International Tables for Crystallography (2006). Vol. C, Section 4.4.5, pp. 454–461.

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

$$\langle j_l(k) \rangle = \int\limits_0^\infty U^2(r) j_l(kr) 4\pi r^2 \, \mathrm{d}r, \qquad (4.4.5.1)$$

Table 4.4.5.2. $\langle j_0 \rangle$ *form factors for 4d atoms and their ions*

Atom or ion	A	a	B	b	C	c	D	e
Y	0.5915	67.608	1.5123	17.900	−1.1130	14.136	0.0080	0.3272
Zr	0.4106	59.996	1.0543	18.648	−0.4751	10.540	0.0106	0.3667
Zr^{+}	0.4532	59.595	0.7834	21.436	−0.2451	9.036	0.0098	0.3639
Nb	0.3946	49.230	1.3197	14.822	−0.7269	9.616	0.0129	0.3659
Nb^{+}	0.4572	49.918	1.0274	15.726	−0.4962	9.157	0.0118	0.3403
Mo	0.1806	49.057	1.2306	14.786	−0.4268	6.987	0.0171	0.4135
Mo^{+}	0.3500	48.035	1.0305	15.060	−0.3929	7.479	0.0139	0.3510
Tc	0.1298	49.661	1.1656	14.131	−0.3134	5.513	0.0195	0.3869
Tc^{+}	0.2674	48.957	0.9569	15.141	−0.2387	5.458	0.0160	0.3412
Ru	0.1069	49.424	1.1912	12.742	−0.3176	4.912	0.0213	0.3597
Ru^{+}	0.4410	33.309	1.4775	9.553	−0.9361	6.722	0.0176	0.2608
Rh	0.0976	49.882	1.1601	11.831	−0.2789	4.127	0.0234	0.3263
Rh^{+}	0.3342	29.756	1.2209	9.438	−0.5755	5.332	0.0210	0.2574
Pd	0.2003	29.363	1.1446	9.599	−0.3689	4.042	0.0251	0.2453
Pd^{+}	0.5033	24.504	1.9982	6.908	−1.5240	5.513	0.0213	0.1909

Table 4.4.5.3. $\langle j_0 \rangle$ *form factors for rare-earth ions*

Ion	A	a	B	b	C	c	D	e
Ce^{2+}	0.2953	17.685	0.2923	6.733	0.4313	5.383	−0.0194	0.0845
Nd^{2+}	0.1645	25.045	0.2522	11.978	0.6012	4.946	−0.0180	0.0668
Nd^{3+}	0.0540	25.029	0.3101	12.102	0.6575	4.722	−0.0216	0.0478
Sm^{2+}	0.0909	25.203	0.3037	11.856	0.6250	4.237	−0.0200	0.0408
Sm^{3+}	0.0288	25.207	0.2973	11.831	0.6954	4.212	−0.0213	0.0510
Eu^{2+}	0.0755	25.296	0.3001	11.599	0.6438	4.025	−0.0196	0.0488
Eu^{3+}	0.0204	25.308	0.3010	11.474	0.7005	3.942	−0.0220	0.0356
Gd^{2+}	0.0636	25.382	0.3033	11.212	0.6528	3.788	−0.0199	0.0486
Gd^{3+}	0.0186	25.387	0.2895	11.142	0.7135	3.752	−0.0217	0.0489
Tb^{2+}	0.0547	25.509	0.3171	10.591	0.6490	3.517	−0.0212	0.0342
Tb^{3+}	0.0177	25.510	0.2921	10.577	0.7133	3.512	−0.0231	0.0512
Dy^{2+}	0.1308	18.316	0.3118	7.665	0.5795	3.147	−0.0226	0.0315
Dy^{3+}	0.1157	15.073	0.3270	6.799	0.5821	3.020	−0.0249	0.0146
Ho^{2+}	0.0995	18.176	0.3305	7.856	0.5921	2.980	−0.0230	0.1240
Ho^{3+}	0.0566	18.318	0.3365	7.688	0.6317	2.943	−0.0248	0.0068
Er^{2+}	0.1122	18.122	0.3462	6.911	0.5649	2.761	−0.0235	0.0207
Er^{3+}	0.0586	17.980	0.3540	7.096	0.6126	2.748	−0.0251	0.0171
Tm^{2+}	0.0983	18.324	0.3380	6.918	0.5875	2.662	−0.0241	0.0404
Tm^{3+}	0.0581	15.092	0.2787	7.801	0.6854	2.793	−0.0224	0.0351
Yb^{2+}	0.0855	18.512	0.2943	7.373	0.6412	2.678	−0.0213	0.0421
Yb^{3+}	0.0416	16.095	0.2849	7.834	0.6961	2.672	−0.0229	0.0344

