6.1. Intensity of diffracted intensities

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6.1.1. X-ray scattering
(By E. N. Maslen, A. G. Fox, and M. A. O'Keefe)

6.1.1.1. *Coherent (Rayleigh) scattering*

An electromagnetic wave incident on a tightly bound electron is scattered coherently. For an incident wave of unit amplitude with the electric vector normal to the plane of the reflection $x0y$ containing the incident and diffracted beams (Fig. 6.1.1.1), the amplitude of the scattered wave at a distance r is

$$r_e/r, \tag{6.1.1.1}$$

where $r_e = (\mu_0/4\pi)(e^2/m)$ is the classical radius of the electron (2.818×10^{-15} m).

For a wave with the electric vector parallel to the plane $x0y$, the amplitude of the scattered wave is

$$\frac{r_e}{r}\cos 2\theta. \tag{6.1.1.2}$$

For unpolarized incident radiation with unit mean amplitude, the amplitude of the scattered wave is given by the Thomson formula

$$\frac{r_e}{r}\left\{\frac{1+\cos^2 2\theta}{2}\right\}^{1/2}. \tag{6.1.1.3}$$

The corresponding intensity of scattering per unit solid angle is

$$I_e = I_o r_e^2\left[\frac{1+\cos^2 2\theta}{2}\right] \tag{6.1.1.4}$$

for an unpolarized incident beam of intensity I_o.

6.1.1.2. *Incoherent (Compton) scattering*

For scattering from a free electron, the quantum nature of the radiation must be considered. Under the impact of a photon with energy hc/λ, momentum h/λ, the recoil of an electron, initially at rest, results in a change in wavelength of

$$\Delta\lambda = \frac{2h}{mc}\sin^2\theta, \tag{6.1.1.5}$$

a geometry similar to that in Fig. 6.1.1.1 being assumed. There is no fixed relationship between the phases of the incident and scattered beams – *i.e.* the scattering is incoherent. The intensity I_e predicted by the Thomson formula is modified by the correction factor $[\lambda/(\lambda+\Delta\lambda)]^3$.

6.1.1.3. *Atomic scattering factor*

For scattering by atomic electrons there are both coherent and incoherent components, with total intensity given by the Thomson formula. The phase for coherent scattering is by convention related to that of a free electron at the nucleus. There is a phase shift of π for scattering from a free electron. The scattering from an element of electron density $\rho(\mathbf{r}_j)$ has a phase difference of $i\mathbf{S}\cdot\mathbf{r}_j$, where

$$\mathbf{S} = 2\pi\mathbf{s}. \tag{6.1.1.6}$$

The total amplitude for coherent scattering from the jth electron is

$$f_j = \int \rho(\mathbf{r}_j)\exp(i\mathbf{S}\cdot\mathbf{r}_j)\,\mathrm{d}\mathbf{r}_j. \tag{6.1.1.7}$$

The intensity of coherent scattering is

$$I_{\rm coh} = I_e f_j^2. \tag{6.1.1.8}$$

The intensity of Compton scattering from that electron is

$$I_{\rm incoh} = I_e - I_{\rm coh} = I_e(1-f_j^2). \tag{6.1.1.9}$$

For an atom with atomic number Z,

$$I_{\rm coh} = I_e\left(\sum_{j=1}^{Z} f_j\right)^2 \tag{6.1.1.10}$$

and

$$I_{\rm incoh} = I_e\left(Z - f_j^2 - \sum_{j,k} f_{jk}\right), \tag{6.1.1.11}$$

where the correction term

$$f_{jk} = \int \psi_j^*\psi_k \exp(i\mathbf{S}\cdot\mathbf{r})\,\mathrm{d}\mathbf{r}, \tag{6.1.1.12}$$

owing to exchange, meets the requirements of the Pauli exclusion principle.

Atomic scattering factors for neutral atoms are listed in Table 6.1.1.1 for the range $0 < (\sin\theta)/\lambda < 6.0$ Å^{-1}. The values for hydrogen are calculated from the analytical solution to the Schrödinger equation and are effectively zero for $(\sin\theta)/\lambda > 1.5$ Å^{-1}. Those for heavier atoms are for relativistic wavefunctions, based on the calculations of Doyle & Turner (1968) using the wavefunctions of Coulthard (1967) (designated RHF in Table 6.1.1.1), or on those of Cromer & Waber (1968) using the wavefunctions of Mann (1968*a*) (designated *RHF). The latter are based on a more exact treatment of potential that allows for the finite size of the nucleus, but the effect on the scattering factors is small. The calculations of Cromer & Waber (1968) were originally made for $0 < (\sin\theta)/\lambda < 2.0$ Å^{-1}, but these have been extended to 6 Å^{-1} by Fox, O'Keefe & Tabbernor (1989); this has been done because there are increasing numbers of applications for high-angle scattering factors.

For a detailed study of the effect of changes in the electron density due to chemical bonding and lattice formation, a more general procedure is necessary, as described in Subsection 6.1.1.4. The changes due to chemical bonding are small in absolute terms, and are relatively small except in the case of hydrogen.

A more approximate treatment is adequate for many purposes. An isotropic approximation to the scattering factor for bonded hydrogen, based on an analysis of the hydrogen molecule by Stewart, Davidson & Simpson (1965), is listed in Table 6.1.1.2.

Scattering for ionic models of solids may be related to the scattering factors for the corresponding free ions. Values for

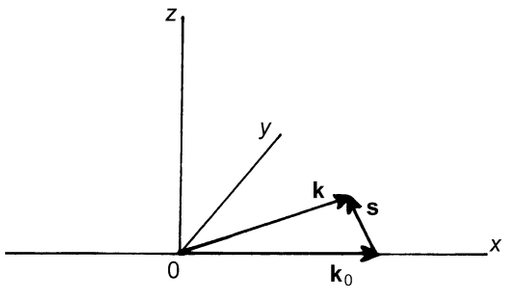

Fig. 6.1.1.1. Scattering by an electron. $\mathbf{k}_0$ and $\mathbf{k}$ are the incident and scattered wavevectors, respectively.

Table 6.1.1.1. *Mean atomic scattering factors in electrons for free atoms*

Methods: E: exact; RHF, *RHF (see text): relativistic Hartree–Fock.

Element	H	He	Li	Be	B	C	N	O	F	Ne
Z	1	2	3	4	5	6	7	8	9	10
Method	E	RHF	RHF	RHF	RHF	RHF	RHF	RHF	RHF	RHF
$(\sin\theta)/\lambda$ (Å^{-1})										
0.00	1.000	2.000	3.000	4.000	5.000	6.000	7.000	8.000	9.000	10.000
0.01	0.998	1.998	2.986	3.987	4.988	5.990	6.991	7.992	8.993	9.993
0.02	0.991	1.993	2.947	3.950	4.954	5.958	6.963	7.967	8.970	9.973
0.03	0.980	1.984	2.884	3.889	4.897	5.907	6.918	7.926	8.933	9.938
0.04	0.966	1.972	2.802	3.807	4.820	5.837	6.855	7.869	8.881	9.891
0.05	0.947	1.957	2.708	3.707	4.724	5.749	6.776	7.798	8.815	9.830
0.06	0.925	1.939	2.606	3.592	4.613	5.645	6.682	7.712	8.736	9.757
0.07	0.900	1.917	2.502	3.468	4.488	5.526	6.574	7.612	8.645	9.672
0.08	0.872	1.893	2.400	3.336	4.352	5.396	6.453	7.501	8.541	9.576
0.09	0.842	1.866	2.304	3.201	4.209	5.255	6.321	7.378	8.427	9.469
0.10	0.811	1.837	2.215	3.065	4.060	5.107	6.180	7.245	8.302	9.351
0.11	0.778	1.806	2.135	2.932	3.908	4.952	6.030	7.103	8.168	9.225
0.12	0.744	1.772	2.065	2.804	3.756	4.794	5.875	6.954	8.026	9.090
0.13	0.710	1.737	2.004	2.683	3.606	4.633	5.714	6.798	7.876	8.948
0.14	0.676	1.701	1.950	2.569	3.459	4.472	5.551	6.637	7.721	8.799
0.15	0.641	1.663	1.904	2.463	3.316	4.311	5.385	6.472	7.560	8.643
0.16	0.608	1.624	1.863	2.365	3.179	4.153	5.218	6.304	7.395	8.483
0.17	0.574	1.584	1.828	2.277	3.048	3.998	5.051	6.134	7.226	8.318
0.18	0.542	1.543	1.796	2.197	2.924	3.847	4.886	5.964	7.055	8.150
0.19	0.511	1.502	1.768	2.125	2.808	3.701	4.723	5.793	6.883	7.978
0.20	0.481	1.460	1.742	2.060	2.699	3.560	4.563	5.623	6.709	7.805
0.22	0.424	1.377	1.693	1.951	2.503	3.297	4.254	5.289	6.362	7.454
0.24	0.373	1.295	1.648	1.864	2.336	3.058	3.963	4.965	6.020	7.102
0.25	0.350	1.254	1.626	1.828	2.263	2.949	3.825	4.808	5.851	6.928
0.26	0.328	1.214	1.604	1.795	2.195	2.846	3.693	4.655	5.685	6.754
0.28	0.287	1.136	1.559	1.739	2.077	2.658	3.445	4.363	5.363	6.412
0.30	0.251	1.060	1.513	1.692	1.979	2.494	3.219	4.089	5.054	6.079
0.32	0.220	0.988	1.465	1.652	1.897	2.351	3.014	3.834	4.761	5.758
0.34	0.193	0.920	1.417	1.616	1.829	2.227	2.831	3.599	4.484	5.451
0.35	0.180	0.887	1.393	1.600	1.799	2.171	2.747	3.489	4.353	5.302
0.36	0.169	0.856	1.369	1.583	1.771	2.120	2.667	3.383	4.225	5.158
0.38	0.148	0.795	1.320	1.551	1.723	2.028	2.522	3.186	3.983	4.880
0.40	0.130	0.738	1.270	1.520	1.681	1.948	2.393	3.006	3.759	4.617
0.42	0.115	0.686	1.221	1.489	1.644	1.880	2.278	2.844	3.551	4.370
0.44	0.101	0.636	1.173	1.458	1.611	1.821	2.178	2.697	3.360	4.139
0.45	0.095	0.613	1.149	1.443	1.596	1.794	2.132	2.629	3.270	4.029
0.46	0.090	0.591	1.125	1.427	1.581	1.770	2.089	2.564	3.183	3.923
0.48	0.079	0.548	1.078	1.395	1.553	1.725	2.011	2.445	3.022	3.722
0.50	0.071	0.509	1.033	1.362	1.526	1.685	1.942	2.338	2.874	3.535
0.55	0.053	0.423	0.924	1.279	1.463	1.603	1.802	2.115	2.559	3.126
0.60	0.040	0.353	0.823	1.195	1.402	1.537	1.697	1.946	2.309	2.517
0.65	0.031	0.295	0.732	1.112	1.339	1.479	1.616	1.816	2.112	2.517
0.70	0.024	0.248	0.650	1.030	1.276	1.426	1.551	1.714	1.956	2.296
0.80	0.015	0.177	0.512	0.876	1.147	1.322	1.445	1.568	1.735	1.971
0.90	0.010	0.129	0.404	0.740	1.020	1.219	1.353	1.463	1.588	1.757
1.00	0.007	0.095	0.320	0.622	0.900	1.114	1.265	1.377	1.482	1.609
1.10	0.005	0.072	0.255	0.522	0.790	1.012	1.172	1.298	1.398	1.502
1.20	0.003	0.055	0.205	0.439	0.690	0.914	1.090	1.221	1.324	1.418
1.30	0.003	0.042	0.165	0.369	0.602	0.822	1.004	1.145	1.254	1.346
1.40	0.002	0.033	0.134	0.311	0.524	0.736	0.921	1.070	1.186	1.280
1.50	0.001	0.026	0.110	0.263	0.457	0.659	0.843	0.997	1.120	1.218
1.60		0.021	0.091	0.223	0.398	0.588	0.769	0.926	1.055	1.158
1.70		0.017	0.075	0.190	0.347	0.525	0.700	0.857	0.990	1.099
1.80		0.014	0.063	0.163	0.304	0.468	0.636	0.792	0.928	1.041
1.90		0.011	0.053	0.139	0.266	0.418	0.578	0.731	0.868	0.984
2.00		0.010	0.044	0.120	0.233	0.373	0.525	0.674	0.810	0.929
2.50		0.004	0.021	0.060	0.126	0.216	0.324	0.443	0.564	0.680
3.00		0.002	0.011	0.033	0.072	0.130	0.204	0.292	0.389	0.489
3.50		0.001	0.006	0.019	0.043	0.081	0.132	0.196	0.270	0.331
4.00		0.001	0.004	0.012	0.027	0.053	0.088	0.134	0.190	0.254
5.00			0.002	0.005	0.012	0.025	0.043	0.067	0.099	0.137
6.00			0.001	0.003	0.006	0.013	0.023	0.037	0.055	0.079

Table 6.1.1.1. *Mean atomic scattering factors for free atoms (cont.)*

Element	Na	Mg	Al	Si	P	S	Cl	Ar	K	Ca
Z	11	12	13	14	15	16	17	18	19	20
Method	RHF	RHF	RHF	RHF	RHF	RHF	RHF	RHF	RHF	RHF
$(\sin\theta)/\lambda$ (Å^{-1})										
0.00	11.000	12.000	13.000	14.000	15.000	16.000	17.000	18.000	19.000	20.000
0.01	10.980	11.978	12.976	13.976	14.977	15.979	16.980	17.981	18.963	19.959
0.02	10.922	11.914	12.903	13.904	14.909	15.915	16.919	17.924	18.854	19.838
0.03	10.830	11.811	12.786	13.787	14.798	15.809	16.820	17.830	18.683	19.645
0.04	10.709	11.674	12.629	13.628	14.646	15.665	16.683	17.700	18.462	19.392
0.05	10.568	11.507	12.439	13.434	14.458	15.484	16.511	17.536	18.204	19.091
0.06	10.412	11.319	12.222	13.209	14.237	15.271	16.306	17.340	17.924	18.758
0.07	10.249	11.116	11.987	12.961	13.990	15.030	16.073	17.116	17.630	18.405
0.08	10.084	10.903	11.739	12.695	13.721	14.764	15.814	16.865	17.332	18.045
0.09	9.920	10.687	11.485	12.417	13.435	14.478	15.533	16.591	17.032	17.685
0.10	9.760	10.472	11.230	12.134	13.138	14.177	15.234	16.298	16.733	17.331
0.11	9.605	10.262	10.978	11.849	12.834	13.865	14.921	15.988	16.436	16.987
0.12	9.455	10.059	10.733	11.567	12.527	13.546	14.597	15.665	16.138	16.655
0.13	9.309	9.864	10.498	11.292	12.223	13.224	14.266	15.331	15.841	16.334
0.14	9.166	9.678	10.273	11.025	11.922	12.902	13.932	14.991	15.543	16.024
0.15	9.027	9.502	10.059	10.769	11.629	12.583	13.597	14.647	15.243	15.723
0.16	8.888	9.334	9.857	10.525	11.345	12.270	13.263	14.301	14.941	15.430
0.17	8.751	9.175	9.667	10.293	11.072	11.964	12.934	13.957	14.638	15.142
0.18	8.613	9.023	9.487	10.074	10.811	11.668	12.611	13.615	14.334	14.859
0.19	8.475	8.876	9.318	9.868	10.563	11.382	12.297	13.279	14.031	14.580
0.20	8.335	8.735	9.158	9.673	10.327	11.109	11.991	12.949	13.728	14.304
0.22	8.052	8.465	8.862	9.319	9.894	10.598	11.413	12.315	13.130	13.760
0.24	7.764	8.205	8.592	9.004	9.510	10.138	10.881	11.721	12.550	13.225
0.25	7.618	8.078	8.465	8.859	9.335	9.927	10.633	11.441	12.268	12.961
0.26	7.471	7.951	8.341	8.722	9.170	9.727	10.398	11.172	11.994	12.701
0.28	7.176	7.698	8.103	8.467	8.869	9.363	9.964	10.671	11.468	12.194
0.30	6.881	7.446	7.873	8.231	8.600	9.039	9.576	10.216	10.977	11.705
0.32	6.588	7.194	7.648	8.011	8.357	8.752	9.231	9.807	10.521	11.240
0.34	6.298	6.943	7.426	7.800	8.134	8.494	8.923	9.441	10.103	10.800
0.35	6.156	6.817	7.316	7.698	8.029	8.376	8.782	9.272	9.908	10.590
0.36	6.015	6.691	7.205	7.597	7.928	8.262	8.649	9.113	9.722	10.388
0.38	5.739	6.442	6.985	7.398	7.733	8.051	8.403	8.820	9.375	10.004
0.40	5.471	6.194	6.766	7.202	7.547	7.856	8.181	8.558	9.061	9.650
0.42	5.214	5.951	6.548	7.008	7.367	7.673	7.979	8.322	8.778	9.324
0.44	4.967	5.712	6.330	6.815	7.190	7.501	7.794	8.110	8.522	9.025
0.45	4.848	5.595	6.222	6.719	7.103	7.417	7.706	8.011	8.403	8.885
0.46	4.731	5.480	6.115	6.622	7.017	7.335	7.621	7.917	8.290	8.752
0.48	4.506	5.253	5.902	6.431	6.845	7.174	7.459	7.739	8.080	8.502
0.50	4.293	5.034	5.692	6.240	6.674	7.017	7.305	7.575	7.889	8.275
0.55	3.811	4.520	5.186	5.769	6.250	6.633	6.941	7.207	7.474	7.788
0.60	3.398	4.059	4.713	5.312	5.829	6.254	6.595	6.875	7.125	7.392
0.65	3.048	3.652	4.277	4.878	5.418	5.877	6.254	6.560	6.814	7.057
0.70	2.754	3.297	3.883	4.470	5.020	5.505	5.915	6.252	6.523	6.762
0.80	2.305	2.729	3.221	3.750	4.284	4.790	5.245	5.639	5.961	6.228
0.90	1.997	2.317	2.712	3.164	3.649	4.138	4.607	5.036	5.406	5.717
1.00	1.784	2.022	2.330	2.702	3.122	3.570	4.023	4.460	4.859	5.209
1.10	1.634	1.812	2.049	2.346	2.698	3.092	3.509	3.931	4.337	4.710
1.20	1.524	1.660	1.841	2.076	2.364	2.699	3.070	3.462	3.855	4.233
1.30	1.438	1.546	1.687	1.872	2.104	2.384	2.704	3.056	3.423	3.791
1.40	1.367	1.459	1.571	1.717	1.903	2.133	2.405	2.713	3.045	3.391
1.50	1.304	1.387	1.481	1.598	1.747	1.935	2.162	2.427	2.722	3.039
1.60	1.247	1.326	1.408	1.505	1.626	1.779	1.967	2.192	2.450	2.733
1.70	1.191	1.270	1.346	1.430	1.530	1.655	1.811	2.000	2.221	2.470
1.80	1.137	1.219	1.292	1.367	1.453	1.557	1.686	1.844	2.033	2.250
1.90	1.084	1.169	1.243	1.313	1.389	1.477	1.585	1.717	1.876	2.063
2.00	1.032	1.120	1.195	1.264	1.333	1.411	1.502	1.614	1.748	1.908
2.50	0.791	0.892	0.979	1.056	1.122	1.182	1.240	1.301	1.367	1.444
3.00	0.591	0.691	0.783	0.867	0.942	1.009	1.069	1.123	1.174	1.225
3.50	0.438	0.527	0.615	0.699	0.777	0.849	0.915	0.974	1.028	1.078
4.00	0.325	0.401	0.478	0.566	0.632	0.705	0.773	0.836	0.895	0.949
5.00	0.183	0.234	0.290	0.349	0.411	0.474	0.536	0.597	0.657	0.715
6.00	0.107	0.141	0.179	0.222	0.268	0.316	0.367	0.419	0.472	0.524

Table 6.1.1.1. *Mean atomic scattering factors for free atoms (cont.)*

Element	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
Z	21	22	23	24	25	26	27	28	29	30
Method	RHF	RHF	RHF	RHF	RHF	RHF	RHF	RHF	RHF	RHF
$(\sin\theta)/\lambda$ (Å^{-1})										
0.00	21.000	22.000	23.000	24.000	25.000	26.000	27.000	28.000	29.000	30.000
0.01	20.962	21.964	22.966	23.971	24.969	25.970	26.972	27.973	28.977	29.975
0.02	20.848	21.856	22.864	23.885	24.876	25.882	26.887	27.892	28.908	29.900
0.03	20.665	21.682	22.698	23.746	24.726	25.738	26.749	27.759	28.794	29.777
0.04	20.422	21.451	22.477	23.558	24.523	25.543	26.562	27.579	28.640	29.609
0.05	20.131	21.171	22.208	23.329	24.274	25.304	26.331	27.356	28.448	29.401
0.06	19.805	20.854	21.902	23.065	23.988	25.026	26.063	27.096	28.223	29.157
0.07	19.455	20.511	21.567	22.772	23.671	24.719	25.764	26.806	27.971	28.883
0.08	19.091	20.150	21.212	22.459	23.331	24.387	25.440	26.490	27.694	28.583
0.09	18.723	19.781	20.846	22.129	22.976	24.038	25.098	26.156	27.397	28.263
0.10	18.356	19.410	20.474	21.789	22.611	23.678	24.744	25.807	27.084	27.927
0.11	17.995	19.041	20.102	21.441	22.240	23.310	24.380	25.448	26.758	27.579
0.12	17.643	18.678	19.733	21.089	21.868	22.939	24.011	25.083	26.422	27.222
0.13	17.301	18.322	19.369	20.734	21.497	22.568	23.641	24.714	26.077	26.859
0.14	16.968	17.974	19.011	20.378	21.128	22.197	23.270	24.344	25.726	26.492
0.15	16.645	17.635	18.661	20.022	20.764	21.829	22.900	23.973	25.370	26.124
0.16	16.330	17.304	18.317	19.667	20.404	21.465	22.533	23.604	25.009	25.754
0.17	16.023	16.980	17.980	19.312	20.049	21.104	22.168	23.237	24.645	25.385
0.18	15.722	16.663	17.649	18.960	19.699	20.748	21.806	22.872	24.278	25.017
0.19	15.426	16.351	17.323	18.609	19.354	20.395	21.448	22.510	23.910	24.649
0.20	15.135	16.044	17.003	18.260	19.012	20.046	21.093	22.150	23.540	24.283
0.22	14.564	15.444	16.376	17.570	18.342	19.359	20.393	21.438	22.798	23.556
0.24	14.006	14.859	15.765	16.893	17.686	18.685	19.704	20.737	22.057	22.836
0.25	13.732	14.572	15.465	16.561	17.364	18.354	19.364	20.390	21.687	22.478
0.26	13.462	14.289	15.169	16.232	17.045	18.025	19.027	20.046	21.319	22.122
0.28	12.933	13.735	14.589	15.588	16.417	17.378	18.361	19.365	20.589	21.417
0.30	12.423	13.198	14.026	14.965	15.806	16.744	17.709	18.696	19.869	20.720
0.32	11.934	12.682	13.482	14.365	15.211	16.127	17.072	18.040	19.162	20.034
0.34	11.467	12.187	12.959	13.790	14.634	15.527	16.450	17.398	18.472	19.359
0.35	11.244	11.949	12.705	13.513	14.353	15.233	16.145	17.084	18.133	19.027
0.36	11.027	11.717	12.458	13.242	14.078	14.945	15.845	16.773	17.799	18.698
0.38	10.613	11.271	11.982	12.720	13.543	14.384	15.260	16.165	17.145	18.051
0.40	10.226	10.852	11.530	12.227	13.031	13.845	14.695	15.576	16.514	17.421
0.42	9.866	10.459	11.105	11.762	12.543	13.328	14.151	15.008	15.904	16.809
0.44	9.534	10.093	10.705	11.326	12.080	12.835	13.630	14.461	15.318	16.216
0.45	9.377	9.920	10.515	11.118	11.858	12.598	13.379	14.196	15.034	15.926
0.46	9.227	9.753	10.332	10.917	11.642	12.367	13.133	13.937	14.757	15.642
0.48	8.946	9.438	9.984	10.536	11.228	11.922	12.659	13.435	14.219	15.090
0.50	8.687	9.148	9.660	10.180	10.840	11.502	12.209	12.956	13.707	14.559
0.55	8.132	8.518	8.952	9.400	9.973	10.557	11.188	11.862	12.533	13.328
0.60	7.682	8.007	8.373	8.756	9.245	9.753	10.309	10.909	11.507	12.235
0.65	7.312	7.588	7.898	8.227	8.639	9.077	9.561	10.090	10.621	11.276
0.70	6.996	7.240	7.506	7.791	8.137	8.512	8.930	9.392	9.861	10.442
0.80	6.460	6.676	6.892	7.118	7.368	7.645	7.955	8.301	8.663	9.108
0.90	5.975	6.200	6.406	6.606	6.808	7.023	7.259	7.519	7.799	8.132
1.00	5.501	5.752	5.972	6.172	6.359	6.545	6.738	6.944	7.166	7.417
1.10	5.030	5.310	5.553	5.768	5.962	6.143	6.318	6.495	6.681	6.879
1.20	4.570	4.872	5.139	5.372	5.586	5.775	5.950	6.118	6.285	6.453
1.30	4.131	4.445	4.730	4.982	5.215	5.420	5.601	5.776	5.939	6.096
1.40	3.722	4.038	4.333	4.597	4.849	5.070	5.270	5.451	5.617	5.775
1.50	3.352	3.660	3.956	4.226	4.490	4.725	4.939	5.133	5.308	5.473
1.60	3.023	3.316	3.604	3.874	4.144	4.388	4.611	4.819	5.005	5.180
1.70	2.733	3.006	3.281	3.545	3.814	4.062	4.295	4.511	4.705	4.892
1.80	2.485	2.734	2.992	3.244	3.506	3.753	3.989	4.211	4.413	4.610
1.90	2.271	2.496	2.733	2.971	3.221	3.463	3.697	3.922	4.128	4.332
2.00	2.090	2.290	2.506	2.727	2.963	3.195	3.424	3.647	3.855	4.063
2.50	1.533	1.637	1.756	1.888	2.037	2.197	2.366	2.543	2.721	2.908
3.00	1.279	1.338	1.404	1.479	1.563	1.658	1.763	1.878	2.001	2.135
3.50	1.125	1.171	1.217	1.266	1.319	1.377	1.441	1.512	1.590	1.677
4.00	0.998	1.044	1.087	1.129	1.171	1.213	1.258	1.306	1.358	1.414
5.00	0.770	0.821	0.869	0.914	0.956	0.995	1.033	1.069	1.105	1.140
6.00	0.577	0.627	0.677	0.724	0.769	0.813	0.853	0.892	0.929	0.964

