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Analytic constants for atomic scattering factors.

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In a paper by Vand, Eiland & Pepinsky (1957), it was shown that the atomic scattering factor, f, could be approximated as a function of $x=\sin\theta$, as far as $\theta=90°$, for Cu $K\alpha$ radiation by the expression

$$f(x)=A\exp(-ax^2)+B\exp(-bx^2)\,.$$

It was also suggested that a better fit, as far as $\theta=90°$, for Mo $K\alpha$ radiation could be obtained by the expression

$$f(x)=A\exp(-ax^2)+B\exp(-bx^2)+C\,.$$

Following this publication, Forsyth & Wells (1959) modified the method of Vand, Eiland & Pepinsky as follows:

(i) The condition that $A+B+C=N$, where N is the number of electrons in the element or ion, was relaxed.
(ii) The reciprocal space variable, $s=\sin\theta/\lambda$ rather than $x=\sin\theta$, was chosen.
(iii) The least-squares weighting factor,

$$\omega_i=\exp[-(s_i-0{\cdot}5)^2]$$

which for Cu $K\alpha$ radiation gives maximum weighting at $\theta=45°$, was used.

As an indication of the fit between the atomic scattering factors calculated from their least-squares analytic constants and the theoretical atomic scattering factors, they included in their tables of A, a, B, b and C, values of

$$\varepsilon=\frac{100}{f_0}\left(\frac{\Sigma\omega_i\delta_i^2}{\Sigma\omega_i}\right)^{\frac{1}{2}}$$

i.e. the error expressed as a percentage of the atomic scattering factor at $s=0$.

It is the intention of the author that this paper should provide new and revised values of the analytical constants A, a, B, b and C for both Cu $K\alpha$ and Mo $K\alpha$ radiation, using the atomic scattering factor tables recently published in *International Tables for X-ray Crystallography* (1962, p. 201).

The least-squares fitting was performed on a Ferranti MERCURY computer programmed to include the above modifications suggested by Forsyth & Wells, but with

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the exception that for Mo $K\alpha$ radiation the weighting factor was altered to

$$\omega_i = \exp\left[-(s_i - 1{\cdot}0)^2\right]$$

to give maximum weighting at $\theta = 45°$.

Tables 1 and 2 give the analytic constants and the error term, ε, determined for atomic scattering factors derived from self-consistent or variational wave functions (*International Tables for X-ray Crystallography*, 1962, Table 3·3·1A, p. 202) and the Thomas–Fermi–Dirac statistical model (*International Tables for X-ray Crystallography*, 1962, Table 3·3·1B, p. 210) respectively.

Table 3 provides a comparison between the least-squares and the theoretical atomic scattering factors corresponding to $\varepsilon = 0{\cdot}01$, $0{\cdot}09$ and $1{\cdot}01$. The examples were calculated from values of A, a, B, b and C determined in three of the steps in the least-squares reiteration calculation for Kr^{8+}. In general, for the same ε, elements or ions with fewer electrons have a slightly better correspondence.

Table 1. *Analytic constants for atomic scattering factors derived from self-consistent or variational wave functions*

