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Dirac–Fock Calculations of X-ray Scattering Factors and Contributions to the Mean Inner Potential for Electron Scattering

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Abstract

Tables of X-ray scattering factors for naturally occurring elements and ions have been calculated using a multiconfiguration Dirac–Fock code. The complete data set takes up about 250 kbytes of space. For accurate values, it is preferable to interpolate directly. For consistency with previous work, parametric fits are also presented with error estimates and a range of validity. The limiting values of the electron scattering factor as $\sin\theta/\lambda$ tends to zero, which are needed to calculate the mean inner potential for electron scattering, are also tabulated. The results show that the mean inner potential can be very sensitive to ionization state.

Introduction

Accurate tables of atomic X-ray and electron scattering factors are essential for structure refinement, diffraction-theory calculations and image simulation. The earliest tables were based on Thomas–Fermi–Dirac models of the atom or on the Hartree–Fock–Slater program of Herman & Skillman (1963). Later calculations (Cromer & Waber, 1965) used the Dirac–Slater program of Liberman, Cromer & Waber (1971). All these results assumed the Slater function of average charge density for the exchange term. The most sophisticated, and probably most quoted, results are those of Doyle & Turner (1968), who used a relativistic-Hartree–Fock program. Unfortunately, they did not completely cover the Periodic Table and the recent edition of Volume C of *International Tables for Crystallography* (Maslen, Fox & O'Keefe, 1992) used their values, as well as some from Cromer & Waber, to give a complete set.

We have used the multiconfiguration Dirac–Fock package of Grant, McKenzie, Norrington, Mayers & Pyper (1980) to calculate charge densities for all naturally occurring elements and many of the most common ionization states. Positive ions can be calculated directly with appropriate input configurations. Negative ions are not only unstable in nature but, also, attempts to calculate charge densities using any of the single-configuration Hartree–Fock programs lead to lack of convergence. A common practice when performing calculations for negative ions is to surround the ion by a sphere of positive charge (Watson, 1958). This simulates the effects of neighbouring ions in a crystal. The resulting charge densities are sensitive to the radius of the Watson sphere and we have selected the published ionic radii for our calculations.

Of course, all atomic calculations (including those presented here) neglect the redistribution of charge caused by bonding. The correct procedure would be to use one of the band-theory computational methods to solve for the ground-state charge density in the solid. This is not practical except in a few limited cases. It is not legitimate to separate the atomic valence charge density and scale it in some simple manner. For some materials, the replacement of atoms by ions is an attempt to approximate the actual solid-state charge density. In a more refined calculation, the potential would be recalculated for each arrangement of ions. Our use of the Watson sphere is an aproximation to model ions that are independent of structure.

Abbreviated atomic X-ray scattering-factor tables that use the same grid as Doyle & Turner (1968) are given in the results section. There is very little difference (less than 0.1%) between our results and

those of Doyle & Turner (1968) except for some heavy elements at high values of $\sin\theta/\lambda$. A more complete set of results, tabulated on a grid of spacing $\sin\theta/\lambda = 0.05$ Å^{-1}, was used for parameterization. We have chosen a fit of four Gaussians to be consistent with Doyle & Turner but have not included a constant because, although it might give better agreement up to a value of 2.0 Å^{-1}, it is intrinsically unphysical. A table of parameters is given along with the value of $f_x(0)$, the χ^2 of the fit and the range of applicability. We have decided to give two tables, one that represents a high-accuracy fit over a range of 0.0 to 2.0 Å^{-1} and another that gives a lower-accuracy fit over an extended range to 6.0 Å^{-1}. In general, we recommend that the original tables are used with cubic spline or even linear interpolation. The space taken by the complete tables is less than 250 kbytes, which is small by the standards of computers today.

Separate electron scattering-factor tables have not been given as we believe it is preferable to use the Mott formula to calculate electron scattering factors from X-ray scattering factors. Recently, there has been a renewed interest in $f_{el}(0)$, from which the mean inner potential, V_{000}, can be calculated. The mean inner potential can now be measured with an accuracy of 0.3 V using electron holography (Gajdardziska-Josifovska, McCartney, de Ruijter, Smith, Weiss & Zuo, 1993) and it is very significant for interpretation of holographic phase imaging and Fresnel fringe contrast (Shih & Stobbs, 1990; Ross & Stobbs, 1991). A table of values for $f_{el}(0)$ is presented and we show that the mean inner potential is sensitive to ionization state.

X-ray scattering factors

Complete details of the atomic multiconfiguration Dirac–Fock package are given by Grant *et al.* (1980). The N-electron wave function is constructed from central-field Dirac orbitals that form an orthonormal set. Configuration state functions are formed by taking linear combinations of these orbitals so as to obtain eigenfunctions of the total angular-momentum operator J^2 and J_z with eigenvalues $J(J+1)$ and M, respectively. The configuration state functions are denoted by a function $\Phi(\gamma,J,M)$, where γ gives all the information about orbital occupation, coupling *etc.* Atomic state functions can now be constructed as linear combinations of configuration state functions that have the same J and M but might have different orbital occupations, as denoted by γ. An eigenvalue equation is solved for the energies of the atomic state functions, derived from the requirement that the energy is stationary for small variations in the mixing coefficients. We take the lowest-energy ground-state charge density that is tabulated on an exponential grid as the input to another program that calculates the X-ray scattering factors according to

$$f_x(s) = 4\pi \int_0^\infty r^2 \rho(r)[\sin(4\pi sr)/(4\pi sr)]\,dr, \qquad (1)$$

where $s = \sin\theta/\lambda$.

Table 1. *Watson-sphere radii used for negative ions*

Ion	Watson-sphere radius (Å)
O^{2-}	1.40
F^-	1.36
Cl^-	1.81
Br^-	1.95
I^-	2.16

All the computations were performed on a VAX system. We input the electrons into the lowest shells available following the table in *The Theory of Atomic Structure and Spectra*, pp. 117–119 (Cowan, 1981). The Dirac–Fock equations were then solved using the extended average level (EAL) model (Grant *et al.*, 1980), with no restrictions on J for all cases except Gd, Sm^{3+} and Eu^{3+}. For these elements and ions, too many configurations were generated and we restricted the calculation to the lowest value of J. Comparison of such a calculation with a calculation for all configurations gave a difference of less than 10^{-5} in the scattering factor for Gd^{3+}, so we feel this approximation is justified. For the positive ions we used the ionized elemental configurations and for the negative ions we modified the program to give a Watson sphere as discussed above. Values for the Watson-sphere radii are given in Table 1.

The complete results are tabulated in Table 2 for $\sin\theta/\lambda$ up to 6.0 Å^{-1}. The differences between these results and those of Doyle & Turner (1968) are less than 0.1% in practically all cases. The greatest difference is for a heavy element such as Au for $s = 4.0$ Å^{-1} and is about 0.7%. A plot showing the Yb scattering factor, which is typical for a heavy element, is given as Fig. 1. The ionized scattering factors are the same as the neutral-atom factors for s greater than about 1.0 Å^{-1}, as can be seen in the comparison between Mg and Mg^{2+}, given as Fig. 2(*a*), and between O and O^{2-}, given as Fig. 2(*b*).

Parameterization

We have parameterized the X-ray scattering factors as a sum of four Gaussians using the Marquardt–Levenberg procedure given in *Numerical Recipes* by Press, Flannery, Teukolsky & Vetterling (1989),

$$f_x(s) = \sum_j a_j \exp(-b_j s^2). \qquad (2)$$

Table 2. *Scattering-factor tables*

s (Å^{-1})	He	Li	Li^+	Be	Be^{2+}	B	C	N	O	O^{2-}	F	F^-
0.00	2.0000	3.0000	2.0000	4.0000	2.0000	5.0000	6.0000	7.0000	8.0000	10.0000	9.0000	10.0000
0.05	1.9572	2.7077	1.9837	3.7069	1.9915	4.7246	5.7518	6.7765	7.7974	9.5884	8.8152	9.7338
0.10	1.8373	2.2153	1.9361	3.0657	1.9663	4.0603	5.1153	6.1810	7.2439	8.5345	8.3011	9.0157
0.15	1.6628	1.9038	1.8607	2.4631	1.9254	3.3166	4.3222	5.3866	6.4706	7.2188	7.5588	8.0324
0.20	1.4607	1.7417	1.7627	2.0602	1.8704	2.6994	3.5698	4.5648	5.6215	5.9558	6.7080	6.9742
0.25	1.2545	1.6262	1.6482	1.8279	1.8032	2.2632	2.9558	3.8268	4.8064	4.8934	5.8499	5.9712
0.30	1.0606	1.5129	1.5236	1.6925	1.7261	1.9793	2.4977	3.2197	4.0872	4.0574	5.0527	5.0878
0.35	0.8877	1.3934	1.3946	1.5998	1.6413	1.7992	2.1734	2.7475	3.4873	3.4190	4.3515	4.3430
0.40	0.7387	1.2707	1.2661	1.5207	1.5514	1.6810	1.9495	2.3929	3.0054	2.9364	3.7581	3.7318
0.45	0.6134	1.1493	1.1418	1.4429	1.4584	1.5960	1.7949	2.1322	2.6279	2.5720	3.2691	3.2389
0.50	0.5093	1.0330	1.0242	1.3626	1.3644	1.5267	1.6851	1.9418	2.3371	2.2963	2.8738	2.8461
0.60	0.3532	0.8237	0.8151	1.1957	1.1798	1.4019	1.5368	1.6974	1.9455	1.9275	2.3086	2.2910
0.70	0.2483	0.6508	0.6435	1.0303	1.0075	1.2761	1.4258	1.5510	1.7144	1.7085	1.9565	1.9475
0.80	0.1774	0.5127	0.5069	0.8768	0.8530	1.1475	1.3224	1.4451	1.5682	1.5678	1.7347	1.7312
0.90	0.1290	0.4045	0.3999	0.7403	0.7182	1.0208	1.2187	1.3533	1.4635	1.4644	1.5881	1.5872
1.00	0.0954	0.3205	0.3169	0.6225	0.6031	0.9007	1.1145	1.2650	1.3772	1.3774	1.4825	1.4825
1.20	0.0546	0.2048	0.2025	0.4389	0.4248	0.6906	0.9141	1.0900	1.2214	1.2191	1.3239	1.3236
1.40	0.0331	0.1345	0.1330	0.3112	0.3012	0.5247	0.7367	0.9218	1.0707	1.0668	1.1868	1.1856
1.60	0.0210	0.0908	0.0898	0.2233	0.2162	0.3984	0.5884	0.7691	0.9261	0.9215	1.0549	1.0530
1.80	0.0139	0.0630	0.0623	0.1625	0.1574	0.3039	0.4687	0.6367	0.7927	0.7881	0.9284	0.9262
2.00	0.0095	0.0448	0.0443	0.1202	0.1164	0.2335	0.3736	0.5251	0.6739	0.6696	0.8103	0.8080
2.50	0.0042	0.0209	0.0207	0.0603	0.0584	0.1258	0.2160	0.3246	0.4434	0.4404	0.5643	0.5625
3.00	0.0021	0.0109	0.0108	0.0328	0.0318	0.0719	0.1296	0.2044	0.2926	0.2907	0.3894	0.3881
3.50	0.0012	0.0062	0.0061	0.0192	0.0186	0.0434	0.0810	0.1324	0.1963	0.1951	0.2703	0.2695
4.00	0.0007	0.0037	0.0037	0.0119	0.0115	0.0275	0.0526	0.0883	0.1345	0.1332	0.1902	0.1895
5.00	0.0003	0.0016	0.0016	0.0052	0.0050	0.0124	0.0245	0.0427	0.0675	0.0686	0.0993	0.0994
6.00	0.0001	0.0008	0.0008	0.0026	0.0025	0.0063	0.0128	0.0227	0.0368	0.0351	0.0552	0.0547

s (Å^{-1})	Ne	Na	Na^+	Mg	Mg^{2+}	Al	Al^{3+}	Si	P	S	Cl	Cl^-
0.00	10.0000	11.0000	10.0000	12.0000	10.0000	13.0000	10.0000	14.0000	15.0000	16.0000	17.0000	18.0000
0.05	9.8303	10.5680	9.8832	11.5076	9.9139	12.4386	9.9336	13.4381	14.4575	15.4828	16.5099	17.3613
0.10	9.3519	9.7607	9.5463	10.4731	9.6625	11.2290	9.7383	12.1415	13.1369	14.1735	15.2319	15.7514
0.15	8.6442	9.0274	9.0262	9.5027	9.2655	10.0592	9.4257	10.7741	11.6278	12.5781	13.5939	13.8027
0.20	7.8062	8.3364	8.3746	8.7364	8.7523	9.1587	9.0137	9.6741	10.3254	11.1041	11.9887	12.0125
0.25	6.9291	7.6196	7.6475	8.0787	8.1571	8.4658	8.5239	8.8586	9.3341	9.9239	10.6318	10.5850
0.30	6.0809	6.8826	6.8961	7.4479	7.5149	7.8743	7.9800	8.2310	8.5998	9.0382	9.5758	9.5215
0.35	5.3039	6.1572	6.1614	6.8183	6.8576	7.3172	7.4053	7.6987	8.0301	8.3760	8.7824	8.7428
0.40	4.6187	5.4730	5.4724	6.1962	6.2115	6.7680	6.8209	7.2041	7.5483	7.8573	8.1821	8.1595
0.45	4.0308	4.8491	4.8464	5.5970	5.5968	6.2243	6.2450	6.7208	7.1055	7.4190	7.7076	7.6978
0.50	3.5365	4.2949	4.2917	5.0354	5.0268	5.6943	5.6916	6.2422	6.6765	7.0194	7.3065	7.3049
0.60	2.7912	3.3989	3.3965	4.0603	4.0480	4.7142	4.6905	5.3146	5.8317	6.2560	6.5968	6.6019
0.70	2.2964	2.7547	2.7535	3.2981	3.2890	3.8849	3.8604	4.4720	5.0215	5.5071	5.9169	5.9222
0.80	1.9720	2.3059	2.3058	2.7296	2.7248	3.2220	3.2040	3.7520	4.2854	4.7914	5.2473	5.2511
0.90	1.7572	1.9975	1.9978	2.3174	2.3160	2.7127	2.7018	3.1653	3.6501	4.1395	4.6085	4.6109
1.00	1.6098	1.7846	1.7852	2.0228	2.0234	2.3311	2.3260	2.7030	3.1232	3.5712	4.0243	4.0258
1.20	1.4180	1.5241	1.5246	1.6601	1.6621	1.8417	1.8427	2.0765	2.3647	2.7001	3.0712	3.0721
1.40	1.2808	1.3671	1.3673	1.4591	1.4605	1.5717	1.5740	1.7171	1.9033	2.1332	2.4054	2.4062
1.60	1.1586	1.2465	1.2464	1.3261	1.3265	1.4085	1.4102	1.5053	1.6264	1.7791	1.9678	1.9685
1.80	1.0416	1.1375	1.1371	1.2190	1.2185	1.2926	1.2931	1.3677	1.4531	1.5572	1.6864	1.6870
2.00	0.9292	1.0330	1.0325	1.1210	1.1198	1.1961	1.1955	1.2648	1.3339	1.4110	1.5026	1.5030
2.50	0.6808	0.7917	0.7909	0.8921	0.8902	0.9799	0.9776	1.0559	1.1225	1.1827	1.2408	1.2408
3.00	0.4896	0.5920	0.5912	0.6912	0.6892	0.7836	0.7808	0.8677	0.9428	1.0094	1.0689	1.0687
3.50	0.3514	0.4393	0.4380	0.5284	0.5260	0.6160	0.6128	0.6997	0.7780	0.8501	0.9156	0.9154
4.00	0.2540	0.3234	0.3247	0.3990	0.3998	0.4769	0.4770	0.5551	0.6315	0.7045	0.7730	0.7721
5.00	0.1377	0.1844	0.1827	0.2372	0.2336	0.2936	0.2890	0.3529	0.4139	0.4759	0.5378	0.5387
6.00	0.0787	0.1067	0.1074	0.1394	0.1409	0.1772	0.1789	0.2195	0.2655	0.3146	0.3656	0.3645