Table 6.1.1.1. *Mean atomic scattering factors for free atoms (cont.)*

Element	Ga	Ge	As	Se	Br	Kr	Rb	Sr	Y	Zr
Z	31	32	33	34	35	36	37	38	39	40
Method	RHF	RHF	RHF	RHF	RHF	RHF	RHF	RHF	*RHF	*RHF
$(\sin\theta)/\lambda$ (Å^{-1})										
0.00	31.000	32.000	33.000	34.000	35.000	36.000	37.000	38.000	39.000	40.000
0.01	30.971	31.970	32.970	33.970	34.971	35.972	36.952	37.946	38.947	39.949
0.02	30.883	31.878	32.879	33.881	34.883	35.886	36.809	37.786	38.792	39.800
0.03	30.740	31.729	32.730	33.734	34.739	35.744	36.583	37.532	38.543	39.559
0.04	30.546	31.526	32.527	33.532	34.540	35.549	36.291	37.197	38.212	39.237
0.05	30.308	31.276	32.274	33.280	34.291	35.304	35.948	36.802	37.816	38.847
0.06	30.031	30.984	31.977	32.982	33.995	35.011	35.571	36.363	37.369	38.403
0.07	29.724	30.657	31.642	32.645	33.658	34.677	35.171	35.897	36.889	37.921
0.08	29.391	30.302	31.276	32.273	33.284	34.305	34.758	35.418	36.387	37.412
0.09	29.040	29.926	30.884	31.872	32.880	33.899	34.336	34.937	35.876	36.887
0.10	28.675	29.534	30.473	31.449	32.450	33.467	33.907	34.458	35.364	36.356
0.11	28.302	29.133	30.049	31.009	32.000	33.011	33.473	33.986	34.855	35.824
0.12	27.924	28.725	29.616	30.557	31.535	32.537	33.034	33.522	34.354	35.296
0.13	27.543	28.316	29.179	30.099	31.060	32.051	32.588	33.066	33.861	34.775
0.14	27.162	27.908	28.742	29.637	30.578	31.555	32.137	32.616	33.378	34.262
0.15	26.783	27.504	28.307	29.175	30.095	31.055	31.681	32.171	32.904	33.758
0.16	26.406	27.104	27.877	28.718	29.613	30.553	31.220	31.730	32.437	33.263
0.17	26.033	26.709	27.454	28.266	29.136	30.053	30.757	31.292	31.977	32.776
0.18	25.663	26.322	27.039	27.822	28.664	29.558	30.293	30.856	31.523	32.298
0.19	25.297	25.941	26.633	27.387	28.202	29.070	29.830	30.421	31.075	31.827
0.20	24.935	25.567	26.235	26.962	27.749	28.590	29.368	29.988	30.631	31.363
0.22	24.121	24.839	25.469	26.145	26.876	27.663	28.459	29.128	29.758	30.454
0.24	23.520	24.135	24.739	25.372	26.052	26.784	27.576	28.280	28.904	29.572
0.25	23.174	23.791	24.386	25.001	25.658	26.364	27.148	27.863	28.485	29.141
0.26	22.830	23.452	24.041	24.641	25.276	25.957	26.729	27.452	28.071	28.716
0.28	22.151	22.787	23.370	23.947	24.545	25.181	25.922	26.648	27.263	27.889
0.30	21.481	22.136	22.724	23.288	23.857	24.453	25.158	25.875	26.483	27.092
0.32	20.820	21.498	22.097	22.656	23.206	23.771	24.437	25.135	25.734	26.327
0.34	20.169	20.870	21.486	22.048	22.587	23.128	23.758	24.430	25.018	25.596
0.35	19.847	20.560	21.185	21.751	22.288	22.820	23.432	24.090	24.673	25.243
0.36	19.527	20.253	20.888	21.459	21.995	22.520	23.116	23.760	24.336	24.899
0.38	18.897	19.645	20.301	20.887	21.425	21.941	22.510	23.125	23.687	24.236
0.40	18.278	19.047	19.725	20.328	20.874	21.388	21.934	22.522	23.071	23.606
0.42	17.673	18.459	19.159	19.780	20.338	20.855	21.386	21.950	22.485	23.008
0.44	17.083	17.882	18.602	19.242	19.816	20.339	20.860	21.404	21.928	22.439
0.45	16.794	17.598	18.326	18.977	19.558	20.087	20.605	21.141	21.660	22.166
0.46	16.508	17.317	18.054	18.713	19.304	19.838	20.354	20.883	21.398	21.899
0.48	15.950	16.765	17.516	18.193	18.801	19.349	19.866	20.383	20.890	21.384
0.50	15.410	16.227	16.989	17.682	18.307	18.870	19.391	19.902	20.404	20.892
0.55	14.142	14.947	15.721	16.444	17.107	17.709	18.252	18.764	19.263	19.745
0.60	12.996	13.770	14.535	15.269	15.958	16.594	17.167	17.696	18.204	18.693
0.65	11.974	12.702	13.440	14.166	14.865	15.524	16.125	16.678	17.203	17.706
0.70	11.073	11.745	12.442	13.145	13.837	14.504	15.126	15.702	16.246	16.767
0.80	9.604	10.151	10.741	11.362	12.001	12.645	13.272	13.872	14.443	14.996
0.90	8.510	8.937	9.411	9.928	10.480	11.057	11.645	12.230	12.798	13.361
1.00	7.702	8.028	8.396	8.809	9.262	9.752	10.270	10.806	11.339	11.883
1.10	7.099	7.348	7.631	7.952	8.312	8.711	9.147	9.612	10.088	10.588
1.20	6.633	6.830	7.050	7.299	7.580	7.898	8.252	8.640	9.046	9.486
1.30	6.254	6.419	6.597	6.795	7.016	7.266	7.548	7.863	8.200	8.574
1.40	5.926	6.076	6.231	6.395	6.574	6.773	6.996	7.249	7.523	7.833
1.50	5.627	5.774	5.917	6.063	6.216	6.380	6.562	6.764	6.985	7.238
1.60	5.342	5.493	5.636	5.775	5.913	6.056	6.210	6.376	6.554	6.760
1.70	5.065	5.224	5.372	5.511	5.645	5.778	5.913	6.055	6.205	6.375
1.80	4.792	4.961	5.117	5.262	5.398	5.528	5.656	5.785	5.914	6.059
1.90	4.523	4.702	4.867	5.020	5.162	5.295	5.420	5.544	5.662	5.790
2.00	4.260	4.447	4.621	4.782	4.932	5.071	5.200	5.323	5.440	5.558
2.50	3.097	3.287	3.475	3.658	3.836	4.007	4.168	4.320	4.460	4.590
3.00	2.277	2.428	2.584	2.745	2.909	3.074	3.239	3.401	3.560	3.720
3.50	1.772	1.876	1.988	2.108	2.235	2.369	2.507	2.649	2.780	2.920
4.00	1.477	1.545	1.621	1.703	1.793	1.890	1.993	2.103	2.215	2.335
5.00	1.176	1.213	1.251	1.292	1.337	1.384	1.436	1.493	1.550	1.620
6.00	0.998	1.030	1.061	1.092	1.123	1.154	1.186	1.219	1.250	1.285

Table 6.1.1.1. *Mean atomic scattering factors for free atoms (cont.)*

Element	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn
Z	41	42	43	44	45	46	47	48	49	50
Method	*RHF	RHF	*RHF	*RHF	*RHF	*RHF	RHF	RHF	RHF	RHF
$(\sin\theta)/\lambda$ (Å^{-1})										
0.00	41.000	42.000	43.000	44.000	45.000	46.000	47.000	48.000	49.000	50.000
0.01	40.956	41.958	42.955	43.960	44.961	45.968	46.964	47.962	48.957	49.955
0.02	40.824	41.831	42.821	43.842	44.847	45.874	46.857	47.848	48.828	49.821
0.03	40.610	41.625	42.603	43.649	44.660	45.718	46.681	47.660	48.618	49.601
0.04	40.323	41.346	42.308	43.386	44.405	45.503	46.440	47.404	48.332	49.303
0.05	39.970	41.003	41.945	43.061	44.088	45.232	46.139	47.085	47.980	48.934
0.06	39.565	40.606	41.526	42.681	43.717	44.908	45.786	46.710	47.570	48.504
0.07	39.116	40.164	41.059	42.254	43.299	44.535	45.385	46.287	47.112	48.022
0.08	38.634	39.686	40.557	41.789	42.842	44.119	44.944	45.822	46.614	47.498
0.09	38.128	39.181	40.028	41.292	42.351	43.663	44.469	45.324	46.086	46.942
0.10	37.606	38.656	39.480	40.770	41.834	43.172	43.964	44.797	45.534	46.361
0.11	37.073	38.117	38.921	40.229	41.296	42.651	43.435	44.248	44.964	45.764
0.12	36.535	37.569	38.355	39.674	40.741	42.105	42.886	43.683	44.383	45.155
0.13	35.994	37.016	37.787	39.108	40.173	41.538	42.322	43.104	43.793	44.541
0.14	35.454	36.461	37.221	38.536	39.597	40.954	41.744	42.517	43.199	43.924
0.15	34.916	35.907	36.658	37.959	39.015	40.357	41.157	41.923	42.603	43.309
0.16	34.382	35.355	36.100	37.381	38.429	39.750	40.563	41.325	42.006	42.696
0.17	33.854	34.806	35.548	36.803	37.841	39.137	39.964	40.726	41.410	42.088
0.18	33.331	34.263	35.003	36.228	37.254	38.520	39.361	40.126	40.817	41.486
0.19	32.814	33.725	34.466	35.655	36.668	37.902	38.758	39.527	40.226	40.891
0.20	32.305	33.195	33.936	35.088	36.086	37.286	38.154	38.930	39.639	40.302
0.22	31.310	32.157	32.900	33.971	34.937	36.064	36.955	37.746	38.478	39.145
0.24	30.348	31.153	31.897	32.886	33.815	34.868	35.774	36.581	37.337	38.016
0.25	29.881	30.665	31.409	32.356	33.267	34.283	35.192	36.007	36.774	37.462
0.26	29.424	30.188	30.930	31.837	32.728	33.708	34.619	35.440	36.218	36.915
0.28	28.538	29.263	29.998	30.829	31.680	32.592	33.498	34.329	35.125	35.841
0.30	27.692	28.382	29.104	29.866	30.675	31.523	32.416	33.251	34.059	34.794
0.32	26.888	27.543	28.250	28.949	29.717	30.505	31.378	32.210	33.025	33.775
0.34	26.126	26.749	27.435	28.079	28.807	29.540	30.387	31.210	32.025	32.786
0.35	25.760	26.368	27.042	27.662	28.370	29.077	29.910	30.725	31.538	32.303
0.36	25.404	25.998	26.660	27.257	27.944	28.628	29.444	30.252	31.060	31.828
0.38	24.721	25.289	25.925	26.480	27.130	27.769	28.551	29.338	30.134	30.902
0.40	24.077	24.620	25.229	25.749	26.363	26.961	27.707	28.468	29.247	30.011
0.42	23.468	23.989	24.571	25.062	25.642	26.202	26.911	27.644	28.401	29.154
0.44	22.892	23.394	23.949	24.415	24.964	25.491	26.163	26.865	27.596	28.334
0.45	22.615	23.109	23.651	24.106	24.640	25.153	25.805	26.492	27.209	27.938
0.46	22.346	22.832	23.361	23.807	24.327	24.825	25.459	26.129	26.832	27.551
0.48	21.829	22.300	22.806	23.235	23.729	24.201	24.800	25.436	26.108	26.805
0.50	21.336	21.796	22.280	22.696	23.167	23.617	24.181	24.784	25.425	26.096
0.55	20.195	20.638	21.080	21.476	21.900	22.307	22.795	23.320	23.881	24.482
0.60	19.156	19.595	20.012	20.403	20.798	21.177	21.607	22.063	22.552	23.081
0.65	18.187	18.635	19.042	19.438	19.820	20.186	20.575	20.978	21.405	21.868
0.70	17.268	17.732	18.142	18.551	18.932	19.296	19.661	20.027	20.408	20.815
0.80	15.533	16.036	16.477	16.922	17.326	17.711	18.069	18.405	18.736	19.073
0.90	13.915	14.448	14.925	15.405	15.845	16.266	16.651	17.000	17.329	17.646
1.00	12.427	12.968	13.466	13.968	14.440	14.893	15.316	15.698	16.053	16.384
1.10	11.098	11.621	12.116	12.620	13.107	13.580	14.035	14.451	14.840	15.201
1.20	9.945	10.430	10.900	11.385	11.866	12.342	12.813	13.253	13.670	14.062
1.30	8.972	9.404	9.833	10.282	10.740	11.200	11.669	12.116	12.548	12.962
1.40	8.169	8.542	8.919	9.323	9.743	10.173	10.623	11.060	11.492	11.913
1.50	7.516	7.831	8.154	8.506	8.880	9.270	9.687	10.101	10.518	10.933
1.60	6.969	7.251	7.521	7.823	8.148	8.492	8.869	9.249	9.639	10.034
1.70	6.564	6.780	7.004	7.258	7.535	7.833	8.165	8.505	8.860	9.227
1.80	6.216	6.397	6.582	6.794	7.028	7.282	7.569	7.867	8.184	8.516
1.90	5.927	6.080	6.234	6.412	6.608	6.824	7.069	7.326	7.603	7.897
2.00	5.680	5.813	5.946	6.097	6.262	6.443	6.651	6.871	7.110	7.367
2.50	4.710	4.827	4.930	5.040	5.140	5.240	5.351	5.461	5.577	5.702
3.00	3.860	3.988	4.110	4.230	4.350	4.460	4.566	4.665	4.761	4.853
3.50	3.065	3.217	3.350	3.485	3.620	3.740	3.862	3.977	4.087	4.192
4.00	2.405	2.581	2.690	2.820	2.940	3.080	3.207	3.330	3.449	3.565
5.00	1.690	1.766	1.840	1.925	2.012	2.100	2.206	2.304	2.406	2.509
6.00	1.327	1.373	1.420	1.470	1.520	1.575	1.635	1.698	1.746	1.835

Table 6.1.1.1. *Mean atomic scattering factors for free atoms (cont.)*

Element	Sb	Te	I	Xe	Cs	Ba	La	Ce	Pr	Nd
Z	51	52	53	54	55	56	57	58	59	60
Method	RHF	*RHF	RHF	RHF	RHF	RHF	*RHF	*RHF	*RHF	*RHF
$(\sin\theta)/\lambda$ (Å^{-1})										
0.00	51.000	52.000	53.000	54.000	55.000	56.000	57.000	58.000	59.000	60.000
0.01	50.955	51.954	52.955	53.956	54.932	55.925	56.926	57.928	58.929	59.931
0.02	50.819	51.818	52.820	53.821	54.732	55.703	56.708	57.715	58.722	59.728
0.03	50.596	51.594	52.597	53.601	54.417	55.350	56.360	57.375	58.392	59.404
0.04	50.293	51.288	52.292	53.297	54.008	54.888	55.900	56.924	57.956	58.977
0.05	49.915	50.906	51.911	52.917	53.527	54.345	55.351	56.385	57.439	58.468
0.06	49.474	50.458	51.460	52.467	52.996	53.743	54.736	55.779	56.861	57.899
0.07	48.977	49.951	50.950	51.954	52.430	53.106	54.076	55.127	56.242	57.288
0.08	48.434	49.395	50.387	51.388	51.839	52.450	53.388	54.446	55.599	56.651
0.09	47.856	48.800	49.781	50.775	51.229	51.786	52.687	53.750	54.943	56.000
0.10	47.250	48.174	49.142	50.125	50.603	51.122	51.982	53.047	54.281	55.342
0.11	46.625	47.526	48.476	49.447	49.963	50.460	51.278	52.345	53.617	54.680
0.12	45.988	46.863	47.793	48.747	49.309	49.802	50.580	51.646	52.952	54.017
0.13	45.344	46.193	47.099	48.033	48.645	49.146	49.888	50.952	52.288	53.354
0.14	44.699	45.519	46.400	47.311	47.971	48.492	49.202	50.263	51.623	52.689
0.15	44.056	44.848	45.702	46.588	47.291	47.839	48.523	49.579	50.957	52.022
0.16	43.419	44.182	45.008	45.868	46.606	47.186	47.849	48.901	50.289	51.353
0.17	42.789	43.526	44.323	45.155	45.921	46.533	47.182	48.227	49.620	50.682
0.18	42.168	42.879	43.648	44.453	45.237	45.882	46.519	47.557	48.950	50.009
0.19	41.556	42.245	42.987	43.763	44.559	45.232	45.862	46.892	48.280	49.334
0.20	40.955	41.623	42.340	43.088	43.888	44.586	45.212	46.233	47.610	48.660
0.22	39.783	40.419	41.091	41.788	42.578	43.309	43.932	44.933	46.278	47.317
0.24	38.652	39.267	39.904	40.557	41.320	42.064	42.686	43.663	44.967	45.989
0.25	38.100	38.709	39.333	39.967	40.713	41.456	42.078	43.042	44.323	45.336
0.26	37.556	38.163	38.776	39.393	40.121	40.859	41.481	42.432	43.688	44.690
0.28	36.495	37.102	37.702	38.294	38.982	39.702	40.321	41.244	42.448	43.428
0.30	35.465	36.079	36.675	37.251	37.904	38.598	39.212	40.104	41.256	42.210
0.32	34.464	35.090	35.690	36.259	36.881	37.546	38.153	39.014	40.113	41.040
0.34	33.491	34.131	34.741	35.310	35.909	36.545	37.145	37.975	39.022	39.920
0.35	33.016	33.663	34.279	34.850	35.440	36.063	36.659	37.474	38.496	39.379
0.36	32.547	33.202	33.824	34.399	34.981	35.593	36.185	36.985	37.982	38.851
0.38	31.631	32.299	32.936	33.520	34.094	34.685	35.270	36.040	36.989	37.830
0.40	30.745	31.424	32.075	32.671	33.241	33.818	34.397	35.139	36.042	36.854
0.42	29.888	30.575	31.238	31.847	32.419	32.986	33.562	34.277	35.137	35.922
0.44	29.063	29.753	30.427	31.047	31.624	32.187	32.760	33.451	34.269	35.029
0.45	28.663	29.352	30.030	30.656	31.236	31.798	32.370	33.051	33.849	34.596
0.46	28.270	28.959	29.640	30.271	30.854	31.415	31.988	32.658	33.437	34.171
0.48	27.511	28.194	28.877	29.517	30.107	30.670	31.243	31.893	32.635	33.347
0.50	26.784	27.458	28.141	28.785	29.382	29.948	30.523	31.154	31.862	32.553
0.55	25.113	25.748	26.412	27.054	27.661	28.238	28.817	29.409	30.040	30.683
0.60	23.646	24.226	24.851	25.470	26.072	26.652	27.231	27.791	28.358	28.960
0.65	22.366	22.885	23.459	24.038	24.619	25.189	25.759	26.289	26.803	27.367
0.70	21.253	21.711	22.228	22.758	23.303	23.851	24.401	24.901	25.370	25.899
0.80	19.424	19.783	20.193	20.618	21.072	21.547	22.031	22.469	22.867	23.325
0.90	17.958	18.262	18.599	18.943	19.310	19.701	20.106	20.481	20.824	21.214
1.00	16.696	16.986	17.293	17.591	17.900	18.224	18.561	18.881	19.182	19.513
1.10	15.537	15.841	16.150	16.438	16.722	17.008	17.300	17.583	17.854	18.139
1.20	14.429	14.759	15.090	15.390	15.676	15.953	16.227	16.491	16.745	17.003
1.30	13.355	13.712	14.072	14.396	14.700	14.988	15.265	15.526	15.776	16.024
1.40	12.321	12.698	13.082	13.432	13.759	14.067	14.362	14.633	14.888	15.138
1.50	11.341	11.726	12.125	12.494	12.845	13.175	13.489	13.776	14.042	14.303
1.60	10.431	10.811	11.214	11.592	11.956	12.305	12.636	12.939	13.218	13.493
1.70	9.602	9.966	10.360	10.736	11.104	11.461	11.807	12.123	12.414	12.704
1.80	8.861	9.201	9.576	9.940	10.303	10.661	11.009	11.333	11.631	11.932
1.90	8.208	8.518	8.868	9.212	9.558	9.907	10.253	10.576	10.878	11.185
2.00	7.642	7.921	8.239	8.556	8.881	9.213	9.550	9.868	10.166	10.473
2.50	5.836	5.980	6.142	6.315	6.502	6.704	6.917	7.117	7.333	7.567
3.00	4.945	5.040	5.132	5.229	5.332	5.440	5.550	5.663	5.800	5.930
3.50	4.295	4.390	4.478	4.566	4.651	4.735	4.820	4.910	5.000	5.090
4.00	3.678	3.780	3.891	3.991	4.087	4.178	4.270	4.360	4.445	4.525
5.00	2.615	2.722	2.828	2.935	3.041	3.146	3.240	3.340	3.435	3.530
6.00	1.909	1.990	2.067	2.150	2.237	2.325	2.410	2.490	2.580	2.670

Table 6.1.1.1. *Mean atomic scattering factors for free atoms (cont.)*

Element	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb
Z	61	62	63	64	65	66	67	68	69	70
Method	*RHF	*RHF	RHF	*RHF	*RHF	*RHF	*RHF	*RHF	*RHF	*RHF
$(\sin\theta)/\lambda$ (Å^{-1})										
0.00	61.000	62.000	63.000	64.000	65.000	66.000	67.000	68.000	69.000	70.000
0.01	60.932	61.934	62.936	63.936	64.938	65.939	66.940	67.941	68.943	69.944
0.02	60.734	61.740	62.746	63.749	64.755	65.760	66.763	67.769	68.773	69.777
0.03	60.417	61.428	62.441	63.447	64.461	65.471	66.476	67.491	68.500	69.509
0.04	59.998	61.017	62.036	63.044	64.071	65.088	66.093	67.120	68.136	69.151
0.05	59.497	60.525	61.552	62.557	63.603	64.627	65.627	66.673	67.696	68.717
0.06	58.936	59.972	61.007	62.004	63.073	64.105	65.096	66.166	67.195	68.223
0.07	58.333	59.377	60.419	61.400	62.499	63.538	64.513	65.613	66.649	67.684
0.08	57.703	58.753	59.801	60.762	61.894	62.940	63.895	65.028	66.070	67.112
0.09	57.057	58.113	59.166	60.102	61.270	62.321	63.251	64.420	65.468	66.516
0.10	56.403	57.463	58.521	59.427	60.634	61.689	62.591	63.798	64.852	65.904
0.11	55.744	56.809	57.869	58.746	59.989	61.049	61.921	63.167	64.224	65.281
0.12	55.084	56.151	57.214	58.061	59.340	60.403	61.247	62.528	63.589	64.650
0.13	54.422	55.491	56.555	57.375	58.686	59.752	60.569	61.884	62.948	64.012
0.14	53.758	54.828	55.893	56.690	58.029	59.097	59.891	61.234	62.301	63.368
0.15	53.091	54.163	55.228	56.005	57.366	58.437	59.212	60.578	61.648	62.718
0.16	52.422	53.493	54.559	55.321	56.699	57.771	58.532	59.917	60.989	62.062
0.17	51.749	52.821	53.886	54.637	56.028	57.101	57.851	59.249	60.324	61.399
0.18	51.074	52.145	53.210	53.953	55.351	56.425	57.169	58.576	59.653	60.729
0.19	50.398	51.467	52.530	53.270	54.670	55.744	56.486	57.897	58.975	60.053
0.20	49.720	50.786	51.847	52.588	53.985	55.059	55.803	57.213	58.292	59.371
0.22	48.367	49.426	50.480	51.227	52.610	53.681	54.435	55.833	56.912	57.992
0.24	47.026	48.074	49.119	49.878	51.234	52.300	53.070	54.445	55.521	56.601
0.25	46.364	47.406	48.444	49.209	50.549	51.611	52.390	53.750	54.825	55.903
0.26	45.710	46.743	47.775	48.546	49.868	50.926	51.714	53.058	54.130	55.206
0.28	44.427	45.443	46.458	47.240	48.523	49.570	50.375	51.683	52.748	53.817
0.30	43.186	44.180	45.176	45.965	47.208	48.240	49.059	50.329	51.384	52.444
0.32	41.991	42.961	43.935	44.729	45.929	46.944	47.772	49.004	50.046	51.095
0.34	40.844	41.789	42.740	43.533	44.690	45.686	46.520	47.712	48.739	49.774
0.35	40.289	41.221	42.160	42.951	44.087	45.073	45.908	47.081	48.099	49.127
0.36	39.747	40.666	41.591	42.380	43.496	44.471	45.305	46.459	47.469	48.488
0.38	38.697	39.589	40.489	41.272	42.346	43.299	44.131	45.246	46.237	47.239
0.40	37.694	38.559	39.433	40.207	41.241	42.171	42.996	44.075	45.046	46.029
0.42	36.735	37.573	38.421	39.184	40.179	41.086	41.903	42.945	43.896	44.859
0.44	35.815	36.627	37.451	38.203	39.160	40.042	40.849	41.857	42.786	43.728
0.45	35.370	36.169	36.980	37.726	38.665	39.536	40.337	41.327	42.246	43.178
0.46	34.933	35.720	36.519	37.259	38.180	39.039	39.834	40.808	41.715	42.637
0.48	34.085	34.848	35.623	36.352	37.237	38.073	38.856	39.797	40.682	41.583
0.50	33.269	34.008	34.761	35.479	36.329	37.143	37.914	38.822	39.686	40.565
0.55	31.349	32.036	32.737	33.428	34.199	34.958	35.699	36.531	37.342	38.169
0.60	29.581	30.222	30.877	31.543	32.243	32.953	33.664	34.425	35.187	35.964
0.65	27.948	28.547	29.161	29.802	30.438	31.103	31.786	32.483	33.198	33.929
0.70	26.442	27.002	27.576	28.192	28.772	29.394	30.049	30.688	31.359	32.045
0.80	23.796	24.281	24.781	25.335	25.822	26.366	26.958	27.497	28.086	28.690
0.30	21.616	22.030	22.459	22.940	23.353	23.821	24.343	24.800	25.311	25.837
1.00	19.853	20.202	20.565	20.970	21.323	21.721	22.167	22.556	22.995	23.447
1.10	18.430	18.728	19.035	19.372	19.675	20.011	20.385	20.718	21.089	21.474
1.20	17.262	17.523	17.789	18.072	18.338	18.623	18.934	19.221	19.535	19.860
1.30	16.266	16.507	16.747	16.995	17.234	17.483	17.746	17.998	18.266	18.542
1.40	15.378	15.613	15.841	16.072	16.296	16.522	16.753	16.980	17.215	17.454
1.50	14.551	14.790	15.020	15.247	15.465	15.680	15.895	16.107	16.321	16.536
1.60	13.755	14.005	14.245	14.477	14.697	14.913	15.123	15.329	15.533	15.735
1.70	12.980	13.243	13.494	13.741	13.968	14.190	14.406	14.612	14.815	15.013
1.80	12.220	12.497	12.763	13.022	13.259	13.491	13.718	13.929	14.137	14.338
1.90	11.481	11.767	12.044	12.317	12.564	12.808	13.047	13.267	13.483	13.691
2.00	10.773	11.064	11.345	11.631	11.886	12.141	12.392	12.621	12.847	13.064
2.50	7.817	8.083	8.348	8.683	8.983	9.267	9.533	9.783	10.033	10.267
3.00	6.088	6.250	6.435	6.588	6.775	6.963	7.163	7.375	7.588	7.788
3.50	5.180	5.280	5.378	5.490	5.610	5.720	5.850	5.980	6.110	6.250
4.00	4.600	4.675	4.750	4.830	4.915	5.000	5.090	5.180	5.280	5.380
5.00	3.625	3.720	3.812	3.905	3.990	4.075	4.155	4.235	4.310	4.380
6.00	2.770	2.865	2.965	3.070	3.170	3.270	3.355	3.440	3.520	3.600

