International Tables for Crystallography (2018). Vol. H, Section 2.3.2.3, pp. 68–69.

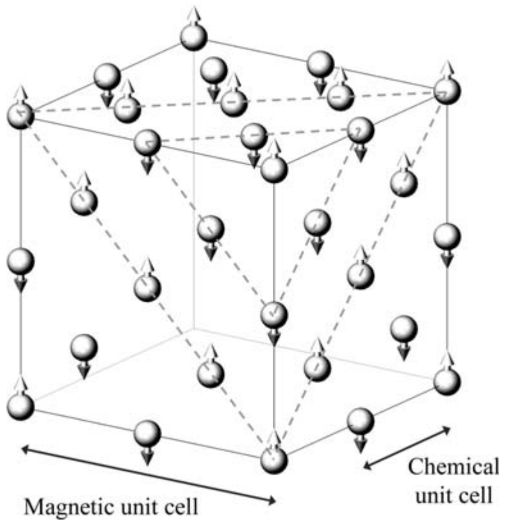

Figure 2.3.4
Magnetic structure for MnO proposed by Shull *et al.* (1951). The figure shows only the Mn atoms, and indeed only those Mn atoms located on the visible faces of the cubic cell. [From Shull *et al.* (1951), redrawn using *ATOMS* (Dowty, 1999).]

2.3.2.2. *Neutron scattering lengths*

The scattering lengths of most interest in neutron powder diffraction are those for coherent elastic scattering, $b_{\rm coh}$, often abbreviated to b. As already mentioned, there is no angle (Q) dependence, since the scattering from the nucleus is isotropic. A selection of scattering lengths for different isotopes and different elements is given in Table 2.3.2.

The first thing to note is the variation in scattering length from element to element and indeed from isotope to isotope. The scattering lengths are in most cases positive real numbers, in which case there is a phase reversal of the neutron on scattering, but for some isotopes the scattering lengths are negative, so there is no change in phase on scattering. The scattering lengths are determined by the details of the neutron–nucleus interaction (Squires, 1978).[5] In the event that the neutron–nucleus system is close to a resonance, such as it is for ^{10}B, ^{155}Gd and ^{157}Gd, scattering lengths will be complex quantities and the scattered neutron will have some different phase relationship with the incident one. The imaginary components imply absorption, which is reflected in the very high absorption cross sections, σ_a, for these isotopes.

The total scattering cross section, σ_s, is given by $\sigma_s = 4\pi b_{\rm coh}^2$ when only coherent scattering from a single isotope is involved, which is very nearly the case for oxygen since 99.76% of naturally occurring oxygen is zero-spin ^{16}O. In most cases there is a more substantial contribution from incoherent scattering, which may be either spin or isotope incoherent scattering. Spin incoherent scattering arises because the scattering length depends on the relative orientation of the neutron and nuclear spins, parallel and antiparallel arrangements giving rise to scattering lengths b_+ and b_-, respectively. Isotope incoherent scattering arises because of the different scattering of neutrons from different isotopes of the same element. In almost all circumstances (except, for example, at the extraordinarily low temperatures mentioned in Section 2.3.1) the distributions of spins and isotopes are truly random, which means that there is no angle dependence in this scattering: this is sometimes described as Laue monotonic scattering.

Table 2.3.1
Properties of the neutron (adapted from Kisi & Howard, 2008)

Mass (m)	1.675×10^{-27} kg
Charge	0
Spin	$\frac{1}{2}$
Magnetic moment (μ_n)	$-1.913\ \mu_N$
Wavelength (λ)	h/mv
Wavevector (**k**)	Magnitude $2\pi/\lambda$
Momentum (**p**)	$\hbar\mathbf{k}$
Energy (E)	$(1/2)mv^2 = h^2/2m\lambda^2$