Table 2 (*cont.*)

s (Å^{-1})	Ar	K	K^+	Ca	Ca^{2+}	Sc	Sc^{3+}	Ti	Ti^{4+}	V	V^{5+}	Cr
0.00	18.0000	19.0000	18.0000	20.0000	18.0000	21.0000	18.0000	22.0000	18.0000	23.0000	18.0000	24.0000
0.05	17.5361	18.2046	17.6487	19.0915	17.7214	20.1312	17.7721	21.1709	17.8093	22.2080	17.8377	23.3268
0.10	16.2988	16.7341	16.6780	17.3321	16.9355	18.3542	17.1207	19.4075	17.2595	20.4716	17.3667	21.7816
0.15	14.6489	15.2444	15.2987	15.7245	15.7755	16.6416	16.1347	17.6297	16.4123	18.6538	16.6314	20.0093
0.20	12.9510	13.7301	13.7618	14.3063	14.4144	15.1315	14.9363	16.0374	15.3561	16.9942	15.6972	18.2458
0.25	11.4426	12.2706	12.2773	12.9634	13.0188	13.7302	13.6534	14.5667	14.1890	15.4567	14.6399	16.5480
0.30	10.2179	10.9786	10.9744	11.7074	11.7149	12.4228	12.3961	13.1953	13.0027	14.0197	13.5342	14.9559
0.35	9.2736	9.9099	9.9031	10.5924	10.5766	11.2449	11.2429	11.9477	11.8707	12.7015	12.4456	13.5062
0.40	8.5592	9.0631	9.0572	9.6518	9.6304	10.2274	10.2375	10.8520	10.8432	11.5283	11.4239	12.2233
0.45	8.0124	8.4047	8.4007	8.8869	8.8685	9.3793	9.3935	9.9208	9.9465	10.5147	10.5016	11.1160
0.50	7.5766	7.8900	7.8879	8.2766	8.2640	8.6891	8.7028	9.1491	9.1870	9.6604	9.6948	10.1795
0.60	6.8762	7.1264	7.1266	7.3930	7.3906	7.6839	7.6921	8.0081	8.0390	8.3736	8.4273	8.7563
0.70	6.2533	6.5243	6.5251	6.7633	6.7654	6.9980	7.0027	7.2418	7.2584	7.5074	7.5440	7.7919
0.80	5.6409	5.9632	5.9639	6.2295	6.2323	6.4614	6.4665	6.6778	6.6881	6.8937	6.9153	7.1190
0.90	5.0373	5.4073	5.4077	5.7186	5.7203	5.9767	5.9840	6.2017	6.2136	6.4075	6.4253	6.6079
1.00	4.4615	4.8603	4.8603	5.2108	5.2113	5.5029	5.5128	5.7538	5.7709	5.9736	5.9961	6.1738
1.20	3.4631	3.8562	3.8560	4.2348	4.2338	4.5719	4.5843	4.8739	4.9000	5.1415	5.1791	5.3747
1.40	2.7138	3.0468	3.0467	3.3926	3.3916	3.7244	3.7359	4.0405	4.0682	4.3355	4.3799	4.5998
1.60	2.1929	2.4500	2.4500	2.7334	2.7329	3.0239	3.0330	3.3171	3.3407	3.6056	3.6468	3.8762
1.80	1.8450	2.0330	2.0333	2.2503	2.2504	2.4857	2.4923	2.7353	2.7531	2.9928	3.0259	3.2459
2.00	1.6145	1.7494	1.7497	1.9098	1.9102	2.0914	2.0959	2.2921	2.3043	2.5076	2.5317	2.7289
2.50	1.3011	1.3682	1.3677	1.4446	1.4446	1.5340	1.5350	1.6379	1.6412	1.7569	1.7647	1.8894
3.00	1.1230	1.1751	1.1746	1.2266	1.2259	1.2804	1.2798	1.3392	1.3390	1.4051	1.4060	1.4795
3.50	0.9747	1.0301	1.0286	1.0806	1.0782	1.1273	1.1250	1.1729	1.1706	1.2192	1.2171	1.2677
4.00	0.8364	0.8933	0.8951	0.9458	0.9487	0.9954	0.9979	1.0415	1.0435	1.0851	1.0865	1.1278
5.00	0.5987	0.6590	0.6578	0.7189	0.7150	0.7737	0.7694	0.8250	0.8206	0.8729	0.8686	0.9164
6.00	0.4179	0.4709	0.4714	0.5229	0.5244	0.5747	0.5765	0.6254	0.6274	0.6747	0.6768	0.7225

s (Å^{-1})	Cr^{4+}	Mn	Mn^{2+}	Fe	Fe^{2+}	Co	Co^{2+}	Ni	Ni^{2+}	Cu	Cu^{2+}	Zn
0.00	20.0000	25.0000	23.0000	26.0000	24.0000	27.0000	25.0000	28.0000	26.0000	29.0000	27.0000	30.0000
0.05	19.8015	24.2739	22.7058	25.3031	23.7101	26.3304	24.7152	27.3557	25.7205	28.3793	26.7260	29.4013
0.10	19.2278	22.6079	21.8713	23.6752	22.8850	24.7418	23.9018	25.8062	24.9200	26.8682	25.9390	27.9278
0.15	18.3389	20.7569	20.6222	21.8228	21.6418	22.8954	22.6685	23.9710	23.6992	25.0479	24.7325	26.1254
0.20	17.2207	19.0021	19.1174	20.0362	20.1310	21.0862	21.1575	22.1461	22.1919	23.2132	23.2323	24.2858
0.25	15.9689	17.3526	17.5077	18.3423	18.4985	19.3554	19.5087	20.3850	20.5324	21.4278	21.5668	22.4812
0.30	14.6743	15.7955	15.9114	16.7335	16.8616	17.7011	17.8382	18.6911	18.8345	19.6997	19.8471	20.7240
0.35	13.4121	14.3450	14.4095	15.2239	15.3031	16.1376	16.2299	17.0791	17.1829	18.0447	18.1582	19.0308
0.40	12.2370	13.0251	13.0493	13.8370	13.8740	14.6884	14.7378	15.5728	15.6340	16.4863	16.5586	17.4253
0.45	11.1824	11.8535	11.8528	12.5919	12.6002	13.3738	13.3917	14.1934	14.2211	15.0468	15.0844	15.9305
0.50	10.2635	10.8369	10.8237	11.4977	11.4899	12.2052	12.2037	12.9543	12.9597	13.7414	13.7542	14.5630
0.60	8.8244	9.2441	9.2275	9.7511	9.7347	10.3067	10.2914	10.9081	10.8946	11.5528	11.5420	12.2384
0.70	7.8281	8.1372	8.1275	8.5114	8.4999	8.9295	8.9165	9.3915	9.3777	9.8971	9.8830	10.4453
0.80	7.1332	7.3692	7.3661	7.6453	7.6403	7.9549	7.9481	8.3010	8.2926	8.6858	8.6759	9.1102
0.90	6.6136	6.8088	6.8093	7.0239	7.0233	7.2592	7.2573	7.5201	7.5168	7.8107	7.8059	8.1340
1.00	6.1804	6.3604	6.3618	6.5466	6.5478	6.7393	6.7399	6.9453	6.9452	7.1702	7.1691	7.4186
1.20	5.3927	5.5876	5.5870	5.7769	5.7770	5.9521	5.9527	6.1196	6.1205	6.2854	6.2865	6.4553
1.40	4.6260	4.8515	4.8485	5.0727	5.0703	5.2720	5.2703	5.4530	5.4519	5.6198	5.6193	5.7766
1.60	3.9033	4.1456	4.1416	4.3899	4.3861	4.6151	4.6115	4.8212	4.8181	5.0095	5.0070	5.1820
1.80	3.2694	3.5075	3.5038	3.7548	3.7509	3.9905	3.9865	4.2124	4.2085	4.4195	4.4158	4.6113
2.00	2.7470	2.9647	2.9619	3.1969	3.1936	3.4259	3.4223	3.6486	3.6447	3.8621	3.8582	4.0649
2.50	1.8962	2.0384	2.0377	2.1980	2.1969	2.3674	2.3658	2.5440	2.5421	2.7255	2.7231	2.9091
3.00	1.4808	1.5640	1.5639	1.6587	1.6584	1.7638	1.7634	1.8789	1.8783	2.0033	2.0025	2.1359
3.50	1.2666	1.3205	1.3196	1.3783	1.3776	1.4424	1.4418	1.5136	1.5130	1.5922	1.5916	1.6785
4.00	1.1289	1.1691	1.1710	1.2119	1.2138	1.2568	1.2585	1.3048	1.3064	1.3568	1.3583	1.4136
5.00	0.9136	0.9596	0.9560	0.9990	0.9957	1.0365	1.0334	1.0726	1.0697	1.1079	1.1052	1.1430
6.00	0.7240	0.7675	0.7691	0.8108	0.8123	0.8518	.8533	.8907	0.8921	0.9276	.9290	0.9627

Table 2 (*cont.*)

s (Å^{-1})	Zn^{2+}	Ga	Ge	As	Se	Br	Br^-	Kr	Rb	Rb^+	Sr	Sr^{2+}
0.00	28.0000	31.0000	32.0000	33.0000	34.0000	35.0000	36.0000	36.0000	37.0000	36.0000	38.0000	36.0000
0.05	27.7315	30.3029	31.2735	32.2677	33.2727	34.2870	35.1146	35.3038	35.9484	35.4350	36.8020	35.5244
0.10	26.9584	28.6670	29.5273	30.4571	31.4297	32.4403	32.8997	33.4680	33.9087	33.8921	34.4593	34.1987
0.15	25.7675	26.7780	27.4940	28.2887	29.1512	30.0828	30.2274	31.0571	31.6830	31.7428	32.1735	32.2827
0.20	24.2770	24.9346	25.5599	26.2223	26.9425	27.7379	27.7224	28.5932	29.3713	29.3959	29.9906	30.0916
0.25	22.6094	23.1771	23.7894	24.3806	24.9905	25.6513	25.5933	26.3670	27.1511	27.1507	27.8666	27.8951
0.30	20.8731	21.4860	22.1389	22.7252	23.2853	23.8558	23.8069	24.4566	25.1616	25.1533	25.8782	25.8641
0.35	19.1526	19.8519	20.5660	21.1907	21.7551	22.2903	22.2614	22.8233	23.4359	23.4277	24.0939	24.0680
0.40	17.5080	18.2836	19.0537	19.7329	20.3347	20.8791	20.8662	21.3913	21.9379	21.9325	22.5258	22.5039
0.45	15.9778	16.7987	17.6054	18.3345	18.9851	19.5647	19.5616	20.0912	20.6090	20.6066	21.1448	21.1318
0.50	14.5836	15.4150	16.2338	16.9962	17.6907	18.3139	18.3160	18.8743	19.3949	19.3948	19.9063	19.9017
0.60	12.2309	12.9999	13.7752	14.5405	15.2755	15.9640	15.9688	16.5982	17.1717	17.1733	17.7003	17.7048
0.70	10.4315	11.0765	11.7485	12.4453	13.1490	13.8419	13.8454	14.5087	15.1308	15.1322	15.7065	15.7119
0.80	9.0992	9.6066	10.1535	10.7432	11.3646	12.0047	12.0066	12.6484	13.2761	13.2768	13.8767	13.8798
0.90	8.1278	8.5121	8.9386	9.4124	9.9291	10.4819	10.4827	11.0601	11.6484	11.6484	12.2339	12.2346
1.00	7.4164	7.7041	8.0294	8.3978	8.8097	9.2639	9.2641	9.7549	10.2734	10.2732	10.8092	10.8084
1.20	6.4563	6.6346	6.8312	7.0512	7.2999	7.5820	7.5819	7.8998	8.2539	8.2536	8.6421	8.6409
1.40	5.7767	5.9279	6.0781	6.2325	6.3964	6.5755	6.5754	6.7748	6.9990	6.9989	7.2514	7.2508
1.60	5.1801	5.3440	5.4949	5.6379	5.7766	5.9151	5.9152	6.0582	6.2107	6.2107	6.3773	6.3773
1.80	4.6080	4.7937	4.9627	5.1188	5.2639	5.4000	5.4001	5.5301	5.6574	5.6577	5.7864	5.7868
2.00	4.0610	4.2624	4.4486	4.6226	4.7842	4.9339	4.9341	5.0729	5.2025	5.2026	5.3255	5.3258
2.50	2.9064	3.0986	3.2883	3.4760	3.6598	3.8377	3.8380	4.0083	4.1706	4.1699	4.3226	4.3218
3.00	2.1347	2.2786	2.4289	2.5852	2.7462	2.9102	2.9106	3.0757	3.2407	3.2400	3.4031	3.4020
3.50	1.6778	1.7741	1.8779	1.9898	2.1095	2.2365	2.2371	2.3699	2.5093	2.5078	2.6521	2.6495
4.00	1.4150	1.4755	1.5442	1.6199	1.7027	1.7929	1.7925	1.8901	1.9919	1.9938	2.0997	2.1034
5.00	1.1406	1.1793	1.2165	1.2550	1.2957	1.3395	1.3411	1.3870	1.4387	1.4378	1.4971	1.4939
6.00	0.9641	.9957	1.0275	1.0587	1.0895	1.1206	1.1196	1.1521	1.1846	1.1852	1.2175	1.2191