Table 4.4.5.4 $\langle j_0 \rangle$ *form factors for actinide ions*

Ion	A	a	B	b	C	c	D	e
U^{3+}	0.5058	23.288	1.3464	7.003	−0.8724	4.868	0.0192	0.1507
U^{4+}	0.3291	23.548	1.0836	8.454	−0.4340	4.120	0.0214	0.1757
U^{5+}	0.3650	19.804	3.2199	6.282	−2.6077	5.301	0.0233	0.1750
Np^{3+}	0.5157	20.865	2.2784	5.893	−1.8163	4.846	0.0211	0.1378
Np^{4+}	0.4206	19.805	2.8004	5.978	−2.2436	4.985	0.0228	0.1408
Np^{5+}	0.3692	18.190	3.1510	5.850	−2.5446	4.916	0.0248	0.1515
Np^{6+}	0.2929	17.561	3.4866	5.785	−2.8066	4.871	0.0267	0.1698
Pu^{3+}	0.3840	16.679	3.1049	5.421	−2.5148	4.551	0.0263	0.1280
Pu^{4+}	0.4934	16.836	1.6394	5.638	−1.1581	4.140	0.0248	0.1242
Pu^{5+}	0.3888	16.559	2.0362	5.657	−1.4515	4.255	0.0267	0.1287
Pu^{6+}	0.3172	16.051	3.4654	5.351	−2.8102	4.513	0.0281	0.1382
Am^{2+}	0.4743	21.776	1.5800	5.690	−1.0779	4.145	0.0218	0.1253
Am^{3+}	0.4239	19.574	1.4573	5.872	−0.9052	3.968	0.0238	0.1054
Am^{4+}	0.3737	17.862	1.3521	6.043	−0.7514	3.720	0.0258	0.1113
Am^{5+}	0.2956	17.372	1.4525	6.073	−0.7755	3.662	0.0277	0.1202
Am^{6+}	0.2302	16.953	1.4864	6.116	−0.7457	3.543	0.0294	0.1323
Am^{7+}	0.3601	12.730	1.9640	5.120	−1.3560	3.714	0.0316	0.1232

Table 4.4.5.5. $\langle j_2 \rangle$ *form factors for 3d transition elements and their ions*

Atom or ion	*A*	*a*	*B*	*b*	*C*	*c*	*D*	*e*
Sc	10.8172	54.327	4.7353	14.847	0.6071	4.218	0.0011	0.1212
Sc^{+}	8.5021	34.285	3.2116	10.994	0.4244	3.605	0.0009	0.1037
Sc^{2+}	4.3683	28.654	3.7231	10.823	0.6074	3.668	0.0014	0.0681
Ti	4.3583	36.056	3.8230	11.133	0.6855	3.469	0.0020	0.0967
Ti^{+}	6.1567	27.275	2.6833	8.983	0.4070	3.052	0.0011	0.0902
Ti^{2+}	4.3107	18.348	2.0960	6.797	0.2984	2.548	0.0007	0.0640
Ti^{3+}	3.3717	14.444	1.8258	5.713	0.2470	2.265	0.0005	0.0491
V	3.7600	21.831	2.4026	7.546	0.4464	2.663	0.0017	0.0556
V^{+}	4.7474	23.323	2.3609	7.808	0.4105	2.706	0.0014	0.0800
V^{2+}	3.4386	16.530	1.9638	6.141	0.2997	2.267	0.0009	0.0565
V^{3+}	2.3005	14.682	2.0364	6.130	0.4099	2.382	0.0014	0.0252
V^{4+}	1.8377	12.267	1.8247	5.458	0.3979	2.248	0.0012	0.0399
Cr	3.4085	20.127	2.1006	6.802	0.4266	2.394	0.0019	0.0662
Cr^{+}	3.7768	20.346	2.1028	6.893	0.4010	2.411	0.0017	0.0686
Cr^{2+}	2.6422	16.060	1.9198	6.253	0.4446	2.372	0.0020	0.0480
Cr^{3+}	1.6262	15.066	2.0618	6.284	0.5281	2.368	0.0023	0.0263
Cr^{4+}	1.0293	13.950	1.9933	6.059	0.5974	2.346	0.0027	0.0366
Mn	2.6681	16.060	1.7561	5.640	0.3675	2.049	0.0017	0.0595
Mn^{+}	3.2953	18.695	1.8792	6.240	0.3927	2.201	0.0022	0.0659
Mn^{2+}	2.0515	15.556	1.8841	6.063	0.4787	2.232	0.0027	0.0306
Mn^{3+}	1.2427	14.997	1.9567	6.118	0.5732	2.258	0.0031	0.0336
Mn^{4+}	0.7879	13.886	1.8717	5.743	0.5981	2.182	0.0034	0.0434
Fe	1.9405	18.473	1.9566	6.323	0.5166	2.161	0.0036	0.0394
Fe^{+}	2.6290	18.660	1.8704	6.331	0.4690	2.163	0.0031	0.0491
Fe^{2+}	1.6490	16.559	1.9064	6.133	0.5206	2.137	0.0035	0.0335
Fe^{3+}	1.3602	11.998	1.5188	5.003	0.4705	1.991	0.0038	0.0374
Fe^{4+}	1.5582	8.275	1.1863	3.279	0.1366	1.107	−0.0022	0.0327
Co	1.9678	14.170	1.4911	4.948	0.3844	1.797	0.0027	0.0452
Co^{+}	2.4097	16.161	1.5780	5.460	0.4095	1.914	0.0031	0.0581
Co^{2+}	1.9049	11.644	1.3159	4.357	0.3146	1.645	0.0017	0.0459
Co^{3+}	1.7058	8.859	1.1409	3.309	0.1474	1.090	−0.0025	0.0462
Co^{4+}	1.3110	8.025	1.1551	3.179	0.1608	1.130	−0.0011	0.0374
Ni	1.0302	12.252	1.4669	4.745	0.4521	1.744	0.0036	0.0338
Ni^{+}	2.1040	14.866	1.4302	5.071	0.4031	1.778	0.0034	0.0561
Ni^{2+}	1.7080	11.016	1.2147	4.103	0.3150	1.533	0.0018	0.0446
Ni^{3+}	1.4683	8.671	0.1794	1.106	1.1068	3.257	−0.0023	0.0373
Ni^{4+}	1.1612	7.700	1.0027	3.263	0.2719	1.378	0.0025	0.0326
Cu	1.9182	14.490	1.3329	4.730	0.3842	1.639	0.0035	0.0617
Cu^{+}	1.8814	13.433	1.2809	4.545	0.3646	1.602	0.0033	0.0590
Cu^{2+}	1.5189	10.478	1.1512	3.813	0.2918	1.398	0.0017	0.0429
Cu^{3+}	1.2797	8.450	1.0315	3.280	0.2401	1.250	0.0015	0.0389
Cu^{4+}	0.9568	7.448	0.9099	3.396	0.3729	1.494	0.0049	0.0330