When b varies from nucleus to nucleus (even considering just a single element), the coherent scattering is determined by the average value of b, that is $b_{\rm coh} = \overline{b}$, $\sigma_{\rm coh} = 4\pi(\overline{b})^2$, and the average incoherent cross section is given by $\sigma_{\rm inc} = 4\pi[\overline{b^2} - (\overline{b})^2]$. The total scattering cross section σ_s is the sum of the two cross sections (Squires, 1978; see also Section 2.3.2 in Kisi & Howard, 2008). For the particular case of a nucleus with spin I, the states $I + 1/2$ and $I - 1/2$ give scattering determined by b_+ and b_-, respectively, and have multiplicities $2I + 2$ and $2I$, respectively, from which it follows that

$$b_{\rm coh} = \overline{b} = \frac{I+1}{2I+1} b_+ + \frac{I}{2I+1} b_-,$$

$$b_{\rm inc}^2 = \left[\overline{b^2} - (\overline{b})^2\right] = \frac{I(I+1)}{(2I+1)^2}(b_+ - b_-)^2.$$

More information, including a comprehensive listing of scattering lengths, can be found in Section 4.4.4 of *International Tables for Crystallography* Volume C (Sears, 2006). This listing presents the spin-dependent scattering lengths *via* $b_{\rm coh}$ and $b_{\rm inc}$ as just defined. Other compilations can be found in the *Neutron Data Booklet* (Rauch & Waschkowski, 2003), and online through the Atominstitut der Österreichischen Universitäten, Vienna, at http://www.ati.ac.at/~neutropt/scattering/table.html. In addition, the majority of computer programs used for the analysis of data from neutron diffraction incorporate, for convenience, a list of $b_{\rm coh}$ values for the elements.

2.3.2.3. *Refractive index for neutrons*

The coherent scattering lengths of the nuclei determine the refractive index for neutrons through the relationship (Squires, 1978)

$$n = 1 - \frac{1}{2\pi}\lambda^2 N b_{\rm coh}, \qquad (2.3.4)$$

where N is the number of nuclei per unit volume. For elements with positive values of the coherent scattering length the refractive index is slightly less than one, and that leads to the possibility of total external reflection of the neutrons by the element in question. In fact, when the coherent scattering length is positive, neutrons will undergo total external reflection for glancing angles less than a critical angle γ_c given by

$$\cos\gamma_c = n = 1 - \frac{1}{2\pi}\lambda^2 N b_{\rm coh}, \qquad (2.3.5)$$

which, since γ_c is small, reduces to

$$\gamma_c = \lambda\left(\frac{N b_{\rm coh}}{\pi}\right)^{1/2}. \qquad (2.3.6)$$

It can be seen that the pertinent material quantity is $Nb_{\rm coh}$, the 'coherent scattering length density'; for materials comprising more than one element this is the quantity that would be

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[5] It is evident from Fig. 2.3 in this reference that even for an attractive interaction between neutron and nucleus positive scattering lengths will predominate.

Table 2.3.2
Coherent scattering lengths and absorption cross sections (for 25 meV neutrons) for selected isotopes

Data are taken from Section 4.4.4 of Volume C (Sears, 2006). Where not stated, the values are for the natural isotopic mix. The X-ray atomic form factors, f, evaluated at $Q = 1.2\pi$ Å^{-1}, are included for comparison.