	CuK_α radiation						MoK_α radiation					
Element	A	a	B	b	C	ε	A	a	B	b	C	ε
H	0.4629	9.077	0.5148	33.154	0.0207	0.167	0.3356	6.381	0.6543	27.870	0.0055	0.300
H^{-1}	1.003	17.616	0.9367	183.64	0.0477	0.959	0.9195	14.275	1.039	151.50	0.0142	0.908
He	1.263	4.808	0.6041	19.319	0.1314	0.071	0.9138	2.930	1.037	13.275	0.0388	0.314
He^{-1}	1.678	7.886	1.073	1147.0	0.2489	0.687	1.746	5.878	1.165	829.12	0.0880	1.468
Li	1.575	3.404	1.064	114.93	0.3564	0.135	1.689	2.601	1.121	101.23	0.1755	0.600
Li^{+1}	1.416	2.466	0.3651	8.636	0.2190	0.011	1.132	1.585	0.7798	5.968	0.0850	0.094
Li^{-1}	1.527	4.633	1.934	309.68	0.5235	1.006	1.742	2.824	2.023	265.05	0.1973	1.060
Be	1.351	2.313	2.032	55.970	0.6032	0.252	1.649	1.501	2.086	53.191	0.2443	0.257
Be^{+1}	1.414	2.205	1.037	44.897	0.5446	0.127	1.637	1.544	1.093	40.979	0.2595	0.276
Be^{+2}	1.469	1.583	0.2155	5.193	0.3159	0.014	1.297	1.046	0.5665	3.626	0.1354	0.029
B	1.093	4.493	2.721	37.281	1.169	0.294	1.576	1.130	3.009	32.460	0.3747	0.400
B^{+1}	1.028	2.521	1.979	28.552	0.9878	0.126	1.566	0.9904	2.098	26.479	0.3218	0.188
B^{+2}	1.184	1.946	0.9906	24.522	0.8232	0.070	1.582	1.041	1.077	22.105	0.3327	0.167
B^{+3}	1.472	1.357	0.0108	11.025	0.5174	0.021	1.404	0.7550	0.4115	2.529	0.1844	0.012
C	1.620	6.785	2.988	28.126	1.380	0.211	1.407	1.119	3.907	21.701	0.6328	0.483
C(valence)	1.721	6.770	2.887	30.278	1.379	0.212	1.469	1.253	3.817	22.785	0.6543	0.531
C^{+2}	0.8815	3.095	1.881	16.337	1.236	0.047	1.519	0.6231	2.159	14.460	0.3119	0.154
C^{+3}	1.003	2.113	0.9051	16.139	1.091	0.029	1.515	0.7724	1.065	13.897	0.4134	0.130
C^{+4}	1.590	0.8103	0.0209	6.088	0.3887	0.022	1.335	0.4187	0.5712	1.465	0.0935	0.024
N	2.708	7.081	2.810	23.810	1.474	0.105	1.385	1.581	4.612	16.297	0.9449	0.470
N^{+3}	1.102	3.734	1.519	13.090	1.379	0.016	1.325	0.6504	2.075	10.645	0.5909	0.146
N^{+4}	0.9469	2.130	0.8156	11.596	1.237	0.014	1.417	0.6427	1.045	9.691	0.5339	0.098
N^{-1}	3.594	9.051	2.855	40.533	1.534	0.292	1.886	3.561	4.817	24.559	1.205	0.651
O	3.811	6.363	2.633	21.191	1.550	0.055	1.841	2.342	4.946	13.822	1.160	0.418
O^{+1}	3.115	5.368	2.390	15.357	1.492	0.029	1.682	2.558	4.065	11.491	1.234	0.179
O^{+2}	2.499	4.673	2.042	12.366	1.459	0.012	1.344	2.009	3.455	9.551	1.190	0.121
O^{+3}	1.921	4.084	1.648	10.358	1.431	0.010	1.091	1.538	2.760	8.187	1.142	0.082
O^{-1}	4.551	7.554	2.818	32.818	1.614	0.198	2.912	4.249	4.686	21.356	1.331	0.467
F	4.884	5.530	2.477	19.362	1.636	0.048	3.340	3.553	4.254	13.813	1.377	0.218
F^{-1}	4.735	5.461	3.612	19.260	1.649	0.039	2.793	2.625	5.917	13.665	1.238	0.387
Ne	5.519	4.558	2.770	15.057	1.708	0.021	3.335	2.467	5.327	10.248	1.302	0.261
Na	7.504	5.179	1.275	107.08	2.203	0.215	7.303	3.753	1.987	39.203	1.553	0.808
Na^{+}	6.298	3.751	1.938	11.842	1.764	0.008	3.956	2.225	4.677	7.640	1.346	0.159
Mg	7.459	3.979	2.272	73.153	2.254	0.110	7.664	3.122	2.657	54.177	1.613	0.546
Mg^{+2}	6.807	3.436	1.183	9.452	2.007	0.048	4.360	1.970	4.240	6.014	1.392	0.069
Al	7.373	3.193	3.246	60.771	2.354	0.160	7.745	2.494	3.569	50.689	1.615	0.437
Al^{+1}	7.458	2.949	2.409	41.721	2.126	0.072	7.610	2.591	2.623	36.554	1.742	0.199
Al^{+2}	7.483	2.990	1.361	32.090	2.154	0.038	7.528	2.436	1.811	22.314	1.627	0.307
Al^{+3}	6.219	2.233	2.111	6.088	1.670	0.023	5.130	1.799	3.418	5.057	1.448	0.033

Table 1 (*cont.*)