Table 4.4.5.6. $\langle j_2 \rangle$ *form factors for 4d atoms and their ions*

Atom or ion	*A*	*a*	*B*	*b*	*C*	*c*	*D*	*e*
Y	14.4084	44.658	5.1045	14.904	−0.0535	3.319	0.0028	0.1093
Zr	10.1378	35.337	4.7734	12.545	−0.0489	2.672	0.0036	0.0912
Zr^{+}	11.8722	34.920	4.0502	12.127	−0.0632	2.828	0.0034	0.0737
Nb	7.4796	33.179	5.0884	11.571	−0.0281	1.564	0.0047	0.0944
Nb^{+}	8.7735	33.285	4.6556	11.605	−0.0268	1.539	0.0044	0.0855
Mo	5.1180	23.422	4.1809	9.208	−0.0505	1.743	0.0053	0.0655
Mo^{+}	7.2367	28.128	4.0705	9.923	−0.0317	1.455	0.0049	0.0798
Tc	4.2441	21.397	3.9439	8.375	−0.0371	1.187	0.0066	0.0645
Tc^{+}	6.4056	24.824	3.5400	8.611	−0.0366	1.485	0.0044	0.0806
Ru	3.7445	18.613	3.4749	7.420	−0.0363	1.007	0.0073	0.0533
Ru^{+}	5.2826	23.683	3.5813	8.152	−0.0257	0.426	0.0131	0.0830
Rh	3.3651	17.344	3.2121	6.804	−0.0350	0.503	0.0146	0.0545
Rh^{+}	4.0260	18.950	3.1663	7.000	−0.0296	0.486	0.0127	0.0629
Pd	3.3105	14.726	2.6332	5.862	−0.0437	1.130	0.0053	0.0492
Pd^{+}	4.2749	17.900	2.7021	6.354	−0.0258	0.700	0.0071	0.0768

Table 4.4.5.7. $\langle j_2 \rangle$ *form factors for rare-earth ions*

Ion	*A*	*a*	*B*	*b*	*C*	*c*	*D*	*e*
Ce^{2+}	0.9809	18.063	1.8413	7.769	0.9905	2.845	0.0120	0.0448
Nd^{2+}	1.4530	18.340	1.6196	7.285	0.8752	2.622	0.0126	0.0461
Nd^{3+}	0.6751	18.342	1.6272	7.260	0.9644	2.602	0.0150	0.0450
Sm^{2+}	1.0360	18.425	1.4769	7.032	0.8810	2.437	0.0152	0.0345
Sm^{3+}	0.4707	18.430	1.4261	7.034	0.9574	2.439	0.0182	0.0510
Eu^{2+}	0.8970	18.443	1.3769	7.005	0.9060	2.421	0.0190	0.0511
Eu^{3+}	0.3985	18.451	1.3307	6.956	0.9603	2.378	0.0197	0.0447
Gd^{2+}	0.7756	18.469	1.3124	6.899	0.8956	2.338	0.0199	0.0441
Gd^{3+}	0.3347	18.476	1.2465	6.877	0.9537	2.318	0.0217	0.0484
Tb^{2+}	0.6688	18.491	1.2487	6.822	0.8888	2.275	0.0215	0.0439
Tb^{3+}	0.2892	18.497	1.1678	6.797	0.9437	2.257	0.0232	0.0458
Dy^{2+}	0.5917	18.511	1.1828	6.747	0.8801	2.214	0.0229	0.0439
Dy^{3+}	0.2523	18.517	1.0914	6.736	0.9345	2.208	0.0250	0.0476
Ho^{2+}	0.5094	18.515	1.1234	6.706	0.8727	2.159	0.0242	0.0560
Ho^{3+}	0.2188	18.516	1.0240	6.707	0.9251	2.161	0.0268	0.0503
Er^{2+}	0.4693	18.528	1.0545	6.649	0.8679	2.120	0.0261	0.0413
Er^{3+}	0.1710	18.534	0.9879	6.625	0.9044	2.100	0.0278	0.0489
Tm^{2+}	0.4198	18.542	0.9959	6.600	0.8593	2.082	0.0284	0.0457
Tm^{3+}	0.1760	18.542	0.9105	6.579	0.8970	2.062	0.0294	0.0468
Yb^{2+}	0.3852	18.550	0.9415	6.551	0.8492	2.043	0.0301	0.0478
Yb^{3+}	0.1570	18.555	0.8484	6.540	0.8880	2.037	0.0318	0.0498