s (Å^{-1})	Y	Y^{3+}	Zr	Zr^{4+}	Nb	Nb^{5+}	Mo	Mo^{6+}	Ru	Rh	Pd	Pd^{2+}
0.00	39.0000	36.0000	40.0000	36.0000	41.0000	36.0000	42.0000	36.0000	44.0000	45.0000	46.0000	44.0000
0.05	37.8157	35.5902	38.8458	35.6412	39.9638	35.6819	40.9967	35.7152	43.0582	44.0870	45.2322	43.4544
0.10	35.3631	34.4325	36.3512	34.6175	37.5864	34.7678	38.6363	34.8924	40.7608	41.8292	43.1745	41.9203
0.15	32.9037	32.7166	33.7519	33.0723	34.8912	33.3687	35.8788	33.6192	37.9441	39.0068	40.3623	39.6620
0.20	30.6344	30.6877	31.3591	31.1988	32.2861	31.6391	33.1680	32.0207	35.0716	36.0779	37.2935	37.0068
0.25	28.4911	28.5776	29.1425	29.1929	29.8731	29.7438	30.6462	30.2357	32.3444	33.2614	34.2936	34.2499
0.30	26.4923	26.5575	27.0987	27.2149	27.6941	27.8277	28.3712	28.3933	29.8603	30.6741	31.5351	31.6049
0.35	24.6836	24.7221	25.2531	25.3701	25.7682	25.9977	26.3651	26.5960	27.6625	28.3726	29.0909	29.1962
0.40	23.0821	23.0999	23.6176	23.7081	24.0893	24.3159	24.6217	24.9125	25.7551	26.3703	26.9749	27.0761
0.45	21.6711	21.6751	22.1783	22.2352	22.6298	22.8054	23.1140	23.3776	24.1162	24.6504	25.1674	25.2484
0.50	20.4149	20.4110	20.9041	20.9303	21.3505	21.4606	21.8026	21.9986	22.7088	23.1790	23.6310	23.6879
0.60	18.2155	18.2066	18.7048	18.6922	19.1696	19.1717	19.6028	19.6517	20.4174	20.8122	21.1909	21.2079
0.70	16.2580	16.2506	16.7791	16.7552	17.2814	17.2345	17.7382	17.6970	18.5663	18.9462	19.3096	19.3046
0.80	14.4558	14.4510	15.0092	14.9882	15.5464	15.4935	16.0416	15.9714	16.9372	17.3404	17.7246	17.7118
0.90	12.8108	12.8078	13.3745	13.3602	13.9277	13.8873	14.4521	14.3877	15.4200	15.8603	16.2803	16.2674
1.00	11.3520	11.3500	11.8966	11.8882	12.4402	12.4151	12.9715	12.9249	13.9825	14.4546	14.9083	14.8987
1.20	9.0582	9.0571	9.4987	9.4962	9.9574	9.9512	10.4315	10.4152	11.3990	11.8813	12.3581	12.3552
1.40	7.5326	7.5319	7.8429	7.8417	8.1797	8.1784	8.5434	8.5386	9.3358	9.7570	10.1885	10.1885
1.60	6.5623	6.5621	6.7686	6.7679	6.9980	6.9968	7.2520	7.2495	7.8339	8.1601	8.5063	8.5066
1.80	5.9212	5.9215	6.0658	6.0657	6.2238	6.2230	6.3978	6.3962	6.8034	7.0380	7.2940	7.2939
2.00	5.4446	5.4452	5.5635	5.5643	5.6858	5.6864	5.8146	5.8148	6.1041	6.2701	6.4531	6.4526
2.50	4.4631	4.4639	4.5938	4.5964	4.7147	4.7201	4.8292	4.8361	5.0425	5.1451	5.2480	5.2480
3.00	3.5596	3.5600	3.7102	3.7129	3.8527	3.8597	3.9896	3.9996	4.2415	4.3567	4.4643	4.4654
3.50	2.7950	2.7937	2.9382	2.9389	3.0789	3.0840	3.2194	3.2277	3.4910	3.6205	3.7434	3.7448
4.00	2.2139	2.2185	2.3328	2.3383	2.4549	2.4620	2.5796	2.5888	2.8324	2.9588	3.0839	3.0859
5.00	1.5593	1.5551	1.6256	1.6214	1.6952	1.6928	1.7703	1.7692	1.9341	2.0221	2.1125	2.1119
6.00	1.2519	1.2545	1.2888	1.2919	1.3288	1.3318	1.3713	1.3745	1.4659	1.5183	1.5744	1.5758

Table 2 (*cont.*)

s (Å^{-1})	Ag	Ag^{2+}	Cd	Cd^{2+}	In	Sn	Sb	Te	I	I^-	Xe	Cs
0.00	47.0000	45.0000	48.0000	46.0000	49.0000	50.0000	51.0000	52.0000	53.0000	54.0000	54.0000	55.0000
0.05	46.1395	44.4625	47.0851	45.4712	47.9647	48.9156	49.8946	50.8883	51.9010	52.6917	52.9174	53.5275
0.10	43.9655	42.9447	44.7986	43.9718	45.5096	46.3221	47.2023	48.1289	49.1172	49.4904	50.1274	50.6045
0.15	41.1604	40.6929	41.9260	41.7315	42.5911	43.2760	44.0113	44.8001	45.6730	45.7384	46.5916	47.2939
0.20	38.1586	38.0185	38.9340	39.0455	39.6417	40.2907	40.9327	41.5956	42.3198	42.2683	43.0923	43.8925
0.25	35.1971	35.2115	36.0122	36.1968	36.7835	37.4684	38.0995	38.7068	39.3266	39.2689	39.9713	40.7172
0.30	32.4213	32.4900	33.2562	33.4061	34.0695	34.8082	35.4777	36.0945	36.6795	36.6461	37.2559	37.9086
0.35	29.9147	29.9888	30.7306	30.8169	31.5467	32.3186	33.0324	33.6881	34.2893	34.2766	34.8553	35.4450
0.40	27.7116	27.7716	28.4735	28.5035	29.2542	30.0236	30.7599	31.4509	32.0868	32.0858	32.6763	33.2468
0.45	25.8099	25.8514	26.4964	26.4884	27.2140	27.9472	28.6744	29.3780	30.0415	30.0459	30.6621	31.2421
0.50	24.1850	24.2098	24.7886	24.7604	25.4287	26.1019	26.7913	27.4798	28.1497	28.1560	28.7902	29.3879
0.60	21.6110	21.6145	22.0675	22.0344	22.5545	23.0824	23.6475	24.2418	24.8559	24.8611	25.4753	26.0776
0.70	19.6652	19.6604	20.0314	20.0127	20.4109	20.8163	21.2535	21.7243	22.2298	22.2326	22.7624	23.3074
0.80	18.0732	18.0670	18.4094	18.4052	18.7401	19.0756	19.4249	19.7953	20.1944	20.1954	20.6227	21.0764
0.90	16.6556	16.6506	17.0043	17.0089	17.3337	17.6499	17.9610	18.2754	18.6021	18.6020	18.9471	19.3144
1.00	15.3210	15.3178	15.7025	15.7104	16.0577	16.3888	16.7013	17.0016	17.2973	17.2967	17.5958	17.9046
1.20	12.8178	12.8169	13.2570	13.2626	13.6747	14.0673	14.4345	14.7768	15.0958	15.0952	15.3954	15.6811
1.40	10.6263	10.6261	11.0637	11.0651	11.4959	11.9180	12.3259	12.7166	13.0871	13.0870	13.4365	13.7647
1.60	8.8716	8.8714	9.2514	9.2509	9.6413	10.0372	10.4346	10.8294	11.2176	11.2178	11.5954	11.9595
1.80	7.5716	7.5713	7.8695	7.8690	8.1857	8.5178	8.8628	9.2176	9.5790	9.5794	9.9431	10.3053
2.00	6.6537	6.6535	6.8733	6.8732	7.1120	7.3693	7.6443	7.9354	8.2412	8.2415	8.5589	8.8850
2.50	5.3533	5.3533	5.4629	5.4631	5.5792	5.7037	5.8383	5.9845	6.1438	6.1440	6.3169	6.5051
3.00	4.5682	4.5683	4.6673	4.6664	4.7628	4.8558	4.9476	5.0398	5.1339	5.1340	5.2313	5.3343
3.50	3.8643	3.8640	3.9797	3.9777	4.0900	4.1948	4.2945	4.3896	4.4805	4.4811	4.5682	4.6546
4.00	3.2075	3.2091	3.3294	3.3298	3.4482	3.5643	3.6772	3.7862	3.8911	3.8901	3.9916	4.0861
5.00	2.2088	2.2070	2.3084	2.3049	2.4107	2.5151	2.6207	2.7271	2.8337	2.8357	2.9402	3.0451
6.00	1.6335	1.6351	1.6961	1.6980	1.7623	1.8321	1.9056	1.9827	2.0635	2.0626	2.1475	2.2346

s (Å^{-1})	Cs^+	Ba	Ba^{2+}	La	La^{3+}	Ce	Ce^{4+}	Pr	Pr^{3+}	Nd	Nd^{3+}	Sm
0.00	54.0000	56.0000	54.0000	57.0000	54.0000	58.0000	54.0000	59.0000	56.0000	60.0000	57.0000	62.0000
0.05	53.0845	54.3449	53.2034	55.3491	53.2943	56.3817	53.3668	57.4382	55.3130	58.4678	56.3229	60.5238
0.10	50.6367	51.1240	51.0255	51.9749	51.3352	53.0372	51.5894	54.2770	53.3936	55.3361	54.4257	57.4542
0.15	47.3485	47.8417	47.9851	48.5159	48.5246	49.5682	48.9868	50.9485	50.6058	52.0094	51.6549	54.1415
0.20	43.9014	44.5901	44.6544	45.2097	45.3397	46.2277	45.9582	47.5983	47.3936	48.6423	48.4381	50.7554
0.25	40.7076	41.4604	41.4507	42.0811	42.1738	43.0436	42.8623	44.3098	44.1401	45.3150	45.1515	47.3681
0.30	37.8982	38.6026	38.5716	39.2184	39.2581	40.1091	39.9415	41.2424	41.0903	42.1882	42.0444	44.1392
0.35	35.4392	36.0686	36.0447	36.6666	36.6704	37.4796	37.3090	38.4833	38.3483	39.3584	39.2312	41.1801
0.40	33.2455	33.8234	33.8134	34.4042	34.3902	35.1444	34.9788	36.0314	35.9179	36.8354	36.7274	38.5199
0.45	31.2436	31.8034	31.8045	32.3764	32.3573	33.0550	32.9109	33.8403	33.7541	34.5797	34.4959	36.1341
0.50	29.3904	29.9543	29.9611	30.5284	30.5112	31.1580	31.0496	31.8562	31.8012	32.5404	32.4846	33.9788
0.60	26.0795	26.6579	26.6648	27.2357	27.2282	27.7939	27.7705	28.3570	28.3606	28.9547	28.9536	30.2045
0.70	23.3077	23.8560	23.8579	24.4055	24.4049	24.9044	24.9425	25.3728	25.4113	25.8992	25.9334	26.9950
0.80	21.0758	21.5511	21.5494	22.0355	22.0373	22.4726	22.5330	22.8712	22.9180	23.3289	23.3737	24.2812
0.90	19.3136	19.7051	19.7024	20.1103	20.1120	20.4849	20.5396	20.8289	20.8674	21.2196	21.2583	22.0336
1.00	17.9041	18.2286	18.2264	18.5647	18.5657	18.8854	18.9228	19.1869	19.2116	19.5183	19.5444	20.2076
1.20	15.6812	15.9580	15.9579	16.2309	16.2307	16.4947	16.5044	16.7499	16.7549	17.0083	17.0142	17.5285
1.40	13.7650	14.0730	14.0738	14.3655	14.3650	14.6367	14.6417	14.8926	14.8949	15.1422	15.1438	15.6181
1.60	11.9597	12.3078	12.3084	12.6407	12.6402	12.9438	12.9548	13.2236	13.2308	13.4990	13.5046	14.0114
1.80	10.3057	10.6632	10.6635	11.0141	11.0137	11.3375	11.3537	11.6370	11.6484	11.9381	11.9481	12.5038
2.00	8.8851	9.2172	9.2172	9.5524	9.5520	9.8699	9.8865	10.1696	10.1818	10.4769	10.4884	11.0693
2.50	6.5042	6.7068	6.7058	6.9224	6.9215	7.1441	7.1505	7.3684	7.3735	7.6061	7.6117	8.0996
3.00	5.3336	5.4434	5.4424	5.5598	5.5588	5.6851	5.6840	5.8183	5.8177	5.9600	5.9599	6.2692
3.50	4.6531	4.7398	4.7368	4.8230	4.8202	4.9085	4.9042	4.9971	4.9933	5.0874	5.0838	5.2797
4.00	4.0880	4.1755	4.1796	4.2621	4.2671	4.3466	4.3511	4.4299	4.4336	4.5105	4.5140	4.6690
5.00	3.0446	3.1514	3.1486	3.2558	3.2515	3.3558	3.3527	3.4519	3.4493	3.5473	3.5446	3.7303
6.00	2.2350	2.3232	2.3244	2.4126	2.4154	2.5032	2.5076	2.5948	2.5977	2.6870	2.6899	2.8719

Table 2 (*cont.*)

s (Å^{-1})	Sm^{3+}	Eu	Eu^{3+}	Gd	Gd^{3+}	Tb	Tb^{3+}	Dy	Dy^{3+}	Ho	Ho^{3+}	Er
0.00	59.0000	63.0000	60.0000	64.0000	61.0000	65.0000	62.0000	66.0000	63.0000	67.0000	64.0000	68.0000
0.05	58.3428	61.5502	59.3525	62.5491	60.3620	63.6014	61.3715	64.6261	62.3810	65.6500	63.3904	66.6733
0.10	56.4916	58.5106	57.5246	59.4001	58.5568	60.6278	59.5896	61.6854	60.6227	62.7419	61.6554	63.7975
0.15	53.7612	55.2064	54.8164	55.9669	55.8711	57.3534	56.9281	58.4275	57.9867	59.5015	59.0453	60.5752
0.20	50.5476	51.8152	51.6092	52.5515	52.6723	53.9653	53.7406	55.0446	54.8135	56.1257	55.8879	57.2080
0.25	47.2117	48.4051	48.2557	49.1785	49.3049	50.5231	50.3633	51.5922	51.4305	52.6659	52.5019	53.7436
0.30	44.0070	45.1332	45.0099	45.9388	46.0226	47.1783	47.0487	48.2179	48.0884	49.2658	49.1361	50.3211
0.35	41.0650	42.1164	42.0102	42.9253	42.9694	44.0563	43.9458	45.0497	44.9404	46.0552	45.9468	47.0718
0.40	38.4215	39.3922	39.3010	40.1805	40.1981	41.2097	41.1146	42.1469	42.0532	43.0993	43.0067	44.0658
0.45	36.0553	36.9432	36.8690	37.6998	37.7026	38.6353	38.5561	39.5127	39.4344	40.4076	40.3298	41.3186
0.50	33.9230	34.7299	34.6757	35.4531	35.4491	36.3026	36.2418	37.1216	37.0605	37.9591	37.8977	38.8140
0.60	30.1967	30.8579	30.8468	31.5229	31.5171	32.2230	32.2030	32.9370	32.9147	33.6694	33.6448	34.4197
0.70	27.0220	27.5679	27.5899	28.1796	28.1762	28.7599	28.7741	29.3845	29.3958	30.0262	30.0346	30.6849
0.80	24.3224	24.7800	24.8170	25.3303	25.3285	25.8164	25.8492	26.3605	26.3913	26.9206	26.9492	27.4967
0.90	22.0727	22.4612	22.4978	22.9397	22.9384	23.3509	23.3872	23.8193	23.8550	24.3027	24.3376	24.8012
1.00	20.2364	20.5695	20.5975	20.9733	20.9720	21.3237	21.3542	21.7216	21.7527	22.1333	22.1647	22.5589
1.20	17.5367	17.7945	17.8031	18.0770	18.0759	18.3414	18.3532	18.6265	18.6398	18.9207	18.9352	19.2247
1.40	15.6189	15.8483	15.8489	16.0771	16.0763	16.3004	16.3020	16.5261	16.5281	16.7534	16.7561	16.9839
1.60	14.0145	14.2510	14.2530	14.4831	14.4823	14.7029	14.7037	14.9181	14.9184	15.1279	15.1280	15.3339
1.80	12.5113	12.7689	12.7750	13.0284	13.0274	13.2648	13.2690	13.4970	13.5003	13.7199	13.7223	13.9343
2.00	11.0791	11.3527	11.3615	11.6358	11.6346	11.8905	11.8979	12.1447	12.1512	12.3892	12.3948	12.6242
2.50	8.1060	8.3528	8.3593	8.6166	8.6151	8.8646	8.8717	9.1210	9.1281	9.3762	9.3832	9.6291
3.00	6.2700	6.4364	6.4376	6.6145	6.6132	6.7939	6.7960	6.9831	6.9857	7.1784	7.1814	7.3791
3.50	5.2765	5.3829	5.3800	5.4914	5.4889	5.6061	5.6037	5.7266	5.7245	5.8534	5.8517	5.9866
4.00	4.6723	4.7483	4.7515	4.8274	4.8317	4.9104	4.9135	4.9944	4.9975	5.0811	5.0842	5.1711
5.00	3.7273	3.8177	3.8146	3.9038	3.8993	3.9848	3.9815	4.0648	4.0613	4.1425	4.1390	4.2184
6.00	2.8748	2.9640	2.9668	3.0554	3.0583	3.1459	3.1488	3.2353	3.2381	3.3234	3.3262	3.4100

