r}), \qquad (4.4.4.1)$$

in which $\mathbf{r}$ is the position of the neutron relative to the nucleus, m the neutrons mass, and b the bound scattering length. The neutron has spin $\mathbf{s}$ and the nucleus spin $\mathbf{I}$ so that, if $I \neq 0$, the Fermi pseudopotential and, hence, the bound scattering length will be spin dependent. Since $s = 1/2$, the most general rotationally invariant expression for b is

$$b = b_c + \frac{2b_i}{\sqrt{I(I+1)}}\,\mathbf{s}\cdot\mathbf{I}, \qquad (4.4.4.2)$$

in which the coefficients b_c and b_i are called the bound coherent and incoherent scattering lengths. If $I = 0$, then $b_i = 0$ by convention.

Table 4.4.4.1. *Bound scattering lengths, b, in fm and cross sections, σ, in barns (1 barn = 100 fm²) of the elements and their isotopes*

Z: atomic number; A: mass number; $I(\pi)$: spin (parity) of the nuclear ground state; c: % natural abundance (for radioisotopes, the half-life is given instead in annums); b_c: bound coherent scattering length; b_i: bound incoherent scattering length; σ_c: bound coherent scattering cross section; σ_i: bound incoherent scattering cross section; σ_s: total bound scattering cross section; σ_a: absorption cross section for 2200 m s^{-1} neutrons (E = 25.30 meV, k = 3.494 Å^{-1}, λ = 1.798 Å); $i = \sqrt{-1}$.

Element	Z	A	$I(\pi)$	c	b_c	b_i	σ_c	σ_i	σ_s	σ_a
H	1				−3.7390(11)		1.7568(10)	80.26(6)	82.02(6)	0.3326(7)
		1	1/2(+)	99.985	−3.7406(11)	25.274(9)	1.7583(10)	80.27(6)	82.03(6)	0.3326(7)
		2	1(+)	0.015	6.671(4)	4.04(3)	5.592(7)	2.05(3)	7.64(3)	0.000519(7)
		3	1/2(+)	(12.32a)	4.792(27)	−1.04(17)	2.89(3)	0.14(4)	3.03(5)	0
He	2				3.26(3)		1.34(2)	0.00	1.34(2)	0.00747(1)
		3	1/2(+)	0.00014	5.74(7)	−2.5(6)	4.42(10)	1.6(4)	6.0(4)	5333.(7.)
					−1.483(2)i	+2.568(3)i				
		4	0(+)	99.99986	3.26(3)	0	1.34(2)	0	1.34(2)	0
Li	3				−1.90(2)		0.454(14)	0.92(3)	1.37(3)	70.5(3)
		6	1(+)	7.5	2.00(11)	−1.89(5)	0.51(5)	0.46(2)	0.97(7)	940.(4.)
					−0.261(1)i	0.257(11)i				
		7	3/2(−)	92.5	−2.22(2)	−2.49(5)	0.619(11)	0.78(3)	1.40(3)	0.0454(3)
Be	4	9	3/2(−)	100	7.79(1)	0.12(3)	7.63(2)	0.0018(9)	7.63(2)	0.0076(8)
B	5				5.30(4)		3.54(5)	1.70(12)	5.24(11)	767.(8.)
					0.213(2)i					
		10	3(+)	20.0	−0.1(3)	−4.7(3)	0.144(8)	3.0(4)	3.1(4)	3835.(9.)
					1.066(3)i	1.231(3)i				
		11	3/2(−)	80.0	6.65(4)	−1.3(2)	5.56(7)	0.22(6)	5.78(9)	0.0055(33)
C	6				6.6460(12)		5.550(2)	0.001(4)	5.551(3)	0.00350(7)
		12	0(+)	98.90	6.6511(16)	0	5.559(3)	0	5.559(3)	0.00353(7)
		13	1/2(−)	1.10	6.19(9)	−0.52(9)	4.81(14)	0.034(12)	4.84(14)	0.00137(4)
N	7				9.36(2)		11.01(5)	0.50(12)	11.51(11)	1.90(3)
		14	1(+)	99.63	9.37(2)	2.0(2)	11.03(5)	0.5(1)	11.53(11)	1.91(3)
		15	1/2(−)	0.37	6.44(3)	−0.02(2)	5.21(5)	0.00005(10)	5.21(5)	0.000024(8)
O	8				5.803(4)		4.232(6)	0.000(8)	4.232(6)	0.00019(2)
		16	0(+)	99.762	5.803(4)	0	4.232(6)	0	4.232(6)	0.00010(2)
		17	5/2(+)	0.038	5.78(12)	0.18(6)	4.20(22)	0.004(3)	4.20(22)	0.236(10)
		18	0(+)	0.200	5.84(7)	0	4.29(10)	0	4.29(10)	0.00016(1)
F	9	19	1/2(+)	100	5.654(10)	−0.082(9)	4.017(17)	0.0008(2)	4.018(14)	0.0096(5)
Ne	10				4.566(6)		2.620(7)	0.008(9)	2.628(6)	0.039(4)
		20	0(+)	90.51	4.631(6)	0	2.695(7)	0	2.695(7)	0.036(4)
		21	3/2(+)	0.27	6.66(19)	±0.6(1)	5.6(3)	0.05(2)	5.7(3)	0.67(11)
		22	0(+)	9.22	3.87(1)	0	1.88(1)	0	1.88(1)	0.046(6)
Na	11	23	3/2(+)	100	3.63(2)	3.59(3)	1.66(2)	1.62(3)	3.28(4)	0.530(5)
Mg	12				5.375(4)		3.631(5)	0.08(6)	3.71(4)	0.063(3)
		24	0(+)	78.99	5.66(3)	0	4.03(4)	0	4.03(4)	0.050(5)
		25	5/2(+)	10.00	3.62(14)	1.48(10)	1.65(13)	0.28(4)	1.93(14)	0.19(3)
		26	0(+)	11.01	4.89(15)	0	3.00(18)	0	3.00(18)	0.0382(8)
Al	13	27	5/2(+)	100	3.449(5)	0.256(10)	1.495(4)	0.0082(7)	1.503(4)	0.231(3)
Si	14				4.1491(10)		2.1633(10)	0.004(8)	2.167(8)	0.171(3)
		28	0(+)	92.23	4.107(6)	0	2.120(6)	0	2.120(6)	0.177(3)
		29	1/2(+)	4.67	4.70(10)	0.09(9)	2.78(12)	0.001(2)	2.78(12)	0.101(14)
		30	0(+)	3.10	4.58(8)	0	2.64(9)	0	2.64(9)	0.107(2)
P	15	31	1/2(+)	100	5.13(1)	0.2(2)	3.307(13)	0.005(10)	3.312(16)	0.172(6)
S	16				2.847(1)		1.0186(7)	0.007(5)	1.026(5)	0.53(1)
		32	0(+)	95.02	2.804(2)	0	0.9880(14)	0	0.9880(14)	0.54(4)
		33	3/2(+)	0.75	4.74(19)	1.5(1.5)	2.8(2)	0.3(6)	3.1(6)	0.54(4)
		34	0(+)	4.21	3.48(3)	0	1.52(3)	0	1.52(3)	0.227(5)
		36	0(+)	0.02	3.(1.) E	0	1.1(8)	0	1.1(8)	0.15(3)