Element		CuK$_\alpha$ radiation						MoK$_\alpha$ radiation					
		A	a	B	b	C	ε	A	a	B	b	C	ε
Si		7.180	2.619	4.299	46.092	2.494	0.150	7.725	2.033	4.576	41.411	1.641	0.289
	Si^{+3}	7.550	2.341	1.403	22.953	2.044	0.029	7.630	2.134	1.587	19.970	1.771	0.095
	Si^{+4}	7.084	2.180	0.9828	5.989	1.934	0.012	5.054	1.439	3.534	3.938	1.412	0.017
P		6.792	2.344	5.297	36.132	2.882	0.150	7.705	1.681	5.588	33.428	1.652	0.204
S		7.545	1.328	6.821	25.877	1.627	0.036	7.700	1.308	6.806	26.003	1.489	0.049
	S^{-1}	8.161	1.135	7.940	27.268	0.8936	0.036	7.688	1.283	7.860	27.675	1.452	0.068
	S^{-2}	13.114	0.6088	8.944	37.448	-4.048	0.069	7.893	1.251	8.740	38.886	1.397	0.159
Cl		7.239	1.138	7.937	22.203	1.819	0.044	7.717	1.070	7.916	22.367	1.367	0.078
	Cl^{-}	7.722	1.002	9.023	23.413	1.246	0.036	7.681	1.069	8.936	23.809	1.385	0.096
Ar		5.394	3.207	7.462	22.232	5.124	0.109	7.479	1.040	8.686	19.039	1.761	0.220
K		9.494	7.981	3.012	64.361	6.461	0.575	7.304	0.9700	9.267	16.525	2.027	0.677
	K^{+1}	5.213	3.254	7.321	16.861	5.457	0.057	7.406	0.8352	8.932	14.310	1.609	0.156
Ca		10.256	7.667	3.060	90.954	6.639	0.358	7.111	1.303	9.073	16.811	3.128	1.170
	Ca^{+1}	9.635	6.878	2.836	45.260	6.490	0.336	7.039	0.9194	9.304	13.407	2.328	0.598
	Ca^{+2}	5.101	2.820	7.432	13.167	5.460	0.035	7.317	0.7105	9.070	11.361	1.576	0.105
Sc		10.966	7.405	3.169	54.359	6.791	0.335	7.053	1.006	10.614	14.092	2.812	0.834
	Sc^{+1}	9.183	5.899	4.287	23.602	6.496	0.140	7.069	0.7983	10.477	12.008	2.256	0.406
	Sc^{+2}	7.056	4.436	5.756	14.789	6.179	0.047	7.211	0.6655	9.955	10.421	1.758	0.191
	Sc^{+3}	5.540	3.235	6.637	11.243	5.820	0.022	7.404	0.5732	9.255	9.187	1.307	0.103
Ti		11.690	6.680	3.408	70.858	6.855	0.257	7.161	1.308	10.512	14.446	3.654	1.129
	Ti^{+1}	10.262	5.769	4.087	23.309	6.625	0.110	6.793	0.8491	11.220	11.024	2.779	0.434
	Ti^{+2}	8.812	4.852	4.782	15.868	6.396	0.043	6.861	0.6988	10.738	9.611	2.298	0.251