Table 6.1.1.1. *Mean atomic scattering factors for free atoms (cont.)*

Element	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg
Z	71	72	73	74	75	76	77	78	79	80
Method	*RHF	*RHF	*RHF	*RHF	*RHF	*RHF	*RHF	*RHF	RHF	RHF
$(\sin\theta)/\lambda$ (Å^{-1})										
0.00	71.000	72.000	73.000	74.000	75.000	76.000	77.000	78.000	79.000	80.000
0.01	70.944	71.945	72.946	73.948	74.949	75.950	76.951	77.955	78.957	79.556
0.02	70.778	71.783	72.788	73.793	74.797	75.801	76.806	77.820	78.826	79.819
0.03	70.509	71.518	72.529	73.539	74.548	75.538	76.567	77.599	78.609	79.595
0.04	70.148	71.161	72.177	73.194	74.209	75.225	76.240	77.295	78.311	79.286
0.05	69.707	70.723	71.745	72.767	73.788	74.810	75.832	76.914	77.936	78.899
0.06	69.202	70.217	71.242	72.269	73.295	74.323	75.352	76.462	77.491	78.439
0.07	68.646	69.656	70.680	71.711	72.740	73.772	74.806	75.946	76.981	77.913
0.08	68.051	69.052	70.072	71.103	72.132	73.167	74.206	75.373	76.414	77.330
0.09	67.429	68.416	69.428	70.455	71.482	72.518	73.558	74.751	75.797	76.696
0.10	66.789	67.757	68.758	69.778	70.799	71.832	72.872	74.086	75.135	76.018
0.11	66.137	67.083	68.069	69.078	70.091	71.119	72.156	73.386	74.437	75.303
0.12	65.477	66.400	67.367	68.363	69.365	70.384	71.416	72.656	73.706	74.559
0.13	64.813	65.711	66.658	67.637	68.625	69.634	70.658	71.902	72.950	73.790
0.14	64.146	65.019	65.944	66.906	67.878	68.874	69.887	71.130	72.173	73.001
0.15	63.478	64.326	65.229	66.172	67.126	68.107	69.108	70.343	71.380	72.198
0.16	62.807	63.634	64.515	65.437	66.372	67.337	68.324	69.546	70.575	71.385
0.17	62.134	62.942	63.802	64.703	65.619	66.566	67.538	68.742	69.761	70.564
0.18	61.460	62.251	63.090	63.972	64.868	65.797	66.752	67.934	68.941	69.740
0.19	60.783	61.560	62.382	63.243	64.121	65.031	65.969	67.125	68.119	68.914
0.20	60.103	60.870	61.675	62.519	63.378	64.269	65.189	66.317	67.296	68.088
0.22	58.739	59.492	60.271	61.082	61.906	62.761	63.645	64.709	65.657	66.447
0.24	57.369	58.119	58.880	59.663	60.457	61.278	62.127	63.125	64.039	64.828
0.25	56.683	57.434	58.189	58.961	59.742	60.548	61.380	62.344	63.241	64.029
0.26	55.998	56.752	57.502	58.265	59.034	59.825	60.641	61.571	62.452	63.239
0.28	54.634	55.396	56.141	56.888	57.637	58.403	59.189	60.056	60.902	61.687
0.30	53.282	54.054	54.799	55.536	56.270	57.013	57.773	58.582	59.395	60.177
0.32	51.950	52.733	53.479	54.210	54.932	55.658	56.395	57.152	57.935	58.711
0.34	50.642	51.435	52.185	52.912	53.627	54.339	55.056	55.769	56.523	57.292
0.35	49.998	50.796	51.548	52.274	52.986	53.692	54.401	55.094	55.835	56.600
0.36	49.363	50.164	50.918	51.644	52.354	53.055	53.756	54.432	55.160	55.920
0.38	48.117	48.924	49.683	50.408	51.114	51.807	52.496	53.141	53.846	54.595
0.40	46.906	47.717	48.479	49.205	49.910	50.596	51.274	51.897	52.581	53.318
0.42	45.731	46.543	47.308	48.036	48.739	49.422	50.091	50.697	51.363	52.088
0.44	44.593	45.405	46.171	46.900	47.603	48.283	48.946	49.540	50.191	50.902
0.45	44.038	44.849	45.615	46.344	47.048	47.726	48.387	48.977	49.622	50.326
0.46	43.492	44.301	45.068	45.797	46.501	47.179	47.837	48.424	49.063	49.761
0.48	42.427	43.232	43.998	44.728	45.432	46.109	46.765	47.347	47.976	48.661
0.50	41.398	42.197	42.962	43.691	44.396	45.072	45.726	46.308	46.929	47.601
0.55	38.970	39.752	40.508	41.236	41.940	42.617	43.269	43.860	44.469	45.113
0.60	36.733	37.494	38.238	38.960	39.662	40.340	40.994	41.601	42.207	42.829
0.65	34.666	35.404	36.132	36.846	37.544	38.222	38.878	39.502	40.110	40.718
0.70	32.752	33.465	34.175	34.878	35.569	36.244	36.901	37.539	38.153	38.753
0.80	29.334	29.992	30.658	31.327	31.993	32.654	33.305	33.958	34.581	35.176
0.90	26.413	27.008	27.618	28.238	28.865	29.495	30.125	30.766	31.387	31.980
1.00	23.950	24.473	25.016	25.576	26.148	26.732	27.323	27.930	28.530	29.112
1.10	21.902	22.352	22.823	23.313	23.821	24.345	24.882	25.437	25.998	26.554
1.20	20.219	20.598	20.998	21.418	21.856	22.314	22.789	23.281	23.789	24.303
1.30	18.842	19.159	19.494	19.847	20.219	20.610	21.019	21.445	21.892	22.354
1.40	17.709	17.975	18.256	18.552	18.864	19.194	19.541	19.902	20.287	20.692
1.50	16.759	16.988	17.228	17.478	17.742	18.019	18.312	18.616	18.943	19.290
1.60	15.939	16.145	16.356	16.575	16.801	17.038	17.287	17.545	17.821	18.116
1.70	15.208	15.403	15.598	15.796	15.998	16.206	16.422	16.644	16.880	17.131
1.80	14.534	14.727	14.916	15.104	15.293	15.483	15.678	15.875	16.081	16.298
1.90	13.894	14.091	14.282	14.469	14.653	14.835	15.018	15.202	15.388	15.581
2.00	13.277	13.481	13.679	13.871	14.057	14.239	14.418	14.595	14.770	14.949
2.50	10.500	10.733	10.950	11.167	11.383	11.583	11.783	11.983	12.168	12.360
3.00	8.013	8.238	8.480	8.706	8.938	9.163	9.400	9.620	9.826	10.049
3.50	6.400	6.560	6.740	6.900	7.080	7.270	7.460	7.650	7.878	8.081
4.00	5.490	5.600	5.710	5.840	5.960	6.080	6.210	6.340	6.489	6.644
5.00	4.450	4.520	4.585	4.650	4.715	4.788	4.860	4.935	5.010	5.090
6.00	3.680	3.755	3.825	3.900	3.970	4.035	4.105	4.175	4.244	4.310

Table 6.1.1.1. *Mean atomic scattering factors for free atoms (cont.)*

Element	Tl	Pb	Bi	Po	At	Rn	Fr	Ra	Ac	Th
Z	81	82	83	84	85	86	87	88	89	90
Method	*RHF	RHF	RHF	*RHF	*RHF	RHF	*RHF	*RHF	*RHF	*RHF
$(\sin\theta)/\lambda$ (Å^{-1})										
0.00	81.000	82.000	83.000	84.000	85.000	86.000	87.000	88.000	89.000	90.000
0.01	80.950	81.949	82.947	83.944	84.944	85.945	86.922	87.915	88.915	89.916
0.02	80.799	81.792	82.784	83.778	84.776	85.777	86.694	87.664	88.664	89.669
0.03	80.553	81.536	82.518	83.506	84.502	85.502	86.332	87.263	88.260	89.269
0.04	80.217	81.186	82.154	83.134	84.125	85.123	85.854	86.734	87.723	88.735
0.05	79.798	80.750	81.700	82.669	83.654	84.649	85.286	86.104	87.077	88.085
0.06	79.305	80.237	81.167	82.121	83.098	84.087	84.647	85.397	86.346	87.344
0.07	78.748	79.656	80.563	81.501	82.466	83.448	83.955	84.638	85.553	86.533
0.08	78.134	79.018	79.901	80.819	81.770	82.742	83.222	83.845	84.719	85.672
0.09	77.473	78.332	79.189	80.086	81.020	81.979	82.457	83.030	83.859	84.779
0.10	76.773	77.607	78.438	79.312	80.226	81.169	81.666	82.202	82.985	83.867
0.11	76.042	76.851	77.657	78.506	79.398	80.322	80.852	81.368	82.105	82.946
0.12	75.284	76.071	76.852	77.677	78.545	79.448	80.018	80.528	81.225	82.025
0.13	74.507	75.274	76.032	76.831	77.674	78.554	79.167	79.685	80.348	81.107
0.14	73.715	74.464	75.202	75.976	76.794	77.648	78.303	78.839	79.474	80.196
0.15	72.912	73.645	74.365	75.117	75.908	76.737	77.430	77.990	78.605	79.294
0.16	72.101	72.822	73.527	74.257	75.023	75.826	76.550	77.138	77.739	78.400
0.17	71.285	71.997	72.689	73.400	74.143	74.920	75.667	76.285	76.879	77.516
0.18	70.467	71.172	71.855	72.549	73.269	74.021	74.785	75.431	76.023	76.642
0.19	69.648	70.349	71.026	71.706	72.405	73.133	73.907	74.578	75.172	75.777
0.20	68.830	69.530	70.203	70.871	71.553	72.258	73.035	73.728	74.326	74.922
0.22	67.205	67.907	68.578	69.232	69.885	70.552	71.320	72.043	72.654	73.242
0.24	65.600	66.310	66.987	67.634	68.269	68.907	69.653	70.389	71.014	71.602
0.25	64.807	65.523	66.204	66.852	67.481	68.109	68.841	69.576	70.208	70.798
0.26	64.022	64.743	65.430	66.080	66.706	67.325	68.043	68.775	69.412	70.005
0.28	62.478	63.210	63.909	64.567	65.193	65.802	66.491	67.210	67.855	68.454
0.30	60.970	61.712	62.425	63.093	63.725	64.332	64.996	65.696	66.345	66.951
0.32	59.503	60.253	60.977	61.658	62.301	62.912	63.556	64.235	64.884	65.497
0.34	58.079	58.833	59.566	60.260	60.915	61.535	62.167	62.826	63.473	64.091
0.35	57.383	58.138	58.875	59.575	60.236	60.862	61.489	62.140	62.785	63.405
0.36	56.698	57.453	58.193	58.899	59.566	60.198	60.823	61.466	62.110	62.731
0.38	55.362	56.116	56.859	57.573	58.253	58.898	59.520	60.151	60.792	61.416
0.40	54.072	54.820	55.563	56.283	56.974	57.631	58.256	58.879	59.517	60.143
0.42	52.826	53.567	54.306	55.029	55.728	56.397	57.026	57.646	58.282	58.910
0.44	51.625	52.356	53.089	53.811	54.515	55.194	55.829	56.448	57.084	57.713
0.45	51.041	51.766	52.495	53.215	53.921	54.604	55.242	55.862	56.497	57.127
0.46	50.467	51.187	51.910	52.629	53.335	54.021	54.663	55.284	55.919	56.550
0.48	49.352	50.058	50.771	51.483	52.189	52.879	53.527	54.151	54.787	55.419
0.50	48.276	48.969	49.669	50.373	51.075	51.767	52.420	53.048	53.684	54.317
0.55	45.753	46.411	47.077	47.752	48.435	49.119	49.777	50.413	51.050	51.684
0.60	43.442	44.069	44.700	45.343	45.997	46.659	47.310	47.948	48.580	49.211
0.65	41.313	41.914	42.517	43.127	43.750	44.384	45.017	45.646	46.268	46.889
0.70	39.337	39.921	40.501	41.085	41.678	42.281	42.891	43.504	44.110	44.716
0.80	35.755	36.322	36.879	37.430	37.980	38.533	39.095	39.664	40.229	40.795
0.90	32.561	33.127	33.680	34.220	34.751	35.277	35.804	36.335	36.863	37.391
1.00	29.687	30.252	30.805	31.344	31.872	32.389	32.900	33.408	33.912	34.413
1.10	27.109	27.662	28.208	28.744	29.271	29.787	30.292	30.790	31.283	31.770
1.20	24.824	25.350	25.875	26.397	26.915	27.426	27.926	28.418	28.906	29.387
1.30	22.827	23.313	23.804	24.298	24.794	25.291	25.779	26.263	26.744	27.219
1.40	21.110	21.546	21.992	22.446	22.909	23.379	23.845	24.312	24.779	25.244
1.50	19.652	20.034	20.429	20.836	21.256	21.689	22.123	22.564	23.008	23.454
1.60	18.424	18.754	19.097	19.453	19.826	20.215	20.608	21.014	21.427	21.846
1.70	17.394	17.674	17.969	18.277	18.602	18.944	19.295	19.660	20.036	20.421
1.80	16.524	16.764	17.017	17.281	17.562	17.859	18.165	18.488	18.823	19.170
1.90	15.780	15.989	16.207	16.435	16.677	16.934	17.199	17.481	17.776	18.083
2.00	15.131	15.317	15.510	15.711	15.922	16.143	16.377	16.623	16.880	17.149
2.50	12.530	12.724	12.896	13.060	13.230	13.386	13.550	13.700	13.860	14.020
3.00	10.270	10.482	10.690	10.900	11.090	11.282	11.460	11.640	11.815	11.980
3.50	8.290	8.495	8.704	8.910	9.120	9.329	9.530	9.730	9.930	10.130
4.00	6.800	6.973	7.145	7.320	7.500	7.686	7.878	8.070	8.255	8.440
5.00	5.175	5.260	5.351	5.440	5.540	5.650	5.755	5.870	5.933	6.118
6.00	4.374	4.441	4.505	4.567	4.630	4.702	4.768	4.840	4.910	4.982

Table 6.1.1.1. *Mean atomic scattering factors for free atoms (cont.)*

Element	Pa	U	Np	Pu	Am	Cm	Bk	Cf
Z	91	92	93	94	95	96	97	98
Method	*RHF	RHF	*RHF	*RHF	*RHF	*RHF	*RHF	*RHF
$(\sin\theta)/\lambda$ (Å^{-1})								
0.00	91.000	92.000	93.000	94.000	95.000	96.000	97.000	98.000
0.01	90.919	91.922	92.922	93.924	94.926	95.926	96.928	97.929
0.02	90.678	91.687	92.691	93.701	94.706	95.708	96.713	97.718
0.03	90.290	91.307	92.318	93.340	94.352	95.354	96.365	97.375
0.04	89.772	90.798	91.817	92.857	93.877	94.877	95.895	96.912
0.05	89.144	90.180	91.208	92.271	93.299	94.294	95.320	96.344
0.06	88.427	89.474	90.510	91.601	92.638	93.623	94.656	95.688
0.07	87.644	88.699	89.742	90.866	91.910	92.879	93.920	94.961
0.08	86.813	87.874	88.923	90.082	91.131	92.081	93.129	94.176
0.09	85.950	87.014	88.067	89.261	90.315	91.241	92.294	93.347
0.10	85.066	86.130	87.186	88.413	89.470	90.371	91.429	92.486
0.11	84.170	85.232	86.288	87.547	88.605	89.479	90.540	91.601
0.12	83.269	84.326	85.380	86.665	87.723	88.573	89.635	90.699
0.13	82.366	83.417	84.467	85.772	86.829	87.656	88.718	89.783
0.14	81.463	82.505	83.550	84.870	85.924	86.731	87.793	88.858
0.15	80.563	81.595	82.632	83.961	85.011	85.802	86.862	87.926
0.16	79.665	80.685	81.715	83.044	84.090	84.869	85.926	86.989
0.17	78.771	79.779	80.799	82.123	83.163	83.934	84.988	86.048
0.18	77.881	78.875	79.885	81.198	82.231	82.998	84.047	85.103
0.19	76.995	77.975	78.973	80.271	81.296	82.062	83.105	84.157
0.20	76.115	77.080	78.066	79.343	80.360	81.126	82.163	83.210
0.22	74.375	75.308	76.267	77.493	78.490	79.263	80.285	81.318
0.24	72.668	73.568	74.496	75.663	76.636	77.419	78.421	79.437
0.25	71.829	72.712	73.624	74.759	75.719	76.507	77.498	78.504
0.26	71.001	71.866	72.763	73.865	74.811	75.603	76.582	77.577
0.28	69.380	70.211	71.074	72.110	73.027	73.824	74.777	75.749
0.30	67.810	68.607	69.436	70.408	71.293	72.091	73.016	73.960
0.32	66.294	67.058	67.853	68.763	69.615	70.409	71.303	72.219
0.34	64.832	65.564	66.326	67.178	67.997	68.783	69.645	70.531
0.35	64.121	64.838	65.584	66.409	67.212	67.991	68.838	69.707
0.36	63.423	64.126	64.857	65.655	66.441	67.214	68.045	68.898
0.38	62.066	62.742	63.443	64.193	64.947	65.705	66.503	67.325
0.40	60.758	61.409	62.083	62.789	63.513	64.254	65.020	65.810
0.42	59.495	60.125	60.775	61.442	62.137	62.859	63.595	64.354
0.44	58.274	58.886	59.514	60.147	60.816	61.519	62.226	62.954
0.45	57.679	58.283	58.901	59.518	60.175	60.869	61.562	62.276
0.46	57.093	57.689	58.298	58.901	59.546	60.231	60.910	61.610
0.48	55.948	56.531	57.124	57.702	58.325	58.992	59.646	60.319
0.50	54.836	55.410	55.989	56.544	57.148	57.798	58.430	59.078
0.55	52.191	52.748	53.303	53.819	54.385	54.998	55.581	56.176
0.60	49.719	50.268	50.808	51.302	51.842	52.427	52.974	53.528
0.65	47.405	47.950	48.483	48.967	49.490	50.052	50.574	51.098
0.70	45.241	45.784	46.312	46.794	47.307	47.850	48.354	48.858
0.80	41.333	41.869	42.390	42.879	43.380	43.894	44.380	44.859
0.90	37.930	38.454	38.966	39.465	39.958	40.449	40.926	41.395
1.00	34.946	35.458	35.961	36.465	36.952	37.426	37.898	38.361
1.10	32.292	32.794	33.289	33.793	34.276	34.740	35.209	35.671
1.20	29.897	30.391	30.879	31.379	31.858	32.318	32.786	33.247
1.30	27.714	28.199	28.680	29.172	29.648	30.106	30.572	31.033
1.40	25.720	26.192	26.662	27.142	27.611	28.068	28.530	28.989
1.50	23.905	24.360	24.813	25.275	25.733	26.184	26.639	27.093
1.60	22.266	22.699	23.128	23.566	24.006	24.446	24.889	25.332
1.70	20.807	21.207	21.609	22.019	22.435	22.857	23.281	23.708
1.80	19.518	19.886	20.253	20.630	21.018	21.415	21.815	22.221
1.90	18.394	18.723	19.055	19.398	19.754	20.121	20.496	20.872
2.00	17.423	17.713	18.012	18.319	18.640	18.975	19.315	19.665
2.50	14.180	14.341	14.503	14.664	14.826	14.988	15.150	15.311
3.00	12.150	12.294	12.475	12.656	12.838	13.019	13.200	13.381
3.50	10.320	10.495	10.695	10.895	11.095	11.295	11.495	11.695
4.00	8.630	8.823	9.008	9.193	9.378	9.563	9.748	9.933
5.00	6.250	6.378	6.489	6.602	6.713	6.825	6.937	7.049
6.00	5.055	5.136	5.206	5.275	5.345	5.414	5.484	5.553

Table 6.1.1.2. *Spherical bonded hydrogen-atom scattering factors from Stewart, Davidson & Simpson (1965)*

$(\sin\theta)/\lambda$ (Å^{-1})	f	$(\sin\theta)/\lambda$ (Å^{-1})	f
0.0000	1.0000	0.7729	0.0254
0.0215	0.9924	0.8158	0.0208
0.0429	0.9704	0.8588	0.0171
0.0644	0.9352	0.9017	0.0140
0.0859	0.8892	0.9447	0.0116
0.1073	0.8350	0.9876	0.0096
0.1288	0.7752	1.0305	0.0080
0.1503	0.7125	1.0735	0.0066
0.1718	0.6492	1.1164	0.0056
0.1932	0.5871	1.1593	0.0047
0.2147	0.5277	1.2023	0.0040
0.2576	0.4201	1.2452	0.0035
0.3006	0.3301	1.2882	0.0031
0.3435	0.2573	1.3311	0.0027
0.3864	0.1998	1.3740	0.0025
0.4294	0.1552	1.4170	0.0022
0.4723	0.1208	1.4599	0.0020
0.5153	0.0945	1.5029	0.0018
0.5582	0.0744	1.5458	0.0016
0.6011	0.0592	1.5887	0.0015
0.6441	0.0474	1.6317	0.0013
0.6870	0.0383	1.6746	0.0011
0.7300	0.0311	1.7176	0.0010

some of the more chemically significant ions are listed in Table 6.1.1.3. For H^-, Li^+ and Be^{2+} these are based on the correlated electron calculations of Thakkar & Smith (1992). For other ions lighter than rubidium, values are based on the Hartree–Fock calculations of Cromer & Mann (1968), using the wavefunctions of Mann (1968*b*). For the heavier ions, the calculations are by Cromer & Waber (1968), based on relativistic Dirac–Slater wavefunctions, which are a good approximation to the corresponding relativistic Hartree–Fock wavefunctions. If ionic scattering factors are required for values of $(\sin\theta)/\lambda$ greater than those shown in Table 6.1.1.3, the free-atom scattering factors of Table 6.1.1.1 can be used because high-angle scattering is dominated by core electrons and is therefore very little affected by ionicity.

6.1.1.3.1. *Scattering-factor interpolation*

A general treatment of interpolation is complicated by possible difficulties resulting from singularities in tabulated functions. The interpolation of scattering factors does not involve such problems, however, and a more restricted treatment suffices.

An iterative method, applicable to a function $f(x)$ tabulated at arbitrary values $x_0, x_1, \ldots, x_n$ is due to Aitken. $f(x|x_0, x_1, \ldots, x_k)$ is the polynominal that coincides with the tabulated values at $x_0, x_1, \ldots, x_k$.

$$f(x|x_0,x_1) = \frac{1}{x_1-x_0}\begin{vmatrix} f_0 x_0 - x & \\ f_1 x_1 - x & \end{vmatrix}$$
$$f(x|x_0,x_1,x_2) = \frac{1}{x_2-x_1}\begin{vmatrix} f(x|x_0,x_1) & x_1-x \\ f(x|x_0,x_2) & x_2-x \end{vmatrix}$$
$$f(x|x_0,x_1,x_2,x_3) = \frac{1}{x_3-x_2}\begin{vmatrix} f(x|x_0,x_1,x_2) & x_2-x \\ f(x|x_0,x_1,x_3) & x_3-x \end{vmatrix}. \quad (6.1.1.13)$$

Iteration is continued until increasing k does not change the interpolated value significantly.

Another interpolation formula, due to Lagrange, is

$$f(x) = \sum_{i=0}^{n} l_i(x) f_i + R_n(x),$$

where

$$l_i(x) = \frac{\pi_n(x)}{(x-x_i)\pi_n'(x_i)}$$

and

$$R_n(x) = \pi_n(x)[x_0, x_1, \ldots, x_n, x]. \quad (6.1.1.14)$$

$\pi_n(x)$ is $(x-x_0)(x-x_1)\ldots(x-x_n)$ and $\pi_n'(x)$ is its derivative, so that

$$\pi_n'(x_k) = (x_k-x_0)(x_k-x_1)\ldots(x_k-x_{k-1}) \times (x_k-x_{k+1})\ldots(x_k-x_n)$$

while

$$[x_0,x_1] = \frac{f_0-f_1}{x_0-x_1}$$
$$[x_0,x_1,x_2] = \frac{[x_0,x_1]-[x_1,x_2]}{x_0-x_2}$$
$$[x_0,x_1\ldots x_n] = \sum_{k=0}^{n}\frac{f_k}{\pi_n'(x_k)}.$$

For the scattering factors of Tables 6.1.1.1 and 6.1.1.3, the expansion

$$f(\sin\theta/\lambda) = \sum_{i=1}^{4} a_i \exp(-b_i \sin^2\theta/\lambda^2) + c \quad (6.1.1.15)$$

has been found to be particularly effective. The coefficients listed in Table 6.1.1.4 give a close fit to the atomic scattering curves over the range $0 < (\sin\theta)/\lambda < 2.0$ Å^{-1}. Table 6.1.1.4 also contains the maximum and minimum deviations from the true curve, and the mean of the magnitude of the deviation. For 2.0 Å$^{-1} < (\sin\theta)/\lambda < 6.0$ Å^{-1}, Fox *et al.* (1989) have shown that (6.1.1.15) is highly inaccurate, and they produced a 'logarithmic polynomial' curve-fitting routine based on the equation

$$\ln\{f[(\sin\theta)/\lambda]\} = \sum_{i=0}^{3} a_i s^i \quad (6.1.1.16)$$

for these high angles. The a_i values listed in Table 6.1.1.5 give a close fit to the atomic scattering factor curves over the range $2.0 < (\sin\theta)/\lambda < 6.0$ Å^{-1}. Because f varies slowly with $(\sin\theta)/\lambda$ at these high angles, four parameters are all that is necessary for accurate fitting. Confirmation of this is given in Table 6.1.1.5 where the correlation coefficients, C, associated with each fit are also shown, and it can be seen that these are close to 1.0 in every case.