Element	Isotope	$b_{\rm coh}$ (fm)	$\sigma_{s({\rm tot})}$ (10^{-24}cm^2)	σ_a (10^{-24}cm^2)	f	Isotopic abundance (%)
H		−3.7390 (11)	82.02 (6)	0.3326 (7)	0.25	
	1	−3.7406 (11)	82.03 (6)	0.3326 (7)		99.985
	2	6.671 (4)	7.64 (3)	0.000519 (7)		0.015
	3	4.792 (27)	3.03 (5)	0		—
B		5.30 (4) − 0.213 (2)i	5.24 (11)	767 (8)	1.99	
	10	−0.1 (3) − 1.066 (3)i	3.1 (4)	3835 (9)		20.0
	11	6.65 (4)	5.78 (9)	0.0055 (33)		80.0
C		6.6460 (12)	5.551 (3)	0.00350 (7)	2.50	
	12	6.6511 (16)	5.559 (3)	0.00353 (7)		98.90
	13	6.19 (9)	4.84 (14)	0.00137 (4)		1.10
O		5.803 (4)	4.232 (6)	0.00019 (2)	4.09	
Ti		−3.370 (13)	4.06 (3)	6.43 (6)	13.2	
	46	4.725 (5)	2.80 (6)	0.59 (18)		8.2
	47	3.53 (7)	3.1 (2)	1.7 (2)		7.4
	48	−5.86 (2)	4.32 (3)	8.30 (9)		73.8
	49	0.98 (5)	3.4 (3)	2.2 (3)		5.4
	50	5.88 (10)	4.34 (15)	0.179 (3)		5.2
V		−0.3824 (12)	5.10 (6)	5.08 (2)	14.0	
Ni		10.3 (1)	18.5 (3)	4.49 (16)	18.7	
	58	14.4 (1)	26.1 (4)	4.6 (3)		68.27
	60	2.8 (1)	0.99 (7)	2.9 (2)		26.10
	61	7.60 (6)	9.2 (3)	2.5 (8)		1.13
	62	−8.7 (2)	9.5 (4)	14.5 (3)		3.59
	64	−0.37 (7)	0.017 (7)	1.52 (3)		0.91
Cu		7.718 (4)	8.03 (3)	3.78 (2)	19.9	
	63	6.43 (15)	5.2 (2)	4.50 (2)		69.17
	65	10.61 (19)	14.5 (5)	2.17 (3)		30.83
Zn		5.680 (5)	4.131 (10)	1.11 (2)	20.8	
Zr		7.16 (3)	6.46 (14)	0.185 (3)	27.0	
Gd		6.5 (5)	180 (2)	49700 (125)	45.9	
	155	6.0 (1) − 17.0 (1)i	66 (6)	61100 (400)		14.8
	157	−1.14 (2) − 71.9 (2)i	1044 (8)	259000 (700)		15.7
Pb		9.405 (3)	11.118 (7)	0.171 (2)	60.9	

computed. Since the critical angle for total external reflection is proportional to the neutron wavelength, it is convenient to express this as degrees per ångstrom of neutron wavelength. These are important considerations in the design and development of neutron guides (Section 2.3.3.4).

2.3.2.4. *Neutron attenuation*

Neutron beams are attenuated by coherent scattering, incoherent scattering and true absorption. The cross sections for all these processes are included in the tables cited above. For powder diffraction, the coherent scattering is usually small because it takes place only in that small fraction of crystallites correctly oriented for Bragg reflection; the other processes, however, take place throughout the sample.

If a particular scattering entity i with scattering cross sections $(\sigma_i)_{\rm inc}$ and $(\sigma_i)_{\rm abs}$ is present at a number density N_i, then the contribution it makes to the linear attenuation coefficient μ is $\mu_i = N_i[(\sigma_i)_{\rm inc} + (\sigma_i)_{\rm abs}]$. If the mass is M_i, then the density is simply $\rho_i = N_i M_i$, so we have the means to evaluate the mass absorption coefficient $(\mu/\rho)_i$. The calculation of absorption for elements, compounds and mixtures commonly proceeds by the manipulation of mass absorption coefficients, in the same manner as is employed for X-rays (see Section 2.4.2 in Kisi & Howard, 2008).

2.3.2.5. *Magnetic form factors and magnetic scattering lengths*

For a complete treatment of the magnetic interaction between the neutron and an atom carrying a magnetic moment, and the resulting scattering, the reader is referred elsewhere [Marshall & Lovesey, 1971; Squires, 1978; Section 6.1.2 of Volume C (Brown, 2006*a*)]. The magnetic moment of an atom is associated with unpaired electrons, but may comprise both spin and orbital contributions. The magnetic interaction between the neutron and the atom depends on the directions of the scattering vector and the magnetic moment vector according to a triple vector product. The direction of polarization of the neutron must also be taken