	Ti^{+3}	7.186	3.917	5.659	11.822	6.150	0.020	6.982	0.6018	10.071	8.541	1.895	0.148
V		12.536	6.298	3.443	65.724	6.976	0.231	7.468	1.532	10.711	13.937	4.173	1.090
	V^{+1}	11.215	5.518	4.027	22.517	6.737	0.088	6.596	0.9651	11.804	10.295	3.390	0.443
	V^{+2}	10.173	4.894	4.270	16.209	6.549	0.034	6.527	0.7751	11.440	8.927	2.918	0.282
	V^{+3}	8.334	3.945	5.402	11.708	6.259	0.023	6.617	0.6470	10.845	7.949	2.473	0.181
Cr		13.530	5.993	3.336	43.358	7.087	0.189	7.343	1.471	11.866	11.864	4.343	0.778
	Cr^{+1}	12.165	5.227	3.991	21.235	6.826	0.071	6.581	1.085	12.338	9.591	3.878	0.434
	Cr^{+2}	11.234	4.694	4.119	15.858	6.638	0.035	6.335	0.9116	11.972	8.389	3.573	0.290
	Cr^{+3}	9.932	4.109	4.623	12.067	6.443	0.013	6.245	0.7527	11.495	7.449	3.190	0.200
Mn		14.310	5.599	3.413	58.160	7.228	0.194	9.191	2.055	10.289	13.782	4.949	0.966
	Mn^{+1}	13.074	4.931	3.985	20.498	6.926	0.062	6.901	1.284	12.529	9.215	4.372	0.427
	Mn^{+2}	12.007	4.411	4.280	14.550	6.707	0.020	6.422	1.289	11.969	8.167	4.515	0.247
	Mn^{+3}	10.997	3.996	4.446	11.713	6.554	0.009	6.129	0.8819	12.021	7.035	3.779	0.201
	Mn^{+4}	9.936	3.661	4.627	9.486	6.435	0.013	5.773	0.8352	11.383	6.375	3.807	0.110
Fe		15.133	5.270	3.444	54.196	7.379	0.179	10.605	2.305	9.642	14.388	5.249	0.885
	Fe^{+1}	14.018	4.693	3.914	19.763	7.055	0.053	7.493	1.467	12.584	8.904	4.739	0.412
	Fe^{+2}	13.224	4.293	3.925	14.841	6.846	0.017	6.712	1.214	12.675	7.588	4.499	0.279
	Fe^{+3}	12.364	3.952	3.950	11.615	6.685	0.014	6.240	1.197	12.101	6.791	4.601	0.166
	Fe^{+4}	10.647	3.386	4.917	9.089	6.436	0.008	5.987	0.8712	11.978	6.028	3.992	0.137
Co		15.994	4.999	3.414	51.767	7.551	0.168	12.022	2.458	9.056	14.861	5.468	0.801
	Co^{+1}	14.852	4.402	3.998	18.694	7.140	0.043	8.336	1.626	12.477	8.689	5.017	0.371
	Co^{+2}	14.052	4.009	4.046	14.069	6.898	0.019	7.326	1.360	12.762	7.318	4.805	0.267
	Co^{+3}	13.088	3.661	4.209	11.042	6.705	0.010	6.637	1.159	12.696	6.391	4.602	0.191