Table 4.4.4.1. *Bound scattering lengths (cont.)*

Element	Z	A	$I(\pi)$	c	b_c	b_i	σ_c	σ_i	σ_s	σ_a
Cl	17				9.5770(8)		11.526(2)	5.3(5)	16.8(5)	33.5(3)
		35	3/2(+)	75.77	11.65(2)	6.1(4)	17.06(6)	4.7(6)	21.8(6)	44.1(4)
		37	3/2(+)	24.23	3.08(6)	0.1(1)	1.19(5)	0.001(3)	1.19(5)	0.433(6)
Ar	18				1.909(6)		0.458(3)	0.22(2)	0.683(4)	0.675(9)
		36	0(+)	0.337	24.90(7)	0	77.9(4)	0	77.9(4)	5.2(5)
		38	0(+)	0.063	3.5(3.5)	0	1.5(3.1)	0	1.5(3.1)	0.8(2)
		40	0(+)	99.600	1.830(6)	0	0.421(3)	0	0.421(3)	0.660(9)
K	19				3.67(2)		1.69(2)	0.27(11)	1.96(11)	2.1(1)
		39	3/2(+)	93.258	3.74(2)	1.4(3)	1.76(2)	0.25(11)	2.01(11)	2.1(1)
		40	4(−)	0.012	3.(1.) *E*		1.1(8)	0.5(5)	1.6(9)	35.(8.)
		41	3/2(+)	6.730	2.69(8)	1.5(1.5)	0.91(5)	0.3(6)	1.2(6)	1.46(3)
Ca	20				4.70(2)		2.78(2)	0.05(3)	2.83(2)	0.43(2)
		40	0(+)	96.941	4.80(2)	0	2.90(2)	0	2.90(2)	0.41(2)
		42	0(+)	0.647	3.36(10)	0	1.42(8)	0	1.42(8)	0.68(7)
		43	7/2(−)	0.135	−1.56(9)	0.31(4)	0.5(5) *E*		0.8(5)	6.2(6)
		44	0(+)	2.086	1.42(6)	0	0.25(2)	0	0.25(2)	0.88(5)
		46	0(+)	0.004	3.6(2)	0	1.6(2)	0	1.6(2)	0.74(7)
		48	0(+)	0.187	0.39(9)	0	0.019(9)	0	0.019(9)	1.09(14)
Sc	21	45	7/2(−)	100	12.29(11)	−6.0(3)	19.0(3)	4.5(5)	23.5(6)	27.5(2)
Ti	22				−3.370(13)		1.427(11)	2.63(3)	4.06(3)	6.43(6)
		46	0(+)	8.2	4.725(5)	0	2.80(6)	0	2.80(6)	0.59(18)
		47	5/2(−)	7.4	3.53(7)	−3.5(2)	1.57(6)	1.5(2)	3.1(2)	1.7(2)
		48	0(+)	73.8	−5.86(2)	0	4.32(3)	0	4.32(3)	8.30(9)
		49	7/2(−)	5.4	0.98(5)	5.1(2)	0.12(1)	3.3(3)	3.4(3)	2.2(3)
		50	0(+)	5.2	5.88(10)	0	4.34(15)	0	4.34(15)	0.179(3)
V	23				−0.3824(12)		0.01838(12)	5.08(6)	5.10(6)	5.08(2)
		50	6(+)	0.250	7.6(6)		7.3(1.1)	0.5(5) *E*	7.8(1.0)	60.(40.)
		51	7/2(−)	99.750	−0.402(2)	6.435(4)	0.0203(2)	5.07(6)	5.09(6)	4.9(1)
Cr	24				3.635(7)		1.660(6)	1.83(2)	3.49(2)	3.05(8)
		50	0(+)	4.35	−4.50(5)	0	2.54(6)	0	2.54(6)	15.8(2)
		52	0(+)	83.79	4.920(10)	0	3.042(12)	0	3.042(12)	0.76(6)
		53	3/2(−)	9.50	−4.20(3)	6.87(10)	2.22(3)	5.93(17)	8.15(17)	18.1(1.5)
		54	0(+)	2.36	4.55(10)	0	2.60(11)	0	2.60(11)	0.36(4)
Mn	25	55	5/2(−)	100	−3.750(18)	1.79(4)	1.77(2)	0.40(2)	2.17(3)	13.3(2)
Fe	26				9.45(2)		11.22(5)	0.40(11)	11.62(10)	2.56(3)
		54	0(+)	5.8	4.2(1)	0	2.2(1)	0	2.2(1)	2.25(18)
		56	0(+)	91.7	9.94(3)	0	12.42(7)	0	12.42(7)	2.59(14)
		57	1/2(−)	2.2	2.3(1)	0.66(6)		0.3(3) *E*	1.0(3)	2.48(30)
		58	0(+)	0.3	15.(7.)	0	28.(26.)	0	28.(26.)	1.28(5)
Co	27	59	7/2(−)	100	2.49(2)	−6.2(2)	0.779(13)	4.8(3)	5.6(3)	37.18(6)
Ni	28				10.3(1)		13.3(3)	5.2(4)	18.5(3)	4.49(16)
		58	0(+)	68.27	14.4(1)	0	26.1(4)	0	26.1(4)	4.6(3)
		60	0(+)	26.10	2.8(1)	0	0.99(7)	0	0.99(7)	2.9(2)
		61	3/2(−)	1.13	7.60(6)	±3.9(3)	7.26(11)	1.9(3)	9.2(3)	2.5(8)
		62	0(+)	3.59	−8.7(2)	0	9.5(4)	0	9.5(4)	14.5(3)
		64	0(+)	0.91	−0.37(7)	0	0.017(7)	0	0.017(7)	1.52(3)
Cu	29				7.718(4)		7.485(8)	0.55(3)	8.03(3)	3.78(2)
		63	3/2(−)	69.17	6.43(15)	0.22(2)	5.2(2)	0.006(1)	5.2(2)	4.50(2)
		65	3/2(−)	30.83	10.61(19)	1.79(10)	14.1(5)	0.40(4)	14.5(5)	2.17(3)
Zn	30				5.60(5)		4.054(7)	0.077(7)	4.131(10)	1.11(2)
		64	0(+)	48.6	5.22(4)	0	3.42(5)	0	3.42(5)	0.93(9)
		66	0(+)	27.9	5.97(5)	0	4.48(8)	0	4.48(8)	0.62(6)
		67	5/2(−)	4.1	7.56(8)	−1.50(7)	7.18(15)	0.28(3)	7.46(15)	6.8(8)
		68	0(+)	18.8	6.03(3)	0	4.57(5)	0	4.57(5)	1.1(1)
		70	0(+)	0.6	6.(1.) *E*	0	4.5(1.5)	0	4.5(1.5)	0.092(5)