Table 4.4.5.8. $\langle j_2 \rangle$ *form factors for actinide ions*

Ion	*A*	*a*	*B*	*b*	*C*	*c*	*D*	*e*
U^{3+}	4.1582	16.534	2.4675	5.952	−0.0252	0.765	0.0057	0.0822
U^{4+}	3.7449	13.894	2.6453	4.863	−0.5218	3.192	0.0009	0.0928
U^{5+}	3.0724	12.546	2.3076	5.231	−0.0644	1.474	0.0035	0.0477
Np^{3+}	3.7170	15.133	2.3216	5.503	−0.0275	0.800	0.0052	0.0948
Np^{4+}	2.9203	14.646	2.5979	5.559	−0.0301	0.367	0.0141	0.0532
Np^{5+}	2.3308	13.654	2.7219	5.494	−0.1357	0.049	0.1224	0.0553
Np^{6+}	1.8245	13.180	2.8508	5.407	−0.1579	0.044	0.1438	0.0585
Pu^{3+}	2.0885	12.871	2.5961	5.190	−0.1465	0.039	0.1343	0.0866
Pu^{4+}	2.7244	12.926	2.3387	5.163	−0.1300	0.046	0.1177	0.0490
Pu^{5+}	2.1409	12.832	2.5664	5.152	−0.1338	0.046	0.1210	0.0491
Pu^{6+}	1.7262	12.324	2.6652	5.066	−0.1695	0.041	0.1550	0.0502
Am^{2+}	3.5237	15.955	2.2855	5.195	−0.0142	0.585	0.0033	0.1120
Am^{3+}	2.8622	14.733	2.4099	5.144	−0.1326	0.031	0.1233	0.0727
Am^{4+}	2.4141	12.948	2.3687	4.945	−0.2490	0.022	0.2371	0.0502
Am^{5+}	2.0109	12.053	2.4155	4.836	−0.2264	0.027	0.2128	0.0414
Am^{6+}	1.6778	11.337	2.4531	4.725	−0.2043	0.034	0.1892	0.0387
Am^{7+}	1.8845	9.161	2.0746	4.042	−0.1318	1.723	0.0020	0.0379

Table 4.4.5.9. $\langle j_4 \rangle$ *form factors for 3d atoms and their ions*

Atom or ion	*A*	*a*	*B*	*b*	*C*	*c*	*D*	*e*
Sc	1.3420	10.200	0.3837	3.079	0.0468	0.118	−0.0328	0.1343
Sc^{+}	7.1167	15.487	−6.6671	18.269	0.4900	2.992	0.0047	0.1624
Sc^{2+}	−1.6684	15.648	1.7742	9.062	0.4075	2.412	0.0042	0.1105
Ti	−2.1515	11.271	2.5149	8.859	0.3555	2.149	0.0045	0.1244
Ti^{+}	−1.0383	16.190	1.4699	8.924	0.3631	2.283	0.0044	0.1270
Ti^{2+}	−1.3242	15.310	1.2042	7.899	0.3976	2.156	0.0051	0.0820
Ti^{3+}	−1.1117	14.635	0.7689	6.927	0.4385	2.089	0.0060	0.0572
V	−0.9633	15.273	0.9274	7.732	0.3891	2.053	0.0063	0.0840
V^{+}	−0.9606	15.545	1.1278	8.118	0.3653	2.097	0.0056	0.1027
V^{2+}	−1.1729	14.973	0.9092	7.613	0.4105	2.039	0.0067	0.0719
V^{3+}	−0.9417	14.205	0.5284	6.607	0.4411	1.967	0.0076	0.0569
V^{4+}	−0.7654	13.097	0.3071	5.674	0.4476	1.871	0.0081	0.0518
Cr	−0.6670	19.613	0.5342	6.478	0.3641	1.905	0.0073	0.0628
Cr^{+}	−0.8309	18.043	0.7252	7.531	0.3828	2.003	0.0073	0.0781
Cr^{2+}	−0.8930	15.664	0.5590	7.033	0.4093	1.924	0.0081	0.0631
Cr^{3+}	−0.7327	14.073	0.3268	5.674	0.4114	1.810	0.0085	0.0505
Cr^{4+}	−0.6748	12.946	0.1805	6.753	0.4526	1.800	0.0098	0.0644
Mn	−0.5452	15.471	0.4406	4.902	0.2884	1.543	0.0059	0.0488
Mn^{+}	−0.7947	17.867	0.6078	7.704	0.3798	1.905	0.0087	0.0737
Mn^{2+}	−0.7416	15.255	0.3831	6.469	0.3935	1.800	0.0093	0.0577
Mn^{3+}	−0.6603	13.607	0.2322	6.218	0.4104	1.740	0.0101	0.0579
Mn^{4+}	−0.5127	13.461	0.0313	7.763	0.4282	1.701	0.0113	0.0693
Fe	−0.5029	19.677	0.2999	3.776	0.2576	1.424	0.0071	0.0292
Fe^{+}	−0.5109	19.250	0.3896	4.891	0.2810	1.526	0.0069	0.0375
Fe^{2+}	−0.5401	17.227	0.2865	3.742	0.2658	1.424	0.0076	0.0278
Fe^{3+}	−0.5507	11.493	0.2153	4.906	0.3468	1.523	0.0095	0.0314
Fe^{4+}	−0.5352	9.507	0.1783	5.175	0.3584	1.469	0.0097	0.0360
Co	−0.4221	14.195	0.2900	3.979	0.2469	1.286	0.0063	0.0400
Co^{+}	−0.4115	14.561	0.3580	4.717	0.2644	1.418	0.0074	0.0541
Co^{2+}	0.4759	14.046	0.2747	3.731	0.2458	1.250	0.0057	0.0282
Co^{3+}	−0.4466	13.391	0.1419	3.011	0.2773	1.335	0.0093	0.0341
Co^{4+}	−0.4091	13.194	−0.0194	3.417	0.3534	1.421	0.0112	0.0622
Ni	−0.4428	14.485	0.0870	3.234	0.2932	1.331	0.0096	0.0554
Ni^{+}	−0.3836	13.425	0.3116	4.462	0.2471	1.309	0.0079	0.0515
Ni^{2+}	−0.3803	10.403	0.2838	3.378	0.2108	1.104	0.0050	0.0474
Ni^{3+}	−0.4014	9.046	0.2314	3.075	0.2192	1.084	0.0060	0.0323
Ni^{4+}	−0.3509	8.157	0.2220	2.106	0.1567	0.925	0.0065	0.0352
Cu	−0.3204	15.132	0.2335	4.021	0.2312	1.196	0.0068	0.0457
Cu^{+}	−0.3572	15.125	0.2336	3.966	0.2315	1.197	0.0070	0.0397
Cu^{2+}	−0.3914	14.740	0.1275	3.384	0.2548	1.255	0.0103	0.0394
Cu^{3+}	−0.3671	14.082	−0.0078	3.315	0.3154	1.377	0.0132	0.0534
Cu^{4+}	−0.2915	14.124	−0.1065	4.201	0.3247	1.352	0.0148	0.0579