s (Å^{-1})	Er^{3+}	Tm	Tm^{3+}	Yb	Yb^{3+}	Lu	Lu^{3+}	Hf	Ta	W	Re	Os
0.00	65.0000	69.0000	66.0000	70.0000	67.0000	71.0000	68.0000	72.0000	73.0000	74.0000	75.0000	76.0000
0.05	64.3994	67.6959	65.4083	68.7180	66.4170	69.7019	67.4255	70.7142	71.7325	72.7531	73.7747	74.7965
0.10	62.6875	64.8521	63.7190	65.9059	64.7499	66.7748	65.7802	67.7292	68.7190	69.7292	70.7529	71.7854
0.15	60.1034	61.6485	61.1611	62.7213	62.2183	63.4617	63.2748	64.2897	65.1726	66.0960	67.0504	68.0292
0.20	56.9631	58.2912	58.0390	59.3750	59.1154	60.0931	60.1919	60.8392	61.6216	62.4409	63.2949	64.1803
0.25	53.5769	54.8245	54.6548	55.9081	55.7352	56.6809	56.8177	57.4176	58.1530	58.9024	59.6735	60.4695
0.30	50.1908	51.3829	51.2515	52.4503	52.3177	53.2868	53.3885	54.0517	54.7836	55.5036	56.2253	56.9574
0.35	46.9637	48.0981	47.9901	49.1335	49.0250	50.0073	50.0676	50.8033	51.5500	52.2664	52.9666	53.6614
0.40	43.9739	45.0451	44.9536	46.0364	45.9448	46.9165	46.9467	47.7299	48.4920	49.2150	49.9103	50.5877
0.45	41.2413	42.2448	42.1676	43.1852	43.1079	44.0492	44.0611	44.8640	45.6339	46.3642	47.0619	47.7340
0.50	38.7522	39.6855	39.6232	40.5727	40.5098	41.4085	41.4111	42.2125	42.9816	43.7157	44.4172	45.0901
0.60	34.3930	35.1873	35.1586	35.9718	35.9411	36.7420	36.7398	37.5056	38.2540	38.9817	39.6856	40.3643
0.70	30.6906	31.3604	31.3634	32.0525	32.0527	32.7595	32.7584	33.4733	34.1862	34.8920	35.5856	36.2633
0.80	27.5231	28.0888	28.1130	28.6969	28.7188	29.3407	29.3403	29.9986	30.6650	31.3348	32.0033	32.6662
0.90	24.8352	25.3151	25.3479	25.8444	25.8759	26.4198	26.4192	27.0137	27.6225	28.2426	28.8701	29.5013
1.00	22.5906	22.9990	23.0307	23.4538	23.4853	23.9558	23.9545	24.4787	25.0204	25.5787	26.1509	26.7342
1.20	19.2405	19.5395	19.5565	19.8656	19.8837	20.2247	20.2227	20.6033	21.0019	21.4203	21.8581	22.3147
1.40	16.9873	17.2186	17.2229	17.4588	17.4639	17.7131	17.7116	17.9796	18.2599	18.5553	18.8669	19.1957
1.60	15.3338	15.5374	15.5372	15.7396	15.7396	15.9429	15.9420	16.1494	16.3609	16.5789	16.8054	17.0419
1.80	13.9361	14.1414	14.1425	14.3421	14.3426	14.5382	14.5376	14.7305	14.9202	15.1086	15.2972	15.4878
2.00	12.6289	12.8500	12.8539	13.0671	13.0703	13.2794	13.2787	13.4844	13.6825	13.8743	14.0608	14.2430
2.50	9.6360	9.8789	9.8856	10.1248	10.1313	10.3737	10.3723	10.6191	10.8598	11.0950	11.3241	11.5466
3.00	7.3824	7.5845	7.5880	7.7936	7.7974	8.0113	8.0097	8.2332	8.4585	8.6861	8.9152	9.1449
3.50	5.9851	6.1260	6.1248	6.2715	6.2707	6.4250	6.4225	6.5854	6.7526	6.9264	7.1064	7.2922
4.00	5.1742	5.2647	5.2678	5.3623	5.3655	5.4640	5.4676	5.5712	5.6841	5.8027	5.9273	6.0581
5.00	4.2148	4.2926	4.2889	4.3655	4.3618	4.4382	4.4336	4.5092	4.5795	4.6495	4.7198	4.7909
6.00	3.4127	3.4949	3.4976	3.5781	3.5808	3.6592	3.6621	3.7384	3.8158	3.8913	3.9649	4.0368

Table 2 (*cont.*)

s (Å^{-1})	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po
0.00	77.0000	78.0000	79.0000	80.0000	81.0000	82.0000	83.0000	84.0000
0.05	75.8233	76.9110	77.9358	78.8983	79.7425	80.6686	81.6272	82.6037
0.10	72.8404	74.0749	75.1371	76.0195	76.6852	77.4471	78.2747	79.1498
0.15	69.0530	70.3248	71.3837	72.2020	72.8694	73.5283	74.2174	74.9467
0.20	65.1231	66.2956	67.3010	68.0934	68.8348	69.4995	70.1352	70.7698
0.25	61.3189	62.3251	63.2474	64.0350	64.8316	65.5494	66.2082	66.8295
0.30	57.7269	58.5686	59.4018	60.1836	60.9957	61.7579	62.4649	63.1218
0.35	54.3735	55.0881	55.8418	56.6067	57.4016	58.1788	58.9212	59.6215
0.40	51.2636	51.8969	52.5879	53.3252	54.0837	54.8473	55.5987	56.3256
0.45	48.3905	48.9818	49.6286	50.3332	51.0477	51.7790	52.5150	53.2442
0.50	45.7386	46.3170	46.9362	47.6082	48.2801	48.9713	49.6761	50.3868
0.60	41.0143	41.6125	42.2137	42.8360	43.4453	44.0633	44.6938	45.3376
0.70	36.9193	37.5510	38.1604	38.7600	39.3422	39.9187	40.4955	41.0773
0.80	33.3183	33.9679	34.5882	35.1833	35.7624	36.3270	36.8810	37.4291
0.90	30.1328	30.7749	31.3942	31.9875	32.5700	33.1363	33.6879	34.2266
1.00	27.3271	27.9369	28.5365	29.1187	29.6968	30.2630	30.8162	31.3560
1.20	22.7908	23.2863	23.7947	24.3093	24.8325	25.3591	25.8858	26.4096
1.40	19.5434	19.9072	20.2923	20.6967	21.1166	21.5510	21.9977	22.4543
1.60	17.2904	17.5492	17.8252	18.1200	18.4298	18.7563	19.0992	19.4578
1.80	15.6818	15.8797	16.0855	16.3022	16.5286	16.7670	17.0187	17.2843
2.00	14.4218	14.5990	14.7755	14.9537	15.1348	15.3208	15.5133	15.7138
2.50	11.7621	11.9714	12.1722	12.3645	12.5502	12.7288	12.9012	13.0684
3.00	9.3744	9.6033	9.8297	10.0524	10.2715	10.4858	10.6949	10.8982
3.50	7.4837	7.6801	7.8806	8.0843	8.2911	8.4992	8.7080	8.9168
4.00	6.1954	6.3397	6.4897	6.6451	6.8055	6.9717	7.1434	7.3200
5.00	4.8635	4.9374	5.0144	5.0948	5.1787	5.2665	5.3580	5.4533
6.00	4.1069	4.1757	4.2431	4.3091	4.3744	4.4388	4.5030	4.5675

s (Å^{-1})	At	Rn	Fr	Ra	Ac	Th	Pa	U
0.00	85.0000	86.0000	87.0000	88.0000	89.0000	90.0600	91.0000	92.0000
0.05	83.6254	84.6483	85.2873	86.1054	87.0680	88.0678	89.1275	90.1546
0.10	80.1508	81.1707	81.6687	82.2057	82.9647	83.8234	85.0251	86.0667
0.15	75.8217	76.7410	77.4340	77.9936	78.5897	79.2520	80.5198	81.5218
0.20	71.4937	72.2631	73.0404	73.7336	74.3250	74.9053	76.0876	77.0215
0.25	67.4621	68.1143	68.8472	69.5828	70.2177	70.8049	71.8168	72.6719
0.30	63.7365	64.3387	65.0035	65.7032	66.3583	66.9708	67.8071	68.5817
0.35	60.2620	60.8690	61.4967	62.1475	62.7984	63.4258	64.1215	64.8221
0.40	57.0015	57.6388	58.2634	58.8869	59.5277	60.1597	60.7591	61.3996
0.45	53.9436	54.6115	55.2503	55.8701	56.5054	57.1382	57.6809	58.2784
0.50	51.0899	51.7746	52.4280	53.0562	53.6909	54.3240	54.8396	55.4101
0.60	46.0000	46.6674	47.3191	47.9566	48.5871	49.2145	49.7268	50.2762
0.70	41.6772	42.2891	42.9005	43.5132	44.1183	44.7218	45.2521	45.7964
0.80	37.9820	38.5410	39.1038	39.6733	40.2386	40.8040	41.3458	41.8826
0.90	34.7576	35.2852	35.8133	36.3445	36.8730	37.4010	37.9424	38.4668
1.00	31.8818	32.3978	32.9091	33.4174	33.9221	34.4236	34.9568	35.4682
1.20	26.9258	27.4336	27.9347	28.4274	28.9153	29.3967	29.9055	30.3973
1.40	22.9179	23.3851	23.8534	24.3206	24.7877	25.2526	25.7268	26.1970
1.60	19.8322	20.2198	20.6169	21.0226	21.4355	21.8542	22.2739	22.7011
1.80	17.3660	17.8628	18.1723	18.4958	18.8309	19.1773	19.5254	19.8873
2.00	15.9250	16.1475	16.3808	16.6267	16.8842	17.1539	17.4279	17.7164
2.50	13.2308	13.3901	13.5484	13.7054	13.8627	14.0218	14.1809	14.3449
3.00	11.0952	11.2858	11.4708	11.6492	11.8215	11.9881	12.1450	12.2993
3.50	9.1251	9.3321	9.5381	9.7415	9.9406	10.1356	10.3197	10.5019
4.00	7.5015	7.6867	7.8730	8.0610	8.2516	8.4441	8.6318	8.8208
5.00	5.5525	5.6562	5.7641	5.8792	6.0002	6.1260	6.2526	6.3856
6.00	4.6328	4.6991	4.7672	4.8363	4.9063	4.9785	5.0549	5.1333

In addition, Doyle & Turner (1968) gave a fit of four Gaussians to the electron scattering factor, though it should be mentioned that this is unphysical at large angles and prone to error. Weickenmeier & Kohl (1991) also published an electron scattering-factor parameterization. However, their scheme is equivalent to using the Doyle–Turner X-ray parameters with $Z = \sum a_j$. As such, it is a better physical representation than the four Gaussians used by Doyle & Turner, though it should be mentioned that fitting the electron scattering factor can hide large errors in the X-ray scattering factor, especially at large angles. We feel that there is no need to present a separate parameterization for the electron scattering factors as they can be calculated using the Mott formula,

$$f_{el}(s) = (me^2/2h^2)\{[Z - f_x(s)]/s^2\}. \quad (3)$$

The *Numerical Recipes* routine was slightly modified to constrain the exponents to be positive numbers less than 200.0. Cases in which any of the constants, a_j, are determined to be negative numbers should also be used with caution. Rather than add an unphysical constant, we have decided to vary the range of the fit to give an acceptable value of χ^2 as defined by

$$\chi^2 = \sum_i \left[f(s_i) - \sum_j a_j \exp(-b_j s_i^2) \right]^2, \quad (4)$$

which acts as a merit function that measures the

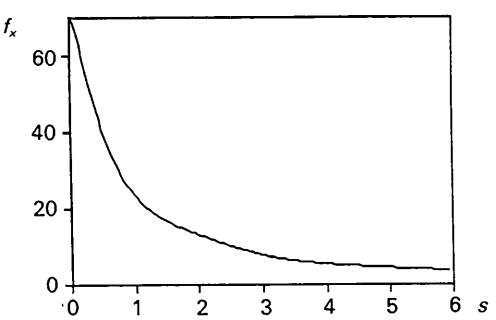
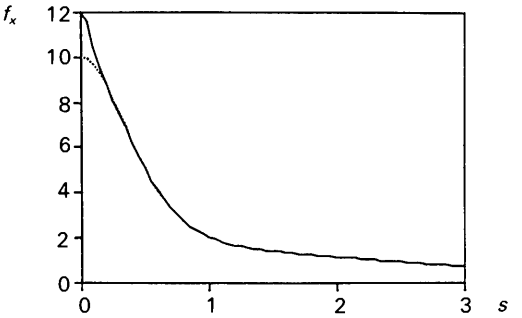


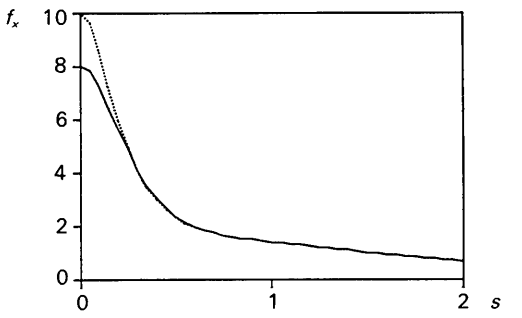
Fig. 1. Atomic X-ray scattering factor for ytterbium.

goodness of fit. Generally, we require that χ^2 be less than 0.1 and that $\sum a_j$ be within 0.1 of Z. The fitting does not give unique values of the parameters, which can vary depending on the starting values assumed. This is indicative of a large number of closely spaced local minima with similar χ^2 values. In Table 3, we give a parameterization using four Gaussians up to 2.0 $Å^{-1}$ starting the fit from the published values of Maslen *et al.* (1992). The summary of $\sum a_j$, the range of fit and χ^2 are given in Table 4.