Table 4.4.4.1. *Bound scattering lengths (cont.)*

Element	Z	A	$I(\pi)$	c	b_c	b_i	σ_c	σ_i	σ_s	σ_a
Ga	31				7.288(2)		6.675(4)	0.16(3)	6.83(3)	2.75(3)
		69	3/2(−)	60.1	7.88(2)	−0.85(5)	7.80(4)	0.091(11)	7.89(4)	2.18(5)
		71	3/2(−)	39.9	6.40(3)	−0.82(4)	5.15(5)	0.084(8)	5.23(5)	3.61(10)
Ge	32				8.185(20)		8.42(4)	0.18(7)	8.60(6)	2.20(4)
		70	0(+)	20.5	10.0(1)	0	12.6(3)	0	12.6(3)	3.0(2)
		72	0(+)	27.4	8.51(10)	0	9.1(2)	0	9.1(2)	0.8(2)
		73	9/2(+)	7.8	5.02(4)	3.4(3)	3.17(5)	1.5(3)	4.7(3)	15.1(4)
		74	0(+)	36.5	7.58(10)	0	7.2(2)	0	7.2(2)	0.4(2)
		76	0(+)	7.8	8.21(1.5)	0	8.(3.)	0	8.(3.)	0.16(2)
As	33	75	3/2(−)	100	6.58(1)	−0.69(5)	5.44(2)	0.060(10)	5.50(2)	4.5(1)
Se	34				7.970(9)		7.98(2)	0.33(6)	8.30(6)	11.7(2)
		74	0(+)	0.9	0.8(3.0)	0	0.1(6)	0	0.1(6)	51.8(1.2)
		76	0(+)	9.0	12.2(1)	0	18.7(3)	0	18.7(3)	85.(7.)
		77	1/2(−)	7.6	8.25(8)	±0.6(1.6)	8.6(2)	0.05(26)	8.65(16)	42.(4.)
		78	0(+)	23.5	8.24(9)	0	8.5(2)	0	8.5(2)	0.43(2)
		80	0(+)	49.6	7.48(3)	0	7.03(6)	0	7.03(6)	0.61(5)
		82	0(+)	9.4	6.34(8)	0	5.05(13)	0	5.05(13)	0.044(3)
Br	35				6.795(15)		5.80(3)	0.10(9)	5.90(9)	6.9(2)
		79	3/2(−)	50.69	6.80(7)	−1.1(2)	5.81(12)	0.15(6)	5.96(13)	11.0(7)
		81	3/2(−)	49.31	6.79(7)	0.6(1)	5.79(12)	0.05(2)	5.84(12)	2.7(2)
Kr	36				7.81(2)		7.67(4)	0.01(14)	7.68(13)	25.(1.)
		78	0(+)	0.35		0		0		6.4(9)
		80	0(+)	2.25		0		0		11.8(5)
		82	0(+)	11.6		0		0		29.(20.)
		83	9/2(+)	11.5		185(30.)				
		84	0(+)	57.0		0		0		0.113(15)
		86	0(+)	17.3	8.1(2)	0	8.2(4)	0	8.2(4)	0.003(2)
Rb	37				7.09(2)		6.32(4)	0.5(4)	6.8(4)	0.38(4)
		85	5/2(−)	72.17	7.03(10)	6.2(2)	0.5(5)	*E*	6.7(5)	0.48(1)
		87	3/2(−)	27.83	7.23(12)	6.6(2)	0.5(5)	*E*	7.1(5)	0.12(3)
Sr	38				7.02(2)		6.19(4)	0.06(11)	6.25(10)	1.28(6)
		84	0(+)	0.56	7.(1.) *E*	0	6.(2.)	0	6.(2.)	0.87(7)
		86	0(+)	9.86	5.67(5)	0	4.04(7)	0	4.04(7)	1.04(7)
		87	9/2(+)	7.00	7.40(7)	6.88(13)	0.5(5)	*E*	7.4(5)	16.(3.)
		88	0(+)	82.58	7.15(6)	0	6.42(11)	0	6.42(11)	0.058(4)
Y	39	89	1/2(−)	100	7.75(2)	1.1(3)	7.55(4)	0.15(8)	7.70(9)	1.28(2)
Zr	40				7.16(3)		6.44(5)	0.02(15)	6.46(14)	0.185(3)
		90	0(+)	51.45	6.4(1)	0	5.1(2)	0	5.1(2)	0.011(5)
		91	5/2(+)	11.32	8.7(1)	−1.08(15)	9.5(2)	0.15(4)	9.7(2)	1.17(10)
		92	0(+)	17.19	7.4(2)	0	6.9(4)	0	6.9(4)	0.22(6)
		94	0(+)	17.28	8.2(2)	0	8.4(4)	0	8.4(4)	0.0499(24)
		96	0(+)	2.76	5.5(1)	0	3.8(1)	0	3.8(1)	0.0229(10)
Nb	41	93	9/2(+)	100	7.054(3)	−0.139(10)	6.253(5)	0.0024(3)	6.255(5)	1.15(5)
Mo	42				6.715(2)		5.67(3)	0.04(5)	5.71(4)	2.48(4)
		92	0(+)	14.84	6.91(8)	0	6.00(14)	0	6.00(14)	0.019(2)
		94	0(+)	9.25	6.80(7)	0	5.81(12)	0	5.81(12)	0.015(2)
		95	5/2(+)	15.92	6.91(6)	6.00(10)	0.5(5)	*E*	6.5(5)	13.1(3)
		96	0(+)	16.68	6.20(6)	0	4.83(9)	0	4.83(9)	0.5(2)
		97	5/2(+)	9.55	7.24(8)	6.59(15)	0.5(5)	*E*	7.1(5)	2.5(2)
		98	0(+)	24.13	6.58(7)	0	5.44(12)	0	5.44(12)	0.127(6)
		100	0(+)	9.63	6.73(7)	0	5.69(12)	0	5.69(12)	0.4(2)
Tc	43									
		99	9/2(+)	$(2.13\times10^5$a)	6.8(3)	5.8(5)	0.5(5)	*E*	6.3(7)	20.(1.)