6.1.1.4. *Generalized scattering factors*

For bound atoms, it may be necessary to account for the perturbation of the electron density by interaction with other atoms, and to analyse its effect on the scattering.

The generalized scattering factor is obtained from the Fourier transform of a perturbed atomic electron-density function. The exponential factor in the transform may be written as an expansion in terms of Legendre polynomials $P_l(\cos\theta)$.†

† Special functions are as given in Abramowitz & Stegun (1964), unless defined otherwise in the text.

Table 6.1.1.3. *Mean atomic scattering factors in electrons for chemically significant ions*

Methods: C: correlated; HF: non-relativistic Hartree–Fock; RHF: relativistic Hartree–Fock; *DS: modified Dirac–Slater.

Element	H^{1-}	Li^{1+}	Be^{2+}	C_{val}	O^{1-}	F^{1-}	Na^{1+}	Mg^{2+}	Al^{3+}	Si_{val}
Z	1	3	4	6	8	9	11	12	13	14
Method	C	C	C	HF	HF	HF	RHF	RHF	HF	HF
$(\sin\theta)/\lambda$ (Å^{-1})										
0.00	2.000	2.000	2.000	6.000	9.000	10.000	10.000	10.000	10.000	14.000
0.01	1.983	1.999	1.999	5.989	8.986	9.988	9.995	9.997	9.997	13.973
0.02	1.933	1.997	1.999	5.956	8.945	9.953	9.981	9.986	9.989	13.894
0.03	1.857	1.994	1.997	5.903	8.878	9.895	9.958	9.969	9.976	13.766
0.04	1.763	1.990	1.995	5.829	8.785	9.816	9.925	9.945	9.957	13.593
0.05	1.659	1.984	1.992	5.738	8.670	9.716	9.883	9.914	9.933	13.381
0.06	1.550	1.977	1.988	5.629	8.534	9.597	9.833	9.876	9.904	13.138
0.07	1.442	1.968	1.983	5.507	8.381	9.461	9.773	9.832	9.870	12.870
0.08	1.338	1.959	1.978	5.372	8.211	9.309	9.705	9.782	9.831	12.586
0.09	1.238	1.948	1.973	5.227	8.029	9.144	9.630	9.725	9.787	12.293
0.10	1.145	1.936	1.966	5.074	7.836	8.967	9.546	9.662	9.738	11.995
0.11	1.058	1.923	1.959	4.916	7.635	8.781	9.455	9.594	9.684	11.700
0.12	0.978	1.909	1.952	4.754	7.429	8.586	9.357	9.519	9.625	11.410
0.13	0.904	1.894	1.944	4.591	7.218	8.386	9.253	9.440	9.563	11.130
0.14	0.836	1.877	1.935	4.428	7.005	8.181	9.142	9.355	9.495	10.862
0.15	0.773	1.860	1.925	4.267	6.792	7.973	9.026	9.265	9.424	10.608
0.16	0.715	1.842	1.915	4.109	6.579	7.762	8.904	9.171	9.349	10.368
0.17	0.661	1.823	1.905	3.954	6.368	7.551	8.777	9.072	9.270	10.143
0.18	0.612	1.804	1.894	3.805	6.160	7.341	8.647	8.969	9.187	9.933
0.19	0.567	1.783	1.882	3.661	5.956	7.131	8.512	8.862	9.101	9.737
0.20	0.526	1.762	1.870	3.523	5.756	6.924	8.374	8.751	9.011	9.553
0.22	0.452	1.718	1.845	3.266	5.371	6.517	8.089	8.521	8.823	9.222
0.24	0.390	1.671	1.817	3.035	5.008	6.126	7.795	8.280	8.623	8.931
0.25	0.362	1.647	1.803	2.930	4.836	5.937	7.646	8.156	8.520	8.798
0.26	0.337	1.623	1.788	2.831	4.670	5.753	7.496	8.030	8.414	8.671
0.28	0.291	1.573	1.758	2.651	4.357	5.399	7.195	7.774	8.198	8.435
0.30	0.253	1.523	1.726	2.495	4.068	5.067	6.894	7.513	7.975	8.214
0.32	0.220	1.471	1.692	2.358	3.804	4.756	6.597	7.251	7.747	8.005
0.34	0.192	1.419	1.658	2.241	3.564	4.467	6.304	6.987	7.515	7.803
0.35	0.179	1.394	1.641	2.188	3.452	4.330	6.160	6.856	7.399	7.704
0.36	0.168	1.368	1.623	2.139	3.345	4.199	6.018	6.725	7.282	7.606
0.38	0.147	1.316	1.587	2.050	3.147	3.951	5.739	6.465	7.047	7.410
0.40	0.129	1.265	1.551	1.974	2.969	3.724	5.471	6.210	6.813	7.215
0.42	0.113	1.215	1.514	1.907	2.808	3.514	5.212	5.959	6.581	7.021
0.44	0.100	1.165	1.476	1.849	2.663	3.322	4.964	5.715	6.350	6.826
0.45	0.094	1.141	1.458	1.822	2.597	3.233	4.845	5.595	6.237	6.729
0.46	0.089	1.117	1.439	1.798	2.533	3.147	4.728	5.477	6.124	6.632
0.48	0.079	1.069	1.401	1.752	2.417	2.987	4.503	5.247	5.901	6.437
0.50	0.070	1.023	1.364	1.711	2.313	2.841	4.290	5.025	5.683	6.244
0.55	0.0526	0.914	1.270	1.624	2.097	2.531	3.808	4.508	5.162	5.766
0.60	0.0401	0.814	1.179	1.552	1.934	2.288	3.395	4.046	4.681	5.303
0.65	0.0311	0.724	1.091	1.488	1.808	2.096	3.046	3.641	4.243	4.865
0.70	0.0243	0.643	1.007	1.428	1.710	1.945	2.753	3.288	3.851	4.455
0.80	0.0155	0.507	0.852	1.315	1.567	1.729	2.305	2.724	3.195	3.734
0.90	0.0102	0.400	0.717	1.204	1.463	1.585	1.997	2.315	2.693	3.150
1.00	0.0070	0.317	0.602	1.096	1.376	1.481	1.785	2.023	2.319	2.691
1.10	0.0049	0.253	0.505	0.992	1.296	1.397	1.635	1.813	2.041	2.338
1.20	0.0036	0.203	0.424	0.894	1.219	1.322	1.524	1.662	1.837	2.069
1.30	0.0026	0.164	0.357	0.802	1.143	1.252	1.438	1.548	1.685	1.867
1.40	0.0020	0.133	0.301	0.718	1.067	1.184	1.367	1.460	1.570	1.713
1.50	0.0015	0.109	0.255	0.642	0.994	1.117	1.304	1.388	1.479	1.595
1.60	0.0012	0.090	0.216				1.246	1.326		
1.70	0.0009	0.075	0.184				1.191	1.270		
1.80	0.0008	0.062	0.157				1.137	1.218		
1.90	0.0006	0.053	0.135				1.084	1.168		
2.00	0.0005	0.044	0.116				1.032	1.119		

Table 6.1.1.3. *Mean atomic scattering factors for chemically significant ions (cont.)*

Element	Si^{4+}	Cl^{1-}	K^{1+}	Ca^{2+}	Sc^{3+}	Ti^{2+}	Ti^{3+}	Ti^{4+}	V^{2+}	V^{3+}
Z	14	17	19	20	21	22	22	22	23	23
Method	HF	RHF	RHF	RHF	HF	HF	HF	HF	RHF	HF
$(\sin\theta)/\lambda$ (Å^{-1})										
0.00	10.000	18.000	18.000	18.000	18.000	20.000	19.000	18.000	21.000	20.000
0.01	9.998	17.972	17.986	17.989	17.991	19.988	18.990	17.992	20.988	19.990
0.02	9.991	17.888	17.943	17.955	17.963	19.951	18.962	17.969	20.952	19.961
0.03	9.981	17.751	17.872	17.899	17.917	19.891	18.914	17.930	20.892	19.913
0.04	9.966	17.563	17.774	17.821	17.853	19.807	18.848	17.877	20.808	19.846
0.05	9.947	17.330	17.649	17.721	17.771	19.701	18.764	17.808	20.702	19.760
0.06	9.924	17.057	17.499	17.601	17.672	19.572	18.662	17.725	20.573	19.657
0.07	9.896	16.750	17.325	17.462	17.556	19.423	18.543	17.628	20.424	19.536
0.08	9.865	16.415	17.129	17.303	17.424	19.253	18.407	17.516	20.255	19.398
0.09	9.829	16.058	16.912	17.127	17.278	19.065	18.255	17.392	20.066	19.244
0.10	9.790	15.685	16.677	16.935	17.116	18.860	18.089	17.255	19.861	19.075
0.11	9.747	15.301	16.426	16.727	16.941	18.639	17.909	17.106	19.639	18.892
0.12	9.700	14.911	16.160	16.506	16.754	18.404	17.716	16.946	19.402	18.695
0.13	9.649	14.519	15.882	16.272	16.555	18.156	17.510	16.775	19.152	18.485
0.14	9.595	14.130	15.594	16.028	16.345	17.896	17.294	16.593	18.890	18.265
0.15	9.537	13.747	15.297	15.774	16.126	17.626	17.067	16.403	18.618	18.033
0.16	9.476	13.371	14.994	15.512	15.898	17.348	16.832	16.205	18.336	17.793
0.17	9.411	13.006	14.688	15.244	15.662	17.062	16.589	15.998	18.047	17.544
0.18	9.343	12.653	14.378	14.970	15.421	16.771	16.339	15.785	17.751	17.287
0.19	9.272	12.313	14.069	14.692	15.173	16.475	16.083	15.566	17.450	17.025
0.20	9.199	11.987	13.760	14.412	14.922	16.176	15.822	15.342	17.146	16.757
0.22	9.043	11.379	13.150	13.850	14.410	15.574	15.291	14.881	16.529	16.210
0.24	8.877	10.832	12.560	13.292	13.893	14.972	14.752	14.408	15.910	15.653
0.25	8.790	10.580	12.275	13.017	13.634	14.673	14.482	14.170	15.602	15.373
0.26	8.701	10.343	11.997	12.745	13.377	14.377	14.213	13.930	15.296	15.093
0.28	8.518	9.908	11.467	12.217	12.869	13.797	13.680	13.452	14.694	14.537
0.30	8.327	9.524	10.972	11.713	12.374	13.236	13.157	12.979	14.107	13.989
0.32	8.131	9.184	10.515	11.235	11.896	12.697	12.650	12.515	13.541	13.455
0.34	7.929	8.884	10.097	10.787	11.438	12.184	12.162	12.064	12.998	12.938
0.35	7.827	8.746	9.901	10.575	11.218	11.938	11.926	11.844	12.736	12.687
0.36	7.724	8.616	9.715	10.370	11.004	11.698	11.696	11.628	12.481	12.441
0.38	7.516	8.377	9.369	9.984	10.595	11.242	11.254	11.211	11.991	11.967
0.40	7.306	8.162	9.056	9.629	10.212	10.815	10.837	10.815	11.530	11.517
0.42	7.095	7.965	8.773	9.303	9.855	10.417	10.446	10.439	11.096	11.092
0.44	6.884	7.785	8.518	9.006	9.524	10.047	10.080	10.086	10.692	10.692
0.45	6.779	7.699	8.399	8.867	9.368	9.873	9.907	9.917	10.500	10.502
0.46	6.674	7.616	8.287	8.734	9.218	9.706	9.740	9.754	10.315	10.318
0.48	6.465	7.457	8.077	8.487	8.937	9.391	9.426	9.445	9.965	9.969
0.50	6.259	7.305	7.886	8.262	8.678	9.102	9.135	9.158	9.641	9.645
0.55	5.755	6.945	7.474	7.781	8.121	8.477	8.503	8.529	8.935	8.936
0.60	5.277	6.600	7.125	7.389	7.670	7.972	7.990	8.012	8.359	8.354
0.65	4.830	6.259	6.814	7.058	7.298	7.560	7.571	7.588	7.889	7.878
0.70	4.418	5.920	6.523	6.764	6.982	7.216	7.222	7.234	7.501	7.485
0.80	3.701	5.248	5.962	6.231	6.445	6.656	6.658	6.664	6.892	6.870
0.90	3.124	4.608	5.406	5.719	5.961	6.179	6.182	6.189	6.407	6.384
1.00	2.673	4.024	4.859	5.209	5.488	5.728	5.734	5.745	5.973	5.950
1.10	2.326	3.509	4.336	4.710	5.017	5.282	5.291	5.306	5.553	5.531
1.20	2.063	3.070	3.854	4.232	4.556	4.840	4.852	4.870	5.137	5.116
1.30	1.864	2.705	3.423	3.790	4.115	4.411	4.425	4.443	4.727	4.705
1.40	1.712	2.405	3.045	3.390	3.706	4.004	4.017	4.035	4.330	4.307
1.50	1.595	2.162	2.722	3.038	3.335	3.626	3.638	3.655	3.952	3.929
1.60		1.968	2.449	2.732					3.600	
1.70		1.811	2.221	2.470					3.278	
1.80		1.686	2.033	2.250					2.989	
1.90		1.585	1.877	2.064					2.731	
2.00		1.502	1.749	1.909					2.505	

Table 6.1.1.3. *Mean atomic scattering factors for chemically significant ions (cont.)*

Element	V^{5+}	Cr^{2+}	Cr^{3+}	Mn^{2+}	Mn^{3+}	Mn^{4+}	Fe^{2+}	Fe^{3+}	Co^{2+}	Co^{3+}
Z	23	24	24	25	25	25	26	26	27	27
Method	HF	HF	HF	RHF	HF	HF	RHF	RHF	RHF	HF
$(\sin\theta)/\lambda$ (Å^{-1})										
0.00	18.000	22.000	21.000	23.000	22.000	21.000	24.000	23.000	25.000	24.000
0.01	17.993	21.988	20.990	22.988	21.990	20.992	23.989	22.991	24.989	23.990
0.02	17.974	21.952	20.961	22.953	21.961	20.968	23.954	22.962	24.954	23.962
0.03	17.941	21.892	20.913	22.894	21.913	20.927	23.895	22.914	24.897	23.914
0.04	17.895	21.808	20.845	22.812	21.846	20.871	23.814	22.848	24.818	23.848
0.05	17.837	21.702	20.759	22.707	21.760	20.799	23.711	22.763	24.716	23.764
0.06	17.766	21.574	20.655	22.581	21.656	20.712	23.587	22.660	24.593	23.661
0.07	17.682	21.425	20.534	22.433	21.534	20.610	23.441	22.539	24.450	23.541
0.08	17.587	21.256	20.395	22.266	21.395	20.493	23.276	22.401	24.287	23.404
0.09	17.480	21.067	20.240	22.080	21.240	20.363	23.091	22.247	24.104	23.250
0.10	17.362	20.861	20.069	21.875	21.070	20.218	22.889	22.078	23.904	23.081
0.11	17.234	20.638	19.884	21.654	20.884	20.061	22.669	21.893	23.687	22.896
0.12	17.095	20.400	19.685	21.418	20.684	19.891	22.435	21.695	23.455	22.698
0.13	16.946	20.148	19.474	21.167	20.472	19.710	22.185	21.483	23.207	22.486
0.14	16.789	19.884	19.250	20.904	20.247	19.517	21.923	21.258	22.946	22.261
0.15	16.622	19.609	19.016	20.629	20.011	19.315	21.648	21.023	22.673	22.024
0.16	16.448	19.324	18.772	20.344	19.765	19.102	21.363	20.776	22.389	21.777
0.17	16.266	19.030	18.519	20.050	19.509	18.881	21.068	20.521	22.095	21.520
0.18	16.078	18.729	18.258	19.748	19.246	18.652	20.765	20.256	21.791	21.253
0.19	15.883	18.423	17.991	19.440	18.975	18.415	20.455	19.984	21.481	20.978
0.20	15.683	18.112	17.718	19.126	18.697	18.172	20.140	19.705	21.164	20.696
0.22	15.268	17.481	17.157	18.488	18.127	17.669	19.494	19.130	20.514	20.114
0.24	14.839	16.845	16.585	17.841	17.543	17.149	18.838	18.538	19.850	19.513
0.25	14.620	16.527	16.297	17.517	17.247	16.884	18.508	18.238	19.516	19.207
0.26	14.399	16.210	16.008	17.193	16.951	16.617	18.178	17.937	19.180	18.899
0.28	13.955	15.584	15.431	16.551	16.357	16.079	17.520	17.331	18.510	18.280
0.30	13.509	14.972	14.862	15.920	15.768	15.540	16.871	16.727	17.845	17.659
0.32	13.067	14.378	14.303	15.304	15.187	15.005	16.234	16.130	17.191	17.043
0.34	12.631	13.805	13.759	14.707	14.619	14.477	15.614	15.543	16.550	16.435
0.35	12.417	13.528	13.494	14.417	14.341	14.217	15.312	15.254	16.236	16.135
0.36	12.205	13.257	13.234	14.132	14.068	13.961	15.014	14.970	15.927	15.838
0.38	11.792	12.734	12.730	13.581	13.536	13.458	14.436	14.414	15.324	15.258
0.40	11.392	12.238	12.248	13.055	13.024	12.972	13.881	13.877	14.743	14.694
0.42	11.010	11.770	11.790	12.556	12.536	12.504	13.352	13.361	14.186	14.151
0.44	10.644	11.330	11.357	12.083	12.072	12.057	12.848	12.868	13.653	13.629
0.45	10.469	11.121	11.150	11.857	11.848	11.841	12.606	12.630	13.396	13.376
0.46	10.298	10.918	10.950	11.638	11.632	11.630	12.370	12.398	13.146	13.129
0.48	9.970	10.533	10.567	11.219	11.216	11.225	11.919	11.953	12.664	12.652
0.50	9.662	10.174	10.210	10.827	10.826	10.843	11.494	11.531	12.207	12.200
0.55	8.973	9.386	9.419	9.954	9.956	9.982	10.542	10.581	11.176	11.171
0.60	8.396	8.737	8.764	9.229	9.223	9.252	9.737	9.772	10.293	10.286
0.65	7.915	8.205	8.224	8.626	8.615	8.641	9.063	9.092	9.546	9.534
0.70	7.515	7.766	7.779	8.128	8.111	8.132	8.501	8.523	8.917	8.900
0.80	6.888	7.091	7.095	7.365	7.341	7.352	7.640	7.651	7.948	7.921
0.90	6.399	6.578	6.580	6.808	6.779	6.785	7.023	7.026	7.257	7.224
1.00	5.968	6.143	6.145	6.360	6.330	6.334	6.546	6.548	6.739	6.703
1.10	5.556	5.738	5.742	5.963	5.933	5.938	6.144	6.145	6.320	6.283
1.20	5.147	5.341	5.348	5.585	5.555	5.562	5.775	5.778	5.951	5.913
1.30	4.741	4.949	4.958	5.213	5.183	5.193	5.419	5.423	5.605	5.566
1.40	4.344	4.564	4.573	4.846	4.815	4.826	5.068	5.074	5.268	5.228
1.50	3.965	4.191	4.202	4.487	4.454	4.467	4.722	4.729	4.936	4.895
1.60				4.140			4.384	4.392	4.609	
1.70				3.810			4.058	4.066	4.291	
1.80				3.502			3.749	3.757	3.985	
1.90				3.218			3.459	3.467	3.694	
2.00				2.960			3.192	3.199	3.421	

Table 6.1.1.3. *Mean atomic scattering factors for chemically significant ions (cont.)*

Element	Ni^{2+}	Ni^{3+}	Cu^{1+}	Cu^{2+}	Zn^{2+}	Ga^{3+}	Ge^{4+}	Br^{1-}	Rb^{1+}	Sr^{2+}
Z	28	28	29	29	30	31	32	35	37	38
Method	RHF	HF	RHF	HF	RHF	HF	HF	RHF	RHF	RHF
$(\sin\theta)/\lambda$ (Å^{-1})										
0.00	26.000	25.000	28.000	27.000	28.000	28.000	28.000	36.000	36.000	36.000
0.01	25.989	24.991	27.987	26.989	27.989	27.991	27.992	35.961	35.977	35.981
0.02	25.955	24.962	27.946	26.956	27.957	27.964	27.969	35.845	35.908	35.923
0.03	25.899	24.915	27.878	26.901	27.903	27.919	27.931	35.656	35.794	35.827
0.04	25.821	24.850	27.783	26.824	27.828	27.856	27.877	35.398	35.635	35.694
0.05	25.721	24.766	27.663	26.726	27.732	27.776	27.808	35.077	35.435	35.524
0.06	25.600	24.665	27.518	26.608	27.615	27.678	27.724	34.703	35.195	35.320
0.07	25.459	24.546	27.349	26.469	27.479	27.564	27.625	34.282	34.917	35.084
0.08	25.299	24.410	27.157	26.311	27.323	27.433	27.512	33.824	34.605	34.816
0.09	25.119	24.258	26.944	26.134	27.149	27.286	27.386	33.336	34.262	34.520
0.10	24.921	24.090	26.711	25.939	26.958	27.123	27.245	32.827	33.891	34.198
0.11	24.707	23.907	26.459	25.728	26.749	26.946	27.091	32.303	33.496	33.851
0.12	24.477	23.709	26.190	25.500	26.525	26.754	26.924	31.771	33.079	33.484
0.13	24.232	23.498	25.905	25.258	26.286	26.548	26.745	31.236	32.646	33.098
0.14	23.973	23.275	25.606	25.001	26.032	26.330	26.554	30.703	32.199	32.696
0.15	23.702	23.039	25.294	24.732	25.766	26.099	26.351	30.175	31.740	32.281
0.16	23.419	22.792	24.972	24.451	25.488	25.856	26.137	29.657	31.275	31.854
0.17	23.126	22.535	24.639	24.159	25.198	25.603	25.913	29.149	30.805	31.420
0.18	22.824	22.268	24.297	23.857	24.899	25.339	25.680	28.654	30.333	30.979
0.19	22.513	21.993	23.949	23.547	24.591	25.066	25.437	28.172	29.862	30.535
0.20	22.195	21.710	23.594	23.229	24.275	24.784	25.185	27.706	29.393	30.089
0.22	21.543	21.125	22.872	22.574	23.622	24.197	24.658	26.817	28.471	29.198
0.24	20.875	20.518	22.139	21.900	22.949	23.585	24.104	25.988	27.579	28.322
0.25	20.536	20.209	21.770	21.558	22.606	23.270	23.818	25.595	27.147	27.892
0.26	20.197	19.897	21.401	21.214	22.261	22.952	23.526	25.215	26.726	27.469
0.28	19.516	19.268	20.666	20.523	21.566	22.305	22.931	24.491	25.916	26.647
0.30	18.839	18.636	19.939	19.832	20.869	21.649	22.321	23.812	25.150	25.861
0.32	18.169	18.005	19.224	19.146	20.175	20.988	21.702	23.170	24.428	25.113
0.34	17.510	17.380	18.524	18.469	19.488	20.327	21.077	22.559	23.749	24.404
0.35	17.187	17.071	18.180	18.135	19.149	19.997	20.764	22.264	23.424	24.064
0.36	16.867	16.765	17.842	17.805	18.812	19.669	20.451	21.975	23.109	23.734
0.38	16.242	16.164	17.180	17.157	18.150	19.019	19.826	21.412	22.503	23.100
0.40	15.637	15.578	16.541	16.528	17.504	18.379	19.205	20.867	21.929	22.500
0.42	15.054	15.010	15.925	15.919	16.876	17.751	18.593	20.335	21.381	21.931
0.44	14.495	14.463	15.333	15.332	16.269	17.139	17.989	19.816	20.857	21.389
0.45	14.224	14.197	15.047	15.046	15.974	16.839	17.692	19.560	20.603	21.128
0.46	13.959	13.936	14.767	14.767	15.683	16.544	17.398	19.306	20.353	20.872
0.48	13.448	13.432	14.225	14.227	15.120	15.967	16.821	18.806	19.865	20.376
0.50	12.962	12.950	13.710	13.711	14.580	15.409	16.259	18.313	19.391	19.898
0.55	11.854	11.847	12.530	12.526	13.331	14.106	14.929	17.114	18.253	18.765
0.60	10.895	10.887	11.502	11.491	12.227	12.937	13.716	15.964	17.169	17.700
0.65	10.075	10.062	10.614	10.597	11.263	11.902	12.625	14.870	16.127	16.684
0.70	9.378	9.360	9.855	9.831	10.429	10.995	11.656	13.840	15.128	15.707
0.80	8.292	8.265	8.659	8.625	9.097	9.526	10.058	12.002	13.273	13.875
0.90	7.516	7.482	7.797	7.757	8.126	8.441	8.853	10.479	11.645	12.231
1.00	6.944	6.906	7.165	7.123	7.414	7.642	7.956	9.261	10.270	10.805
1.10	6.497	6.457	6.681	6.637	6.879	7.045	7.286	8.311	9.147	9.611
1.20	6.119	6.078	6.285	6.240	6.455	6.582	6.774	7.580	8.251	8.638
1.30	5.776	5.734	5.939	5.892	6.096	6.203	6.365	7.016	7.548	7.862
1.40	5.450	5.407	5.617	5.568	5.775	5.872	6.021	6.573	6.997	7.249
1.50	5.131	5.086	5.307	5.256	5.472	5.569	5.715	6.216	6.561	6.764
0.60	4.816		5.003		5.178			5.913	6.209	6.375
1.70	4.507		4.704		4.890			5.645	5.913	6.056
1.80	4.207		4.411		4.606			5.398	5.656	5.785
1.90	3.918		4.127		4.329			5.162	5.421	5.545
2.00	3.643		3.853		4.059			4.932	5.201	5.324

Table 6.1.1.3. *Mean atomic scattering factors for chemically significant ions (cont.)*