Table 1 (*cont.*)

Element		CuK$_\alpha$ radiation						MoK$_\alpha$ radiation					
		A	a	B	b	C	ε	A	a	B	b	C	ε
Ni		16.859	4.749	3.365	49.734	7.734	0.160	13.358	2.529	8.580	15.113	5.643	0.730
	Ni^{+1}	15.762	4.191	3.936	17.856	7.294	0.031	9.383	1.758	12.224	8.501	5.242	0.332
	Ni^{+2}	14.982	3.815	4.008	13.447	7.006	0.016	8.133	1.492	12.711	7.091	5.058	0.239
	Ni^{+3}	14.274	3.583	3.851	11.011	6.877	0.009	7.299	1.303	12.739	6.189	4.900	0.179
Cu		17.815	4.537	3.239	33.810	7.907	0.127	12.957	2.264	10.084	11.554	5.654	0.519
	Cu^{+1}	16.595	3.896	4.051	17.041	7.346	0.034	11.819	2.175	10.367	9.250	5.703	0.254
	Cu^{+2}	15.988	3.665	3.851	13.139	7.161	0.011	9.155	1.609	12.481	6.927	5.276	0.221
	Cu^{+3}	15.043	3.337	4.054	10.299	6.902	0.009	8.158	1.418	12.657	5.991	5.127	0.157
Zn		18.543	4.299	3.260	46.229	8.156	0.135	15.864	2.520	7.855	15.264	5.915	0.610
	Zn^{+2}	16.892	3.421	3.901	12.782	7.205	0.013	11.821	2.001	10.395	7.501	5.720	0.160
Ga		18.653	3.890	4.003	47.443	8.291	0.147	18.212	2.628	6.376	23.516	6.113	0.598
	Ga^{+1}	18.509	3.674	3.491	31.007	7.978	0.067	16.341	2.331	7.501	13.645	5.932	0.435
	Ga^{+3}	17.277	3.114	3.499	10.420	7.224	0.009	10.844	1.639	11.599	5.901	5.507	0.133
Ge		18.762	3.483	4.884	43.735	8.311	0.122	18.997	2.495	6.591	27.676	6.194	0.514
	Ge^{+2}	18.678	3.243	3.436	24.385	7.876	0.038	17.211	2.220	6.645	12.779	5.991	0.346
	Ge^{+4}	16.955	2.638	4.129	7.880	6.917	0.008	12.034	1.708	10.222	5.384	5.723	0.066
As		18.766	3.106	5.892	37.993	8.300	0.101	19.320	2.301	7.287	27.846	6.222	0.413
	As^{+1}	18.575	3.244	5.098	36.062	8.300	0.092	18.619	2.410	6.786	23.989	6.432	0.380
	As^{+2}	18.524	3.158	4.336	28.190	8.128	0.047	18.123	2.327	6.393	17.823	6.353	0.321
	As^{+3}	18.425	3.038	3.683	20.998	7.886	0.023	17.283	2.204	6.372	12.589	6.241	0.250
	As^{+5}	17.779	2.502	3.193	7.192	7.028	0.006	12.012	1.566	10.270	4.628	5.702	0.043
Se		18.662	2.849	6.835	33.858	8.465	0.095	19.531	2.113	8.105	26.700	6.218	0.330
	Se^{+6}	17.364	2.179	3.799	5.708	6.837	0.009	12.165	1.454	10.136	4.069	5.690	0.031
Br		18.394	2.644	7.807	29.824	8.766	0.086	19.594	1.923	9.055	24.568	6.225	0.263
	Br^{+7}	19.069	2.222	1.685	6.459	7.249	0.009	12.523	1.374	9.765	3.642	5.708	0.022
	Br^{-1}	18.251	2.846	8.393	35.668	9.287	0.157	19.796	1.959	9.743	28.767	6.271	0.322
Kr		18.032	2.507	8.753	26.563	9.183	0.081	19.637	1.755	10.053	22.454	6.195	0.207
	Kr^{+8}	14.567	0.5346	13.268	3.007	0.166	0.007	12.435	1.251	9.923	3.224	5.640	0.011
	Rb^{+1}	17.861	2.211	9.099	20.791	9.025	0.041	19.493	1.606	10.221	18.450	6.221	0.115
	Zr^{+4}	17.348	1.740	9.630	13.539	9.016	0.015	19.313	1.251	10.701	12.471	5.957	0.080
	Mo^{+1}	17.301	3.817	8.790	28.572	14.824	0.209	19.941	1.193	14.207	16.386	6.455	0.384
Ag		20.137	4.645	9.296	24.870	17.493	0.128	18.850	1.088	19.051	12.979	8.652	0.442
	Ag^{+1}	19.105	3.899	10.204	16.346	16.662	0.045	18.551	0.9246	19.534	10.306	7.698	0.245
W		36.594	3.647	9.202	42.974	28.065	0.244	38.655	1.579	17.935	16.338	16.500	0.459
	Au^{+}	35.524	3.050	13.033	21.945	29.372	0.079	39.445	1.339	21.104	13.806	17.049	0.267
Hg		36.733	3.453	11.590	29.761	31.546	0.133	39.928	1.442	20.536	15.477	18.855	0.408
	Hg^{+2}	35.913	3.109	11.917	20.264	30.171	0.079	38.680	1.310	21.310	12.107	17.713	0.248
	Tl^{+1}	36.608	3.436	11.577	25.681	31.706	0.129	39.463	1.261	22.529	12.894	17.391	0.335
	Tl^{+3}	34.663	2.491	15.112	14.748	28.202	0.027	38.676	1.149	22.695	10.657	16.420	0.151
	Pb^{+3}	36.265	3.028	11.951	17.737	30.805	0.067	39.019	1.144	22.895	10.551	16.822	0.215
	U^{+6}	39.990	2.222	14.811	17.162	31.191	0.008	42.286	1.348	20.421	12.535	23.051	0.252