Table 4.4.4.1. *Bound scattering lengths (cont.)*

Element	Z	A	$I(\pi)$	c	b_c	b_i	σ_c	σ_i	σ_s	σ_a
Ru	44				7.03(3)		6.21(5)	0.4(1)	6.6(1)	2.56(13)
		96	0(+)	5.5	0	0	0.28(2)			
		98	0(+)	1.9	0	0	<8.0			
		99	5/2(+)	12.7	6.9(1.0)					
		100	0(+)	12.6	0	0	4.8(6)			
		101	5/2(+)	17.0	3.3(9)					
		102	0(+)	31.6	0	0	1.17(7)			
		104	0(+)	18.7	0	0	0.31(2)			
Rh	45	103	1/2(−)	100	5.88(4)	4.34(6)	0.3(3)	*E*	4.6(3)	144.8(7)
Pd	46				5.91(6)		4.39(9)	0.093(9)	4.48(9)	6.9(4)
		102	0(+)	1.02	7.7(7) *E*	0	7.5(1.4)	0	7.5(1.4)	3.4(3)
		104	0(+)	11.14	7.7(7) *E*	0	7.5(1.4)	0	7.5(1.4)	0.6(3)
		105	5/2(+)	22.33	5.5(3)	−2.6(1.6)	3.8(4)	0.8(1.0)	4.6(1.1)	20.(3.)
		106	0(+)	27.33	6.4(4)	0	5.1(6)	0	5.1(6)	0.304(29)
		108	0(+)	26.46	4.1(3)	0	2.1(3)	0	2.1(3)	8.5(5)
		110	0(+)	11.72	7.7(7)*E*	0	7.5(1.4)	0	7.5(1.4)	0.226(31)
Ag	47				5.922(7)		4.407(10)	0.58(3)	4.99(3)	63.3(4)
		107	1/2(−)	51.839	7.555(11)	1.00(13)	7.17(2)	0.13(3)	7.30(4)	37.6(1.2)
		109	1/2(−)	48.161	4.165(11)	−1.60(13)	2.18(1)	0.32(5)	2.50(5)	91.0(1.0)
Cd	48				4.87(5)		3.04(6)	3.46(13)	6.50(12)	2520.(50.)
					−0.70(1)*i*					
		106	0(+)	1.25	5.(2.) *E*	0	3.1(2.5)	0	3.1(2.5)	1.
		108	0(+)	0.89	5.4(1)	0	3.7(1)	0	3.7(1)	1.1(3)
		110	0(+)	12.51	5.9(1)	0	4.4(1)	0	4.4(1)	11.(1.)
		111	1/2(+)	12.81	6.5(1)	5.3(2)	0.3(3)	*E*	5.6(4)	24(3.)
		112	0(+)	24.13	6.4(1)	0	5.1(2)	0	5.1(2)	2.2(5)
		*113	1/2(+)	12.22	−8.0(2)	12.1(4)	0.3(3) *E*	12.4(5)		20600(400.)
					−5.73(11)*i*					
		114	0(+)	28.72	7.5(1)	0	7.1(2)	0	7.1(2)	0.34(2)
		116	0(+)	7.47	6.3(1)	0	5.0(2)	0	5.0(2)	0.075(13)
In	49			4.065(20)	2.08(2)	0.54(11)	2.62(11)	193.8(1.5)		
					−0.0539(4)*i*					
		113	9/2(+)	43	5.39(6)	±0.017(1)	3.65(8)	0.000037(5)	3.65(8)	12.0(1.1)
		115	9/2(+)	957	4.01(2)	−2.1(2)	2.02(2)	0.55(11)	2.57(11)	202(2.)
					−0.0562(6)*i*					
Sn	50				6.225(2)		4.870(3)	0.022(5)	4.892(6)	0.626(9)
		112	0(+)	1.0	6.1(1.) *E*	0	4.5(1.5)	0	4.5(1.5)	1.01(11)
		114	0(+)	0.7	6.2(3)	0	4.8(5)	0	4.8(5)	0.114(30)
		115	1/2(+)	0.4	6.(1.) *E*	4.5(1.5)	0.3(3) *E*	4.8(1.5)	30(7.)	
		116	0(+)	14.7	5.93(5)	0	4.42(7)	0	4.42(7)	0.14(3)
		117	1/2(+)	7.7	6.48(5)	5.28(8)	0.3(3) *E*	5.6(3)	2.3(5)	
		118	0(+)	24.3	6.07(5)	0	4.63(8)	0	4.63(8)	0.22(5)
		119	1/2(+)	8.6	6.12(5)	4.71(8)	0.3(3) *E*	5.0(3)	2.2(5)	
		120	0(+)	32.4	6.49(5)	0	5.29(8)	0	5.29(8)	0.14(3)
		122	0(+)	4.6	5.74(5)	0	4.14(7)	0	4.14(7)	0.18(2)
		124	0(+)	5.6	5.97(5)	0	4.48(8)	0	4.48(8)	0.133(5)
Sb	51				5.57(3)		3.90(4)	0.00(7)	3.90(6)	4.91(5)
		121	7/2(+)	57.3	5.71(6)	−0.05(15)	4.10(9)	0.0003(19)	4.10(9)	5.75(12)
		123	5/2(+)	42.7	5.38(7)	−0.10(15)	3.64(9)	0.001(4)	3.64(9)	3.8(2)
Te	52				5.80(3)		4.23(4)	0.09(1)	4.32(4)	4.05(5)
		120	0(+)	0.096	5.3(5)	0	3.5(7)	0	3.4(7)	2.3(3)
		122	0(+)	2.60	3.8(2)	0	1.8(2)	0	1.8(2)	3.4(5)
		123	1/2(+)	0.908	−0.05(25)	−2.04(9)	0.002(3)	0.52(5)	0.52(5)	418(30.)
					−0.116(8)*i*					
		124	0(+)	4.816	7.96(10)	0	8.0(2)	0	8.0(2)	6.8(1.3)
		125	1/2(+)	7.14	5.02(8)	−0.26(13)	3.17(10)	0.008(8)	3.18(10)	1.55(16)
		126	0(+)	18.95	5.56(7)	0	3.88(10)	0	3.88(10)	1.04(15)
		128	0(+)	31.69	5.89(7)	0	4.36(10)	0	4.36(10)	0.215(8)
		130	0(+)	33.80	6.02(7)	0	4.55(11)	0	4.55(11)	0.29(6)