Element	Y^{3+}	Zr^{4+}	Nb^{3+}	Nb^{5+}	Mo^{3+}	Mo^{5+}	Mo^{6+}	Ru^{3+}	Ru^{4+}	Rh^{3+}
Z	39	40	41	41	42	42	42	44	44	45
Method	*DS	*DS	*DS	*DS	*DS	*DS	*DS	*DS	*DS	*DS
$(\sin\theta)/\lambda$ (Å^{-1})										
0.00	36.000	36.000	38.000	36.000	39.000	37.000	36.000	41.000	40.000	42.000
0.01	35.983	35.985	37.981	35.987	38.981	36.986	35.988	40.980	39.983	41.980
0.02	35.933	35.942	37.925	35.948	38.923	36.946	35.954	40.922	39.933	41.922
0.03	35.850	35.869	37.832	35.884	38.827	36.878	35.897	40.824	39.849	41.824
0.04	35.735	35.768	37.702	35.795	38.695	36.783	35.817	40.689	39.733	41.689
0.05	35.588	35.640	37.537	35.681	38.526	36.663	35.715	40.517	39.585	41.516
0.06	35.411	35.484	37.339	35.543	38.323	36.517	35.591	40.309	39.406	41.308
0.07	35.204	35.302	37.109	35.381	38.087	36.347	35.446	40.067	39.197	41.066
0.08	34.970	35.096	36.849	35.197	37.820	36.152	35.280	39.793	38.959	40.791
0.09	34.710	34.865	36.560	34.991	37.523	35.936	35.095	39.489	38.695	40.485
0.10	34.425	34.612	36.246	34.765	37.200	35.697	34.890	39.156	38.404	40.150
0.11	34.118	34.338	35.908	34.519	36.853	35.438	34.667	38.798	38.090	39.789
0.12	33.791	34.045	35.548	34.254	36.483	35.160	34.428	38.416	37.754	39.404
0.13	33.445	33.734	35.170	33.973	36.094	34.865	34.172	38.012	37.397	38.997
0.14	33.082	33.406	34.775	33.675	35.688	34.553	33.900	37.590	37.022	38.569
0.15	32.705	33.064	34.366	33.363	35.266	34.226	33.615	37.151	36.630	38.125
0.16	32.316	32.708	33.945	33.038	34.832	33.886	33.317	36.698	36.223	37.665
0.17	31.916	32.341	33.514	32.701	34.388	33.533	33.006	36.233	35.804	37.193
0.18	31.509	31.964	33.076	32.353	33.936	33.170	32.685	35.758	35.374	36.710
0.19	31.094	31.580	32.632	31.997	33.478	32.798	32.354	35.276	34.934	36.218
0.20	30.675	31.188	32.184	31.632	33.016	32.418	32.015	34.789	34.488	35.720
0.22	29.830	30.392	31.284	30.885	32.086	31.640	31.316	33.804	33.579	34.713
0.24	28.986	29.586	30.388	30.121	31.159	30.847	30.595	32.819	32.659	33.701
0.25	28.567	29.182	29.945	29.736	30.701	30.448	30.229	32.329	32.199	33.198
0.26	28.152	28.781	29.506	29.351	30.246	30.048	29.862	31.844	31.741	32.697
0.28	27.337	27.985	28.646	28.582	29.356	29.252	29.123	30.889	30.833	31.711
0.30	26.548	27.205	27.814	27.821	28.494	28.465	28.387	29.962	29.943	30.751
0.32	25.789	26.447	27.013	27.074	27.664	27.695	27.658	29.067	29.078	29.823
0.34	25.063	25.716	26.248	26.346	26.871	26.944	26.941	28.210	28.242	28.932
0.35	24.712	25.360	25.878	25.990	26.488	26.578	26.589	27.796	27.836	28.500
0.36	24.370	25.012	25.518	25.640	26.115	26.218	26.241	27.392	27.439	28.079
0.38	23.712	24.339	24.824	24.960	25.397	25.518	25.562	26.614	26.671	27.268
0.40	23.086	23.696	24.167	24.306	24.717	24.847	24.904	25.878	25.940	26.499
0.42	22.492	23.083	23.543	23.680	24.073	24.205	24.270	25.181	25.245	25.772
0.44	21.927	22.500	22.953	23.081	23.464	23.592	23.662	24.524	24.586	25.086
0.45	21.654	22.218	22.669	22.792	23.172	23.296	23.366	24.209	24.271	24.757
0.46	21.388	21.944	22.393	22.509	22.888	23.007	23.078	23.904	23.963	24.438
0.48	20.874	21.414	21.861	21.963	22.342	22.450	22.518	23.319	23.374	23.829
0.50	20.382	20.907	21.355	21.442	21.825	21.920	21.983	22.767	22.817	23.254
0.55	19.231	19.731	20.187	20.235	20.638	20.697	20.744	21.516	21.549	21.957
0.60	18.166	18.658	19.128	19.142	19.573	19.599	19.627	20.416	20.434	20.826
0.65	17.163	17.659	18.148	18.137	18.597	18.598	18.608	19.430	19.436	19.824
0.70	16.208	16.716	17.224	17.198	17.685	17.668	17.664	18.528	18.525	18.918
0.80	14.415	14.952	15.492	15.458	15.985	15.955	15.937	16.884	16.872	17.292
0.90	12.784	13.333	13.886	13.858	14.405	14.377	14.357	15.367	15.354	15.807
1.00	11.340	11.873	12.414	12.395	12.939	12.918	12.902	13.939	13.929	14.407
1.10	10.100	10.592	11.099	11.088	11.606	11.593	11.581	12.605	12.597	13.086
1.20	9.067	9.501	9.958	9.951	10.427	10.418	10.411	11.382	11.378	11.859
1.30	8.225	8.595	8.992	8.988	9.410	9.405	9.400	10.291	10.288	10.744
1.40	7.548	7.856	8.193	8.190	8.554	8.551	8.547	9.339	9.338	9.756
1.50	7.008	7.261	7.541	7.539	7.846	7.843	7.841	8.528	8.527	8.899
1.60	6.575	6.782	7.013	7.011	7.267	7.265	7.263	7.847	7.846	8.171
1.70	6.222	6.394	6.584	6.583	6.795	6.793	6.792	7.282	7.282	7.559
1.80	5.927	6.074	6.234	6.233	6.409	6.408	6.407	6.817	6.817	7.051
1.90	5.672	5.802	5.941	5.940	6.090	6.089	6.089	6.433	6.433	6.631
2.00	5.443	5.565	5.689	5.690	5.820	5.820	5.820	6.114	6.114	6.281

Table 6.1.1.3. *Mean atomic scattering factors for chemically significant ions (cont.)*

Element	Rh^{4+}	Pd^{2+}	Pd^{4+}	Ag^{1+}	Ag^{2+}	Cd^{2+}	In^{3+}	Sn^{2+}	Sn^{4+}	Sb^{3+}
Z	45	46	46	47	47	48	49	50	50	51
Method	*DS	*DS	*DS	*DS	*DS	*DS	*DS	RHF	RHF	*DS
$(\sin\theta)/\lambda$ (Å^{-1})										
0.00	41.000	44.000	42.000	46.000	45.000	46.000	46.000	48.000	46.000	48.000
0.01	40.983	43.977	41.983	45.974	44.978	45.978	45.981	47.975	45.984	47.978
0.02	40.932	43.909	41.932	45.894	44.911	45.912	45.924	47.898	45.934	47.911
0.03	40.848	43.796	41.847	45.764	44.799	45.802	45.829	47.771	45.852	47.801
0.04	40.730	43.640	41.729	45.582	44.645	45.650	45.697	47.596	45.737	47.647
0.05	40.581	43.441	41.579	45.353	44.448	45.456	45.529	47.373	45.590	47.452
0.06	40.400	43.201	41.396	45.076	44.211	45.222	45.325	47.106	45.411	47.218
0.07	40.188	42.923	41.184	44.757	43.936	44.950	45.087	46.797	45.203	46.945
0.08	39.948	42.608	40.942	44.397	43.624	44.641	44.816	46.449	44.964	46.636
0.09	39.680	42.258	40.671	43.999	43.277	44.298	44.513	46.066	44.698	46.293
0.10	39.385	41.877	40.375	43.567	42.898	43.923	44.181	45.650	44.404	45.920
0.11	39.067	41.467	40.053	43.105	42.490	43.517	43.821	45.206	44.084	45.517
0.12	38.725	41.031	39.708	42.616	42.056	43.085	43.435	44.736	43.739	45.089
0.13	38.363	40.572	39.341	42.103	41.597	42.628	43.024	44.244	43.371	44.638
0.14	37.981	40.092	38.955	41.570	41.117	42.148	42.591	43.733	42.981	44.167
0.15	37.582	39.595	38.551	41.020	40.618	41.649	42.138	43.206	42.572	43.677
0.16	37.168	39.083	38.131	40.457	40.103	41.134	41.667	42.667	42.143	43.172
0.17	36.740	38.558	37.696	39.883	39.575	40.603	41.180	42.117	41.698	42.655
0.18	36.301	38.024	37.249	39.301	39.036	40.061	40.678	41.560	41.237	42.127
0.19	35.852	37.483	36.792	38.713	38.489	39.509	40.165	40.998	40.763	41.590
0.20	35.395	36.936	36.326	38.122	37.935	38.949	39.641	40.431	40.276	41.047
0.22	34.463	35.836	35.374	36.940	36.817	37.816	38.570	39.296	39.274	39.950
0.24	33.518	34.739	34.406	35.768	35.697	36.677	37.481	38.164	38.242	38.847
0.25	33.045	34.195	33.921	35.191	35.141	36.110	36.933	37.604	37.718	38.298
0.26	32.572	33.657	33.435	34.620	34.589	35.545	36.385	37.047	37.192	37.750
0.28	31.635	32.601	32.471	33.503	33.502	34.431	35.295	35.950	36.135	36.668
0.30	30.715	31.577	31.521	32.424	32.445	33.344	34.220	34.878	35.082	35.605
0.32	29.819	30.592	30.594	31.389	31.425	32.291	33.167	33.836	34.041	34.569
0.34	28.951	29.649	29.695	30.400	30.446	31.276	32.145	32.826	33.019	33.561
0.35	28.530	29.194	29.257	29.924	29.973	30.785	31.647	32.333	32.517	33.069
0.36	28.117	28.751	28.828	29.460	29.511	30.305	31.158	31.850	32.023	32.585
0.38	27.318	27.899	27.998	28.569	28.622	29.379	30.209	30.910	31.057	31.643
0.40	26.557	27.093	27.204	27.727	27.780	28.500	29.302	30.008	30.127	30.737
0.42	25.833	26.333	26.450	26.933	26.984	27.667	28.438	29.144	29.235	29.866
0.44	25.148	25.617	25.735	26.186	26.233	26.881	27.618	28.318	28.383	29.031
0.45	24.819	25.275	25.391	25.829	25.874	26.505	27.224	27.920	27.972	28.628
0.46	24.499	24.944	25.057	25.484	25.527	26.140	26.842	27.532	27.571	28.234
0.48	23.886	24.311	24.418	24.825	24.863	25.443	26.109	26.785	26.802	27.472
0.50	23.307	23.716	23.814	24.206	24.239	24.788	25.418	26.075	26.074	26.747
0.55	21.995	22.378	22.450	22.817	22.839	23.319	23.865	24.464	24.430	25.088
0.60	20.850	21.221	21.267	21.623	21.635	22.061	22.533	23.067	23.019	23.634
0.65	19.835	20.205	20.228	20.583	20.588	20.974	21.389	21.859	21.810	22.367
0.70	18.919	19.295	19.300	19.660	19.660	20.021	20.394	20.810	20.767	21.261
0.80	17.282	17.683	17.668	18.051	18.046	18.392	18.724	19.074	19.052	19.433
0.90	15.795	16.229	16.208	16.622	16.616	16.979	17.315	17.649	17.646	17.957
1.00	14.396	14.859	14.840	15.284	15.278	15.673	16.034	16.386	16.395	16.684
1.10	13.078	13.557	13.542	14.006	14.002	14.425	14.818	15.203	15.215	15.516
1.20	11.853	12.331	12.321	12.790	12.788	13.230	13.649	14.063	14.074	14.403
1.30	10.740	11.201	11.194	11.654	11.653	12.099	12.530	12.962	12.970	13.329
1.40	9.754	10.183	10.180	10.616	10.616	11.050	11.479	11.913	11.917	12.300
1.50	8.898	9.288	9.286	9.688	9.688	10.098	10.510	10.932	10.933	11.326
1.60	8.170	8.514	8.513	8.875	8.876	9.251	9.637	10.033	10.033	10.422
1.70	7.559	7.858	7.857	8.176	8.176	8.513	8.864	9.227	9.225	9.599
1.80	7.051	7.307	7.306	7.582	7.582	7.878	8.191	8.515	8.513	8.863
1.90	6.630	6.847	6.847	7.083	7.083	7.339	7.613	7.897	7.896	8.215
2.00	6.281	6.464	6.464	6.665	6.665	6.884	7.122	7.367	7.366	7.652

Table 6.1.1.3. *Mean atomic scattering factors for chemically significant ions (cont.)*

Element	Sb^{5+}	I^{1-}	Cs^{1+}	Ba^{2+}	La^{3+}	Ce^{3+}	Ce^{4+}	Pr^{3+}	Pr^{4+}	Nd^{3+}
Z	51	53	55	56	57	58	58	59	59	60
Method	*DS	RHF	RHF	*DS	*DS	*DS	*DS	*DS	*DS	*DS
$(\sin\theta)/\lambda$ (Å^{-1})										
0.00	46.000	54.000	54.000	54.000	54.000	55.000	54.000	56.000	55.000	57.000
0.01	45.985	53.943	53.963	53.967	53.971	54.972	53.974	55.972	54.975	56.972
0.02	45.940	53.772	53.850	53.869	53.885	54.886	53.897	55.888	54.898	56.889
0.03	45.865	53.493	53.665	53.708	53.742	54.745	53.769	55.748	54.772	56.752
0.04	45.760	53.114	53.408	53.484	53.544	54.549	53.592	55.555	54.597	56.561
0.05	45.627	52.646	53.084	53.200	53.293	54.300	53.366	55.309	54.373	56.318
0.06	45.464	52.101	52.698	52.861	52.991	54.001	53.094	55.013	54.104	56.026
0.07	45.274	51.492	52.254	52.468	52.640	53.654	52.778	54.669	53.791	55.686
0.08	45.057	50.834	51.758	52.027	52.245	53.261	52.420	54.280	53.436	55.302
0.09	44.813	50.136	51.217	51.543	51.808	52.827	52.022	53.850	53.042	54.876
0.10	44.544	49.413	50.635	51.018	51.332	52.355	51.589	53.381	52.612	54.411
0.11	44.251	48.672	50.020	50.460	50.823	51.848	51.122	52.878	52.148	53.911
0.12	43.935	47.924	49.377	49.872	50.284	51.310	50.625	52.343	51.654	53.380
0.13	43.596	47.175	48.714	49.259	49.718	50.745	50.102	51.781	51.133	52.821
0.14	43.237	46.432	48.035	48.627	49.130	50.158	49.555	51.195	50.588	52.237
0.15	42.859	45.698	47.345	47.980	48.524	49.551	48.988	50.589	50.022	51.632
0.16	42.462	44.978	46.651	47.322	47.903	48.928	48.404	49.966	49.439	51.010
0.17	42.049	44.273	45.955	46.657	47.272	48.294	47.807	49.331	48.841	50.374
0.18	41.621	43.585	45.262	45.989	46.633	47.651	47.199	48.686	48.231	49.727
0.19	41.178	42.916	44.575	45.321	45.989	47.002	46.583	48.034	47.613	49.073
0.20	40.723	42.265	43.897	44.657	45.344	46.351	45.963	47.378	46.989	48.414
0.22	39.781	41.019	42.577	43.348	44.061	45.052	44.718	46.066	45.733	47.091
0.24	38.806	39.841	41.312	42.077	42.801	43.771	43.481	44.767	44.481	45.778
0.25	38.309	39.276	40.703	41.459	42.183	43.142	42.871	44.128	43.861	45.129
0.26	37.807	38.726	40.110	40.855	41.576	42.522	42.268	43.497	43.248	44.489
0.28	36.796	37.665	38.971	39.688	40.396	41.315	41.088	42.266	42.046	43.235
0.30	35.780	36.650	37.893	38.579	39.267	40.157	39.950	41.080	40.882	42.025
0.32	34.770	35.676	36.872	37.525	38.190	39.050	38.859	39.945	39.763	40.863
0.34	33.771	34.735	35.902	36.525	37.166	37.996	37.817	38.860	38.692	39.750
0.35	33.278	34.276	35.434	36.043	36.673	37.488	37.314	38.337	38.174	39.213
0.36	32.790	33.824	34.977	35.574	36.192	36.992	36.823	37.826	37.669	38.688
0.38	31.834	32.941	34.091	34.668	35.266	36.037	35.877	36.842	36.693	37.675
0.40	30.905	32.082	33.240	33.802	34.384	35.127	34.977	35.903	35.763	36.708
0.42	30.009	31.248	32.419	32.972	33.541	34.258	34.118	35.007	34.876	35.785
0.44	29.146	30.437	31.625	32.173	32.734	33.427	33.298	34.150	34.028	34.903
0.45	28.729	30.040	31.238	31.785	32.342	33.025	32.901	33.736	33.619	34.476
0.46	28.321	29.650	30.856	31.403	31.959	32.630	32.513	33.329	33.218	34.057
0.48	27.532	28.887	30.110	30.659	31.212	31.863	31.759	32.541	32.440	33.246
0.50	26.782	28.149	29.385	29.939	30.492	31.124	31.034	31.782	31.693	32.465
0.55	25.073	26.418	27.664	28.231	28.789	29.382	29.329	29.996	29.939	30.631
0.60	23.590	24.855	26.074	26.649	27.211	27.771	27.753	28.348	28.323	28.943
0.65	22.310	23.460	24.620	25.189	25.748	26.278	26.290	26.822	26.826	27.380
0.70	21.205	22.227	23.303	23.854	24.398	24.899	24.933	25.411	25.437	25.936
0.80	19.397	20.191	21.071	21.555	22.039	22.479	22.532	22.927	22.976	23.387
0.90	17.947	18.598	19.309	19.709	20.117	20.495	20.543	20.881	20.927	21.275
1.00	16.690	17.292	17.900	18.227	18.568	18.892	18.926	19.222	19.256	19.559
1.10	15.529	16.150	16.721	17.003	17.299	17.585	17.605	17.874	17.895	18.166
1.20	14.416	15.091	15.676	15.941	16.218	16.485	16.495	16.749	16.760	17.012
1.30	13.339	14.072	14.701	14.970	15.249	15.513	15.519	15.769	15.775	16.020
1.40	12.305	13.082	13.760	14.048	14.341	14.614	14.620	14.875	14.880	15.126
1.50	11.328	12.126	12.844	13.154	13.467	13.754	13.763	14.027	14.034	14.288
1.60	10.422	11.214	11.956	12.285	12.616	12.919	12.931	13.207	13.217	13.481
1.70	9.597	10.360	11.104	11.447	11.791	12.105	12.120	12.407	12.419	12.695
1.80	8.860	9.577	10.302	10.649	10.997	11.319	11.335	11.629	11.644	11.928
1.90	8.213	8.868	9.559	9.902	10.246	10.568	10.585	10.881	10.897	11.186
2.00	7.650	8.239	8.882	9.213	9.545	9.860	9.877	10.171	10.187	10.476

Table 6.1.1.3. *Mean atomic scattering factors for chemically significant ions (cont.)*

Element	Pm^{3+}	Sm^{3+}	Eu^{2+}	Eu^{3+}	Gd^{3+}	Tb^{3+}	Dy^{3+}	Ho^{3+}	Er^{3+}	Tm^{3+}
Z	61	62	63	63	64	65	66	67	68	69
Method	*DS	*DS	*DS	*DS	*DS	*DS	*DS	*DS	*DS	*DS
$(\sin\theta)/\lambda$ (Å^{-1})										
0.00	58.000	59.000	61.000	60.000	61.000	62.000	63.000	64.000	65.000	66.000
0.01	57.973	58.973	60.970	59.973	60.974	61.974	62.975	63.975	64.975	65.976
0.02	57.891	58.892	60.881	59.894	60.895	61.896	62.898	63.900	64.901	65.903
0.03	57.755	58.759	60.732	59.762	60.765	61.767	62.772	63.775	64.779	65.782
0.04	57.567	58.573	60.527	59.579	60.585	61.588	62.596	63.602	64.608	65.613
0.05	57.328	58.337	60.266	59.347	60.355	61.360	62.373	63.382	64.391	65.399
0.06	57.039	58.052	59.952	59.066	60.077	61.086	62.102	63.115	64.128	65.139
0.07	56.704	57.721	59.587	58.739	59.754	60.766	61.787	62.804	63.821	64.836
0.08	56.324	57.345	59.175	58.368	59.387	60.403	61.429	62.451	63.472	64.491
0.09	55.902	56.929	58.718	57.956	58.980	60.000	61.031	62.058	63.083	64.107
0.10	55.442	56.473	58.222	57.505	58.534	59.559	60.595	61.626	62.657	63.685
0.11	54.947	55.982	57.688	57.019	58.053	59.082	60.124	61.160	62.195	63.228
0.12	54.420	55.460	57.122	56.501	57.539	58.574	59.620	60.660	61.701	62.739
0.13	53.864	54.908	56.527	55.954	56.996	58.036	59.086	60.131	61.176	62.219
0.14	53.284	54.330	55.906	55.380	56.427	57.471	58.525	59.574	60.624	61.671
0.15	52.681	53.731	55.264	54.784	55.834	56.883	57.940	58.993	60.047	61.099
0.16	52.061	53.112	54.604	54.168	55.222	56.274	57.334	58.391	59.448	60.504
0.17	51.425	52.478	53.930	53.536	54.592	55.647	56.710	57.769	58.830	59.889
0.18	50.778	51.831	53.245	52.890	53.948	55.006	56.070	57.132	58.196	59.258
0.19	50.122	51.175	52.552	52.234	53.292	54.353	55.417	56.481	57.547	58.611
0.20	49.461	50.512	51.854	51.570	52.628	53.689	54.754	55.819	56.886	57.953
0.22	48.130	49.175	50.454	50.228	51.283	52.344	53.407	54.471	55.540	56.608
0.24	46.804	47.839	49.062	48.884	49.933	50.989	52.046	53.107	54.174	55.241
0.25	46.148	47.176	48.374	48.216	49.260	50.312	51.366	52.424	53.489	54.554
0.26	45.499	46.519	47.694	47.553	48.591	49.639	50.688	51.742	52.804	53.866
0.28	44.226	45.228	46.361	46.246	47.270	48.306	49.344	50.389	51.442	52.498
0.30	42.993	43.975	45.069	44.973	45.980	47.001	48.025	49.057	50.099	51.145
0.32	41.805	42.764	43.825	43.741	44.728	45.731	46.738	47.755	48.783	49.817
0.34	40.666	41.600	42.629	42.553	43.519	44.501	45.489	46.489	47.501	48.520
0.35	40.115	41.036	42.050	41.977	42.931	43.902	44.880	45.871	46.874	47.884
0.36	39.576	40.484	41.484	41.412	42.354	43.314	44.282	45.263	46.256	47.258
0.38	38.534	39.416	40.387	40.319	41.236	42.172	43.118	44.078	45.052	46.035
0.40	37.540	38.395	39.338	39.271	40.163	41.075	41.998	42.936	43.889	44.853
0.42	36.590	37.418	38.333	38.268	39.135	40.021	40.921	41.837	42.768	43.711
0.44	35.681	36.483	37.371	37.307	38.149	39.010	39.887	40.780	41.689	42.611
0.45	35.241	36.031	36.904	36.842	37.671	38.520	39.385	40.267	41.164	42.075
0.46	34.810	35.587	36.447	36.386	37.203	38.040	38.893	39.764	40.649	41.550
0.48	33.975	34.728	35.560	35.503	36.295	37.108	37.938	38.786	39.649	40.527
0.50	33.172	33.902	34.707	34.653	35.423	36.212	37.019	37.844	38.685	39.542
0.55	31.287	31.965	32.702	32.663	33.379	34.113	34.866	35.637	36.424	37.228
0.60	29.555	30.188	30.861	30.838	31.506	32.191	32.894	33.615	34.352	35.106
0.65	27.955	28.547	29.160	29.155	29.779	30.420	31.078	31.753	32.444	33.151
0.70	26.475	27.029	27.589	27.599	28.183	28.784	29.400	30.032	30.680	31.344
0.80	23.858	24.342	24.811	24.840	25.351	25.876	26.416	26.970	27.540	28.123
0.90	21.681	22.098	22.494	22.528	22.969	23.424	23.892	24.374	24.870	25.380
1.00	19.905	20.260	20.599	20.626	21.003	21.392	21.793	22.207	22.634	23.074
1.10	18.464	18.768	19.061	19.080	19.400	19.730	20.072	20.424	20.787	21.163
1.20	17.277	17.544	17.805	17.815	18.092	18.373	18.666	18.966	19.276	19.595
1.30	16.267	16.512	16.753	16.758	17.004	17.252	17.508	17.768	18.035	18.309
1.40	15.370	15.607	15.839	15.840	16.071	16.298	16.531	16.764	17.000	17.241
1.50	14.538	14.778	15.010	15.011	15.237	15.457	15.678	15.896	16.114	16.332
1.60	13.743	13.993	14.231	14.233	14.463	14.685	14.904	15.118	15.327	15.534
1.70	12.970	13.232	13.480	13.483	13.724	13.953	14.178	14.394	14.604	14.809
1.80	12.215	12.490	12.748	12.753	13.005	13.245	13.479	13.703	13.919	14.127
1.90	11.481	11.765	12.032	12.039	12.302	12.554	12.798	13.032	13.257	13.473
2.00	10.774	11.063	11.336	11.344	11.616	11.878	12.132	12.376	12.610	12.836

Table 6.1.1.3. *Mean atomic scattering factors for chemically significant ions (cont.)*