Table 2. *Analytic constants for atomic scattering factors derived from Thomas–Fermi–Dirac statistics*

Element	CuK_α radiation						MoK_α radiation					
	A	a	B	b	C	ε	A	a	B	b	C	ε
Ca	9.625	4.447	4.752	36.621	5.609	0.164	9.092	1.951	7.399	20.738	3.291	0.711
Ca^{+1}	8.707	3.082	5.565	20.201	4.733	0.033						
Ca^{+2}	8.932	1.339	7.056	11.919	2.013	0.020						
Sc	10.115	4.429	4.899	36.471	5.971	0.151	9.561	1.928	7.704	20.424	3.504	0.705
Sc^{+1}	9.211	3.066	5.769	20.372	5.027	0.030						
Sc^{+2}	9.605	1.324	7.348	12.110	2.049	0.020						
Sc^{+3}	67.014	0.0782	8.542	8.107	-57.555	0.014						
Ti	10.586	4.382	5.072	36.264	6.323	0.161	10.063	1.920	7.966	20.345	3.729	0.693
Ti^{+1}	9.691	3.144	5.875	20.747	5.440	0.030						
Ti^{+2}	9.646	1.539	7.397	12.539	2.963	0.025						
Ti^{+3}	55.927	0.1055	8.801	8.340	-45.728	0.013						
V	11.075	4.347	5.230	36.060	6.674	0.159	10.521	1.894	8.281	20.017	3.941	0.693
V^{+1}	10.200	3.137	6.056	20.948	5.754	0.033						
V^{+2}	9.974	1.624	7.588	12.749	3.442	0.026						
V^{+3}	71.040	0.0875	9.195	8.460	-60.235	0.011						
Cr	11.550	4.324	5.381	35.943	7.046	0.162	11.009	1.877	8.563	19.839	4.159	0.688
Cr^{+1}	10.653	3.205	6.172	21.206	6.181	0.032						
Cr^{+2}	10.303	1.754	7.681	13.099	4.021	0.028						
Cr^{+3}	17.330	0.4676	9.166	8.823	-5.494	0.015						
Mn	12.043	4.333	5.492	36.078	7.443	0.158	11.485	1.860	8.851	19.614	4.383	0.682
Mn^{+1}	11.153	3.183	6.363	21.361	6.493	0.031						
Mn^{+2}	10.785	1.800	7.859	13.316	4.362	0.022						
Mn^{+3}	16.119	0.5699	9.336	9.066	-3.452	0.014						
Mn^{+4}	181.856	0.0279	10.089	6.723	-170.942	0.015						
Fe	12.517	4.293	5.651	35.880	7.806	0.157	11.986	1.851	9.108	19.513	4.614	0.676
Fe^{+1}	11.639	3.196	6.510	21.504	6.857	0.023						
Fe^{+2}	11.143	1.904	7.969	13.595	4.893	0.023						
Fe^{+3}	19.639	0.4759	9.728	9.163	-6.363	0.012						
Fe^{+4}	151.727	0.0358	10.451	6.846	-140.176	0.013						
Co	12.992	4.275	5.791	35.728	8.188	0.161	12.448	1.831	9.404	19.268	4.841	0.671
Co^{+1}	12.147	3.243	6.603	21.861	7.259	0.027						
Co^{+2}	11.684	1.901	8.196	13.733	5.125	0.019						
Co^{+3}	13.149	0.9294	9.523	9.583	1.333	0.018						
Ni	13.467	4.234	5.952	35.577	8.555	0.155	12.954	1.820	9.662	19.181	5.073	0.667
Ni^{+1}	12.608	3.253	6.760	21.937	7.638	0.025						
Ni^{+2}	12.250	1.910	8.382	13.926	5.374	0.020						
Ni^{+3}	17.779	0.6352	10.132	9.523	-2.910	0.014						
Cu	13.943	4.234	6.069	35.505	8.958	0.159	13.414	1.806	9.949	18.949	5.310	0.661
Cu^{+1}	13.095	3.235	6.934	22.049	7.977	0.018						
Cu^{+2}	12.643	1.973	8.529	14.097	5.830	0.019						
Cu^{+3}	15.243	0.8504	10.213	9.730	0.5434	0.016						
Zn	14.425	4.198	6.218	35.382	9.327	0.161	13.906	1.795	10.210	18.823	5.547	0.660
Zn^{+2}	13.539	1.697	9.250	13.509	5.207	0.094						
Ga	14.908	4.202	6.319	35.463	9.741	0.162	14.388	1.783	10.476	18.659	5.786	0.655
Ga^{+1}	14.047	3.285	7.169	22.422	8.790	0.017						
Ga^{+3}	14.405	1.136	10.313	10.239	3.285	0.009						

Table 2 (*cont.*)