Table 4.4.4.1. *Bound scattering lengths (cont.)*

Element	Z	A	$I(\pi)$	c	b_c	b_i	σ_c	σ_i	σ_s	σ_a
I	53	127	5/2(+)	100	5.28(2)	1.58(15)	3.50(3)	0.31(6)	3.81(7)	6.15(6)
Xe	54				4.92(3)		3.04(4)			23.9(1.2)
		124	0(+)	0.10		0		0		165.(20.)
		126	0(+)	0.09		0		0		3.5(8)
		128	0(+)	1.91		0		0		< 8.
		129	1/2(+)	26.4						21.(5.)
		130	0(+)	4.1		0		0		< 26.
		131	3/2(+)	21.2						85.(10.)
		132	0(+)	26.9		0		0		0.45(6)
		134	0(+)	10.4		0		0		0.265(20)
		136	0(+)	8.9		0		0		0.26(2)
Cs	55	133	7/2(+)	100	5.42(2)	1.29(15)	3.69(3)	0.21(5)	3.90(6)	29.0(1.5)
Ba	56				5.07(3)		3.23(4)	0.15(11)	3.38(10)	1.1(1)
		130	0(+)	0.11	−3.6(6)	0	1.6(5)	0	1.6(5)	30(5.)
		132	0(+)	0.10	7.8(3)	0	7.6(6)	0	7.6(6)	7.0(8)
		134	0(+)	2.42	5.7(1)	0	4.08(14)	0	4.08(14)	2.0(1.6)
		135	3/2(+)	6.59	4.67(10)		2.74(12)	0.5(5) *E*	3.2(5)	5.8(9)
		136	0(+)	7.85	4.91(8)	0	3.03(10)	0	3.03(10)	0.68(17)
		137	3/2(+)	11.23	6.83(10)		5.86(17)	0.5(5) *E*	6.4(5)	3.6(2)
		138	0(+)	71.70	4.84(8)	0	2.94(10)	0	2.94(10)	0.27(14)
La	57				8.24(4)		8.53(8)	1.13(19)	9.66(17)	8.97(5)
		138	5(+)	0.09	8.(2.) *E*	8.(4.)	0.5(5) *E*	8.5(4.0)	57.(6.)	
		139	7/2(+)	99.91	8.24(4)	3.0(2)	8.53(8)	1.13(15)	9.66(17)	8.93(4)
Ce	58				4.84(2)		2.94(2)	0.00(10)	2.94(10)	0.63(4)
		136	0(+)	0.19	5.80(9)	0	4.23(13)	0	4.23(13)	7.3(1.5)
		138	0(+)	0.25	6.70(9)	0	5.64(15)	0	5.64(15)	1.1(3)
		140	0(+)	88.48	4.84(9)	0	2.94(11)	0	2.94(11)	0.57(4)
		142	0(+)	11.08	4.75(9)	0	2.84(11)	0	2.84(11)	0.95(5)
Pr	59	141	5/2(+)	100	4.58(5)	−0.35(3)	2.64(6)	0.015(3)	2.66(6)	11.5(3)
Nd	60				7.69(5)		7.43(10)	9.2(8)	16.6(8)	50.5(1.2)
		142	0(+)	27.16	7.7(3)	0	7.5(6)	0	7.5(6)	18.7(7)
		143	7/2(−)	12.18	14.2(5) *E*	±21.1(6)	25.(7.)	55.(7.)	80.(2.)	334.(10.)
		144	0(+)	23.80	2.8(3)	0	1.0(2)	0	1.0(2)	3.6(3)
		145	7/2(−)	8.29	14.2(5)	*E*	25.(7.)	5.(5.) *E*	30.(9.)	42.(2.)
		146	0(+)	17.19	8.7(2)	0	9.5(4)	0	9.5(4)	1.4(1)
		148	0(+)	5.75	5.7(3)	0	4.1(4)	0	4.1(4)	2.5(2)
		150	0(+)	5.63	5.3(2)	0	3.5(3)	0	3.5(3)	1.2(2)
Pm	61									
		147	7/2(+)	(2.62a)	12.6(4)	±3.2(2.5)	20.0(1.3)	1.3(2.0)	21.3(1.5)	168.4(3.5)
Sm	62				0.80(2) −1.65(2)*i*		0.422(9)	39.(3.)	39.(3.)	5922.(56.)
		144	0(+)	3.1	−3.(4.) *E*	0	1.(3.)	0	1.(3.)	0.7(3)
		147	7/2(−)	15.1	14(3.)	±11.(7.)	25.(11.)	14.(19.)	39(16.)	57(3.)
		148	0(+)	11.3	−3.(4.) *E*	0	1.(3.)	0	1.(3.)	2.4(6)
		*149	7/2(−)	13.9	−19.2(1) −11.7(1)*i*	±31.4(6) −10.3(1)*i*	63.5(6)	137.(5.)	200.(5.)	42080.(400.)
		150	0(+)	7.4	14(3.)	0	25(11.)	0	25(11.)	104(4.)
		152	0(+)	26.6	−5.0(6)	0	3.1(8)	0	3.1(8)	206.(6.)
		154	0(+)	22.6	9.3(1.0)	0	11.(2.)	0	11.(2.)	8.4(5)
Eu	63				7.22(2) −1.26(1)*i*		6.75(4)	2.5(4)	9.2(4)	4530.(40.)
		*151	5/2(+)	47.8	6.13(14) −2.53(3)*i*	±4.5(4) −2.14(2)*i*	5.5(2)	3.1(4)	8.4(4)	9100(100.)
		153	5/2(+)	52.2	8.22(12)	±3.2(9)	8.5(2)	1.3(7)	9.8(7)	312.(7.)