Element	Yb^{2+}	Yb^{3+}	Lu^{3+}	Hf^{4+}	Ta^{5+}	W^{6+}	Os^{4+}	Ir^{3+}	Ir^{4+}	Pt^{2+}
Z	70	70	71	72	73	74	76	77	77	78
Method	*DS	*DS	*DS	*DS	*DS	*DS	*DS	*DS	*DS	*DS
$(\sin\theta)/\lambda$ (Å^{-1})										
0.00	68.000	67.000	68.000	68.000	68.000	68.000	72.000	74.000	73.000	76.000
0.01	67.973	66.976	67.976	67.979	67.981	67.982	71.976	73.972	72.975	75.968
0.02	67.892	66.904	67.905	67.915	67.922	67.929	71.904	73.889	72.902	75.874
0.03	67.759	66.785	67.788	67.809	67.826	67.840	71.784	73.752	72.780	75.717
0.04	67.573	66.619	67.624	67.661	67.691	67.716	71.617	73.561	72.611	75.499
0.05	67.337	66.407	67.415	67.472	67.519	67.557	71.404	73.318	72.395	75.222
0.06	67.051	66.151	67.161	67.243	67.309	67.365	71.147	73.024	72.133	74.889
0.07	66.719	65.851	66.866	66.976	67.065	67.139	70.847	72.682	71.828	74.502
0.08	66.342	65.511	66.529	66.670	66.785	66.881	70.506	72.294	71.481	74.065
0.09	65.922	65.131	66.154	66.329	66.471	66.592	70.125	71.863	71.094	73.580
0.10	65.464	64.714	65.741	65.953	66.126	66.272	69.707	71.392	70.669	73.052
0.11	64.968	64.262	65.294	65.544	65.749	65.923	69.254	70.883	70.208	72.485
0.12	64.439	63.777	64.814	65.103	65.343	65.546	68.769	70.339	69.715	71.881
0.13	63.879	63.262	64.303	64.634	64.908	65.142	68.253	69.764	69.190	71.245
0.14	63.292	62.719	63.765	64.138	64.448	64.713	67.711	69.162	68.638	70.582
0.15	62.679	62.151	63.201	63.616	63.963	64.260	67.143	68.534	68.060	69.894
0.16	62.046	61.561	62.615	63.071	63.455	63.785	66.552	67.884	67.460	69.185
0.17	61.393	60.950	62.008	62.505	62.926	63.290	65.942	67.215	66.839	68.459
0.18	60.724	60.321	61.383	61.921	62.378	62.775	65.313	66.530	66.200	67.719
0.19	60.043	59.678	60.742	61.319	61.812	62.242	64.670	65.832	65.546	66.968
0.20	59.350	59.022	60.088	60.703	61.231	61.693	64.014	65.123	64.879	66.210
0.22	57.943	57.679	58.749	59.433	60.028	60.553	62.671	63.684	63.515	64.679
0.24	56.521	56.312	57.382	58.127	58.783	59.367	61.302	62.228	62.124	63.144
0.25	55.809	55.624	56.693	57.465	58.149	58.760	60.612	61.500	61.423	62.381
0.26	55.098	54.935	56.002	56.799	57.509	58.146	59.920	60.773	60.721	61.621
0.28	53.687	53.560	54.622	55.460	56.216	56.901	58.537	59.328	59.319	60.121
0.30	52.297	52.198	53.253	54.123	54.917	55.643	57.164	57.905	57.927	58.652
0.32	50.937	50.858	51.903	52.796	53.620	54.381	55.809	56.510	56.555	57.220
0.34	49.611	49.548	50.580	51.487	52.334	53.122	54.478	55.148	55.209	55.830
0.35	48.962	48.904	49.930	50.842	51.696	52.496	53.823	54.481	54.548	55.151
0.36	48.323	48.270	49.288	50.203	51.064	51.873	53.175	53.823	53.894	54.483
0.38	47.076	47.030	48.032	48.947	49.817	50.641	51.906	52.538	52.613	53.182
0.40	45.871	45.828	46.813	47.723	48.597	49.430	50.671	51.293	51.369	51.925
0.42	44.707	44.667	45.633	46.534	47.406	48.244	49.473	50.089	50.163	50.714
0.44	43.585	43.545	44.491	45.381	46.247	47.086	48.312	48.926	48.995	49.545
0.45	43.038	42.999	43.935	44.818	45.681	46.518	47.745	48.359	48.425	48.977
0.46	42.502	42.463	43.389	44.265	45.122	45.957	47.187	47.802	47.865	48.419
0.48	41.458	41.419	42.325	43.184	44.031	44.860	46.099	46.717	46.773	47.333
0.50	40.450	40.412	41.297	42.140	42.974	43.795	45.046	45.668	45.717	46.286
0.55	38.080	38.046	38.880	39.680	40.479	41.271	42.562	43.197	43.227	43.820
0.60	35.901	35.874	36.658	37.419	38.181	38.942	40.270	40.918	40.932	41.549
0.65	33.890	33.873	34.610	35.335	36.064	36.793	38.147	38.805	38.807	39.443
0.70	32.029	32.022	32.716	33.409	34.106	34.806	36.172	36.835	36.830	37.479
0.80	28.709	28.722	29.335	29.970	30.612	31.258	32.602	33.261	33.249	33.905
0.90	25.880	25.904	26.442	27.018	27.605	28.199	29.471	30.104	30.094	30.732
1.00	23.501	23.527	23.994	24.506	25.033	25.572	26.734	27.324	27.317	27.918
1.10	21.528	21.551	21.952	22.396	22.858	23.336	24.368	24.902	24.898	25.447
1.20	19.908	19.926	20.267	20.645	21.042	21.456	22.350	22.821	22.820	23.307
1.30	18.580	18.591	18.883	19.202	19.538	19.890	20.652	21.057	21.058	21.481
1.40	17.480	17.486	17.738	18.009	18.293	18.592	19.234	19.579	19.581	19.942
1.50	16.550	16.553	16.777	17.011	17.255	17.510	18.054	18.347	18.348	18.654
1.60	15.740	15.741	15.947	16.158	16.374	16.597	17.066	17.315	17.317	17.578
1.70	15.009	15.010	15.208	15.406	15.605	15.808	16.225	16.443	16.444	16.670
1.80	14.330	14.330	14.528	14.722	14.914	15.106	15.493	15.691	15.691	15.893
1.90	13.681	13.682	13.884	14.081	14.274	14.463	14.838	15.024	15.024	15.211
2.00	13.051	13.053	13.263	13.467	13.666	13.858	14.234	14.417	14.416	14.597

Table 6.1.1.3. *Mean atomic scattering factors for chemically significant ions (cont.)*

Element	Pt^{4+}	Au^{1+}	Au^{3+}	Hg^{1+}	Hg^{2+}	Tl^{1+}	Tl^{3+}	Pb^{2+}	Pb^{4+}	Bi^{3+}
Z	78	79	79	80	80	81	81	82	82	83
Method	*DS	*DS	*DS	*DS	*DS	*DS	*DS	*DS	*DS	*DS
$(\sin\theta)/\lambda$ (Å^{-1})										
0.00	74.000	78.000	76.000	79.000	78.000	80.000	78.000	80.000	78.000	80.000
0.01	73.975	77.964	75.972	78.962	77.968	79.961	77.975	79.966	77.975	79.969
0.02	73.901	77.855	75.888	78.850	77.875	79.845	77.891	79.864	77.899	79.878
0.03	73.778	77.676	75.750	78.664	77.719	79.653	77.753	79.695	77.774	79.727
0.04	73.606	77.428	75.557	78.406	77.503	79.388	77.560	79.461	77.599	79.516
0.05	73.387	77.113	75.311	78.080	77.229	79.052	77.314	79.164	77.376	79.249
0.06	73.123	76.736	75.015	77.689	76.897	78.650	77.017	78.807	77.106	78.926
0.07	72.814	76.299	74.669	77.238	76.512	78.186	76.670	78.392	76.790	78.550
0.08	72.462	75.807	74.276	76.731	76.076	77.665	76.276	77.924	76.430	78.124
0.09	72.070	75.264	73.839	76.173	75.591	77.093	75.836	77.406	76.028	77.651
0.10	71.639	74.676	73.361	75.570	75.062	76.474	75.355	76.843	75.586	77.134
0.11	71.173	74.046	72.843	74.925	74.492	75.814	74.833	76.238	75.106	76.577
0.12	70.673	73.380	72.290	74.245	73.884	75.119	74.275	75.597	74.590	75.983
0.13	70.141	72.683	71.705	73.535	73.243	74.394	73.683	74.922	74.041	75.355
0.14	69.581	71.958	71.089	72.798	72.571	73.644	73.060	74.220	73.461	74.698
0.15	68.995	71.211	70.448	72.041	71.874	72.873	72.409	73.493	72.853	74.014
0.16	68.386	70.446	69.783	71.266	71.153	72.085	71.733	72.745	72.220	73.308
0.17	67.756	69.665	69.097	70.477	70.413	71.286	71.035	71.981	71.563	72.581
0.18	67.107	68.874	68.395	69.679	69.658	70.477	70.319	71.204	70.885	71.839
0.19	66.443	68.075	67.678	68.874	68.889	69.663	69.586	70.417	70.190	71.083
0.20	65.766	67.271	66.949	68.065	68.111	68.847	68.841	69.623	69.479	70.317
0.22	64.380	65.658	65.466	66.445	66.536	67.214	67.320	68.023	68.020	68.764
0.24	62.968	64.054	63.965	64.836	64.952	65.597	65.776	66.425	66.527	67.199
0.25	62.256	63.260	63.213	64.040	64.162	64.797	65.001	65.631	65.772	66.416
0.26	61.543	62.472	62.462	63.251	63.376	64.005	64.226	64.841	65.015	65.636
0.28	60.119	60.923	60.969	61.698	61.821	62.448	62.685	63.284	63.501	64.090
0.30	58.707	59.413	59.499	60.184	60.296	60.931	61.163	61.759	61.995	62.569
0.32	57.315	57.947	58.058	58.714	58.810	59.458	59.670	60.275	60.509	61.081
0.34	55.951	56.529	56.653	57.290	57.367	58.031	58.214	58.833	59.052	59.631
0.35	55.281	55.839	55.965	56.596	56.663	57.335	57.502	58.128	58.336	58.922
0.36	54.619	55.161	55.288	55.914	55.972	56.651	56.800	57.436	57.629	58.223
0.38	53.323	53.841	53.967	54.586	54.625	55.318	55.432	56.085	56.247	56.858
0.40	52.065	52.571	52.689	53.306	53.327	54.032	54.110	54.781	54.908	55.538
0.42	50.847	51.348	51.457	52.073	52.079	52.792	52.837	53.523	53.614	54.263
0.44	49.669	50.172	50.269	50.885	50.879	51.596	51.613	52.309	52.367	53.033
0.45	49.095	49.600	49.691	50.308	50.296	51.015	51.018	51.719	51.762	52.435
0.46	48.531	49.040	49.124	49.742	49.725	50.444	50.435	51.140	51.167	51.847
0.48	47.431	47.950	48.021	48.640	48.615	49.332	49.304	50.013	50.014	50.704
0.50	46.370	46.899	46.958	47.578	47.548	48.261	48.217	48.927	48.905	49.602
0.55	43.871	44.432	44.464	45.085	45.050	45.742	45.677	46.377	46.318	47.018
0.60	41.573	42.163	42.175	42.795	42.764	43.429	43.364	44.040	43.969	44.653
0.65	39.447	40.062	40.060	40.679	40.656	41.294	41.241	41.888	41.822	42.481
0.70	37.470	38.103	38.093	38.709	38.696	39.311	39.275	39.895	39.844	40.473
0.80	33.885	34.534	34.518	35.131	35.133	35.718	35.714	36.293	36.278	36.857
0.90	30.713	31.352	31.338	31.944	31.952	32.523	32.538	33.096	33.108	33.657
1.00	27.905	28.513	28.504	29.090	29.100	29.659	29.679	30.227	30.249	30.784
1.10	25.440	26.000	25.996	26.549	26.557	27.097	27.114	27.648	27.669	28.194
1.20	23.305	23.807	23.806	24.315	24.319	24.828	24.839	25.349	25.364	25.871
1.30	21.482	21.921	21.923	22.378	22.379	22.846	22.850	23.325	23.332	23.811
1.40	19.945	20.322	20.325	20.723	20.722	21.139	21.138	21.568	21.568	22.009
1.50	18.658	18.978	18.981	19.324	19.322	19.686	19.682	20.062	20.058	20.453
1.60	17.580	17.853	17.856	18.148	18.146	18.460	18.454	18.784	18.778	19.124
1.70	16.672	16.907	16.909	17.160	17.157	17.426	17.420	17.705	17.697	17.997
1.80	15.894	16.101	16.102	16.320	16.319	16.550	16.546	16.790	16.784	17.043
1.90	15.211	15.401	15.401	15.597	15.596	15.800	15.797	16.010	16.005	16.229
2.00	14.596	14.777	14.777	14.958	14.958	15.143	15.141	15.332	15.329	15.527

Table 6.1.1.3. *Mean atomic scattering factors for chemically significant ions (cont.)*

Element	Bi^{5+}	Ra^{2+}	Ac^{3+}	Th^{4+}	U^{3+}	U^{4+}	U^{6+}	Np^{3+}	Np^{4+}	Np^{6+}
Z	83	88	89	90	92	92	92	93	93	93
Method	*DS	*DS	*DS	*DS	*DS	*DS	*DS	*DS	*DS	*DS
$(\sin\theta)/\lambda$ (Å^{-1})										
0.00	78.000	86.000	86.000	86.000	89.000	88.000	86.000	90.000	89.000	87.000
0.01	77.977	85.957	85.961	85.965	88.961	87.965	85.970	89.962	88.965	86.970
0.02	77.908	85.829	85.846	85.860	88.846	87.860	85.881	89.847	88.860	86.881
0.03	77.793	85.616	85.655	85.686	88.654	87.686	85.733	89.657	88.687	86.733
0.04	77.633	85.323	85.390	85.444	88.389	87.444	85.527	89.393	88.446	86.527
0.05	77.428	84.951	85.054	85.137	88.051	87.137	85.264	89.058	88.140	86.265
0.06	77.180	84.506	84.651	84.767	87.646	86.766	84.947	88.654	87.770	85.947
0.07	76.889	83.993	84.183	84.337	87.175	86.335	84.577	88.185	87.340	85.577
0.08	76.558	83.417	83.656	83.851	86.643	85.847	84.157	87.656	86.853	85.157
0.09	76.187	82.783	83.074	83.313	86.054	85.305	83.689	87.069	86.312	84.688
0.10	75.778	82.099	82.441	82.725	85.414	84.714	83.176	86.430	85.721	84.174
0.11	75.333	81.371	81.765	82.094	84.727	84.077	82.622	85.744	85.084	83.618
0.12	74.854	80.605	81.048	81.423	83.998	83.399	82.029	85.015	84.405	83.023
0.13	74.342	79.808	80.298	80.717	83.233	82.685	81.401	84.249	83.688	82.392
0.14	73.800	78.985	79.519	79.981	82.436	81.938	80.741	83.449	82.939	81.729
0.15	73.231	78.142	78.716	79.218	81.612	81.163	80.052	82.623	82.160	81.036
0.16	72.635	77.285	77.895	78.433	80.766	80.364	79.339	81.773	81.357	80.318
0.17	72.016	76.418	77.059	77.631	79.903	79.546	78.605	80.904	80.533	79.578
0.18	71.376	75.546	76.213	76.815	79.027	78.712	77.852	80.021	79.693	78.818
0.19	70.716	74.673	75.362	75.990	78.142	77.866	77.084	79.129	78.840	78.043
0.20	70.039	73.803	74.508	75.158	77.253	77.013	76.305	78.230	77.977	77.255
0.22	68.643	72.080	72.805	73.488	75.471	75.294	74.722	76.426	76.237	75.652
0.24	67.204	70.396	71.125	71.827	73.705	73.578	73.125	74.634	74.497	74.032
0.25	66.474	69.572	70.300	71.006	72.834	72.727	72.327	73.748	73.634	73.221
0.26	65.739	68.762	69.485	70.193	71.972	71.884	71.532	72.872	72.776	72.413
0.28	64.260	67.184	67.893	68.598	70.286	70.227	69.957	71.154	71.089	70.810
0.30	62.781	65.663	66.355	67.050	68.654	68.616	68.413	69.489	69.447	69.236
0.32	61.312	64.200	64.873	65.554	67.081	67.057	66.908	67.882	67.856	67.701
0.34	59.863	62.791	63.446	64.112	65.569	65.555	65.448	66.337	66.322	66.209
0.35	59.149	62.105	62.753	63.410	64.835	64.825	64.736	65.587	65.576	65.482
0.36	58.442	61.432	62.072	62.722	64.117	64.109	64.036	64.853	64.845	64.767
0.38	57.055	60.120	60.748	61.384	62.723	62.720	62.672	63.429	63.426	63.374
0.40	55.706	58.850	59.470	60.094	61.383	61.384	61.357	62.062	62.063	62.032
0.42	54.398	57.619	58.235	58.850	60.095	60.099	60.090	60.749	60.753	60.739
0.44	53.134	56.424	57.037	57.646	58.854	58.861	58.867	59.487	59.492	59.493
0.45	52.518	55.839	56.452	57.059	58.251	58.259	58.271	58.873	58.880	58.887
0.46	51.914	55.262	55.875	56.481	57.657	57.667	57.686	58.271	58.279	58.292
0.48	50.740	54.130	54.746	55.350	56.501	56.513	56.544	57.097	57.108	57.133
0.50	49.611	53.028	53.647	54.252	55.381	55.397	55.439	55.964	55.978	56.013
0.55	46.974	50.396	51.023	51.633	52.725	52.749	52.815	53.283	53.305	53.363
0.60	44.584	47.932	48.561	49.176	50.251	50.282	50.364	50.795	50.823	50.898
0.65	42.407	45.632	46.255	46.869	47.938	47.972	48.062	48.474	48.507	48.591
0.70	40.409	43.490	44.100	44.706	45.774	45.807	45.895	46.306	46.338	46.423
0.80	36.830	39.649	40.220	40.794	41.860	41.882	41.942	42.384	42.408	42.472
0.90	33.663	36.318	36.851	37.387	38.443	38.449	38.468	38.958	38.966	38.992
1.00	30.807	33.389	33.896	34.402	35.443	35.435	35.419	35.948	35.943	35.933
1.10	28.219	30.771	31.264	31.753	32.776	32.762	32.724	33.272	33.259	33.227
1.20	25.890	28.404	28.890	29.370	30.373	30.357	30.314	30.861	30.846	30.805
1.30	23.821	26.256	26.734	27.206	28.184	28.170	28.132	28.665	28.651	28.612
1.40	22.011	24.314	24.777	25.238	26.183	26.173	26.146	26.652	26.642	26.612
1.50	20.449	22.574	23.015	23.456	24.357	24.352	24.335	24.810	24.803	24.784
1.60	19.117	21.033	21.443	21.858	22.703	22.701	22.695	23.133	23.130	23.121
1.70	17.989	19.685	20.058	20.439	21.219	21.220	21.221	21.621	21.621	21.620
1.80	17.035	18.516	18.849	19.194	19.902	19.904	19.910	20.272	20.274	20.278
1.90	16.223	17.510	17.804	18.111	18.745	18.748	18.756	19.080	19.083	19.090
2.00	15.523	16.646	16.904	17.174	17.736	17.740	17.748	18.036	18.039	18.047

Table 6.1.1.3. *Mean atomic scattering factors for chemically significant ions (cont.)*

Element Z Method $(\sin\theta)/\lambda$ (Å^{-1})	Pu^{3+} 94 *DS	Pu^{4+} 94 *DS	Pu^{6+} 94 *DS
0.00	91.000	90.000	88.000
0.01	90.962	89.965	87.970
0.02	90.848	89.861	87.881
0.03	90.660	89.689	87.734
0.04	90.398	89.450	87.528
0.05	90.066	89.145	87.267
0.06	89.665	88.777	86.950
0.07	89.199	88.349	86.580
0.08	88.673	87.863	86.160
0.09	88.089	87.324	85.692
0.10	87.453	86.734	85.178
0.11	86.769	86.098	84.621
0.12	86.041	85.419	84.025
0.13	85.275	84.703	83.393
0.14	84.475	83.952	82.727
0.15	83.646	83.171	82.032
0.16	82.794	82.365	81.310
0.17	81.921	81.537	80.565
0.18	81.033	80.691	79.800
0.19	80.134	79.832	79.019
0.20	79.227	78.962	78.224
0.22	77.403	77.204	76.604
0.24	75.587	75.441	74.963
0.25	74.688	74.565	74.140
0.26	73.797	73.695	73.320
0.28	72.048	71.979	71.690
0.30	70.351	70.305	70.088
0.32	68.711	68.683	68.522
0.34	67.133	67.116	66.999
0.35	66.367	66.354	66.256
0.36	65.616	65.607	65.525
0.38	64.161	64.157	64.102
0.40	62.765	62.765	62.731
0.42	61.425	61.428	61.411
0.44	60.138	60.143	60.140
0.45	59.513	59.519	59.522
0.46	58.900	58.907	58.916
0.48	57.708	57.717	57.736
0.50	56.557	56.569	56.598
0.55	53.845	53.864	53.915
0.60	51.337	51.363	51.430
0.65	49.004	49.034	49.113
0.70	46.828	46.860	46.942
0.80	42.898	42.922	42.989
0.90	39.463	39.474	39.506
1.00	36.445	36.443	36.440
1.10	33.763	33.752	33.724
1.20	31.346	31.331	31.293
1.30	29.142	29.128	29.090
1.40	27.121	27.109	27.078
1.50	25.264	25.257	25.235
1.60	23.567	23.564	23.552
1.70	22.030	22.029	22.025
1.80	20.650	20.651	20.653
1.90	19.424	19.427	19.433
2.00	18.346	18.349	18.357

Table 6.1.1.4. *Coefficients for analytical approximation to the scattering factors of Tables 6.1.1.1 and 6.1.1.3*