Element	CuK_α radiation						MoK_α radiation					
	A	a	B	b	C	ε	A	a	B	b	C	ε
Ge	15.384	4.171	6.460	35.371	10.120	0.160	14.868	1.768	10.746	18.509	6.021	0.656
Ge^{+2}	13.944	2.165	8.840	14.777	7.224	0.022						
Ge^{+4}	61.544	0.1385	12.182	7.654	−45.723	0.012						
As	15.838	4.151	6.604	35.146	10.522	0.158	15.360	1.761	10.999	18.417	6.271	0.645
As^{+1}	15.023	3.265	7.473	22.587	9.509	0.028						
As^{+2}	14.484	2.145	9.068	14.857	7.457	0.023						
As^{+3}	16.605	1.024	10.974	10.360	2.424	0.015						
Se	16.322	4.144	6.708	35.224	10.932	0.154	15.856	1.752	11.244	18.303	6.516	0.644
Br	16.794	4.112	6.854	35.038	11.314	0.151	16.339	1.740	11.505	18.174	6.763	0.641
Kr	17.267	4.084	6.994	34.903	11.702	0.153	16.823	1.732	11.759	18.061	7.017	0.639
Rb	17.724	4.073	7.116	34.766	12.118	0.154	17.317	1.723	12.005	17.974	7.267	0.633
Rb^{+1}	16.926	3.303	7.950	23.088	11.129	0.023						
Sr	18.196	4.068	7.222	34.757	12.540	0.153	17.790	1.712	12.272	17.827	7.516	0.630
Y	18.666	4.067	7.315	34.842	12.976	0.154	18.275	1.700	12.523	17.687	7.764	0.625
Zr	19.128	4.033	7.466	34.563	13.361	0.155	18.776	1.695	12.754	17.633	8.027	0.619
Zr^{+4}	22.716	0.7120	13.535	8.695	−0.2476	0.010						
Nb	19.604	4.028	7.563	34.636	13.789	0.153	19.243	1.683	13.019	17.472	8.280	0.620
Mo	20.052	3.994	7.719	34.363	14.180	0.152	19.732	1.675	13.263	17.394	8.537	0.614
Mo^{+1}	19.295	3.315	8.545	23.535	13.165	0.027						
Tc	20.520	4.009	7.782	34.514	14.648	0.154	20.216	1.667	13.508	17.277	8.797	0.610
Ru	21.003	3.994	7.886	34.506	15.062	0.157	20.694	1.656	13.762	17.144	9.052	0.610
Rh	21.446	3.957	8.049	34.203	15.452	0.153	21.194	1.652	13.982	17.107	9.325	0.605
Pd	21.934	3.957	8.122	34.370	15.893	0.149	21.683	1.644	14.220	17.004	9.586	0.605
Ag	22.368	3.933	8.268	34.120	16.312	0.148	22.171	1.638	14.453	16.945	9.860	0.598
Ag^{+1}	21.643	3.291	9.164	23.747	15.196	0.030						
Cd	22.825	3.936	8.344	34.125	16.773	0.152	22.652	1.629	14.692	16.832	10.125	0.594
In	23.299	3.905	8.479	33.954	17.162	0.149	23.146	1.624	14.915	16.760	10.398	0.592
Sn	23.762	3.901	8.572	33.992	17.608	0.148	23.628	1.618	15.150	16.682	10.673	0.591
Sb	24.199	3.891	8.685	33.872	18.057	0.150	24.117	1.610	15.384	16.608	10.943	0.585
Te	24.677	3.884	8.770	33.901	18.495	0.146	24.591	1.603	15.626	16.498	11.214	0.585
I	25.122	3.871	8.881	33.759	18.934	0.145	25.080	1.597	15.854	16.420	11.487	0.580
Xe	25.583	3.853	8.993	33.730	19.361	0.144	25.578	1.590	16.073	16.367	11.761	0.579
Cs	26.033	3.842	9.097	33.634	19.804	0.146	26.069	1.587	16.286	16.309	12.048	0.575
Ba	26.491	3.834	9.195	33.604	20.249	0.144	26.534	1.579	16.532	16.213	12.327	0.574
La	26.939	3.825	9.291	33.579	20.705	0.145	27.052	1.577	16.721	16.207	12.616	0.570
Ce	27.382	3.814	9.399	33.529	21.154	0.143	27.529	1.569	16.962	16.118	12.887	0.569
Pr	27.833	3.807	9.487	33.462	21.611	0.143	28.009	1.562	17.188	16.033	13.169	0.563
Nd	28.296	3.805	9.560	33.496	22.074	0.143	28.495	1.557	17.408	15.956	13.452	0.562
Pm	28.749	3.794	9.659	33.471	22.521	0.140	28.990	1.554	17.612	15.932	13.746	0.561
Sm	29.196	3.769	9.794	33.248	22.936	0.141	29.467	1.547	17.843	15.843	14.028	0.557
Eu	29.642	3.758	9.894	33.212	23.390	0.140	29.969	1.543	18.044	15.806	14.317	0.554
Gd	30.074	3.757	9.980	33.140	23.872	0.139	30.436	1.535	18.290	15.713	14.596	0.551
Tb	30.525	3.739	10.092	33.050	24.308	0.140	30.930	1.532	18.491	15.675	14.893	0.548
Dy	30.985	3.733	10.169	33.072	24.770	0.137	31.421	1.528	18.697	15.619	15.187	0.548
Ho	31.430	3.723	10.271	32.991	25.222	0.137	31.902	1.523	18.915	15.563	15.480	0.544
Er	31.886	3.716	10.351	32.977	25.686	0.138	32.378	1.518	19.135	15.489	15.773	0.543
Tm	32.319	3.706	10.446	32.887	26.152	0.139	32.869	1.514	19.336	15.442	16.069	0.539
Yb	32.764	3.693	10.550	32.842	26.603	0.135	33.366	1.509	19.540	15.402	16.360	0.538
Lu	33.203	3.687	10.657	32.800	27.076	0.136	33.853	1.504	19.750	15.352	16.656	0.535

Table 2 (*cont.*)