The limitations of the restricted range of the Doyle & Turner (1968) parameters have been recognised by Fox, O'Keefe & Tabbernor (1989). They published an extended parameterization based on a linear fit of a second-order polynomial to $\ln f_x(s)$ in the range 2.0 to 6.0. We have decided to present another table of parameters, this time generated using separate parameterizations in terms of two Gaussians in an inner and an outer region. The parameters of the four Gaussians are then refined together. The parameters are given in Table 5, and Table 6 shows χ^2 and $\sum a_j$ values. Examination of the results of Tables 4 and 6 reveals that some elements or ions are very difficult to fit. Particularly bad cases are light elements such as lithium and beryllium and their ions, ions such as potassium and calcium, second-row transition elements such as silver and some of the heavier elements close to lead and bismuth. Similar problems have been found by Doyle & Turner.



(*a*)



(*b*)

Fig. 2. (*a*) Atomic X-ray scattering factor for magnesium. The lower line is for Mg^{2+}. (*b*) Atomic X-ray scattering factor for oxygen. The higher line is for O^{2-}.

In general, we recommend direct use of the tables of scattering factors, rather than use of any parameterization. The complete tables take up less than 250 kbytes, a negligible amount of space on computers today, and one could use either a cubic spline or linear interpolation.

Electron scattering factors

As mentioned above, electron scattering factors can be calculated using the Mott formula. This does not help in evaluating $f_{el}(0)$, which has recently become of considerable interest owing to advances in holography and the use of Fresnel imaging to characterize interfaces. We have calculated atomic or ionic values by taking the limit of (3) as s tends to zero. This is done by calculating the coefficient of s^2 that fits the charge density near $s=0$. The values of $f_{el}(0)$ are tabulated as Table 7 and are shown graphically for neutral atoms as a function of Z in Fig. 3. The mean inner potential for a finite crystal can be derived from $f_{el}(0)$ using the expression

$$V_{000} = (\hbar^2\pi/2\varepsilon_0 m e V_c)\sum_j n_j f^j_{el}(0), \qquad (5)$$

where V_c is the unit-cell size and the n_j are the occupation numbers for atoms of type j, with the assumption that there is no charge overlap between atoms. The mean inner potential is a measure of the average value of r^2 (Ibers, 1958) and as such is very sensitive to charge redistribution. These effects of charge redistribution and surface dipole layers on V_{000} are discussed by O'Keeffe & Spence (1994). The above V_{000} is the mean of the electrostatic or Coulomb potential (including the nuclear contribution) and so should be distinguished from the much smaller mean inner potential of surface physics, which usually refers to pseudopotentials or valence-electron potentials. Using the values given in Table 7, we have calculated mean inner potentials for elements and compounds where accurate values have been measured recently by electron holography (Gajdardziska-Josifovska *et al.*, 1993). The results are shown in Table 8. Particularly striking is the

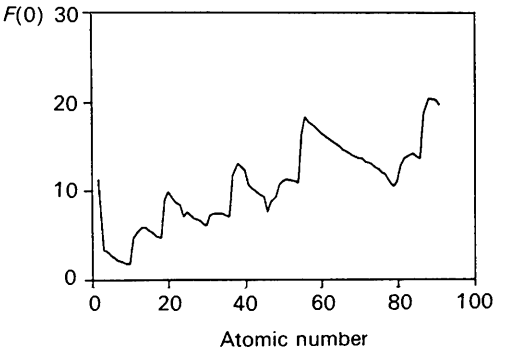


Fig. 3. Variation of neutral-atom electron scattering factor with atomic number.

Table 3. *Parameterization over range up to* 2.0 $Å^{-1}$

He	2	.9293	8.6243	.6200	2.8879	.3318	22.3531	.1188	.6748
Li	3	1.3569	3.3246	.5338	.6856	.4316	66.4053	.6778	149.9503
Li^+	3	1.3211	3.8304	.6282	.7630	.1267	73.7337	-.0735	199.4269
Be	4	1.5242	42.3109	1.2628	1.7276	.6125	97.9345	.6004	.4090
Be^{2+}	4	.0128	67.7350	1.3494	1.8375	.0703	124.1407	.5661	0.3875
B	5	2.0730	23.3127	1.2077	1.0718	1.0773	60.7133	.6411	0.2699
C	6	2.6158	11.3632	.2279	3.0830	1.5983	.3787	1.5602	49.7088
N	7	.4743	.1041	2.9082	9.1890	2.2778	27.0869	1.3332	0.4612
O	8	3.4716	11.9964	1.8289	4.7941	1.7198	.2372	.9790	31.9917
O^{2-}	8	4.2977	16.4438	2.2263	5.2614	1.7313	.2415	1.7412	49.7371
F	9	3.8364	9.8148	2.3728	3.8835	1.7299	.1904	1.0600	25.9693
F^-	9	4.1803	10.9872	2.5253	4.0129	1.7360	.1923	1.5564	33.0471
Ne	10	4.2156	8.1154	2.9030	3.1648	1.7341	.1553	1.1463	21.5835
Na	11	4.1946	2.8601	3.8961	7.9204	1.7637	.1346	1.1391	125.7209
Na^+	11	4.4278	5.2355	2.4274	2.2658	1.7182	.1272	1.4258	12.6031
Mg	12	4.5028	2.3277	2.2123	77.7413	1.7687	.1146	3.5049	5.9035
Mg^{2+}	12	4.3643	2.1618	3.9083	5.9459	1.6872	.0879	0.0382	.0000
Al	13	6.9497	2.4785	1.9692	.1286	1.1904	12.5062	2.8774	66.1402
Al^{3+}	13	4.0707	1.7260	4.1517	4.2883	1.7051	.0859	.0706	32.8254
Si	14	7.1620	1.9861	.9286	13.9567	1.8869	.0966	4.0099	51.3981
P	15	7.1583	1.7276	3.4832	23.7455	2.0781	.1140	2.2770	57.1173
S	16	7.1301	1.4247	5.0712	21.7545	2.0611	.0994	1.7369	54.2128
Cl	17	1.9223	.0722	7.1697	1.1600	6.1830	18.3275	1.7250	46.8148
Cl^-	17	1.8908	.0682	7.2032	1.1532	6.1851	18.8805	2.7190	51.3334
Ar	18	1.7760	.0484	7.2215	.9567	7.3061	15.6234	1.6972	41.1982
K	19	8.3113	9.9767	8.0220	.3899	1.1654	166.1394	1.4898	36.3604
K^+	19	8.6078	12.8738	7.9831	.7329	.8931	.0000	.4937	54.3035
Ca	20	7.5005	7.3264	7.8568	.4028	2.8393	29.2324	1.8036	142.0442
Ca^{2+}	20	8.4026	10.2488	7.7343	.6274	1.0077	.0000	.8573	25.4419
Sc	21	8.6967	6.0531	7.6978	.3439	2.0208	133.3668	2.5917	31.1311
Sc^{3+}	21	8.7769	8.6343	7.6660	.5467	.5349	28.8159	1.0211	.0000
Ti	22	8.2824	5.9317	7.8778	.3228	3.4763	15.7854	2.3563	102.1476
Ti^{4+}	22	9.1121	6.0140	7.8109	.2649	.8270	21.0441	.2673	108.4904
V	23	9.4200	5.6518	7.9252	.2790	3.5777	19.8076	2.0762	106.9938
V^{5+}	23	7.9780	5.9050	7.0702	.4154	1.3997	11.2548	1.5534	.0454
Cr	24	2.1592	1.7563	7.5070	.2563	11.5180	7.6002	2.7799	58.4816
Cr^{4+}	24	9.4679	4.7481	7.8807	.2349	2.5940	13.4095	.0610	99.5152
Mn	25	4.6706	3.2004	7.8910	.2479	9.3545	7.8654	3.0602	64.8640
Mn^{2+}	25	9.2787	4.4959	8.0358	.2537	5.4444	12.3213	.2410	56.4882
Fe	26	8.7267	3.8443	8.0070	.2319	6.4440	9.4874	2.8058	65.8373
Fe^{2+}	26	9.9708	4.1647	8.0590	.2340	5.6730	10.8269	.2955	39.6599
Co	27	10.4470	3.7376	8.0361	.2146	5.8114	9.9259	2.6910	64.0058
Co^{2+}	27	10.8328	3.8579	8.0675	.2159	5.7728	10.1789	.3248	31.3142
Ni	28	11.5224	3.5052	8.0427	.1984	5.7846	9.7491	2.6363	61.2607
Ni^{2+}	28	11.6115	3.5609	8.0660	.1994	5.9757	9.6026	.3446	27.4704
Cu	29	12.4034	3.2588	8.0407	.1838	5.9379	9.3595	2.6040	58.4193
Cu^{2+}	29	12.2599	3.2668	8.0489	.1840	6.3163	8.9438	.3720	18.5527
Zn	30	13.1577	3.0177	8.0333	.1706	6.2005	8.8438	2.5942	55.4451
Zn^{2+}	30	13.0154	3.0266	8.0424	.1707	6.5544	8.4540	.3850	22.8068
Ga	31	14.4553	2.8296	8.0236	.1584	5.3320	8.9052	3.1660	58.7737
Ge	32	15.3565	2.6125	7.9946	.1468	4.5606	8.5906	4.0649	51.2258
As	33	16.2740	2.4201	7.9707	.1365	3.8167	8.9871	4.9167	44.1949
Se	34	17.0384	2.2387	7.9488	.1273	3.5070	10.5104	5.4877	39.2994
Br	35	17.4960	2.0529	4.2115	13.0028	7.9096	.1185	5.3711	36.6126
Br^-	35	17.6056	2.0679	4.9704	15.1006	7.9344	.1193	5.4763	45.3025
Kr	36	17.7085	1.8641	5.9137	14.7862	7.8321	.1092	4.5393	35.6792
Rb	37	17.8838	1.7076	9.7227	16.9358	7.7948	.1022	1.5830	160.2323
Rb^+	37	17.7741	1.6811	7.1450	14.1155	7.7094	.0992	3.3697	29.2349
Sr	38	17.8443	1.5272	9.8506	13.9829	7.6087	.0909	2.6842	131.9738
Sr^{2+}	38	17.8275	1.5184	8.8646	13.3203	7.5690	.0896	1.7393	27.4135
Y	39	17.9239	1.3862	10.2998	12.7104	7.4713	.0821	3.2877	104.2218
Y^{3+}	39	17.9540	1.3676	10.4284	12.3604	7.3322	.0767	.2810	43.2583
Zr	40	18.0241	1.2627	10.9315	11.8383	7.3288	.0739	3.6934	87.5310
Zr^{4+}	40	17.9264	1.2420	10.7051	10.8094	7.2110	.0700	.1594	38.4892
Nb	41	18.1801	1.1578	11.9696	11.6375	7.1992	.0666	3.6219	69.8068
Nb^{5+}	41	17.9918	1.1230	10.9034	9.4967	6.9753	.0596	.1308	35.6515
Mo	42	6.9981	.0579	18.2939	1.0546	12.8488	10.9149	3.8270	61.7489
Mo^{6+}	42	6.4551	.0465	18.2451	1.0042	11.1601	8.2190	.1377	16.2605
Ru	44	20.3021	.4099	6.7634	2.5572	13.6174	11.2459	3.2945	59.7656
Rh	45	19.8137	.2815	12.9693	3.6398	11.9072	14.2137	.3117	.1072
Pd	46	20.1415	.3688	12.6027	4.1475	11.5709	14.8191	.6406	.0000

Table 3 (*cont.*)