		a_1	b_1	a_2	b_2	a_3	b_3	a_4	b_4	c	Maximum error	$\sin\theta/\lambda$ (Å^{-1})	Mean error
H	SDS	0.493002	10.5109	0.322912	26.1257	0.140191	3.14236	0.040810	57.7997	0.003038	0.000	0.00	0.000
H	HF	0.489918	20.6593	0.262003	7.74039	0.196767	49.5519	0.049879	2.20159	0.001305	0.000	0.17	0.000
H^{1-}	HF	0.897661	53.1368	0.565616	15.1870	0.415815	186.576	0.116973	3.56709	0.002389	0.002	0.09	0.001
He	RHF	0.873400	9.10370	0.630900	3.35680	0.311200	22.9276	0.178000	0.982100	0.006400	0.001	1.01	0.000
Li	RHF	1.12820	3.95460	0.750800	1.05240	0.617500	85.3905	0.465300	168.261	0.037700	0.005	2.00	0.001
Li^{1+}	RHF	0.696800	4.62370	0.788800	1.95570	0.341400	0.631600	0.156300	10.0953	0.016700	0.001	1.78	0.000
Be	RHF	1.59190	43.6427	1.12780	1.86230	0.539100	103.483	0.702900	0.542000	0.038500	0.003	0.56	0.001
Be^{2+}	RHF	6.26030	0.002700	0.884900	0.831300	0.799300	2.27580	0.164700	5.11460	−6.1092	0.001	1.97	0.000
B	RHF	2.05450	23.2185	1.33260	1.02100	1.09790	60.3498	0.706800	0.140300	−0.19320	0.002	0.75	0.001
C	RHF	2.31000	20.8439	1.02000	10.2075	1.58860	0.568700	0.865000	51.6512	0.215600	0.006	2.00	0.001
C_{val}	HF	2.26069	22.6907	1.56165	0.656665	1.05075	9.75618	0.839259	55.5949	0.286977	0.001	0.16	0.000
N	RHF	12.2126	0.005700	3.13220	9.89330	2.01250	28.9975	1.16630	0.582600	−11.529	0.007	0.11	0.002
O	RHF	3.04850	13.2771	2.28680	5.70110	1.54630	0.323900	0.867000	32.9089	0.250800	0.001	0.22	0.000
O^{1-}	HF	4.19160	12.8573	1.63969	4.17236	1.52673	47.0179	−20.307	−0.01404	21.9412	0.011	1.50	0.004
F	RHF	3.53920	10.2825	2.64120	4.29440	1.51700	0.261500	1.02430	26.1476	0.277600	0.001	0.01	0.000
F^{1-}	HF	3.63220	5.27756	3.51057	14.7353	1.26064	0.442258	0.940706	47.3437	0.653396	0.003	0.09	0.001
Ne	RHF	3.95530	8.40420	3.11250	3.42620	1.45460	0.230600	1.12510	21.7184	0.351500	0.002	0.25	0.001
Na	RHF	4.76260	3.28500	3.17360	8.84220	1.26740	0.313600	1.11280	129.424	0.676000	0.009	0.13	0.002
Na^{1+}	RHF	3.25650	2.66710	3.93620	6.11530	1.39980	0.200100	1.00320	14.0390	0.404000	0.001	0.70	0.000
Mg	RHF	5.42040	2.82750	2.17350	79.2611	1.22690	0.380800	2.30730	7.19370	0.858400	0.015	0.08	0.003
Mg^{2+}	RHF	3.49880	2.16760	3.83780	4.75420	1.32840	0.185000	0.849700	10.1411	0.485300	0.001	1.34	0.000
Al	RHF	6.42020	3.03870	1.90020	0.742600	1.59360	31.5472	1.96460	85.0886	1.11510	0.018	2.00	0.005
Al^{3+}	HF	4.17448	1.93816	3.38760	4.14553	1.20296	0.228753	0.528137	8.28524	0.706786	0.000	1.50	0.000
Si_v	RHF	6.29150	2.43860	3.03530	32.3337	1.98910	0.678500	1.54100	81.6937	1.14070	0.009	2.00	0.002
Si_{val}	HF	5.66269	2.66520	3.07164	38.6634	2.62446	0.916946	1.39320	93.5458	1.24707	0.001	0.53	0.001
Si^{4+}	HF	4.43918	1.64167	3.20345	3.43757	1.19453	0.214900	0.416530	6.65365	0.746297	0.000	1.50	0.000
P	RHF	6.43450	1.90670	4.17910	27.1570	1.78000	0.526000	1.49080	68.1645	1.11490	0.003	0.65	0.001
S	RHF	6.90530	1.46790	5.20340	22.2151	1.43790	0.253600	1.58630	56.1720	0.866900	0.005	0.67	0.002
Cl	RHF	11.4604	0.010400	7.19640	1.16620	6.25560	18.5194	1.64550	47.7784	−9.5574	0.007	0.78	0.003
Cl^{1-}	RHF	18.2915	0.006600	7.20840	1.17170	6.53370	19.5424	2.33860	60.4486	−16.378	0.007	0.76	0.003
Ar	RHF	7.48450	0.907200	6.77230	14.8407	0.653900	43.8983	1.64420	33.3929	1.44450	0.029	2.00	0.006
K	RHF	8.21860	12.7949	7.43980	0.774800	1.05190	213.187	0.865900	41.6841	1.42280	0.011	0.90	0.005
K^{1+}	RHF	7.95780	12.6331	7.49170	0.767400	6.35900	−0.00200	1.19150	31.9128	−4.9978	0.011	0.91	0.005
Ca	RHF	8.62660	10.4421	7.38730	0.659900	1.58990	85.7484	1.02110	178.437	1.37510	0.016	0.99	0.006
Ca^{2+}	RHF	15.6348	−0.00740	7.95180	0.608900	8.43720	10.3116	0.853700	25.9905	−14.875	0.017	2.00	0.004
Sc	RHF	9.18900	9.02130	7.36790	0.572900	1.64090	136.108	1.46800	51.3531	1.33290	0.014	1.07	0.006
Sc^{3+}	HF	13.4008	0.298540	8.02730	7.96290	1.65943	−0.28604	1.57936	16.0662	−6.6667	0.002	1.50	0.000
Ti	RHF	9.75950	7.85080	7.35580	0.500000	1.69910	35.6338	1.90210	116.105	1.28070	0.014	2.00	0.006
Ti^{2+}	HF	9.11423	7.52430	7.62174	0.457585	2.27930	19.5361	0.087899	61.6558	0.897155	0.006	1.50	0.001
Ti^{3+}	HF	17.7344	0.220610	8.73816	7.04716	5.25691	−0.15762	1.92134	15.9768	−14.652	0.001	0.00	0.000
Ti^{4+}	HF	19.5114	0.178847	8.23473	6.67018	2.01341	−0.29263	1.52080	12.9464	−13.280	0.002	1.50	0.000
V	RHF	10.2971	6.86570	7.35110	0.438500	2.07030	26.8938	2.05710	102.478	1.21990	0.014	2.00	0.005
V^{2+}	RHF	10.1060	6.88180	7.35410	0.440900	2.28840	20.3004	0.022300	115.122	1.22980	0.015	2.00	0.004
V^{3+}	HF	9.43141	6.39535	7.74190	0.383349	2.15343	15.1908	0.016865	63.9690	0.656565	0.004	1.50	0.001
V^{5+}	HF	15.6887	0.679003	8.14208	5.40135	2.03081	9.97278	−9.5760	0.940464	1.71430	0.000	0.34	0.000
Cr	RHF	10.6406	6.10380	7.35370	0.392000	3.32400	20.2626	1.49220	98.7399	1.18320	0.011	2.00	0.004
Cr^{2+}	HF	9.54034	5.66078	7.75090	0.344261	3.58274	13.3075	0.509107	32.4224	0.616898	0.002	1.50	0.000
Cr^{3+}	HF	9.68090	5.59463	7.81136	0.334393	2.87603	12.8288	0.113575	32.8761	0.518275	0.002	1.50	0.000
Mn	RHF	11.2819	5.34090	7.35730	0.343200	3.01930	17.8674	2.24410	83.7543	1.08960	0.009	2.00	0.004
Mn^{2+}	RHF	10.8061	5.27960	7.36200	0.343500	3.52680	14.3430	0.218400	41.3235	1.08740	0.009	2.00	0.002
Mn^{3+}	HF	9.84521	4.91797	7.87194	0.294393	3.56531	10.8171	0.323613	24.1281	0.393974	0.001	1.50	0.000
Mn^{4+}	HF	9.96253	4.84850	7.97057	0.283303	2.76067	10.4852	0.054447	27.5730	0.251877	0.001	1.50	0.000
Fe	RHF	11.7695	4.76110	7.35730	0.307200	3.52220	15.3535	2.30450	76.8805	1.03690	0.011	0.08	0.004
Fe^{2+}	RHF	11.0424	4.65380	7.37400	0.305300	4.13460	12.0546	0.439900	31.2809	1.00970	0.008	2.00	0.002
Fe^{3+}	RHF	11.1764	4.61470	7.38630	0.300500	3.39480	11.6729	0.072400	38.5566	0.970700	0.008	2.00	0.002
Co	RHF	12.2841	4.27910	7.34090	0.278400	4.00340	13.5359	2.34880	71.1692	1.01180	0.013	0.08	0.004
Co^{2+}	RHF	11.2296	4.12310	7.38830	0.272600	4.73930	10.2443	0.710800	25.6466	0.932400	0.006	2.00	0.001
Co^{3+}	HF	10.3380	3.90969	7.88173	0.238668	4.76795	8.35583	0.725591	18.3491	0.286667	0.000	1.50	0.000
Ni	RHF	12.8376	3.87850	7.29200	0.256500	4.44380	12.1763	2.38000	66.3421	1.0341	0.014	0.08	0.004
Ni^{2+}	RHF	11.4166	3.67660	7.40050	0.244900	5.34420	8.87300	0.977300	22.1626	0.861400	0.003	2.00	0.001
Ni^{3+}	HF	10.7806	3.54770	7.75868	0.223140	5.22746	7.64468	0.847114	16.9673	0.386044	0.000	0.57	0.000
Cu	RHF	13.3380	3.58280	7.16760	0.247000	5.61580	11.3966	1.67350	64.8126	1.19100	0.015	0.08	0.005
Cu^{1+}	RHF	11.9475	3.36690	7.35730	0.227400	6.24550	8.66250	1.55780	25.8487	0.89000	0.003	0.24	0.001
Cu^{2+}	HF	11.8168	3.37484	7.11181	0.244078	5.78135	7.98760	1.14523	19.8970	1.14431	0.001	0.26	0.000
Zn	RHF	14.0743	3.26550	7.03180	0.233300	5.16520	10.3163	2.41000	58.7097	1.30410	0.016	0.08	0.005
Zn^{2+}	RHF	11.9719	2.99460	7.38620	0.203100	6.46680	7.08260	1.39400	18.0995	0.780700	0.001	0.62	0.000
Ga	RHF	15.2354	3.06690	6.70060	0.241200	4.35910	10.7805	2.96230	61.4135	1.71890	0.025	0.08	0.008
Ga^{3+}	HF	12.6920	2.81262	6.69883	0.227890	6.06692	6.36441	1.00660	14.4122	1.53545	0.008	1.45	0.000
Ge	RHF	16.0816	2.85090	6.37470	0.251600	3.70680	11.4468	3.68300	54.7625	2.13130	0.024	0.08	0.008
Ge^{4+}	HF	12.9172	2.53718	6.70003	0.205855	6.06791	5.47913	0.859041	11.6030	1.45572	0.000	0.32	0.000

Table 6.1.1.4. *Coefficients for analytical approximation to scattering factors (cont.)*

		a_1	b_1	a_2	b_2	a_3	b_3	a_4	b_4	c	Maximum error	$\sin\theta/\lambda$ (Å^{-1})	Mean error
As	RHF	16.6723	2.63450	6.07010	0.264700	3.43130	12.9479	4.27790	47.7972	2.53100	0.019	0.09	0.008
Se	RHF	17.0006	2.40980	5.81960	0.272600	3.97310	15.2372	4.35430	43.8163	2.84090	0.016	2.00	0.006
Br	RHF	17.1789	2.17230	5.23580	16.5796	5.63770	0.260900	3.98510	41.4328	2.95570	0.012	2.00	0.004
Br^{1-}	RHF	17.1718	2.20590	6.33380	19.3345	5.57540	0.287100	3.72720	58.1535	3.17760	0.016	2.00	0.006
Kr	RHF	17.3555	1.93840	6.72860	16.5623	5.54930	0.226100	3.53750	39.3972	2.82500	0.008	2.00	0.002
Rb	RHF	17.1784	1.78880	9.64350	17.3151	5.13990	0.274800	1.52920	164.934	3.48730	0.028	0.12	0.008
Rb^{1+}	RHF	17.5816	1.71390	7.65980	14.7957	5.89810	0.160300	2.78170	31.2087	2.07820	0.002	1.99	0.001
Sr	RHF	17.5663	1.55640	9.81840	14.0988	5.42200	0.166400	2.66940	132.376	2.50640	0.021	0.13	0.005
Sr^{2+}	RHF	18.0874	1.49070	8.13730	12.6963	2.56540	24.5651	−34.193	−0.01380	41.4025	0.008	2.00	0.002
Y	*RHF	17.7760	1.40290	10.2946	12.8006	5.72629	0.125599	3.26588	104.354	1.91213	0.028	0.07	0.006
Y^{3+}	*DS	17.9268	1.35417	9.15310	11.2145	1.76795	22.6599	−33.108	−0.01319	40.2602	0.005	2.00	0.001
Zr	*RHF	17.8765	1.27618	10.9480	11.9160	5.41732	0.117622	3.65721	87.6627	2.06929	0.035	0.07	0.008
Zr^{4+}	*DS	18.1668	1.21480	10.0562	10.1483	1.01118	21.6054	−2.6479	−0.10276	9.41454	0.004	2.00	0.001
Nb	*RHF	17.6142	1.18865	12.0144	11.7660	4.04183	0.204785	3.53346	69.7957	3.75591	0.042	0.08	0.011
Nb^{3+}	*DS	19.8812	0.019175	18.0653	1.13305	11.0177	10.1621	1.94715	28.3389	−12.912	0.006	2.00	0.002
Nb^{5+}	*DS	17.9163	1.12446	13.3417	0.028781	10.7990	9.28206	0.337905	25.7228	−6.3934	0.007	2.00	0.003
Mo	RHF	3.70250	0.277200	17.2356	1.09580	12.8876	11.0040	3.74290	61.6584	4.38750	0.046	0.08	0.012
Mo^{3+}	*DS	21.1664	0.014734	18.2017	1.03031	11.7423	9.53659	2.30951	26.6307	−14.421	0.009	2.00	0.003
Mo^{5+}	*DS	21.0149	0.014345	18.0992	1.02238	11.4632	8.78809	0.740625	23.3452	−14.316	0.010	2.00	0.003
Mo^{6+}	*DS	17.8871	1.03649	11.1750	8.48061	6.57891	0.058881	0.000000	0.000000	0.344941	0.014	0.00	0.006
Tc	*RHF	19.1301	0.864132	11.0948	8.14487	4.64901	21.5707	2.71263	86.8472	5.40428	0.061	2.00	0.011
Ru	*RHF	19.2674	0.808520	12.9182	8.43467	4.86337	24.7997	1.56756	94.2928	5.37874	0.041	2.00	0.006
Ru^{3+}	*DS	18.5638	0.847329	13.2885	8.37164	9.32602	0.017662	3.00964	22.8870	−3.1892	0.013	2.00	0.004
Ru^{4+}	*DS	18.5003	0.844582	13.1787	8.12534	4.71304	0.36495	2.18535	20.8504	1.42357	0.014	2.00	0.004
Rh	*RHF	19.2957	0.751536	14.3501	8.21758	4.73425	25.8749	1.28918	98.6062	5.32800	0.021	2.00	0.004
Rh^{3+}	*DS	18.8785	0.764252	14.1259	7.84438	3.32515	21.2487	−6.1989	−0.01036	11.8678	0.014	2.00	0.004
Rh^{4+}	*DS	18.8545	0.760825	13.9806	7.62436	2.53464	19.3317	−5.6526	−0.01020	11.2835	0.014	2.00	0.003
Pd	*RHF	19.3319	0.698655	15.5017	7.98929	5.29537	25.2052	0.605844	76.8986	5.26593	0.012	1.08	0.005
Pd^{2+}	*DS	19.1701	0.696219	15.2096	7.55573	4.32234	22.5057	0.000000	0.000000	5.29160	0.011	2.00	0.004
Pd^{4+}	*DS	19.2493	0.683839	14.7900	7.14833	2.89289	17.9144	−7.9492	0.005127	13.0174	0.014	2.00	0.003
Ag	RHF	19.2808	0.644600	16.6885	7.47260	4.80450	24.6605	1.04630	99.8156	5.17900	0.016	1.14	0.007
Ag^{1+}	*DS	19.1812	0.646179	15.9719	7.19123	5.27475	21.7326	0.357534	66.1147	5.21572	0.012	1.13	0.005
Ag^{2+}	*DS	19.1643	0.645643	16.2456	7.18544	4.37090	21.4072	0.000000	0.000000	5.21404	0.011	1.14	0.005
Cd	RHF	19.2214	0.594600	17.6444	6.90890	4.46100	24.7008	1.60290	87.4825	5.06940	0.020	2.00	0.008
Cd^{2+}	*DS	19.1514	0.597922	17.2535	6.80639	4.47128	20.2521	0.000000	0.000000	5.11937	0.014	1.17	0.007
In	RHF	19.1624	0.547600	18.5596	6.37760	4.29480	25.8499	2.03960	92.8029	4.93910	0.027	2.00	0.009
In^{3+}	*DS	19.1045	0.551522	18.1108	6.32470	3.78897	17.3595	0.000000	0.000000	4.99635	0.022	2.00	0.007
Sn	RHF	19.1889	5.83030	19.1005	0.503100	4.45850	26.8909	2.46630	83.9571	4.78210	0.032	2.00	0.009
Sn^{2+}	RHF	19.1094	0.503600	19.0548	5.83780	4.56480	23.3752	0.487000	62.2061	4.78610	0.032	2.00	0.009
Sn^{4+}	RHF	18.9333	5.76400	19.7131	0.465500	3.41820	14.0049	0.019300	−0.75830	3.91820	0.016	2.00	0.004
Sb	RHF	19.6418	5.30340	19.0455	0.460700	5.03710	27.9074	2.68270	75.2825	4.59090	0.035	2.00	0.009
Sb^{3+}	*DS	18.9755	0.467196	18.9330	5.22126	5.10789	19.5902	0.288753	55.5113	4.69626	0.028	2.00	0.007
Sb^{5+}	*DS	19.8685	5.44853	19.0302	0.467973	2.41253	14.1259	0.000000	0.000000	4.69263	0.030	2.00	0.008
Te	*RHF	19.9644	4.81742	19.0138	0.420885	6.14487	28.5284	2.52390	70.8403	4.35200	0.038	2.00	0.009
I	RHF	20.1472	4.34700	18.9949	0.381400	7.51380	27.7660	2.27350	66.8776	4.07120	0.037	2.00	0.009
I^{1-}	RHF	20.2332	4.35790	18.9970	0.381500	7.80690	29.5259	2.88680	84.9304	4.07140	0.038	2.00	0.009
Xe	RHF	20.2933	3.92820	19.0298	0.344000	8.97670	26.4659	1.99000	64.2658	3.71180	0.038	2.00	0.009
Cs	RHF	20.3892	3.56900	19.1062	0.310700	10.6620	24.3879	1.49530	213.904	3.33520	0.032	2.00	0.010
Cs^{1+}	RHF	20.3524	3.55200	19.1278	0.308600	10.2821	23.7128	0.961500	59.4565	3.27910	0.037	2.00	0.009
Ba	RHF	20.3361	3.21600	19.2970	0.275600	10.8880	20.2073	2.69590	167.202	2.77310	0.032	2.00	0.009
Ba^{2+}	*DS	20.1807	3.21367	19.1136	0.283310	10.9054	20.0558	0.77634	51.7460	3.02902	0.029	2.00	0.007
La	*RHF	20.5780	2.94817	19.5990	0.244475	11.3727	18.7726	3.28719	133.124	2.14678	0.032	2.00	0.009
La^{3+}	*DS	20.2489	2.92070	19.3763	0.250698	11.6323	17.8211	0.336048	54.9453	2.40860	0.028	2.00	0.007
Ce	*RHF	21.1671	2.81219	19.7695	0.226836	11.8513	17.6083	3.33049	127.113	1.86264	0.026	2.00	0.008
Ce^{3+}	*DS	20.8036	2.77691	19.5590	0.231540	11.9369	16.5408	0.612376	43.1692	2.09013	0.023	2.00	0.005
Ce^{4+}	*DS	20.3235	2.65941	19.8186	0.218850	12.1233	15.7992	0.144583	62.2355	1.59180	0.026	2.00	0.007
Pr	*RHF	22.0440	2.77393	19.6697	0.222087	12.3856	16.7669	2.82428	143.644	2.05830	0.021	0.12	0.007
Pr^{3+}	*DS	21.3727	2.64520	19.7491	0.214299	12.1329	15.3230	0.975180	36.4065	1.77132	0.019	2.00	0.004
Pr^{4+}	*DS	20.9413	2.54467	20.0539	0.202481	12.4668	14.8137	0.296689	45.4643	1.24285	0.021	2.00	0.005
Nd	*RHF	22.6845	2.66248	19.6847	0.210628	12.7740	15.8850	2.85137	137.903	1.98486	0.024	0.13	0.007
Nd^{3+}	*DS	21.9610	2.52722	19.9339	0.199237	12.1200	14.1783	1.51031	30.8717	1.47588	0.015	2.00	0.003
Pm	*RHF	23.3405	2.56270	19.6095	0.202088	13.1235	15.1009	2.87516	132.721	2.02876	0.026	0.13	0.008
Pm^{3+}	*DS	22.5527	2.41740	20.1108	0.185769	12.0671	13.1275	2.07492	27.4491	1.19499	0.012	2.00	0.002
Sm	*RHF	24.0042	2.47274	19.4258	0.196451	13.4396	14.3996	2.89604	128.007	2.20963	0.029	0.13	0.009
Sm^{3+}	*DS	23.1504	2.31641	20.2599	0.174081	11.9202	12.1571	2.71488	24.8242	0.954586	0.009	2.00	0.002
Eu	RHF	24.6274	2.38790	19.0886	0.194200	13.7603	13.7546	2.92270	123.174	2.57450	0.031	0.14	0.010
Eu^{2+}	*DS	24.0063	2.27783	19.9504	0.173530	11.8034	11.6096	3.87243	26.5156	1.36389	0.004	2.00	0.002
Eu^{3+}	*DS	23.7497	2.22258	20.3745	0.163940	11.8509	11.3110	3.26503	22.9966	0.759344	0.006	2.00	0.001
Gd	*RHF	25.0709	2.25341	19.0798	0.181951	13.8518	12.9331	3.54545	101.398	2.41960	0.036	0.15	0.011
Gd^{3+}	*DS	24.3466	2.13553	20.4208	0.155525	11.8708	10.5782	3.71490	21.7029	0.645089	0.004	2.00	0.001

Table 6.1.1.4. *Coefficients for analytical approximation to scattering factors (cont.)*

		a_1	b_1	a_2	b_2	a_3	b_3	a_4	b_4	c	Maximum error	$\sin\theta/\lambda$ (Å^{-1})	Mean error
Tb	*RHF	25.8976	2.24256	18.2185	0.196143	14.3167	12.6648	2.95354	115.362	3.58324	0.035	0.14	0.012
Tb^{3+}	*DS	24.9559	2.05601	20.3271	0.149525	12.2471	10.0499	3.77300	21.2773	0.691967	0.005	0.00	0.001
Dy	*RHF	26.5070	2.18020	17.6383	0.202172	14.5596	12.1899	2.96577	111.874	4.29728	0.037	0.15	0.013
Dy^{3+}	*DS	25.5395	1.98040	20.2861	0.143384	11.9812	9.34972	4.50073	19.5810	0.689690	0.003	0.00	0.001
Ho	*RHF	26.9049	2.07051	17.2940	0.197940	14.5583	11.4407	3.63837	92.6566	4.56796	0.040	0.15	0.013
Ho^{3+}	*DS	26.1296	1.91072	20.0994	0.139358	11.9788	8.80018	4.93676	18.5908	0.852795	0.003	0.00	0.001
Er	*RHF	27.6563	2.07356	16.4285	0.223545	14.9779	11.3604	2.98233	105.703	5.92046	0.040	0.15	0.015
Er^{3+}	*DS	26.7220	1.84659	19.7748	0.137290	12.1506	8.36225	5.17379	17.8974	1.17613	0.003	0.00	0.001
Tm	*RHF	28.1819	2.02859	15.8851	0.238849	15.1542	10.9975	2.98706	102.961	6.75621	0.041	0.15	0.016
Tm^{3+}	*DS	27.3083	1.78711	19.3320	0.136974	12.3339	7.96778	5.38348	17.2922	1.63929	0.003	0.00	0.001
Yb	*RHF	28.6641	1.98890	15.4345	0.257119	15.3087	10.6647	2.98963	100.417	7.56672	0.042	0.15	0.016
Yb^{2+}	*DS	28.1209	1.78503	17.6817	0.159970	13.3335	8.18304	5.14657	20.3900	3.70983	0.008	0.00	0.003
Yb^{3+}	*DS	27.8917	1.73272	18.7614	0.138790	12.6072	7.64412	5.47647	16.8153	2.26001	0.003	0.00	0.002
Lu	*RHF	28.9476	1.90182	15.2208	9.98519	15.1000	0.261033	3.71601	84.3298	7.97628	0.043	0.16	0.016
Lu^{3+}	*DS	28.4628	1.68216	18.1210	0.142292	12.8429	7.33727	5.59415	16.3535	2.97573	0.004	0.14	0.002
Hf	*RHF	29.1440	1.83262	15.1726	9.59990	14.7586	0.275116	4.30013	72.0290	8.58154	0.047	0.08	0.016
Hf^{4+}	*DS	28.8131	1.59136	18.4601	0.128903	12.7285	6.76232	5.59927	14.0366	2.39699	0.002	0.00	0.001
Ta	*RHF	29.2024	1.77333	15.2293	9.37046	14.5135	0.295977	4.76492	63.3644	9.24354	0.049	0.08	0.017
Ta^{5+}	*DS	29.1587	1.50711	18.8407	0.116741	12.8268	6.31524	5.38695	12.4244	1.78555	0.002	2.00	0.001
W	*RHF	29.0818	1.72029	15.4300	9.22590	14.4327	0.321703	5.11982	57.0560	9.88750	0.051	0.09	0.017
W^{6+}	*DS	29.4936	1.42755	19.3763	0.104621	13.0544	5.93667	5.06412	11.1972	1.01074	0.001	0.00	0.000
Re	*RHF	28.7621	1.67191	15.7189	9.09227	14.5564	0.350500	5.44174	52.0861	10.4720	0.052	0.09	0.017
Os	*RHF	28.1894	1.62903	16.1550	8.97948	14.9305	0.382661	5.67589	48.1647	11.0005	0.051	0.09	0.017
Os^{4+}	*DS	30.4190	1.37113	15.2637	6.84706	14.7458	0.165191	5.06795	18.0030	6.49804	0.006	0.29	0.003
Ir	*RHF	27.3049	1.59279	16.7296	8.86553	15.6115	0.417916	5.83377	45.0011	11.4722	0.050	0.09	0.017
Ir^{3+}	*DS	30.4156	1.34323	15.8620	7.10909	13.6145	0.204633	5.82008	20.3254	8.27903	0.009	0.28	0.004
Ir^{4+}	*DS	30.7058	1.30923	15.5512	6.71983	14.2326	0.167252	5.53672	17.4911	6.96824	0.006	0.29	0.003
Pt	*RHF	27.0059	1.51293	17.7639	8.81174	15.7131	0.424593	5.78370	38.6103	11.6883	0.046	0.10	0.016
Pt^{2+}	*DS	29.8429	1.32927	16.7224	7.38979	13.2153	0.263297	6.35234	22.9426	9.85329	0.014	0.00	0.006
Pt^{4+}	*DS	30.9612	1.24813	15.9829	6.60834	13.7348	0.168640	5.92034	16.9392	7.39534	0.006	0.14	0.003
Au	RHF	16.8819	0.461100	18.5913	8.62160	25.5582	1.48260	5.86000	36.3956	12.0658	0.045	0.10	0.015
Au^{1+}	*DS	28.0109	1.35321	17.8204	7.73950	14.3359	0.356752	6.58077	26.4043	11.2299	0.023	0.12	0.009
Au^{3+}	*DS	30.6886	1.21990	16.9029	6.82872	12.7801	0.212867	6.52354	18.6590	9.09680	0.009	0.14	0.004
Hg	RHF	20.6809	0.545000	19.0417	8.44840	21.6575	1.57290	5.96760	38.3246	12.6089	0.046	0.10	0.017
Hg^{1+}	*DS	25.0853	1.39507	18.4973	7.65105	16.8883	0.443378	6.48216	28.2262	12.0205	0.027	0.12	0.011
Hg^{2+}	*DS	29.5641	1.21152	18.0600	7.05639	12.8374	0.284738	6.89912	20.7482	10.6268	0.013	0.00	0.006
Tl	*RHF	27.5446	0.655150	19.1584	8.70751	15.5380	1.96347	5.52593	45.8149	13.1746	0.059	0.09	0.021
Tl^{1+}	*DS	21.3985	1.47110	20.4723	0.517394	18.7478	7.43463	6.82847	28.8482	12.5258	0.028	0.12	0.011
Tl^{3+}	*DS	30.8695	1.10080	18.3481	6.53852	11.9328	0.219074	7.00574	17.2114	9.80270	0.008	0.01	0.004
Pb	RHF	31.0617	0.690200	13.0637	2.35760	18.4420	8.61800	5.96960	47.2579	13.4118	0.060	2.00	0.021
Pb^{2+}	*DS	21.7886	1.33660	19.5682	0.488383	19.1406	6.77270	7.01107	23.8132	12.4734	0.020	2.00	0.008
Pb^{4+}	*DS	32.1244	1.00566	18.8003	6.10926	12.0175	0.147041	6.96886	14.7140	8.08428	0.005	0.31	0.002
Bi	RHF	33.3689	0.704000	12.9510	2.92380	16.5877	8.79370	6.46920	48.0093	13.5782	0.065	2.00	0.020
Bi^{3+}	*DS	21.8053	1.23560	19.5026	6.24149	19.1053	0.469999	7.10295	20.3185	12.4711	0.015	2.00	0.006
Bi^{5+}	*DS	33.5364	0.916540	25.0946	0.39042	19.2497	5.71414	6.91555	12.8285	−6.7994	0.003	0.00	0.001
Po	*RHF	34.6726	0.700999	15.4733	3.55078	13.1138	9.55642	7.02588	47.0045	13.6770	0.066	2.00	0.018
At	*RHF	35.3163	0.685870	19.0211	3.97458	9.49887	11.3824	7.42518	45.4715	13.7108	0.062	2.00	0.015
Rn	RHF	35.5631	0.663100	21.2816	4.06910	8.00370	14.0422	7.44330	44.2473	13.6905	0.054	2.00	0.012
Fr	*RHF	35.9299	0.646453	23.0547	4.17619	12.1439	23.1052	2.11253	150.645	13.7247	0.055	2.00	0.017
Ra	*RHF	35.7630	0.616341	22.9064	3.87135	12.4739	19.9887	3.21097	142.325	13.6211	0.037	2.00	0.012
Ra^{2+}	*DS	35.2150	0.604909	21.6700	3.57670	7.91342	12.6010	7.65078	29.8436	13.5431	0.029	2.00	0.006
Ac	*RHF	35.6597	0.589092	23.1032	3.65155	12.5977	18.5990	4.08655	117.020	13.5266	0.030	0.06	0.009
Ac^{3+}	*DS	35.1736	0.579689	22.1112	3.41437	8.19216	12.9187	7.05545	25.9443	13.4637	0.021	2.00	0.004
Th	*RHF	35.5645	0.563359	23.4219	3.46204	12.7473	17.8309	4.80703	99.1722	13.4314	0.031	0.07	0.008
Th^{4+}	*DS	35.1007	0.555054	22.4418	3.24498	9.78554	13.4661	5.29444	23.9533	13.3760	0.014	2.00	0.002
Pa	*RHF	35.8847	0.547751	23.2948	3.41519	14.1891	16.9235	4.17287	105.251	13.4287	0.033	0.06	0.010
U	RHF	36.0228	0.529300	23.4128	3.32530	14.9491	16.0927	4.18800	100.613	13.3966	0.035	0.07	0.010
U^{3+}	*DS	35.5747	0.520480	22.5259	3.12293	12.2165	12.7148	5.37073	26.3394	13.3092	0.009	2.00	0.002
U^{4+}	*DS	35.3715	0.516598	22.5326	3.05053	12.0291	12.5723	4.79840	23.4582	13.2671	0.007	2.00	0.001
U^{6+}	*DS	34.8509	0.507079	22.7584	2.89030	14.0099	13.1767	1.21457	25.2017	13.1665	0.003	2.00	0.001
Np	*RHF	36.1874	0.511929	23.5964	3.25396	15.6402	15.3622	4.18550	97.4908	13.3573	0.037	0.07	0.011
Np^{3+}	*DS	35.7074	0.502322	22.6130	3.03807	12.9898	12.1449	5.43227	25.4928	13.2544	0.006	2.00	0.002
Np^{4+}	*DS	35.5103	0.498626	22.5787	2.96627	12.7766	11.9484	4.92159	22.7502	13.2116	0.005	2.00	0.001
Np^{6+}	*DS	35.0136	0.489810	22.7286	2.81099	14.3884	12.3300	1.75669	22.6581	13.1130	0.002	2.00	0.001
Pu	*RHF	36.5254	0.499384	23.8083	3.26371	16.7707	14.9455	3.47947	105.980	13.3812	0.038	0.14	0.013
Pu^{3+}	*DS	35.8400	0.484938	22.7169	2.96118	13.5807	11.5331	5.66016	24.3992	13.1991	0.005	2.00	0.001
Pu^{4+}	*DS	35.6493	0.481422	22.6460	2.89020	13.3595	11.3160	5.18831	21.8301	13.1555	0.003	2.00	0.001
Pu^{6+}	*DS	35.1736	0.473204	22.7181	2.73848	14.7635	11.5530	2.28678	20.9303	13.0582	0.001	1.36	0.001
Am	*RHF	36.6706	0.483629	24.0992	3.20647	17.3415	14.3136	3.49331	102.273	13.3592	0.040	0.07	0.013
Cm	*RHF	36.6488	0.465154	24.4096	3.08997	17.3990	13.4346	4.21665	88.4834	13.2887	0.041	0.07	0.013
Bk	*RHF	36.7881	0.451018	24.7736	3.04619	17.8919	12.8946	4.23284	86.0030	13.2754	0.042	0.07	0.014
Cf	*RHF	36.9185	0.437533	25.1995	3.00775	18.3317	12.4044	4.24391	83.7881	13.2674	0.043	0.07	0.014

