International Tables for Crystallography (2006). Vol. C, Section 4.4.4.3, pp. 452–453.

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

Element	Z	A	I(π)	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,

$$b = b' - ib''. \qquad (4.4.4.3)$$

The total bound scattering cross section is then given by

$$\sigma_s = 4\pi\langle |b|^2\rangle, \qquad (4.4.4.4)$$

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

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

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

$$\sigma_s = \sigma_c + \sigma_i, \qquad (4.4.4.6)$$

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

$$\sigma_c = 4\pi|b_c|^2, \quad \sigma_i = 4\pi|b_i|^2. \qquad (4.4.4.7)$$

Also,

$$b_c = \langle b\rangle, \qquad (4.4.4.8)$$

so that the absorption cross section is given by

$$\sigma_a = \frac{4\pi}{k}\, b''_c. \qquad (4.4.4.9)$$

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 $k = 3.494\,\text{Å}^{-1}$, a wavelength $\lambda = 1.798\,\text{Å}$, 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

Copyright © 2006 International Union of Crystallography

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

$$\sum_l c_l = 1, \qquad (4.4.4.10)$$

then, for an isotopic mixture,

$$b_c = \sum_l c_l b_{cl}, \qquad (4.4.4.11)$$

$$\sigma_s = \sum_l c_l \sigma_{sl}, \qquad (4.4.4.12)$$

and

$$\sigma_a = \sum_l c_l \sigma_{al}. \qquad (4.4.4.13)$$

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

$$\sigma_c = 4\pi |b_c|^2, \qquad (4.4.4.14)$$

while the bound incoherent scattering cross section is defined as

$$\sigma_i = \sigma_s - \sigma_c. \qquad (4.4.4.15)$$

Hence, it follows that

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

in which the contribution from spin incoherence is given by

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

and that from isotope incoherence is given by

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

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

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

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)

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

with $q_0 = \gamma Z^{1/3}$. The value $\gamma = 1.90 \pm 0.07\,\text{Å}^{-1}$ 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

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

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.*

$$q = 2k \sin\theta_{hkl}, \qquad (4.4.4.22)$$

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

references