Pd^{2+}	46	16.1822	4.3496	20.0860	.3223	6.9823	17.1340	.7390	50.2893
Ag	47	21.1966	.3532	5.3046	2.3773	17.2072	9.1072	3.2655	48.9088
Ag^{2+}	47	19.5768	.3374	12.3058	3.4367	12.7143	13.6319	.4101	.0000
Cd	48	14.5758	4.1905	21.0830	.3158	10.4040	15.0058	1.9299	77.0010
Cd^{2+}	48	12.4737	3.1756	19.8570	.2840	14.1977	13.2315	-.5169	143.9014
In	49	20.6912	.2776	16.4798	3.9721	10.0509	17.6620	1.7346	77.0257
Sn	50	17.9200	3.2798	19.7597	.2388	9.4954	17.6874	2.8286	79.0376
Sb	51	16.4937	3.3219	20.2786	.2406	9.6340	11.6278	4.5839	61.6158
Te	52	18.5053	3.8099	21.5711	.2659	5.1871	12.5504	6.7321	54.3996
I	53	17.2389	3.0732	20.6465	.2293	7.9860	8.3218	7.0956	29.2052
I^-	53	18.1749	3.1761	20.7046	.2302	7.9271	10.9205	7.1573	39.0555
Xe	54	19.5398	3.1997	20.9701	.2253	7.0143	13.8671	6.4594	28.5326
Cs	55	20.6321	3.1994	21.2392	.2210	11.1858	21.4501	1.9196	162.2653
Cs^+	55	20.8999	3.0687	20.8074	.1884	11.5422	21.2422	.7355	114.7388
Ba	56	20.5353	2.9691	21.1736	.2098	11.3434	18.6103	2.9339	153.0169
Ba^{2+}	56	20.5981	2.9632	21.1416	.2090	11.6447	19.1679	.6058	23.2442
La	57	20.7434	2.7935	21.1245	.1995	11.6063	17.7161	3.5099	125.7274
La^{3+}	57	20.5986	2.7704	21.0931	.1989	11.9651	17.3313	.3382	50.8389
Ce	58	21.2963	2.6974	21.1410	.1911	12.0325	16.8378	3.5137	121.6763
Ce^{4+}	58	20.5950	2.5854	21.0107	.1888	12.2608	15.6874	.1319	75.7027
Pr	59	22.1528	2.6599	21.2189	.1843	12.6707	16.1512	2.9420	137.7915
Pr^{3+}	59	21.7820	2.5911	21.1240	.1827	12.7803	15.7833	.3081	33.6002
Nd	60	22.7714	2.5670	21.2153	.1766	13.0452	15.3993	2.9515	133.2029
Nd^{3+}	60	22.2780	2.4905	21.1058	.1749	11.8492	14.0760	1.7687	27.0830
Sm	62	24.0711	2.3917	21.1887	.1623	13.7362	14.0288	2.9846	124.2208
Sm^{3+}	62	23.8814	2.1944	20.3552	.1414	14.2543	13.0766	.4986	106.9538
Eu	63	24.7357	2.3078	21.1681	.1557	14.0669	13.4144	3.0084	119.8020
Eu^{3+}	63	24.3908	2.2549	21.0594	.1540	14.0814	12.9944	.4599	20.7019
Gd	64	25.1591	2.1888	21.0662	.1483	14.0582	12.5610	3.6924	99.2170
Gd^{3+}	64	25.0280	2.1736	21.0264	.1477	14.3312	12.2977	.6055	26.5919
Tb	65	26.1301	2.1547	21.1263	.1437	14.6682	12.2899	3.0512	111.7726
Tb^{3+}	65	25.7586	2.0985	20.9680	.1411	14.6912	11.8161	.5715	17.2401
Dy	66	26.8408	2.0825	21.1052	.1382	14.9523	11.7814	3.0755	107.9034
Dy^{3+}	66	26.4722	2.0192	20.8747	.1341	14.9981	11.2512	.6429	15.2869
Ho	67	27.5569	2.0136	21.0861	.1331	15.2280	11.3052	3.1009	104.1453
Ho^{3+}	67	26.5512	1.9230	20.8447	.1299	11.2764	8.7474	5.3265	17.5901
Er	68	28.2815	1.9485	21.0719	.1283	15.4941	10.8670	3.1227	100.8027
Er^{3+}	68	27.1701	1.8540	20.7960	.1247	11.3136	8.2221	5.7187	16.8295
Tm	69	29.0083	1.8865	21.0624	.1239	15.7519	10.4545	3.1460	97.4986
Tm^{3+}	69	27.7854	1.7880	20.7472	.1198	11.3841	7.7420	6.0813	16.1400
Yb	70	29.7372	1.8277	21.0586	.1197	16.0018	10.0678	3.1692	94.3403
Yb^{3+}	70	28.4011	1.7251	11.5159	7.3150	20.6991	.1152	6.3815	15.5395
Lu	71	30.1535	1.7412	15.9083	9.3789	20.9541	.1146	3.9485	80.2529
Lu^{3+}	71	29.0169	1.6654	11.6805	6.9293	20.6528	.1108	6.6470	14.9929
Hf	72	30.6276	1.6628	15.8438	8.9350	20.8615	.1098	4.6278	68.4901
Ta	73	31.1117	1.5895	15.8592	8.6359	20.7732	.1054	5.2133	59.9094
W	74	31.5764	1.5194	15.9855	8.4277	20.6846	.1011	5.7081	53.5131
Re	75	32.0060	1.4520	16.2421	8.2768	20.5922	.0971	6.1127	48.6201
Os	76	32.3895	1.3864	16.6370	8.1544	20.4917	.0932	6.4338	44.7634
Ir	77	32.7046	1.3211	17.2579	8.0409	20.3732	.0892	6.6160	41.6406
Pt	78	33.0384	1.2529	18.1877	8.0552	20.1682	.0845	6.5607	35.7778
Au	79	20.4657	.0868	19.0318	8.0375	33.0170	1.2144	6.4440	34.2724
Hg	80	20.5235	.0856	33.0365	1.1646	19.7804	7.7629	6.6155	35.7598
Tl	81	21.0729	.0903	32.8891	1.1444	21.0487	7.8442	5.9110	45.0760
Pb	82	33.4861	1.0481	21.9052	7.2688	20.0114	.0752	6.5187	47.3250
Bi	83	19.8360	.0718	22.2914	6.7590	33.4300	.9928	7.3714	46.5293
Po	84	25.2534	.1335	21.3651	6.7141	29.3111	1.1521	8.0167	45.9357
At	85	34.3560	.2268	23.2498	1.6437	18.5641	7.0127	8.7901	42.2189
Rn	86	37.9584	.2565	22.4154	1.9675	16.0144	7.2076	9.5697	37.2747
Fr	87	44.7473	.3309	26.8048	3.4800	12.8901	20.8008	2.5239	128.5198
Ra	88	38.4087	.2379	27.6504	2.1955	16.2526	11.9072	5.5831	80.4273
Ac	89	33.5966	.1825	28.1785	1.5549	18.8469	8.2662	8.2096	59.0710
Th	90	28.0936	.1293	29.7756	1.1087	21.3586	6.2033	10.5524	47.6686
Pa	91	29.6569	.1379	29.3781	1.1586	21.7312	6.6084	9.9984	45.4293
U	92	31.1742	.1454	28.9718	1.2121	21.9075	6.8891	9.7265	45.5549

large difference between ionic and atomic MgO. Changing the Watson sphere radius for the O^{2-} ion by 1 Å can change the ionic mean inner potential by 0.7 V. The accuracy of holographic measurements of mean inner potential is about 0.3 V (Gajdardziska-Josifovska *et al.*, 1993). In this system, one might be able to measure a transfer of 0.06 e from one atom to another. It would be interesting to see if this could be

Table 4. *Summary of range, $\sum a_j$ and χ^2 for Table 3*

	Z	Range	$\sum a_j$	χ^2		Z	Range	$\sum a_j$	χ^2
He	2	2.0	2.00	1.4780e-05	Ru	44	1.2	43.98	7.0410e-03
Li	3	2.0	3.00	1.2550e-03	Rh	45	1.6	45.00	6.4770e+01
Li^+	3	1.8	2.00	2.2810e-03	Pd	46	1.6	44.96	3.1350e+00
Be	4	2.0	4.00	3.1040e-04	Pd^{2+}	46	1.8	43.99	3.4550e+00
Be^{2+}	4	2.6	2.00	1.6190e-02	Ag	47	1.4	46.97	8.6180e-02
B	5	2.0	5.00	2.6870e-05	Ag^{2+}	47	1.8	45.01	5.0170e+00
C	6	2.0	6.00	1.1680e-01	Cd	48	1.8	47.99	1.0220e+00
N	7	5.0	6.99	1.4400e-03	Cd^{2+}	48	2.0	46.01	2.8840e+00
O	8	2.0	8.00	2.5230e-03	In	49	1.8	48.96	2.9330e+00
O^{2-}	8	2.0	10.00	3.5060e-03	Sn	50	2.0	50.00	5.9320e+00
F	9	2.0	9.00	5.2300e-04	Sb	51	2.0	50.99	2.4110e+00
F^-	9	2.0	10.00	7.4700e-04	Te	52	1.8	52.00	9.0360e-01
Ne	10	2.0	10.00	4.2920e-04	I	53	2.0	52.97	7.8090e+00
Na	11	2.0	10.99	9.4310e-04	I^-	53	2.0	53.96	3.6060e+00
Na^+	11	2.0	10.00	2.0760e-05	Xe	54	2.0	53.98	3.4120e+00
Mg	12	2.0	11.99	1.2900e-03	Cs	55	2.0	54.98	1.4310e-01
Mg^{2+}	12	2.0	10.00	2.3170e-01	Cs^+	55	2.0	53.99	1.3150e+01
Al	13	2.0	12.99	1.3220e-02	Ba	56	2.0	55.99	6.5530e-02
Al^{3+}	13	2.6	10.00	1.6690e-02	Ba^{2+}	56	2.0	53.99	2.3980e-01
Si	14	2.5	13.99	6.8750e-02	La	57	2.0	56.98	3.0910e-02
P	15	2.0	15.00	2.0970e-03	La^{3+}	57	2.0	54.00	3.0060e-02
S	16	2.0	16.00	3.7070e-04	Ce	58	2.0	57.98	1.8660e-02
Cl	17	2.4	17.00	7.8720e-04	Ce^{4+}	58	2.0	54.00	1.1060e-02
Cl^-	17	2.6	18.00	1.5540e-03	Pr	59	2.0	58.98	1.5510e-02
Ar	18	2.0	18.00	1.1140e-03	Pr^{3+}	59	2.0	55.99	2.4710e-02
K	19	1.6	18.99	6.5930e+00	Nd	60	2.0	59.98	1.1380e-02
K^+	19	1.6	17.98	9.5280e-01	Nd^{3+}	60	2.0	57.00	4.7110e-03
Ca	20	1.8	20.00	3.7730e-01	Sm	62	2.0	61.98	9.6460e-03
Ca^{2+}	20	2.0	18.00	7.5580e-01	Sm^{3+}	62	2.0	58.99	1.7260e+00
Sc	21	2.0	21.01	1.0000e+00	Eu	63	2.0	62.98	1.0480e-02
Sc^{3+}	21	2.2	18.00	6.7720e-01	Eu^{3+}	63	2.0	59.99	8.7270e-02
Ti	22	2.0	21.99	3.7870e-01	Gd	64	2.0	63.98	9.6490e-03
Ti^{4+}	22	2.0	18.02	5.7870e+00	Gd^{3+}	64	2.0	60.99	5.4740e-02
V	23	2.0	23.00	8.4800e-01	Tb	65	2.0	64.98	1.3910e-02
V^{5+}	23	1.8	18.00	7.8270e-01	Tb^{3+}	65	2.0	61.99	1.7010e-01
Cr	24	2.0	23.96	3.4280e-02	Dy	66	2.0	65.97	1.6240e-02
Cr^{4+}	24	2.0	20.00	2.6070e+00	Dy^{3+}	66	2.0	62.99	2.6650e-01
Mn	25	2.0	24.98	2.3450e-02	Ho	67	2.0	66.97	1.8840e-02
Mn^{2+}	25	2.0	23.00	6.7330e-02	Ho^{3+}	67	2.0	64.00	7.7740e-05
Fe	26	2.0	25.98	1.3970e-02	Er	68	2.0	67.97	2.1660e-02
Fe^{2+}	26	2.0	24.00	1.7990e-02	Er^{3+}	68	2.0	65.00	5.0680e-05
Co	27	2.0	26.99	8.1720e-03	Tm	69	2.0	68.97	2.4760e-02
Co^{2+}	27	2.0	25.00	1.9420e-02	Tm^{3+}	69	2.0	66.00	7.3600e-05
Ni	28	2.0	27.99	5.3970e-03	Yb	70	2.0	69.97	2.7860e-02
Ni^{2+}	28	2.0	26.00	1.8350e-02	Yb^{3+}	70	2.0	67.00	1.0480e-04
Cu	29	2.0	28.99	4.2320e-03	Lu	71	2.0	70.96	2.4770e-02
Cu^{2+}	29	2.0	27.00	4.6550e-02	Lu^{3+}	71	2.0	68.00	2.0860e-04
Zn	30	2.0	29.99	3.9060e-03	Hf	72	2.0	71.96	2.5390e-02
Zn^{2+}	30	2.0	28.00	1.9900e-02	Ta	73	2.0	72.96	2.6990e-02
Ga	31	2.0	30.98	6.7310e-03	W	74	2.0	73.95	2.8560e-02
Ge	32	2.0	31.98	6.9310e-03	Re	75	2.0	74.95	2.9570e-02
As	33	2.0	32.98	6.8840e-03	Os	76	2.0	75.95	3.0120e-02
Se	34	2.0	33.98	6.0920e-03	Ir	77	2.0	76.95	2.9790e-02
Br	35	2.0	34.99	4.0350e-03	Pt	78	2.0	77.96	2.3850e-02
Br^-	35	2.0	35.99	5.5470e-03	Au	79	1.8	78.96	1.9790e-02
Kr	36	2.0	35.99	1.7240e-03	Hg	80	1.8	79.96	2.4030e-02
Rb	37	2.0	36.98	7.4330e-03	Tl	81	1.8	80.92	5.8630e-02
Rb^+	37	2.0	36.00	2.4820e-04	Pb	82	2.0	81.92	7.0110e-02
Sr	38	2.0	37.99	2.1930e-03	Bi	83	2.0	82.93	6.2750e-02
Sr^{2+}	38	2.0	36.00	5.4980e-05	Po	84	1.6	83.95	3.7440e-02
Y	39	2.0	38.98	3.6610e-03	At	85	1.4	84.96	2.0890e-02
Y^{3+}	39	2.0	36.00	3.3040e-03	Rn	86	1.2	85.96	5.2570e-01
Zr	40	2.0	39.98	5.9080e-03	Fr	87	1.2	86.97	3.2630e-02
Zr^{4+}	40	2.0	36.00	2.3410e-03	Ra	88	1.6	87.89	2.7130e-01
Nb	41	2.0	40.97	9.2790e-03	Ac	89	1.8	88.83	4.5320e-01
Nb^{5+}	41	2.0	36.00	1.0530e-03	Th	90	2.0	89.78	5.9250e-01
Mo	42	2.0	41.97	1.1090e-02	Pa	91	2.0	90.76	6.3950e-01
Mo^{6+}	42	2.0	36.00	3.7600e-01	U	92	2.0	91.78	6.2400e-01