Element	CuK_α radiation						MoK_α radiation					
	A	*a*	*B*	*b*	*C*	*ε*	*A*	*a*	*B*	*b*	*C*	*ε*
Hf	33.650	3.678	10.727	32.737	27.537	0.135	34.348	1.501	19.947	15.318	16.958	0.534
Ta	34.087	3.671	10.816	32.661	28.008	0.136	34.811	1.496	20.179	15.232	17.252	0.530
W	34.536	3.660	10.909	32.607	28.465	0.136	35.302	1.491	20.384	15.181	17.545	0.528
Re	34.969	3.652	11.004	32.564	28.937	0.134	35.784	1.487	20.591	15.139	17.849	0.527
Os	35.409	3.656	11.054	32.638	29.448	0.134	36.271	1.482	20.797	15.085	18.146	0.525
Ir	35.859	3.631	11.190	32.440	29.860	0.133	36.758	1.480	20.992	15.049	18.458	0.523
Pt	36.300	3.626	11.267	32.440	30.340	0.133	37.245	1.475	21.198	14.999	18.756	0.521
Au	36.729	3.611	11.383	32.280	30.794	0.132	37.724	1.472	21.399	14.961	19.070	0.518
Au^+	36.197	3.200	12.339	24.720	29.454	0.041						
Hg	37.156	3.612	11.444	32.316	31.304	0.132	38.124	1.469	21.624	14.878	19.431	0.532
Hg^{2+}	36.104	2.715	13.921	18.924	27.984	0.009						
Tl	37.593	3.615	11.488	32.416	31.822	0.132	38.683	1.462	21.809	14.856	19.680	0.514
Tl^{+1}	37.059	3.186	12.553	24.652	30.375	0.044						
Tl^{+3}	36.339	2.178	16.088	14.748	25.585	0.012						
Pb	38.034	3.590	11.629	32.214	32.238	0.132	39.028	1.461	22.052	14.757	20.078	0.538
Pb^{+3}	36.749	2.178	16.238	14.746	26.022	0.009						
Bi	38.461	3.599	11.671	32.314	32.773	0.132	39.761	1.538	21.490	15.480	20.974	0.462
Po	38.891	3.586	11.776	32.170	33.236	0.130	40.136	1.452	22.407	14.736	20.610	0.509
At	39.319	3.586	11.836	32.208	33.747	0.131	40.621	1.448	22.608	14.696	20.915	0.506
Rn	39.764	3.575	11.927	32.157	34.211	0.129	41.111	1.445	22.800	14.655	21.224	0.506
Fr	40.189	3.564	12.030	32.043	34.680	0.129	41.590	1.442	22.997	14.622	21.543	0.502
Ra	40.625	3.556	12.114	32.006	35.158	0.130	42.086	1.439	23.176	14.595	21.859	0.500
Ac	41.071	3.545	12.204	31.962	35.622	0.128	42.562	1.434	23.389	14.539	22.161	0.501
Th	41.483	3.542	12.283	31.889	36.130	0.128	43.042	1.430	23.593	14.496	22.471	0.497
Pa	41.915	3.534	12.365	31.875	36.613	0.126	43.534	1.428	23.768	14.475	22.795	0.496
U	42.362	3.525	12.450	31.845	37.081	0.126	44.011	1.425	23.962	14.434	23.115	0.495
Np	42.775	3.525	12.516	31.792	37.601	0.127	44.495	1.422	24.160	14.392	23.426	0.492
Pu	43.217	3.520	12.578	31.843	38.095	0.127	44.985	1.419	24.336	14.364	23.751	0.491
Am	43.646	3.511	12.671	31.745	38.571	0.127	45.461	1.416	24.535	14.321	24.068	0.489
Cm	44.093	3.499	12.763	31.721	39.036	0.123	45.952	1.413	24.716	14.295	24.391	0.489
Bk	44.505	3.501	12.819	31.744	39.568	0.123	46.438	1.410	24.907	14.263	24.707	0.487
Cf	44.939	3.492	12.901	31.693	40.048	0.125	46.930	1.408	25.076	14.240	25.038	0.484
Es	45.342	3.487	12.992	31.583	40.552	0.123	47.394	1.404	25.295	14.188	25.347	0.483
Fm	45.789	3.477	13.071	31.581	41.026	0.123	47.887	1.402	25.464	14.167	25.677	0.482
Md	46.200	3.475	13.144	31.544	41.541	0.123	48.367	1.398	25.659	14.133	25.996	0.479
No	46.630	3.465	13.229	31.467	42.022	0.123	48.855	1.396	25.834	14.102	26.326	0.478
Lr	47.052	3.460	13.304	31.442	42.526	0.121	49.340	1.393	26.023	14.071	26.644	0.475
– 104	47.484	3.452	13.387	31.394	43.013	0.121	49.822	1.391	26.204	14.041	26.977	0.475

Table 3. *Correspondence between theoretical and least-squares atomic scattering factors*

$\sin\theta/\lambda$		0·0	0·1	0·2	0·3	0·4	0·5	0·6	0·7
f (theoretical)		28·00	27·53	26·19	24·17	21·74	19·17	16·68	14·42
f (least squares)	$\varepsilon=0{\cdot}01$	28·00	27·53	26·19	24·17	21·74	19·17	16·68	14·42
	$\varepsilon=0{\cdot}09$	28·00	27·53	26·20	24·20	21·78	19·21	16·71	14·46
	$\varepsilon=1{\cdot}01$	28·00	27·53	26·22	24·26	21·94	19·51	17·20	15·12

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