Table 4.4.5.10. $\langle j_4 \rangle$ *form factors for 4d atoms and their ions*

Atom or ion	*A*	*a*	*B*	*b*	*C*	*c*	*D*	*e*
Y	−8.0767	32.201	7.9197	25.156	1.4067	6.827	−0.0001	0.1031
Zr	−5.2697	32.868	4.1930	24.183	1.5202	6.048	−0.0002	0.0855
Zr^{+}	−5.6384	33.607	4.6729	22.338	1.3258	5.924	−0.0003	0.0674
Nb	−3.1377	25.595	2.3411	16.569	1.2304	4.990	−0.0005	0.0615
Nb^{+}	−3.3598	25.820	2.8297	16.427	1.1203	4.982	−0.0005	0.0724
Mo	−2.8860	20.572	1.8130	14.628	1.1899	4.264	−0.0008	0.0410
Mo^{+}	−3.2618	25.486	2.3596	16.462	1.1164	4.491	−0.0007	0.0592
Tc	−2.7975	20.159	1.6520	16.261	1.1726	3.943	−0.0008	0.0657
Tc^{+}	−2.0470	19.683	1.6306	11.592	0.8698	3.769	−0.0010	0.0723
Ru	−1.5042	17.949	0.6027	9.961	0.9700	3.393	−0.0010	0.0338
Ru^{+}	1.6278	18.506	1.1828	10.189	0.8138	3.418	−0.0009	0.0673
Rh	−1.3492	17.577	0.4527	10.507	0.9285	3.155	−0.0009	0.0483
Rh^{+}	−1.4673	17.957	0.7381	9.944	0.8485	3.126	−0.0012	0.0487
Pd	−1.1955	17.628	0.3183	11.309	0.8696	2.909	−0.0006	0.0555
Pd^{+}	−1.4098	17.765	0.7927	9.999	0.7710	2.930	−0.0006	0.0530

Table 4.4.5.11. $\langle j_4 \rangle$ *form factors for rare-earth ions*

Ion	*A*	*a*	*B*	*b*	*C*	*c*	*D*	*e*
Ce^{2+}	−0.6468	10.533	0.4052	5.624	0.3412	1.535	0.0080	0.0522
Nd^{2+}	−0.5416	12.204	0.3571	6.169	0.3154	1.485	0.0098	0.0519
Nd^{3+}	−0.4053	14.014	0.0329	7.005	0.3759	1.707	0.0209	0.0372
Sm^{2+}	−0.4150	14.057	0.1368	7.032	0.3272	1.582	0.0192	0.0319
Sm^{3+}	−0.4288	10.052	0.1782	5.019	0.2833	1.236	0.0088	0.0328
Eu^{2+}	−0.4145	10.193	0.2447	5.164	0.2661	1.205	0.0065	0.0516
Eu^{3+}	−0.4095	10.211	0.1485	5.175	0.2720	1.237	0.0131	0.0494
Gd^{2+}	−0.3824	10.344	0.1955	5.306	0.2622	1.203	0.0097	0.0363
Gd^{3+}	−0.3621	10.353	0.1016	5.310	0.2649	1.219	0.0147	0.0494
Tb^{2+}	−0.3443	10.469	0.1481	5.416	0.2575	1.182	0.0104	0.0280
Tb^{3+}	−0.3228	10.476	0.0638	5.419	0.2566	1.196	0.0159	0.0439
Dy^{2+}	−0.3206	12.071	0.0904	8.026	0.2616	1.230	0.0143	0.0767
Dy^{3+}	−0.2829	9.525	0.0565	4.429	0.2437	1.066	0.0092	0.0181
Ho^{2+}	−0.2976	9.719	0.1224	4.635	0.2279	1.005	0.0063	0.0452
Ho^{3+}	−0.2717	9.731	0.0474	4.638	0.2292	1.047	0.0124	0.0310
Er^{2+}	−0.2975	9.829	0.1189	4.741	0.2116	1.004	0.0117	0.0524
Er^{3+}	−0.2568	9.834	0.0356	4.741	0.2172	1.028	0.0148	0.0434
Tm^{2+}	−0.2677	9.888	0.0925	4.784	0.2056	0.990	0.0124	0.0396
Tm^{3+}	−0.2292	9.895	0.0124	4.785	0.2108	1.007	0.0151	0.0334
Yb^{2+}	−0.2393	9.947	0.0663	4.823	0.2009	0.965	0.0122	0.0311
Yb^{3+}	−0.2121	8.197	0.0325	3.153	0.1975	0.884	0.0093	0.0435