Table 5. *Parameterization over range up to* 6.0 $Å^{-1}$

He	2	.9642	8.2337	.5874	2.6488	.3519	21.9356	.0961	.5921
Li	3	1.4093	3.1474	.4692	.6160	.3313	56.9003	.7903	137.29
Li^+	3	.4707	6.7143	-.8101	.4681	1.1574	2.4978	1.1819	.4903
Be	4	.8232	30.1555	1.4326	1.4665	1.3491	71.9798	.3929	.2888
Be^{2+}	4	.0307	.0327	.2364	6.0628	1.1969	1.5873	.5328	.4564
B	5	1.6847	20.1203	1.4201	.8912	1.5004	52.2289	.3918	.1803
C	6	1.7401	38.1927	2.4357	13.7125	1.3245	.6520	.4960	.1488
N	7	.4743	.1041	2.9082	9.1890	2.2778	27.0869	1.3332	.4612
O	8	3.5531	6.8702	2.6162	21.0743	1.2120	.3871	.6107	.0960
O^{2-}	8	4.0627	31.7973	4.0629	7.7817	1.2299	.4065	.6247	.0965
F	9	3.1620	16.2253	4.0183	5.0974	1.2647	.2885	.5433	.0685
F^-	9	3.5691	21.4312	4.5619	5.6541	1.1716	.3285	.6780	.0805
Ne	10	3.5800	13.1434	4.5889	4.0251	1.1999	.2466	.6167	.0606
Na	11	1.5468	70.9392	7.1834	4.6170	1.0440	.4927	1.1717	.0767
Na^+	11	7.4010	4.5309	.4787	43.9221	.9428	.3435	1.1356	.0754
Mg	12	7.1773	3.5565	2.5089	63.2541	1.0098	.4906	1.2662	.0688
Mg^{2+}	12	1.1002	16.6083	6.6744	3.2353	.9324	.3778	1.2525	.0686
Al	13	3.4553	54.4948	7.1181	2.8378	1.0330	.5062	1.3472	.0621
Al^{3+}	13	3.5632	4.8494	4.6573	1.8876	1.0703	.1459	.7038	.0396
Si	14	4.4794	43.2573	7.0199	2.2811	1.0516	.4950	1.4002	.0557
P	15	5.5289	34.2841	6.9083	1.8577	1.0702	.4743	1.4395	.0500
S	16	6.5881	27.6154	6.7734	1.5353	1.1051	.4580	1.4747	.0452
Cl	17	7.7055	22.3647	7.1936	1.1964	.7594	.1885	1.2716	.0348
Cl^-	17	8.5770	25.5594	7.1869	1.2286	.7985	.2157	1.3288	.0365
Ar	18	8.7309	18.8014	6.6457	1.0670	1.0425	.3810	1.5076	.0367
K	19	9.3143	16.3323	6.8249	.9278	1.6199	.0357	.8062	.2976
K^+	19	8.8588	14.4381	1.2845	1.4519	6.1602	.7240	1.6526	.0381
Ca	20	9.8335	15.1591	5.5728	.9519	1.8247	.0369	2.0799	.5351
Ca^{2+}	20	9.0581	11.3375	4.2886	.7810	2.9800	.5783	1.6410	.0341
Sc	21	10.9222	13.2580	6.7601	.7123	1.6516	.0287	.9302	.2098
Sc^{3+}	21	6.9714	10.3241	2.2388	5.2961	7.0999	.6016	1.6601	.0316
Ti	22	4.7939	25.4898	7.2348	7.3826	7.8591	.5846	1.6990	.0293
Ti^{4+}	22	9.2375	7.5947	.0841	35.8416	7.0609	.5233	1.6186	.0271
V	23	11.9445	11.4230	.5501	1.5124	7.7024	.5619	2.0564	.0388
V^{5+}	23	9.4907	6.3917	.5520	1.2279	6.2476	.4171	1.6924	.0265
Cr	24	13.6852	9.2123	.7821	.0000	7.2815	.5517	1.5997	.0967
Cr^{4+}	24	7.6562	7.5449	3.4733	4.8525	7.2003	.4341	1.6410	.0234
Mn	25	14.2140	8.5904	.7519	1.6230	7.3544	.4327	1.7816	.0250
Mn^{2+}	25	7.6888	5.9716	6.0578	8.7513	7.2130	.4234	1.7974	.0268
Fe	26	15.2456	7.6240	1.0394	.0000	7.2502	.4810	1.5785	.1017
Fe^{2+}	26	9.2568	4.3145	6.2209	10.8026	6.8432	.3454	1.6267	.0200
Co	27	4.0297	41.6879	14.2511	4.9187	7.0022	.3260	1.6448	.0186
Co^{2+}	27	4.4550	11.1211	11.9578	4.4875	6.9272	.3201	1.6193	.0180
Ni	28	4.2213	37.2296	15.0617	4.4844	6.9819	.2999	1.6518	.0174
Ni^{2+}	28	3.9701	13.4440	13.4941	4.1236	6.9074	.2940	1.6207	.0167
Cu	29	4.4189	33.3559	15.8641	4.1015	6.9608	.2770	1.6609	.0164
Cu^{2+}	29	4.3975	12.2564	14.0954	3.7432	6.8794	.2701	1.6178	.0155
Zn	30	4.6165	30.0488	16.6623	3.7653	6.9356	.2573	1.6787	.0158
Zn^{2+}	30	14.6954	3.4107	4.8261	11.2241	6.8522	.2490	1.6140	.0144
Ga	31	4.9552	34.5383	17.3270	3.4280	6.9107	.2381	1.6831	.0149
Ge	32	5.6938	34.7231	17.6620	3.0728	6.8586	.2191	1.6771	.0139
As	33	20.6740	4.3699	.8757	.0000	7.1331	.3114	2.3157	.0643
Se	34	7.6260	29.0738	17.9310	2.4432	6.7671	.1822	1.5845	.0105
Br	35	8.6899	25.8428	17.9735	2.1847	6.7300	.1659	1.5205	.0087
Br^-	35	9.5044	29.5231	18.0951	2.2072	6.7400	.1673	1.5412	.0090
Kr	36	9.7841	22.9658	17.9894	1.9594	6.7141	.1504	1.4294	.0064
Rb	37	10.3402	21.3340	18.1665	1.7963	6.7107	.1393	1.3887	.0051
Rb^+	37	10.0470	18.4947	17.9002	1.7491	6.7603	.1338	1.2411	.0018
Sr	38	10.8557	20.8810	18.4417	1.6734	6.6905	.1318	1.4186	.0054
Sr^{2+}	38	10.2747	15.2738	17.8345	1.5644	6.7740	.1175	1.0784	.0000
Y	39	11.6721	20.2317	18.6197	1.5493	6.6650	.1240	1.4264	.0053
Y^{3+}	39	10.5873	12.7800	17.4857	1.4209	6.8869	.1104	1.0122	.0000
Zr	40	12.6121	19.1188	18.7164	1.4279	6.6475	.1157	1.4006	.0045
Zr^{4+}	40	10.1933	11.7534	13.0407	1.6115	6.0546	.7428	6.7084	.0646
Nb	41	13.8863	17.3651	18.6686	1.2944	6.7223	.1036	1.1946	.0004
Nb^{5+}	41	10.7405	9.8271	17.7219	1.1881	6.1471	.0947	1.3873	.0103
Mo	42	-0.5335	.1503	13.8022	18.0808	19.3549	1.2497	8.5288	.0914

Table 5 (*cont.*)

Mo^{6+}	42	10.0471	8.4888	18.1673	1.1430	4.4638	.1275	3.2409	.0255
Ru	44	17.4492	13.7038	16.1683	1.1046	4.7256	.2453	5.0909	.0380
Rh	45	18.1565	12.7117	4.0808	.0298	18.6671	.9224	3.5577	.1104
Pd	46	19.5358	11.5978	18.5378	.8609	5.6868	.0793	1.8561	.0117
Pd^{2+}	46	18.3818	9.8735	-9.3923	.8350	27.7999	.8146	7.0317	.0509
Ag	47	20.3106	10.8851	18.4263	.8146	5.3383	.0846	2.3717	.0164
Ag^{2+}	47	19.6756	9.0682	-8.7103	.6998	27.0629	.7277	6.7662	.0449
Cd	48	21.1359	10.2153	18.5320	.7619	5.5077	.0743	2.0855	.0141
Cd^{2+}	48	20.7330	8.5338	-9.2791	.6669	27.5694	.6752	6.7691	.0430
In	49	21.7709	9.6786	18.4687	.7285	4.0382	.0937	3.7334	.0243
Sn	50	22.5247	9.1608	1.0443	.0105	18.7391	.6779	6.4719	.0580
Sb	51	6.4346	48.0462	20.0969	5.8287	17.8000	.5467	6.6281	.0366
Te	52	7.4566	43.6783	20.1616	5.3336	17.6778	.5172	6.6699	.0356
I	53	8.6191	38.5578	20.1638	4.8469	17.5864	.4834	6.6000	.0334
I^-	53	4.3633	91.1901	23.0389	6.3113	18.2650	.5024	6.6951	.0341
Xe	54	9.8156	34.2058	20.1178	4.4184	17.4902	.4534	6.5479	.0316
Cs	55	4.4687	56.0653	23.3078	5.8031	18.7438	.4597	6.7143	.0315
Cs^+	55	5.1679	52.7785	22.0885	5.7789	18.8128	.4609	6.7191	.0316
Ba	56	10.6045	34.1617	21.2072	3.9127	17.7637	.3884	6.0052	.0228
Ba^{2+}	56	10.3729	23.6162	19.8569	3.7060	17.3077	.4019	6.4702	.0286
La	57	11.3144	33.9508	21.4338	3.7166	17.5797	.3777	6.2639	.0252
La^{3+}	57	10.5829	20.3557	19.7768	3.4197	17.2374	.3788	6.4196	.0270
Ce	58	11.6706	31.6855	22.1380	3.5454	17.5765	.3571	6.1848	.0234
Ce^{4+}	58	10.7722	17.8107	19.7126	3.1661	17.1748	.3573	6.3634	.0255
Pr	59	11.6506	28.2975	23.0290	3.4642	17.4261	.3498	6.4301	.0250
Pr^{3+}	59	11.4023	18.2377	21.0979	3.1246	17.1725	.3410	6.3375	.0243
Nd	60	11.9758	26.6197	23.7533	3.3107	17.3930	.3328	6.3962	.0237
Nd^{3+}	60	11.7652	17.3350	21.8081	2.9920	17.1424	.3239	6.2913	.0230
Sm	62	12.5808	23.7524	25.2547	3.0305	17.3293	.3018	6.3196	.0214
Sm^{3+}	62	12.4419	15.7504	23.2835	2.7491	17.0873	.2928	6.1874	.0205
Eu	63	12.8794	22.5220	26.0120	2.9011	17.3003	.2876	6.2771	.0203
Eu^{3+}	63	12.7665	15.0459	24.0378	2.6372	17.0629	.2786	6.1291	.0193
Gd	64	13.1663	22.9855	26.7602	2.7813	17.2983	.2746	6.2370	.0193
Gd^{3+}	64	13.0945	14.3909	24.7894	2.5298	17.0415	.2653	6.0670	.0182
Tb	65	13.4219	20.3272	27.5856	2.6664	17.2455	.2618	6.1835	.0182
Tb^{3+}	65	13.4004	13.7797	25.5644	2.4305	17.0235	.2527	6.0000	.0170
Dy	66	13.9049	18.9990	28.4442	2.5072	17.6410	.2346	5.4181	.0109
Dy^{3+}	66	13.7016	13.2073	26.3450	2.3347	17.0083	.2408	5.9294	.0159
Ho	67	14.0474	18.3051	29.1991	2.4342	17.3447	.2328	5.8088	.0141
Ho^{3+}	67	14.0008	12.6695	27.1278	2.2437	16.9973	.2295	5.8541	.0148
Er	68	14.2414	17.5723	29.9762	2.3520	17.2146	.2269	5.9565	.0147
Er^{3+}	68	14.2988	12.1636	27.9117	2.1573	16.9904	.2189	5.7744	.0137
Tm	69	14.5077	16.7820	30.7710	2.2596	17.2020	.2169	5.8924	.0138
Tm^{3+}	69	14.5962	11.6865	28.6960	2.0752	16.9882	.2089	5.6904	.0126
Yb	70	14.7438	16.0821	31.5613	2.1771	17.1483	.2090	5.9061	.0134
Yb^{3+}	70	14.8939	11.2354	29.4796	1.9972	16.9907	.1994	5.6017	.0115
Lu	71	14.7680	16.6802	32.5059	2.1102	17.1721	.2013	5.8792	.0127
Lu^{3+}	71	15.1919	10.8089	30.2626	1.9231	16.9981	.1903	5.5083	.0105
Hf	72	15.1022	17.0254	33.2289	2.0291	17.1739	.1932	5.8327	.0120
Ta	73	15.6912	16.9875	33.7761	1.9352	17.2119	.1834	5.6780	.0105
W	74	16.4071	16.7085	34.1624	1.8441	17.1371	.1762	5.6710	.0102
Re	75	17.2631	16.1902	34.4590	1.7492	17.1138	.1676	5.5558	.0092
Os	76	18.2027	15.5503	34.6842	1.6565	17.0958	.1591	5.4184	.0081
Ir	77	19.2410	14.7568	34.8269	1.5657	17.0846	.1506	5.2556	.0069
Pt	78	20.7882	13.4703	34.6716	1.4567	17.0825	.1401	4.9448	.0049
Au	79	21.9097	12.7452	34.7505	1.3764	17.1147	.1320	4.7183	.0034
Hg	80	22.5800	12.4460	35.0588	1.3212	17.1486	.1265	4.6216	.0026
Tl	81	23.1403	12.0702	35.3335	1.2691	17.1758	.1215	4.5398	.0020
Pb	82	23.6202	11.8888	35.6786	1.2275	17.1696	.1180	4.5592	.0020
Bi	83	24.0197	11.8672	36.0709	1.1957	17.0953	.1162	4.7286	.0028
Po	84	24.3714	11.9587	36.4725	1.1713	16.9209	.1164	5.0776	.0045
At	85	24.7639	12.1368	36.8392	1.1530	16.5994	.1190	5.6662	.0073
Rn	86	37.1227	1.1421	25.1332	12.3717	16.0681	.1254	6.6038	.0111
Fr	87	8.7590	.0189	25.2084	12.3929	36.9843	1.1436	14.7208	.1465
Ra	88	25.3995	12.4247	37.1106	1.1325	14.6082	.1526	9.3365	.0200
Ac	89	14.2009	30.5812	26.3130	3.6535	31.6265	.5949	16.3369	.0394
Th	90	14.3941	32.3516	26.5082	3.6866	32.1473	.5887	16.4889	.0389
Pa	91	14.9246	28.6636	26.3076	3.6981	32.6541	.5806	16.6101	.0383
U	92	29.8398	10.3246	37.5857	.9066	15.2780	.1074	7.3550	.0132