Table 4.4.4.1.*Bound scattering lengths (cont.)*

Element	Z	A	$I(\pi)$	c	b_c	b_i	σ_c	σ_i	σ_s	σ_a
Gd	64				6.5(5) −13.82(3)*i*		29.3(8)	151.(2.)	180.(2.)	49700.(125.)
		152	0(+)	0.2	10.(3.) *E*	0	13.(8.)	0	13.(8.)	735.(20.)
		154	0(+)	2.1	10.(3.) *E*	0	13.(8.)	0	13.(8.)	85.(12.)
		*155	3/2(−)	14.8	6.0(1) −17.0(1)*i*	±5.(5.) *E* −13.16(9)*i*	40.8(4.)	25.(6.)	66.(6.)	61100.(400.)
		156	0(+)	20.6	6.3(4)	0	5.0(6)	0	5.0(6)	1.5(1.2)
		*157	3/2(−)	15.7	−1.14(2) −71.9(2)*i*	±5.(5.) *E* −55.8(2)*i*	650(4.)	394.(7.)	1044.(8.)	259000.(700.)
		158	0(+)	24.8	9.(2.)	0	10.(5.)	0	10.(5.)	2.2(2)
		160	0(+)	21.8	9.15(5)	0	10.52(11)	0	10.52(11)	0.77(2)
Tb	65	159	3/2(+)	100	7.38(3)	−0.17(7)	6.84(6)	0.004(3)	6.84(6)	23.4(4)
Dy	66				16.9(2) −0.276(4)*i*		35.9(8)	54.4(1.2)	90.3(9)	994.(13.)
		156	0(+)	0.06	6.1(5)	0	4.7(8)	0	4.7(8)	33.(3.)
		158	0(+)	0.10	6.(4.) *E*	0	5.(6.)	0	5.(6.)	43.(6.)
		160	0(+)	2.34	6.7(4)	0	5.6(7)	0	5.6(7)	56.(5.)
		161	5/2(+)	19.0	10.3(4)	±4.9(8)	13.3(1.0)	3.(1.)	16.(1.)	600.(25.)
		162	0(+)	25.5	−1.4(5)	0	0.25(18)	0	0.25(18)	194.(10.)
		163	5/2(−)	24.9	5.0(4)	1.3(3)	3.1(5)	0.21(10)	3.3(5)	124.(7.)
		164	0(+)	28.1	49.4(5) −0.79(1)*i*	0	307.(3.)	0	307.(3.)	2840.(40.)
Ho	67	165	7/2(−)	100	8.01(8)	−1.70(8)	8.06(16)	0.36(3)	8.42(16)	64.7(1.2)
Er	68				7.79(2)		7.63(4)	1.1(3)	8.7(3)	159.(4.)
		162	0(+)	0.14	8.8(2)	0	9.7(4)	0	9.7(4)	19.(2.)
		164	0(+)	1.56	8.2(2)	0	8.4(4)	0	8.4(4)	13.(2.)
		166	0(+)	33.4	10.6(2)	0	14.1(5)	0	14.1(5)	19.6(1.5)
		167	7/2(+)	22.9	3.0(3)	1.0(3)	1.1(2)	0.13(8)	1.2(2)	659.(16.)
		168	0(+)	27.1	7.4(4)	0	6.8(7)	0	6.9(7)	2.74(8)
		170	0(+)	14.9	9.6(5)	0	11.6(1.2)	0	11.6(1.2)	5.8(3)
Tm	69	169	1/2(+)	100	7.07(3)	0.9(3)	6.28(5)	0.10(7)	6.38(9)	100.(2.)
Yb	70				12.43(3)		19.42(9)	4.0(2)	23.05(18)	34.8(8)
		168	0(+)	0.14	−4.07(2) −0.62(1)*i*	0	2.13(2)	0	2.13(2)	2230.(40.)
		170	0(+)	3.06	6.77(10)	0	5.8(2)	0	5.8(2)	11.4(1.0)
		171	1/2(−)	143	9.66(10)	−5.59(17)	11.7(2)	3.9(2)	15.6(3)	48.6(2.5)
		172	0(+)	21.9	9.43(10)	0	11.2(2)	0	11.2(2)	0.8(4)
		173	5/2(−)	16.1	9.56(7)	−5.3(2)	11.5(2)	3.5(3)	15.0(4)	17.1(1.3)
		174	0(+)	31.8	19.3(1)	0	46.8(5)	0	46.8(5)	69.4(5.0)
		176	0(+)	12.7	8.72(10)	0	9.6(2)	0	9.6(2)	2.85(5)
Lu	71				7.21(3)		6.53(5)	0.7(4)	7.2(4)	74.(2.)
		175	7/2(+)	97.39	7.24(3)	±2.2(7)	6.59(5)	0.6(4)	7.2(4)	21.(3.)
		*176	7(−)	2.61	6.1(1) −0.57(1)*i*	±3.0(4) +0.61(1)*i*	4.7(2)	1.2(3)	5.9(4)	2065.(35.)
Hf	72				7.77(14)		7.6(3)	2.6(5)	10.2(4)	104.1(0.5)
		174	0(+)	0.2	10.9(1.1)	0	15.(3.)	0	15.(3.)	561.(35.)
		176	0(+)	5.2	6.61(18)	0	5.5(3)	0	5.5(3)	23.5(3.1)
		177	7/2(−)	18.6	0.8(1.0) *E*	±0.9(1.3)	0.1(2)	0.1(3)	0.2(2)	373.(10.)
		178	0(+)	27.1	5.9(2)	0	4.4(3)	0	4.4(3)	84.(4.)
		179	9/2(+)	13.7	7.46(16)	±1.06(8)	7.0(3)	0.14(2)	7.1(3)	41.(3.)
		180	0(+)	35.2	13.2(3)	0	21.9(1.0)	0	21.9(1.0)	13.04(7)
Ta	73				6.91(7)		6.00(12)	0.01(17)	6.01(12)	20.6(5)
		*180	9(−)	0.012	7.(2.) *E*	6.2(3.5)	0.5(5)	*E*	7.(4.)	563.(60.)
		181	7/2(+)	99.988	6.91(7)	−0.29(3)	6.00(12)	0.011(2)	6.01(12)	20.5(5)