Table 4.4.5.12. $\langle j_4 \rangle$ *form factors for actinide ions*

Ion	*A*	*a*	*B*	*b*	*C*	*c*	*D*	*e*
U^{3+}	−0.9859	16.601	0.6116	6.515	0.6020	2.597	−0.0010	0.0599
U^{4+}	−1.0540	16.605	0.4339	6.512	0.6746	2.599	−0.0011	0.0471
U^{5+}	−0.9588	16.485	0.1576	6.440	0.7785	2.640	−0.0010	0.0493
Np^{3+}	0.9029	16.586	0.4006	6.470	0.6545	2.563	−0.0004	0.0470
Np^{4+}	−0.9887	12.441	0.5918	5.294	0.5306	2.263	−0.0021	0.0583
Np^{5+}	−0.8146	16.581	−0.0055	6.475	0.7956	2.562	−0.0004	0.0600
Np^{6+}	0.6738	16.553	−0.2297	6.505	0.8513	2.553	−0.0003	0.0623
Pu^{3+}	−0.7014	16.369	−0.1162	6.697	0.7778	2.450	0.0000	0.0546
Pu^{4+}	−0.9160	12.203	0.4891	5.127	0.5290	2.149	−0.0022	0.0520
Pu^{5+}	−0.7035	16.360	−0.0979	6.706	0.7726	2.447	0.0000	0.0610
Pu^{6+}	−0.5560	16.322	−0.3046	6.768	0.8146	2.426	0.0001	0.0596
Am^{2+}	−0.7433	16.416	0.3481	6.788	0.6014	2.346	0.0000	0.0566
Am^{3+}	0.8092	12.854	0.4161	5.459	0.5476	2.172	−0.0011	0.0530
Am^{4+}	−0.8548	12.226	0.3037	5.909	0.6173	2.188	−0.0016	0.0456
Am^{5+}	−0.6538	15.462	−0.0948	5.997	0.7295	2.297	0.0000	0.0594
Am^{6+}	−0.5390	15.449	−0.2689	6.017	0.7711	2.297	0.0002	0.0729
Am^{7+}	−0.4688	12.019	−0.2692	7.042	0.7297	2.164	−0.0011	0.0262

Table 4.4.5.13. $\langle j_6 \rangle$ *form factors for rare-earth ions*

Ion	A	a	B	b	C	c	D	e
Ce^{2+}	−0.1212	7.994	−0.0639	4.024	0.1519	1.096	0.0078	0.0388
Nd^{2+}	−0.1600	8.009	0.0272	4.028	0.1104	1.068	0.0139	0.0363
Nd^{3+}	0.0416	8.014	−0.1261	4.040	0.1400	1.087	0.0102	0.0367
Sm^{2+}	0.1428	6.041	0.0723	2.033	0.0550	0.513	0.0081	0.0450
Sm^{3+}	−0.0944	6.030	−0.0498	2.074	0.1372	0.645	−0.0132	0.0387
Eu^{2+}	−0.1252	6.049	0.0507	2.085	0.0572	0.646	0.0132	0.0403
Eu^{3+}	−0.0817	6.039	−0.0596	2.120	0.1243	0.764	−0.0001	0.0206
Gd^{2+}	−0.1351	5.030	0.0828	2.025	0.0315	0.503	0.0187	0.0453
Gd^{3+}	−0.0662	6.031	−0.0850	2.154	0.1323	0.891	0.0048	0.0371
Th^{2+}	−0.0758	6.032	−0.0540	2.158	0.1199	0.890	0.0051	0.0488
Tb^{3+}	−0.0559	6.031	−0.1020	2.237	0.1264	1.107	0.0167	0.0170
Dy^{2+}	−0.0568	6.032	−0.1003	2.240	0.1401	1.106	0.0109	0.0463
Dy^{3+}	−0.0423	6.038	−0.1248	2.244	0.1359	1.200	0.0188	0.0350
Ho^{2+}	−0.0725	6.045	−0.0318	2.243	0.0738	1.202	0.0252	0.0634
Ho^{3+}	−0.0289	6.050	−0.1545	2.230	0.1550	1.260	0.0177	0.0351
Er^{2+}	0.0648	6.056	−0.0515	2.230	0.0825	1.264	0.0250	0.0409
Er^{3+}	−0.0110	6.061	−0.1954	2.224	0.1818	1.296	0.0149	0.0455
Tm^{2+}	0.0842	4.070	0.0807	0.849	−0.2087	0.039	0.2095	0.0360
Tm^{3+}	0.0727	4.073	0.0243	0.689	3.9459	0.002	−3.9076	0.0502
Yb^{2+}	−0.0739	5.031	0.0140	2.030	0.0351	0.508	0.0174	0.0434
Yb^{3+}	−0.0345	5.007	−0.0677	2.020	0.0985	0.549	−0.0076	0.0359