Table 6. *Summary of range, Σa_j and χ^2 for Table 5*

	Z	Range	Σa_j	χ^2		Z	Range	Σa_j	χ^2
He	2	6.0	2.00	9.3750e-05	Ru	44	6.0	43.43	3.6570e+00
Li	3	6.0	3.00	4.4170e-03	Rh	45	6.0	44.46	3.2170e+00
Li^+	3	3.0	2.00	2.4740e-03	Pd	46	5.8	45.62	1.3240e+00
Be	4	6.0	4.00	4.9070e-03	Pd^{2+}	46	4.8	43.82	3.5150e-01
Be^{2+}	4	5.0	2.00	3.4520e-03	Ag	47	5.8	46.45	1.9380e+00
B	5	6.0	5.00	3.9200e-03	Ag^{2+}	47	5.8	44.79	1.3670e+00
C	6	4.0	6.00	7.2670e-04	Cd	48	5.8	47.26	3.0570e+00
N	7	6.0	6.99	3.3310e-03	Cd^{2+}	48	5.8	45.79	7.5990e-01
O	8	4.4	7.99	1.8640e-03	In	49	5.8	48.01	4.8170e+00
O^{2-}	8	4.8	9.98	5.9140e-03	Sn	50	6.0	48.78	9.0120e+00
F	9	5.8	8.99	2.8820e-03	Sb	51	6.0	50.96	2.7480e-01
F^-	9	5.0	9.98	5.8750e-03	Te	52	5.0	51.97	2.2490e-01
Ne	10	5.8	9.99	3.9390e-03	I	53	5.0	52.97	2.6140e-01
Na	11	6.0	10.95	9.8470e-02	I^-	53	4.6	52.36	1.0350e+01
Na^+	11	5.8	9.96	2.3900e-01	Xe	54	6.0	53.97	3.0940e-01
Mg	12	6.0	11.96	6.9050e-02	Cs	55	5.4	53.23	9.7570e+00
Mg^{2+}	12	5.4	9.96	2.5850e-01	Cs^+	55	5.2	52.79	1.1190e+01
Al	13	6.0	12.95	5.7290e-02	Ba	56	4.2	55.58	9.6830e-01
Al^{3+}	13	5.8	9.99	7.8060e-04	Ba^{2+}	56	5.8	54.01	3.8260e-01
Si	14	6.0	13.95	4.4830e-02	La	57	4.8	56.59	1.1490e+00
P	15	6.0	14.95	3.7790e-02	La^{3+}	57	5.8	54.02	4.2260e-01
S	16	5.9	15.94	3.6510e-02	Ce	58	4.8	57.57	1.2190e+00
Cl	17	6.0	16.93	4.8670e-02	Ce^{4+}	58	5.8	54.02	4.5840e-01
Cl^-	17	5.9	17.89	1.1230e-01	Pr	59	6.0	58.54	1.2770e+00
Ar	18	6.0	17.93	4.8530e-02	Pr^{3+}	59	5.8	56.01	4.3140e-01
K	19	6.0	18.57	7.0960e-01	Nd	60	6.0	59.52	1.3410e+00
K^+	19	4.8	17.96	5.0510e-02	Nd^{3+}	60	5.8	57.01	4.3150e-01
Ca	20	5.8	19.31	2.0760e+00	Sm	62	6.0	61.48	1.4610e+00
Ca^{2+}	20	4.8	17.97	2.3780e-02	Sm^{3+}	62	5.8	59.00	4.2210e-01
Sc	21	5.8	20.26	3.5910e+00	Eu	63	6.0	62.47	1.5200e+00
Sc^{3+}	21	4.8	17.97	2.4100e-01	Eu^{3+}	63	5.8	60.00	4.1290e-01
Ti	22	5.8	21.59	3.9000e+00	Gd	64	6.0	63.46	1.7690e+00
Ti^{4+}	22	5.8	18.00	1.2450e-02	Gd^{3+}	64	5.8	60.99	4.0060e-01
V	23	5.4	22.25	6.7060e+00	Tb	65	6.0	64.44	1.6320e+00
V^{5+}	23	5.8	17.98	6.3790e-01	Tb^{3+}	65	5.8	61.99	3.8720e-01
Cr	24	5.4	23.35	2.8030e+00	Dy	66	4.8	65.41	1.5770e+00
Cr^{4+}	24	5.8	19.97	1.7010e-01	Dy^{3+}	66	5.8	62.98	3.7220e-01
Mn	25	6.0	24.10	3.7890e+00	Ho	67	5.4	66.40	1.6920e+00
Mn^{2+}	25	4.6	22.76	3.3990e-01	Ho^{3+}	67	5.8	63.98	3.5620e-01
Fe	26	5.8	25.11	6.4740e+00	Er	68	5.8	67.39	1.7930e+00
Fe^{2+}	26	4.6	23.95	4.4840e-02	Er^{3+}	68	5.8	64.98	3.3960e-01
Co	27	6.0	26.93	6.8160e-02	Tm	69	5.8	68.37	1.8520e+00
Co^{2+}	27	5.8	24.96	9.9490e-02	Tm^{3+}	69	5.8	65.97	3.2300e-01
Ni	28	6.0	27.92	8.7510e-02	Yb	70	6.0	69.36	1.9250e+00
Ni^{2+}	28	5.8	25.99	6.5680e-03	Yb^{3+}	70	5.8	66.97	3.0760e-01
Cu	29	6.0	28.90	1.1050e-01	Lu	71	6.0	70.33	2.4360e+00
Cu^{2+}	29	5.8	26.99	6.6100e-03	Lu^{3+}	71	5.8	67.96	2.9110e-01
Zn	30	5.8	29.89	1.3700e-01	Hf	72	6.0	71.34	2.6850e+00
Zn^{2+}	30	5.8	27.99	6.8830e-03	Ta	73	5.8	72.36	2.7880e+00
Ga	31	6.0	30.88	1.8260e-01	W	74	6.0	73.38	2.8340e+00
Ge	32	5.8	31.89	1.6530e-01	Re	75	6.0	74.39	2.8410e+00
As	33	5.8	31.00	2.1140e+01	Os	76	6.0	75.40	2.8380e+00
Se	34	5.8	33.91	1.0950e-01	Ir	77	6.0	76.41	2.8120e+00
Br	35	6.0	34.91	9.0860e-02	Pt	78	6.0	77.49	2.1970e+00
Br^-	35	5.8	35.88	1.5800e-01	Au	79	6.0	78.49	2.1670e+00
Kr	36	6.0	35.92	7.9860e-02	Hg	80	6.0	79.41	2.8020e+00
Rb	37	6.0	36.61	5.0630e-01	Tl	81	6.0	80.19	3.9990e+00
Rb^+	37	5.8	35.95	3.9370e-02	Pb	82	6.0	81.03	5.6250e+00
Sr	38	6.0	37.41	1.3630e+00	Bi	83	6.0	81.91	7.4980e+00
Sr^{2+}	38	5.8	35.96	1.2360e-01	Po	84	6.0	82.84	9.4760e+00
Y	39	6.0	38.38	1.7140e+00	At	85	6.0	83.87	1.0790e+01
Y^{3+}	39	5.8	35.97	4.8750e-01	Rn	86	6.0	84.93	1.1790e+01
Zr	40	6.0	39.38	1.9100e+00	Fr	87	5.8	85.67	1.3230e+01
Zr^{4+}	40	4.8	36.00	6.4970e-01	Ra	88	6.0	86.45	1.5540e+01
Nb	41	6.0	40.47	1.4470e+00	Ac	89	6.0	88.48	1.2340e+01
Nb^{5+}	41	4.8	36.00	1.2340e-01	Th	90	6.0	89.54	1.0740e+01
Mo	42	6.0	41.15	4.1250e+01	Pa	91	6.0	90.50	9.4760e+00
Mo^{6+}	42	4.8	35.92	1.8600e+00	U	92	6.0	90.06	2.1770e+01

Table 7. *Electron scattering factors for $s = 0$ with error estimates*

	Z	Number of electrons	$f_{el}(0)$	Estimated error
He	2	2.0	.4173	3.8916E-05
Li	3	3.0	3.2556	2.8129E-03
Li^+	3	2.0	.1569	5.2706E-06
Be	4	4.0	3.0383	1.3486E-03
Be^{2+}	4	2.0	.0817	1.4034E-06
B	5	5.0	2.7850	8.4544E-04
C	6	6.0	2.4709	5.3145E-04
N	7	7.0	2.2034	3.5427E-04
O	8	8.0	1.9839	2.4833E-04
O^{2-}	8	10.0	4.0992	8.9507E-04
F	9	9.0	1.8017	1.8092E-04
F^-	9	10.0	2.6159	3.7702E-04
Ne	10	10.0	1.6494	1.3603E-04
Na	11	11.0	4.7387	3.7538E-03
Na^+	11	10.0	1.1285	5.7620E-05
Mg	12	12.0	5.1781	2.7491E-03
Mg^{2+}	12	10.0	.8300	2.9536E-05
Al	13	13.0	5.8665	2.9083E-03
Al^{3+}	13	10.0	.6392	1.6927E-05
Si	14	14.0	5.7535	2.1630E-03
P	15	15.0	5.4738	1.5953E-03
S	16	16.0	5.1640	1.2010E-03
Cl	17	17.0	4.8566	9.2179E-04
Cl^-	17	18.0	6.3858	1.5298E-03
Ar	18	18.0	4.5712	7.2232E-04
K	19	19.0	8.8966	8.3276E-03
K^+	19	18.0	3.4300	3.7103E-04
Ca	20	20.0	9.8371	6.9986E-03
Ca^{2+}	20	18.0	2.7075	2.1868E-04
Sc	21	21.0	9.2502	5.6518E-03
Sc^{3+}	21	18.0	2.2078	1.3993E-04
Ti	22	22.0	8.7270	4.7373E-03
Ti^{4+}	22	18.0	1.8429	9.4739E-05
V	23	23.0	8.2633	4.0568E-03
V^{5+}	23	18.0	1.5658	6.6885E-05
Cr	24	24.0	6.9550	3.0578E-03
Cr^{4+}	24	20.0	1.9167	9.2242E-05
Mn	25	25.0	7.4772	3.0987E-03
Mn^{2+}	25	23.0	2.8554	2.1291E-04
Fe	26	26.0	7.1403	2.7477E-03
Fe^{2+}	26	24.0	2.8109	1.9600E-04
Co	27	27.0	6.8305	2.4537E-03
Co^{2+}	27	25.0	2.7595	1.7988E-04
Ni	28	28.0	6.5466	2.2048E-03
Ni^{2+}	28	26.0	2.7057	1.6514E-04
Cu	29	29.0	6.2851	1.9917E-03
Cu^{2+}	29	27.0	2.6507	1.5178E-04
Zn	30	30.0	6.0434	1.8075E-03
Zn^{2+}	30	28.0	2.5957	1.3972E-04
Ga	31	31.0	7.1413	2.7662E-03
Ge	32	32.0	7.3741	2.4313E-03
As	33	33.0	7.3686	2.0464E-03
Se	34	34.0	7.2661	1.7198E-03
Br	35	35.0	7.0805	1.4342E-03
Br-	35	36.0	8.8736	2.2562E-03
Kr	36	36.0	6.8811	1.2090E-03
Rb	37	37.0	11.6690	1.0518E-02
Rb+	37	36.0	5.5344	6.9338E-04
Sr	38	38.0	13.0052	9.5547E-03
Sr^{2+}	38	36.0	4.6353	4.4984E-04
Y	39	39.0	12.5953	7.6528E-03
Y^{3+}	39	36.0	3.9802	3.1337E-04
Zr	40	40.0	12.1094	6.3672E-03
Zr^{4+}	40	36.0	3.4772	2.2891E-04
Nb	41	41.0	10.6991	4.6565E-03
Nb^{5+}	41	36.0	3.0772	1.7305E-04
Mo	42	42.0	10.2830	4.0237E-03
Mo^{6+}	42	36.0	2.7508	1.3430E-04
Ru	44	44.0	9.5521	3.1557E-03
Rh	45	45.0	9.2244	2.8416E-03
Pd	46	46.0	7.5645	1.2037E-03
Pd^{2+}	46	45.0	6.2132	6.7643E-04
Ag	47	47.0	8.6414	2.3620E-03
Ag^{2+}	47	45.0	5.2211	4.1702E-04
Cd	48	48.0	9.2024	2.5729E-03
Cd^{2+}	48	46.0	5.1324	3.8261E-04
In	49	49.0	10.5928	4.0541E-03
Sn	50	50.0	11.0376	3.8385E-03
Sb	51	51.0	11.1772	3.4339E-03
Te	52	52.0	11.1747	3.0381E-03
I	53	53.0	10.9811	2.6087E-03
I^-	53	54.0	13.1951	3.8319E-03
Xe	54	54.0	10.7652	2.2614E-03
Cs	55	55.0	16.3483	1.5084E-02
Cs^+	55	54.0	9.0154	1.3983E-03
Ba	56	56.0	18.1123	1.4382E-02
Ba^{2+}	56	54.0	7.8000	9.6292E-04
La	57	57.0	17.7054	1.1768E-02
La^{3+}	57	54.0	6.8841	7.0536E-04
Ce	58	58.0	17.2940	1.1121E-02
Ce^{4+}	58	54.0	6.1598	5.3826E-04
Pr	59	59.0	16.8631	1.1987E-02
Pr^{3+}	59	56.0	6.6906	6.2747E-04
Nd	60	60.0	16.4897	1.1389E-02
Nd^{3+}	60	57.0	6.5894	5.9248E-04
Sm	62	62.0	15.7949	1.0344E-02
Sm^{3+}	62	59.0	6.3881	5.3018E-04
Eu	63	63.0	15.4700	9.8674E-03
Eu^{3+}	63	60.0	6.2897	5.0251E-04
Gd	64	64.0	15.2591	8.3286E-03
Gd^{3+}	64	61.0	6.1954	4.7726E-04
Tb	65	65.0	14.8526	9.0420E-03
Tb^{3+}	65	62.0	6.0994	4.5316E-04
Dy	66	66.0	14.5577	8.6608E-03
Dy^{3+}	66	63.0	6.0041	4.3068E-04
Ho	67	67.0	14.2730	8.3015E-03
Ho^{3+}	67	64.0	5.9111	4.0975E-04
Er	68	68.0	13.9978	7.9620E-03
Er^{3+}	68	65.0	5.8204	3.9024E-04
Tm	69	69.0	13.7312	7.6404E-03
Tm^{3+}	69	66.0	5.7320	3.7202E-04
Yb	70	70.0	13.4728	7.3350E-03
Yb^{3+}	70	67.0	5.6458	3.5498E-04
Lu	71	71.0	13.4834	6.3382E-03
Lu^{3+}	71	68.0	5.5618	3.3902E-04
Hf	72	72.0	13.2202	5.3929E-03
Ta	73	73.0	12.9316	4.6792E-03
W	74	74.0	12.6434	4.1191E-03
Re	75	75.0	12.3627	3.6659E-03
Os	76	76.0	12.0917	3.2907E-03
Ir	77	77.0	11.7793	2.9537E-03
Pt	78	78.0	10.8225	2.2698E-03
Au	79	79.0	10.5466	2.0467E-03
Hg	80	80.0	10.9356	2.2127E-03
Tl	81	81.0	12.8045	4.5944E-03
Pb	82	82.0	13.5344	4.6469E-03
Bi	83	83.0	13.8911	4.3559E-03
Po	84	84.0	14.0629	4.0044E-03
At	85	85.0	13.7529	3.3840E-03
Rn	86	86.0	13.4546	2.9122E-03
Fr	87	87.0	18.5513	1.4183E-02
Ra	88	88.0	20.3926	1.4190E-02
Ac	89	89.0	20.4678	1.2092E-02
Th	90	90.0	20.2022	1.0261E-02
Pa	91	91.0	19.6404	1.0418E-02
U	92	92.0	19.2909	9.8434E-03

Table 8. *Mean inner potentials in* V *calculated using Doyle–Turner electron scattering factors, the Herman–Skillman Hartree–Slater program and the Grant et al.* (1980) *Dirac–Fock program*

	Doyle–Turner	Herman–Skillman	Dirac–Fock
Aluminium	17.10	15.59	17.04
Silicon	14.02	13.42	13.84
Copper	22.06	21.51	24.35
Germanium	15.58	14.64	15.57
Silver	24.44	23.24	24.36
Gold	29.80	27.90	29.73
SiO_2 neutral	6.87	10.16	6.89
MgO neutral	18.34	17.45	18.40
MgO ions		11.48	12.64
GaAs	15.19	14.41	15.40

applied to other systems, such as intermetallics, and how the results would compare with measurements from energy-loss fine structure.

Concluding remarks

We have presented X-ray scattering-factor tables for a complete range of elements and ions calculated using a multiconfiguration Dirac–Fock computer code. The results are within less than 1% of the relativistic Hartree–Fock results of Doyle & Turner (1968). We have also given two parameterizations in terms of four Gaussians, one of higher accuracy over a range of about 2.0 $Å^{-1}$ and the other of lower accuracy over an extended range of 6.0 $Å^{-1}$. In general, we recommend direct use of the tables rather than use of the parameterizations. The electron scattering factors can be calculated from the X-ray scattering factors using the Mott formula. The limiting case of $f_{el}(0)$ has been tabulated directly and can be used to calculate the mean inner potential. We show that the mean inner potential can be very sensitive to charge transfer and we give estimates for a number of compounds for which measurements are available.

Information on how to obtain the complete tables is available from DR at the address given above.

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Use of Tilted Bragg Reflections in X-ray Standing-Wave Experiments and X-ray Optics Applications

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Abstract

This paper studies in detail 'tilted reflections', which are defined here as Bragg reflections where the incident vector $\mathbf{k}_o^{(a)}$, the diffraction vector $\mathbf{h}$ and the normal $\mathbf{n}$ to the surface are not coplanar. Such reflections are especially useful when it is necessary to work in Bragg geometry with reflecting planes