Table 4.4.4.1. *Bound scattering lengths (cont.)*

Element	Z	A	$I(\pi)$	c	b_c	b_i	σ_c	σ_i	σ_s	σ_a
W	74				4.86(2)		2.97(2)	1.63(6)	4.60(6)	18.3(2)
		180	0(+)	0.1	5.(3.) *E*	0	3.(4.)	0	3.(4.)	30.(20.)
		182	0(+)	26.3	6.97(14)	0	6.10(7)	0	6.10(7)	20.7(5)
		183	1/2(−)	14.3	6.53(4)		5.36(7)	0.3(3) *E*	5.7(3)	10.1(3)
		184	0(+)	30.7	7.48(6)	0	7.03(11)	0	7.03(11)	1.7(1)
		186	0(+)	28.6	−0.72(4)	0	0.065(7)	0	0.065(7)	37.9(0.6)
Re	75				9.2(2)		10.6(5)	0.9(6)	11.5(3)	89.7(1.0)
		185	5/2(+)	37.40	9.0(3)	±2.0(1.8)	10.2(7)	0.5(9)	10.7(6)	112.(2.)
		187	5/2(+)	62.60	9.3(3)	±2.8(1.1)	10.9(7)	1.0(8)	11.9(4)	76.4(1.0)
Os	76				10.7(2)		14.4(5)	0.3(8)	14.7(6)	16.0(4)
		184	0(+)	0.02	10.(2.) *E*	0	13.(5.)	0	13.(5.)	3000.(150.)
		186	0(+)	1.58	11.6(1.7)	0	17.(5.)	0	17.(5.)	80.(13.)
		187	1/2(−)	1.6	10.(2.) *E*	13.(5.)	0.3(3)	*E*	13.(5.)	320(10.)
		188	0(+)	13.3	7.6(3)	0	7.3(6)	0	7.3(6)	4.7(5)
		189	3/2(−)	16.1	10.7(3)		14.4(8)	0.5(5) *E*	14.9(9)	25(4.)
		190	0(+)	26.4	11.0(3)	0	15.2(9)	0	15.2(8)	13.1(3)
		192	0(+)	41.0	11.5(4)	0	16.6(1.2)	0	16.6(1.2)	2.0(1)
Ir	77				10.6(3)		14.1(8)	0.(3.)	14.(3.)	425.3(2.4)
		191	3/2(+)	37.3						954.(10.)
		193	3/2(+)	62.7						111.(5.)
Pt	78				9.60(1)		11.58(2)	0.13(11)	11.71(11)	10.3(3)
		190	0(+)	0.01	9.0(1.0)	0	10.(2.)	0	10.(2.)	152.(4.)
		192	0(+)	0.79	9.9(5)	0	12.3(1.2)	0	12.3(1.2)	10.0(2.5)
		194	0(+)	32.9	10.55(8)	0	14.0(2)	0	14.0(2)	1.44(19)
		195	1/2(−)	33.8	8.83(9)	−1.00(17)	9.8(2)	0.13(4)	9.9(2)	27.5(1.2)
		196	0(+)	25.3	9.89(8)	0	12.3(2)	0	12.3(2)	0.72(4)
		198	0(+)	7.2	7.8(1)	0	7.7(2)	0	7.6(2)	3.66(19)
Au	79	197	3/2(+)	100	7.63(6)	−1.84(10)	7.32(12)	0.43(5)	7.75(13)	98.65(9)
Hg	80				12.692(15)		20.24(5)	6.6(1)	26.8(1)	372.3(4.0)
		196	0(+)	0.2	30.3(1.0)	0	115(8.)	0	115(8.)	3080(180.)
		198	0(+)	10.1		0		0		2.0(3)
		199	1/2(−)	17.0	16.9(4)	±15.5(8)	36.(2.)	30.(3.)	66.(2.)	2150.(48.)
		200	0(+)	23.1		0		0		<60.
		201	3/2(−)	13.2			7.8(2.0)			
		202	0(+)	29.6		0		0		4.89(5)
		204	0(+)	6.8		0		0		0.43(10)
Tl	81				8.776(5)		9.678(11)	0.21(15)	9.89(15)	3.43(6)
		203	1/2(+)	29.524	6.99(16)	1.06(14)	6.14(28)	0.14(4)	6.28(28)	11.4(2)
		205	1/2(+)	70.476	9.52(7)	−0.242(17)	11.39(17)	0.007(1)	11.40(17)	0.104(17)
Pb	82				9.405(3)		11.115(7)	0.0030(7)	11.118(7)	0.171(2)
		204	0(+)	1.4	9.90(10)	0	12.3(2)	0	12.3(2)	0.65(7)
		206	0(+)	24.1	9.22(5)	0	10.68(12)	0	10.68(12)	0.0300(8)
		207	1/2(−)	22.1	9.28(4)	0.14(6)	10.82(9)	0.002(2)	10.82(9)	0.699(10)
		208	0(+)	52.4	9.50(2)	0	11.34(5)	0	11.34(5)	0.00048(3)
Bi	83	209	9/2(−)	100	8.532(2)	0.259(15)	9.148(4)	0.0084(10)	9.156(4)	0.0338(7)
Po	84									
At	85									
Rn	86									
Fr	87									
Ra	88									
		226	0(+)	$(1.60\times10^3$a)	10.0(1.0)	0	13.(3.)	0	13.(3.)	12.8(1.5)