Table 4.4.5.14. $\langle j_6 \rangle$ *form factors for actinide ions*

Ion	A	a	B	b	C	c	D	e
U^{3+}	−0.3797	9.953	0.0459	5.038	0.2748	1.607	0.0016	0.0345
U^{4+}	−0.1793	11.896	−0.2269	5.428	0.3291	1.701	0.0030	0.0472
U^{5+}	−0.0399	11.891	−0.3458	5.580	0.3340	1.645	0.0029	0.0444
Np^{3+}	−0.2427	11.844	−0.1129	5.377	0.2848	1.568	0.0022	0.0368
Np^{4+}	−0.2436	9.599	−0.1317	4.101	0.3029	1.545	0.0019	0.0500
Np^{5+}	−0.1157	9.565	−0.2654	4.260	0.3298	1.549	0.0025	0.0495
Np^{6+}	−0.0128	9.569	−0.3611	4.304	0.3419	1.541	0.0032	0.0520
Pu^{3+}	−0.0364	9.572	−0.3181	4.342	0.3210	1.523	0.0041	0.0496
Pu^{4+}	−0.2394	7.837	−0.0785	4.024	0.2643	1.378	0.0012	0.0414
Pu^{5+}	−0.1090	7.819	−0.2243	4.100	0.2947	1.404	0.0015	0.0477
Pu^{6+}	−0.0001	7.820	−0.3354	4.144	0.3097	1.403	0.0020	0.0513
Am^{2+}	−0.3176	7.864	0.0771	4.161	0.2194	1.339	0.0018	0.0374
Am^{3+}	−0.3159	6.982	0.0682	3.995	0.2141	1.188	−0.0015	0.0281
Am^{4+}	−0.1787	7.880	−0.1274	4.090	0.2565	1.315	0.0017	0.0419
Am^{5+}	−0.0927	6.073	−0.2227	3.784	0.2916	1.372	0.0026	0.0485
Am^{6+}	0.0152	6.079	−0.3549	3.861	0.3125	1.403	0.0036	0.0732
Am^{7+}	0.1292	6.082	−0.4689	3.879	0.3234	1.393	0.0042	0.0475

in which $U(r)$ is the radial wavefunction for the unpaired electrons in the atom, k is the length of the scattering vector, and $j_l(kr)$ is the lth-order spherical Bessel function.

Tables 4.4.5.1–4.4.5.8 give the coefficients in an analytical approximation to the $\langle j_0 \rangle$ magnetic form factors for the 3*d* and 4*d* transition series, the 4*f* electrons of rare-earth ions, and the 5*f* electrons of some actinide ions. The approximation has the form used by Forsyth & Wells (1959) but allowing three instead of two exponential terms:

$$\langle j_0(s) \rangle = A\exp(-as^2) + B\exp(-bs^2) + C\exp(-cs^2) + D, \qquad (4.4.5.2)$$

where s is the value of $(\sin\theta)/\lambda$ in Å^{-1}.

Tables 4.4.5.9–4.4.5.14 give coefficients in the approximation used by Lisher & Forsyth (1971) to the $\langle j_2 \rangle$, $\langle j_4 \rangle$, and $\langle j_6 \rangle$ form factors for the same series of atoms and ions, again using three rather than two exponential terms, *viz* for $l \neq 0$:

$$\langle j_l(s) \rangle = As^2\exp(-as^2) + Bs^2\exp(-bs^2) + Cs^2\exp(-cs^2) + Ds^2. \qquad (4.4.5.3)$$

For the transition-metal series, the coefficients of the approximation have been obtained by fitting to form factors calculated from the Hartree–Fock wavefunctions given by Clementi & Roetti (1974) in terms of Slater-type functions in the form

$$U(r) = \sum_{nj} N_{nl}\, r^2 A_{nlj} \exp(-a_{nlj}\, r) \qquad (4.4.5.4)$$

by using the identity:

$$\int_0^\infty j_l(kr) r^n \exp(-pr) 4\pi r^2 \,\mathrm{d}r$$
$$= \frac{\pi^{3/2}\Gamma(n+l+3)k^l}{2^{l-1}\Gamma(l+3/2)(k^2+p^2)^{(n+l+3)/2}}$$
$$\times {}_2F_1\left(\frac{n+l+3}{2};\ \frac{l-n+3}{2};\ l+\frac{3}{2};\ \frac{k^2}{k^2+p^2}\right). \quad (4.4.5.5)$$

The form factors have been calculated from these relationships in the range $(\sin\theta)/\lambda = 0$ to $1.5\,\text{Å}^{-1}$ at intervals of $0.05\,\text{Å}^{-1}$, and the coefficients of the exponential expansion fitted by a least-squares procedure at the calculated points.