Table 4.4.4.1. *Bound scattering lengths (cont.)*

Element	Z	A	$I(\pi)$	c	b_c	b_i	σ_c	σ_i	σ_s	σ_a
Ac	89									
Th	90	232	0(+)	100	10.31(3)	0	13.36(8)	0	13.36(8)	7.37(6)
Pa	91									
		231	3/2(−)	(3.28×10^4a)	9.1(3)	1	0.4(7)	0.1(3.3)	10.5(3.2)	200.6(2.3)
U	92				8.417(5)		8.903(11)	0.005(16)	8.908(11)	7.57(2)
		233	5/2(+)	(1.59×10^5a)	10.1(2)	±1.(3.)	12.8(5)	0.1(6)	12.9(3)	574.7(1.0)
		234	0(+)	0.005	12.4(3)	0	19.3(9)	0	19.3(9)	100.1(1.3)
		235	7/2(−)	0.720	10.47(3)	±1.3(6)	13.78(11)	0.2(2)	14.0(2)	680.9(1.1)
		238	0(+)	99.275	8.402(5)	0	8.871(11)	0	8.871(11)	2.68(2)
Np	93									
		237	5/2(+)	(2.14×10^6a)	10.55(10)		14.0(3)	0.5(5)*E*	14.5(6)	175.9(2.9)
Pu	94									
		238	0(+)	(87.74a)	14.1(5)	0	25.0(1.8)	0	25.0(1.8)	558.(7.)
		239	1/2(+)	(2.41×10^4a)	7.7(1)	±1.3(1.9)	7.5(2)	0.2(6)	7.7(6)	1017.3(2.1)
		240	0(+)	(6.56×10^3a)	3.5(1)	0	1.54(9)	0	1.54(9)	289.6(1.4)
		242	0(+)	(3.76×10^5a)	8.1(1)	0	8.2(2)	0	8.2(2)	18.5(5)
Am	95									
		243	5/2(−)	(7.37×10^3a)	8.3(2)	±2.(7.)	8.7(4)	0.3(2.6)	9.0(2.6)	75.3(1.8)
Cm	96									
		244	0(+)	(18.10a)	9.5(3)	0	11.3(7)	0	11.3(7)	16.2(1.2)
		246	0(+)	(4.7×10^3a)	9.3(2)	0	10.9(5)	0	10.9(5)	1.36(17)
		248	0(+)	(3.5×10^5a)	7.7(2)	0	7.5(4)	0	7.5(4)	3.00(26)

4.4.4.2. *Scattering and absorption cross sections*

When a thermal neutron collides with a nucleus, it may be either scattered or absorbed. By absorption, we mean reactions such as (n,γ), (n,p), or (n,α), in which there is no neutron in the final state. The effect of absorption can be included by allowing the bound scattering length to be complex,

$$b = b' - ib''. \tag{4.4.4.3}$$

The total bound scattering cross section is then given by

$$\sigma_s = 4\pi\langle|b|^2\rangle, \tag{4.4.4.4}$$

in which $\langle\,\rangle$ denotes a statistical average over the neutron and nuclear spins and the absorption cross section is given by

$$\sigma_a = \frac{4\pi}{k}\langle b''\rangle, \tag{4.4.4.5}$$

where $k = 2\pi/\lambda$ is the wavevector of the incident neutron and λ is the wavelength.

If the neutron and/or the nucleus is unpolarized, then the total bound scattering cross section is of the form

$$\sigma_s = \sigma_c + \sigma_i, \tag{4.4.4.6}$$

in which σ_c and σ_i are called the bound coherent and incoherent scattering cross sections and are given by

$$\sigma_c = 4\pi|b_c|^2, \quad \sigma_i = 4\pi|b_i|^2. \tag{4.4.4.7}$$

Also,

$$b_c = \langle b\rangle, \tag{4.4.4.8}$$

so that the absorption cross section is given by

$$\sigma_a = \frac{4\pi}{k}\, b_c''. \tag{4.4.4.9}$$

The absorption cross section is therefore uniquely determined by the imaginary part of the bound coherent scattering length. It is only when the neutron and the nucleus are both polarized that the imaginary part of the bound incoherent scattering length contributes to the value of σ_a.

For most nuclides, the scattering lengths and, hence, the scattering cross sections are constant in the thermal-neutron region, and the absorption cross sections are inversely proportional to k. Since k is proportional to the neutron velocity v, the absorption is said to obey a $1/v$ law. By convention, absorption cross sections are tabulated for a velocity $v = 2200\ \mathrm{m\,s^{-1}}$, which corresponds to a wavevector $k = 3.494\ \mathrm{\AA^{-1}}$, a wavelength $\lambda = 1.798$ Å, or an energy $E = 25.30$ meV.

The only major deviations from the $1/v$ law are for a few heavy nuclides (specifically, ^{113}Cd, ^{149}Sm, ^{151}Eu, ^{155}Gd, ^{157}Gd, ^{176}Lu, and ^{180}Ta), which have an (n,γ) resonance at thermal-neutron energies. For these nuclides (which are indicated by the symbol * in Table 4.4.4.1), the scattering lengths and cross sections are strongly energy dependent. The scattering lengths of the resonant rare-earth nuclides have been tabulated as a function of energy by Lynn & Seeger (1990).

4.4.4.3. *Isotope effects*

The coefficients b_c and b_i in (4.4.4.2) for the bound scattering length depend on the particular isotope under consideration, and this provides an additional source of incoherence in the scattering of neutrons by a mixture of isotopes. If $\langle\,\rangle$ is now taken to denote an average over both the spin and isotope distributions, then the expressions (4.4.4.8) for b_c, (4.4.4.4) for σ_s, and (4.4.4.5) for

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 ($\sim$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 ($\sim$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 $\pm$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

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