For the atoms of the rare-earth and actinide series, the wavefunctions and form factors have been calculated by Freeman & Desclaux (1979) and Desclaux & Freeman (1978) using Dirac–Fock theory. The constants given in Tables 4.4.5.3, 4.4.5.4, 4.4.5.7, 4.4.5.8, and 4.4.5.11–4.4.5.14 have been fitted to the results of these calculations. For the rare-earth ions, the form factors are given in the range $(\sin\theta)/\lambda = 0$ to $0.5\,\text{Å}^{-1}$ at intervals of $0.5\,\text{Å}^{-1}$ and in the range 0.5 to $1.2\,\text{Å}^{-1}$ at intervals of $0.1\,\text{Å}^{-1}$. For the actinide ions, the calculations extend to $1.5\,\text{Å}^{-1}$. All the values given in the publications cited were included in the fitting procedure. The accuracy with which the exponential expansions fit the theoretical form factors can be judged from the value of the parameter e given in the tables, and defined by:

$$e = 100\left(\frac{\sum_i \delta_i^2}{N}\right)^{1/2}, \quad (4.4.5.6)$$

where δ_i is the difference between the ith fitted point and its theoretical value. The sum is over the N points included in the fitting procedure.

4.4.6. Absorption coefficients for neutrons (By B. T. M. Willis)

The cross sections σ discussed in Section 4.4.4 represent the area of each nucleus as seen by the neutron. To calculate the beam attenuation arising from absorption it is more convenient to use the macroscopic cross section Σ, which is the cross section per unit volume in units of cm^{-1}. Σ is derived by multiplying σ for the element by the number of atoms per unit volume. Thus, for element j, with density ρ_j and atomic weight A_j,

$$\Sigma_j = N_A \rho_j \sigma_j / A_j,$$

where N_A is Avogadro's number.

Table 4.4.6.1 gives the macroscopic absorption cross sections Σ_a of the elements. They are tabulated for a neutron velocity $v = 2200\ \text{m s}^{-1}$, corresponding to a wavelength of 1.80 Å. The cross sections are larger at longer wavelengths (Section 4.4.4). Apart from a few exceptions, such as boron and cadmium, the absorption cross section is vastly smaller than for X-rays. The $1/e$ penetration depth (l) is listed separately – most metals, for example, have a penetration depth of several cm. The data in Table 4.4.6.1 have been derived from the review article by Hutchings & Windsor (1987).

Table 4.4.6.1. *Absorption of the elements for neutrons ($\lambda = 1.80$ Å)*

Atom	Σ_a (cm^{-1})	l (cm)	Atom	Σ_a (cm^{-1})	l (cm)
H	0.0141	0.288	Rh	10.544	0.092
D	0.0000	6.17	Pd	0.4687	1.29
He	0.0001	20.22	Ag	3.7120	0.249
Li	3.2698	0.300	Cd	116.80	0.008
Be	0.0009	1.059	In	7.4135	0.133
B	105.41	0.009	Sn	0.0231	4.87
C	0.0004	1.58	Sb	0.1689	3.20
N	0.0662	2.14	Te	0.1386	4.01
O	0.0001	5.52	I	0.1458	4.36
F	0.0003	6.82	Xe	0.3904	2.27
Ne	0.0017	8.71	Cs	0.2458	3.57
Na	0.0135	10.22	Ba	0.0189	13.39
Mg	0.0027	6.11	La	0.2402	2.00
Al	0.0139	9.48	Ce	0.0182	9.60
Si	0.0085	8.45	Pr	0.3333	2.46
P	0.0061	8.04	Nd	1.4763	0.496
S	0.0208	16.14	Sm	171.23	0.005
Cl	0.9109	0.731	Eu	95.715	0.010
Ar	0.0143	2.03	Gd	1474.1	0.000
K	0.0279	18.12	Tb	0.7334	1.05
Ca	0.0099	12.35	Dy	29.731	0.030
Sc	1.0906	0.491	Ho	2.0791	0.424
Ti	0.3453	1.74	Er	5.1861	0.182
V	0.3658	1.35	Tm	3.4919	0.269
Cr	0.2558	1.82	Yb	0.8513	0.717
Mn	1.0900	0.789	Lu	2.5889	0.354
Fe	0.2174	0.82	Hf	4.6648	0.195
Co	3.3440	0.260	Ta	1.1434	0.676
Ni	0.4104	0.475	W	1.1609	0.681
Cu	0.3202	1.00	Re	6.1692	0.143
Zn	0.0730	2.89	Os	1.1444	0.442
Ga	0.1480	2.04	Ir	30.064	0.032
Ge	0.1016	2.07	Pt	0.6843	0.682
As	0.2091	2.15	Au	5.8181	0.159
Se	0.4292	1.36	Hg	15.146	0.061
Br	0.1623	3.31	Tl	0.1200	2.15
Kr	0.3882	1.97	Pb	0.0056	2.68
Rb	0.0041	13.09	Bi	0.0009	3.84
Sr	0.0227	7.44	Ra	0.1706	2.95
Y	0.0388	3.66	Th	0.2244	1.68
Zr	0.0079	3.42	Pa	8.0405	0.118
Nb	0.0640	2.42	U	0.3650	1.26
Mo	0.1637	1.75	Np	9.0534	0.10
Tc	1.4281	0.542	Pu	14.481	0.069
Ru	0.1886	1.48	Am	2.5522	0.351

references