Table 6.1.1.5. *Coefficients for analytical approximation to the scattering factors of Table 6.1.1.1 for the range* $2.0 < (\sin\theta)/\lambda < 6.0\ \text{Å}^{-1}$ *[equation (6.1.1.16)]*

Z	Symbol	a_0	a_1	a_2 (×10)	a_3 (×100)	C
2	He	0.52543	−3.43300	4.80070	−2.54760	1.0000
3	Li	0.89463	−2.43660	2.32500	−0.71949	1.0000
4	Be	1.25840	−1.94590	1.30460	−0.04297	1.0000
5	B	1.66720	−1.85560	1.60440	−0.65981	1.0000
6	C	1.70560	−1.56760	1.18930	−0.42715	1.0000
7	N	1.54940	−1.20190	0.51064	0.02472	1.0000
8	O	1.30530	−0.83742	−0.16738	0.47500	1.0000
9	F	1.16710	−0.63203	−0.40207	0.54352	1.0000
10	Ne	1.09310	−0.50221	−0.53648	0.60957	0.9995
11	Na	0.84558	−0.26294	−0.87884	0.76974	1.0000
12	Mg	0.71877	−0.13144	−1.20900	0.82738	1.0000
13	Al	0.67975	−0.08756	−0.95431	0.72294	1.0000
14	Si	0.70683	−0.09888	−0.98356	0.55631	1.0000
15	P	0.85532	−0.21262	−0.37390	0.20731	1.0000
16	S	1.10400	−0.40325	0.20094	−0.26058	1.0000
17	Cl	1.42320	−0.63936	0.84722	−0.76135	0.9995
18	Ar	1.82020	−0.92776	1.59220	−1.32510	0.9995
19	K	2.26550	−1.24530	2.38330	−1.91290	0.9990
20	Ca	2.71740	−1.55670	3.13170	−2.45670	0.9990
21	Sc	3.11730	−1.81380	3.71390	−2.85330	0.9990
22	Ti	3.45360	−2.01150	4.13170	−3.11710	0.9995
23	V	3.71270	−2.13920	4.34610	−3.22040	0.9995
24	Cr	3.87870	−2.19000	4.38670	−3.17520	1.0000
25	Mn	3.98550	−2.18850	4.27960	−3.02150	1.0000
26	Fe	3.99790	−2.11080	3.98170	−2.71990	1.0000
27	Co	3.95900	−1.99650	3.60630	−2.37050	1.0000
28	Ni	3.86070	−1.88690	3.12390	−1.94290	1.0000
29	Cu	3.72510	−1.65500	2.60290	−1.49760	0.9995
30	Zn	3.55950	−1.45100	2.03390	−1.02160	0.9995
31	Ga	3.37560	−1.23910	1.46160	−0.55471	0.9995
32	Ge	3.17800	−1.02230	0.89119	−0.09884	0.9995
33	As	2.97740	−0.81038	0.34861	0.32231	0.9995
34	Se	2.78340	−0.61110	−0.14731	0.69837	0.9995
35	Br	2.60610	−0.43308	−0.57381	1.00950	0.9995
36	Kr	2.44280	−0.27244	−0.95570	1.27070	0.9995
37	Rb	2.30990	−0.14328	−1.22600	1.45320	1.0000
38	Sr	2.21070	−0.04770	−1.41100	1.55410	1.0000
39	Y	2.14220	0.01935	−1.52240	1.59630	1.0000
40	Zr	2.12690	0.08618	−1.49190	1.51820	1.0000
41	Nb	2.12120	0.05381	−1.50070	1.50150	1.0000
42	Mo	2.18870	−0.00655	−1.25340	1.24010	1.0000
43	Tc	2.25730	−0.05737	−1.07450	1.06630	1.0000
44	Ru	2.37300	−0.15040	−0.77694	0.79060	0.9995
45	Rh	2.50990	−0.25906	−0.44719	0.49443	0.9995
46	Pd	2.67520	−0.39137	−0.05894	0.15404	0.9995
47	Ag	2.88690	−0.56119	0.42189	−0.25659	0.9990
48	Cd	3.08430	−0.71450	0.84482	−0.60990	0.9990
49	In	3.31400	−0.89697	1.35030	−1.03910	0.9990
50	Sn	3.49840	−1.02990	1.68990	−1.29860	0.9990
51	Sb	3.70410	−1.18270	2.08920	−1.61640	0.9990
52	Te	3.88240	−1.30980	2.41170	−1.86420	0.9990
53	I	4.08010	−1.45080	2.76730	−2.13920	0.9990
54	Xe	4.24610	−1.56330	3.04200	−2.34290	0.9990
55	Cs	4.38910	−1.65420	3.25450	−2.49220	0.9995
56	Ba	4.51070	−1.72570	3.41320	−2.59590	0.9995
57	La	4.60250	−1.77070	3.49970	−2.64050	0.9995
58	Ce	4.69060	−1.81790	3.60280	−2.70670	0.9995
59	Pr	4.72150	−1.81390	3.56480	−2.65180	0.9995
60	Nd	4.75090	−1.80800	3.51970	−2.59010	1.0000
61	Pm	4.74070	−1.76600	3.37430	−2.44210	1.0000
62	Sm	4.71700	−1.71410	3.20800	−2.28170	1.0000
63	Eu	4.66940	−1.64140	2.98580	−2.07460	1.0000
64	Gd	4.61010	−1.55750	2.73190	−1.84040	0.9995
65	Tb	4.52550	−1.45520	2.43770	−1.57950	0.9995
66	Dy	4.45230	−1.36440	2.17540	−1.34550	0.9990
67	Ho	4.37660	−1.27460	1.92540	−1.13090	0.9990
68	Er	4.29460	−1.18170	1.67060	−0.91467	0.9990
69	Tm	4.21330	−1.09060	1.42390	−0.70804	0.9990
70	Yb	4.13430	−1.00310	1.18810	−0.51120	0.9990
71	Lu	4.04230	−0.90518	0.92889	−0.29820	0.9990
72	Hf	3.95160	−0.80978	0.68951	−0.09620	0.9990
73	Ta	3.85000	−0.70599	0.41103	0.11842	0.9990
74	W	3.76510	−0.61807	0.18568	0.29787	0.9990
75	Re	3.67600	−0.52688	−0.04706	0.48180	0.9995
76	Os	3.60530	−0.45420	−0.22529	0.61700	0.9995
77	Ir	3.53130	−0.37856	−0.41174	0.75967	0.9995
78	Pt	3.47070	−0.31534	−0.56487	0.87492	0.9995
79	Au	3.41630	−0.25987	−0.69030	0.96224	0.9995
80	Hg	3.37350	−0.21428	−0.79013	1.02850	1.0000
81	Tl	3.34590	−0.18322	−0.84911	1.05970	1.0000
82	Pb	3.32330	−0.15596	−0.89878	1.08380	1.0000
83	Bi	3.31880	−0.14554	−0.90198	1.06850	1.0000
84	Po	3.32030	−0.13999	−0.89333	1.04380	1.0000
85	At	3.34250	−0.15317	−0.83350	0.97641	1.0000
86	Rn	3.37780	−0.17800	−0.74320	0.88510	1.0000
87	Fr	3.41990	−0.20823	−0.64000	0.78354	0.9995
88	Ra	3.47530	−0.25005	−0.50660	0.65836	0.9995
89	Ac	3.49020	−0.25109	−0.49651	0.64340	0.9995
90	Th	3.61060	−0.35409	−0.18926	0.36849	0.9995
91	Pa	3.68630	−0.41329	−0.01192	0.20878	0.9995
92	U	3.76650	−0.47542	0.16850	0.05060	0.9990
93	Np	3.82870	−0.51955	0.29804	−0.06566	0.9990
94	Pu	3.88970	−0.56296	0.42597	−0.18080	0.9990
95	Am	3.95060	−0.60554	0.54967	−0.29112	0.9985
96	Cm	4.01470	−0.65062	0.67922	−0.40588	0.9985
97	Bk	4.07780	−0.69476	0.80547	−0.51729	0.9985
98	Cf	4.14210	−0.73977	0.93342	−0.62981	0.9980

$$\exp(i\mathbf{S}\cdot\mathbf{r}) = \sum_{l=0}^{\infty}(2l+1)i^l j_l(Sr)P_l\left[\cos\left(\frac{\mathbf{S}\cdot\mathbf{r}}{Sr}\right)\right],$$

where j_l is a spherical Bessel function of order l and $S = |\mathbf{S}|$. The addition theorem enables this to be expressed as

$$\exp(i\mathbf{S}\cdot\mathbf{r}) = 4\pi\sum_{l=0} i^l j_l(Sr)\sum_{m=-l}^{l} Y_{lm}(\theta_S,\varphi_S)Y^*_{lm}(\theta,\varphi). \quad (6.1.1.17)$$

The $Y_{lm}(\theta,\varphi)$ are spherical (surface) harmonics

$$\begin{aligned} Y_{lm}(\theta,\varphi) &= \left[\frac{(2l+1)(l+m)!}{4\pi(l-m)!}\right]^{1/2}\frac{(-)^l e^{im\varphi}}{2^l l!(\sin\theta)^m} \\ &\quad\times\frac{\mathrm{d}^{l-m}}{\mathrm{d}(\cos\theta)^{l-m}}(\sin\theta)^{2l} \\ &= \left[\frac{(2l+1)(l-m)!}{4\pi(l+m)!}\right]^{1/2}(-)^m e^{im\varphi}P_l^m(\cos\theta) \quad m\geq 0, \end{aligned} \quad (6.1.1.18)$$

where $P_l^m(\cos\theta)$ is an associated Legendre polynomial.

With this definition of the spherical harmonics,

$$Y_{l-m} = (-)^m Y^*_{lm}. \quad (6.1.1.19)$$

Spherical harmonics with alternative phase conventions can be defined. The relationship between those in common use is given by Normand (1980). With the convention given in (6.1.1.18), the spherical harmonics up to fourth order are

$$
\begin{aligned}
Y_{00} &= (4\pi)^{-1/2} \\
Y_{1\pm1} &= \mp(3/8\pi)^{1/2} \sin\theta\, e^{\pm i\varphi} \\
Y_{10} &= (3/4\pi)^{1/2} \cos\theta \\
Y_{2\pm2} &= \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta\, e^{\pm 2i\varphi} \\
Y_{2\pm1} &= \mp\left(\frac{15}{8\pi}\right)^{1/2} \sin\theta\cos\theta\, e^{\pm i\varphi} \\
Y_{20} &= \left(\frac{5}{16\pi}\right)^{1/2} (3\cos^2\theta - 1) \\
Y_{3\pm3} &= \mp\left(\frac{35}{64\pi}\right)^{1/2} \sin^3\theta\, e^{\pm 3i\varphi} \\
Y_{3\pm2} &= \left(\frac{105}{32\pi}\right)^{1/2} \cos\theta\sin^2\theta\, e^{\pm 2i\varphi} \\
Y_{3\pm1} &= \mp\left(\frac{21}{64\pi}\right)^{1/2} \sin\theta(4 - 5\sin^2\theta)\, e^{\pm i\varphi} \\
Y_{30} &= \left(\frac{7}{16\pi}\right)^{1/2} \cos\theta(2 - 5\sin^2\theta) \\
Y_{4\pm4} &= \left(\frac{315}{512\pi}\right)^{1/2} \sin^4\theta\, e^{\pm 4i\varphi} \\
Y_{4\pm3} &= \mp\left(\frac{315}{64\pi}\right)^{1/2} \cos\theta\sin^3\theta\, e^{\pm 3i\varphi} \\
Y_{4\pm2} &= \left(\frac{45}{128\pi}\right)^{1/2} \sin^2\theta(6 - 7\sin^2\theta)\, e^{\pm 2i\varphi} \\
Y_{4\pm1} &= \mp\left(\frac{45}{64\pi}\right)^{1/2} \cos\theta\sin\theta(4 - 7\sin^2\theta)\, e^{\pm i\varphi} \\
Y_{40} &= \left(\frac{9}{256\pi}\right)^{1/2} (3 - 30\sin^2\theta + 35\sin^4\theta).
\end{aligned}
\tag{6.1.1.20}
$$

The perturbed electron density may be written as a multipole expansion in spherical polar coordinates r, θ, φ, each term having the form

$$\rho_{lm\pm}(r) = \rho_{lm\pm}(r)\mathbf{y}(\theta, \varphi), \tag{6.1.1.21}$$

where $\mathbf{y}$ is a suitably normalized real function of the polar coordinates. A common choice is the real form of the spherical harmonics

$$Y_{lm\pm(\theta,\varphi)} = \left[\frac{(2l+1)(l-m)!}{2\pi(l+m)!(1+\delta_{0m})}\right]^{1/2} P_l^m(\cos\theta) \begin{matrix}\cos m\varphi \\ \sin m\varphi\end{matrix}, \tag{6.1.1.22}$$

where $m = 0, 1, 2, \ldots$.

These harmonics can also be expressed in terms of Cartesian components of a unit vector q_x, q_y, q_z.

The normalization in (6.1.1.17) is appropriate to wavefunctions. The physical significance of the normalization for the spherical harmonics depends on the context in which they are utilized. The implications for density functions are not the same as those for wavefunctions. A normalizing condition on the real form of the spherical harmonics that expresses the properties of the functions under integration is

$$\int |y(\theta, \varphi)|\, \mathrm{d}(\cos\theta)\, \mathrm{d}\varphi = 2 - \delta_{l0}. \tag{6.1.1.23}$$

We assume the radial function to be constant in sign, and normalized to unity. The scalar function, with $l = 0$, does not change sign. Integration over the angular coordinates gives the electron content of the scalar function. The multipole terms with $l > 0$ integrate to zero. Taking the modulus of the angular function, and then integrating, gives twice the electron transfer from the electron-deficient to the electron-enriched volume for that multipole. With this normalization, the angle-dependent factors in the expansion, in terms of the associated Legendre polynomials and in terms of direction cosines, are given in Table 6.1.1.6. For the alternative normalization such that

$$\int |y_{lmp}|^2\, \mathrm{d}(\cos\theta)\, \mathrm{d}\varphi = 1,$$

the factor multiplying the angle-dependent term is as given in (6.1.1.22).

The site symmetry of the atom restricts multipole terms to those that are invariant under the operations of the relevant point group. The restrictions for the 27 non-cubic crystallographic point groups are given in Table 6.1.1.7.

For the five cubic point groups, the functions allowed are the linear combinations of the $Y_{lmp}(\theta, \varphi)$ known as the cubic harmonics $K_{lj}(\theta, \varphi)$ (Altmann & Cracknell, 1965). These are listed in Table 6.1.1.8. The normalization constant N_{lj}^2 is given by

$$N_{lj}^2 = \int K_{lj}^2\, \mathrm{d}(\cos\theta)\, \mathrm{d}\varphi.$$

The derivation of Tables 6.1.1.7 and 6.1.1.8 is described by Kurki-Suonio (1977).

The generalized scattering factor for a particular multipole involves evaluating the Fourier transform of the density

$$\int \exp(i\mathbf{S}\cdot\mathbf{r})\rho_{lm\pm}(r)Y_{lm\pm}(\theta, \varphi)\, \mathrm{d}\mathbf{r} = f_{lm\pm}(S)Y_{lm}(\theta_S, \varphi_S),$$

where the right-hand side is obtained by substituting (6.1.1.17) and integrating over the angular coordinates for the direct-space variables. The term

$$f_{lm\pm}(S) = \int_0^\infty j_l(Sr)\rho_{lm\pm}(r)r^2\, \mathrm{d}r \tag{6.1.1.24}$$

gives the radial variation of the generalized scattering factor.

The density function $\rho_{lm\pm}(r_a)$ may be derived from atomic basis functions, which asymptotically have the form of simple exponential functions $A_n r^n \exp(-\alpha r)$. Expansions in terms of Gaussian functions $B_n r^n \exp(-\beta r^2)$ or of Laguerre functions $C_n r^l L_n^{2l+2} \exp(-\gamma r/2)$, where L is a Laguerre polynomial of order n and degree $2l+2$, are also convenient for some purposes. A_n, B_n and C_n are normalizing factors, which, when specified as

$$
\begin{gathered}
A_n = \frac{\alpha^{l+n+3}}{4\pi(l+n+2)!}, \quad B_n = \frac{2^{\beta(l+n+3)/2}}{\Gamma[(l+n+3)/2]}, \\
C_n = \frac{(-)^n n!(\gamma/2)^{2l+3}}{4\pi(2l+n+2)!},
\end{gathered}
\tag{6.1.1.25}
$$

impose the normalization condition (Stewart, 1980*a*)

$$\int_0^\infty \rho_{lm}(r_a)r_a^{l+2}\, \mathrm{d}r_a = 1. \tag{6.1.1.26}$$

With this normalization, the Fourier–Bessel transforms are, for the simple exponential,

Table 6.1.1.6. *Angle dependence of multipole functions, normalized as in equation (6.1.1.23); $\omega = \cos\theta$ and S, D, Q, O, H denote scalar, dipole, quadrupole, octupole, and hexadecapole terms, respectively*

Pole	Real spherical harmonic	Cartesian representation
S 1	$\frac{1}{4\pi}P_0^0(\omega)$	$\frac{1}{4\pi}$
D 1	$\frac{1}{\pi}P_1^1(\omega)\cos\varphi$	$\frac{1}{\pi}q_x$
D 2	$\frac{1}{\pi}P_1^1(\omega)\sin\varphi$	$\frac{1}{\pi}q_y$
D 3	$\frac{1}{\pi}P_1^0(\omega)$	$\frac{1}{\pi}q_z$
Q 1	$\frac{1}{8}P_2^2(\omega)\cos 2\varphi$	$\frac{3}{8}(q_x^2 - q_y^2)$
Q 2	$\frac{1}{8}P_2^2(\omega)\sin 2\varphi$	$\frac{3}{4}q_xq_y$
Q 3	$\frac{1}{4}P_2^1(\omega)\cos\varphi$	$\frac{3}{4}q_xq_z$
Q 4	$\frac{1}{4}P_2^1(\omega)\sin\varphi$	$\frac{3}{4}q_yq_z$
Q 5	$\frac{3\sqrt{3}}{4\pi}P_2^0(\omega)$	$\frac{9\sqrt{2}}{8\pi}(q_z^2 - \frac{1}{3})$
O 1	$\frac{4}{45\pi}P_3^3(\omega)\cos 3\varphi$	$\frac{4}{3\pi}(q_x^2 - 3q_y^2)q_x$
O 2	$\frac{4}{45\pi}P_3^3(\omega)\sin 3\varphi$	$\frac{4}{3\pi}(3q_x^2 - q_y^2)q_y$
O 3	$\frac{1}{15}P_3^2(\omega)\cos 2\varphi$	$(q_x^2 - q_y^2)q_z$
O 4	$\frac{1}{15}P_3^2(\omega)\sin 2\varphi$	$2q_xq_yq_z$
O 5	$\frac{2}{3}\left[\tan^{-1}2 + \frac{14}{5} - \frac{\pi}{4}\right]^{-1}P_3^1(\omega)\cos\varphi$	$\left[\tan^{-1}2 + \frac{14}{5} - \frac{\pi}{4}\right]^{-1}(5q_z^2 - 1)q_x$
O 6	$\frac{2}{3}\left[\tan^{-1}2 + \frac{14}{5} - \frac{\pi}{4}\right]^{-1}P_3^1(\omega)\sin\varphi$	$\left[\tan^{-1}2 + \frac{14}{5} - \frac{\pi}{4}\right]^{-1}(5q_z^2 - 1)q_y$
O 7	$\frac{20}{13\pi}P_3^0(\omega)$	$\frac{10}{13\pi}(5q_z^2 - 3)q_z$
H 1	$\frac{1}{224}P_4^4(\omega)\cos 4\varphi$	$\frac{105}{224}(q_x^4 - 6q_x^2q_y^2 + q_y^4)$
H 2	$\frac{1}{224}P_4^4(\omega)\sin 4\varphi$	$\frac{420}{224}(q_x^2 - q_y^2)q_xq_y$
H 3	$\frac{1}{84}P_4^3(\omega)\cos 3\varphi$	$\frac{105}{84}(q_x^2 - 3q_y^2)q_xq_z$
H 4	$\frac{1}{84}P_4^3(\omega)\sin 3\varphi$	$\frac{105}{84}(3q_x^2 - q_y^2)q_yq_z$
H 5	$\left(\frac{7\sqrt{7}}{272 + 56\sqrt{7}}\right)P_4^2(\omega)\cos 2\varphi$	$\frac{15}{2}\left(\frac{7\sqrt{7}}{272 + 56\sqrt{7}}\right)(7q_z^2 - 1)(q_x^2 - q_y^2)$
H 6	$\left(\frac{7\sqrt{7}}{272 + 56\sqrt{7}}\right)P_4^2(\omega)\sin 2\varphi$	$\frac{15}{2}\left(\frac{7\sqrt{7}}{272 + 56\sqrt{7}}\right)(7q_z^2 - 1)q_xq_y$
H 7	$\left(\frac{21\sqrt{7}}{256 + 14\sqrt{7}}\right)P_4^1(\omega)\cos\varphi$	$\frac{5}{2}\left(\frac{21\sqrt{7}}{256 + 14\sqrt{7}}\right)(7q_z^2 - 3)q_xq_z$
H 8	$\left(\frac{21\sqrt{7}}{256 + 14\sqrt{7}}\right)P_4^1(\omega)\sin\varphi$	$\frac{5}{2}\left(\frac{21\sqrt{7}}{256 + 14\sqrt{7}}\right)(7q_z^2 - 3)q_xq_z$
H 9	$0.55534P_4^0(\omega)$	$\frac{5}{8}(0.55534)(7q_z^4 - 6q_z^2 + \frac{3}{5})$
$^*H_{\rm cubic}$	$\frac{160}{27\sqrt{3}\pi}\left[\frac{1}{420}P_4^4(\omega)\cos 4\varphi + \frac{2}{5}P_4^0(\omega)\right]$	$\frac{160}{27\sqrt{3}\pi}(q_x^4 + q_y^4 + q_z^4 - 3/5)$

$^*H_{\rm cubic}$ is the fourth-order hexadecapole appropriate to cubic site symmetry.

$$f_{nl}(\alpha, S) = \frac{S}{(2l+1)!![1+(S/\alpha)^2]^{n+2}} \times {}_2F_1\left[\frac{l-n-1}{2}, \frac{l-n}{2}; l+\frac{3}{2}; -(S/\alpha)^2\right]; \quad (6.1.1.27)$$

for the Gaussian function,

$$g_{nl}(\beta, S) = \frac{S^1}{(2l+1)!!}\exp(-S^2/4\beta){}_1F_1\left[\frac{l-n}{2}; l+\frac{3}{2}; \frac{S^2}{4\beta}\right]; \quad (6.1.1.28)$$

and, for the Laguerre function,

$$h_{nl}(\gamma, S) = \frac{(-)^n n! 2^n S^l}{[2(l+n)+1]!![1+(2S/\gamma)^2]^{l+2}} P_n^{(l+\frac{3}{2}, l+\frac{1}{2})}(t);$$

where the Jacobi polynomial is given by

$$\begin{aligned} P_n^{(a,b)}(x) &= 2^{-n}\sum_{m=0}^{n}\binom{n+a}{m}\binom{n+b}{n-m}(x-1)^{n-m}(x+1)^m \\ &= \frac{\Gamma(a+n+1)}{n!\Gamma(a+b+n+1)} \\ &\quad \times \sum_{m=0}^{n}\binom{n}{m}\frac{\Gamma(a+b+n+m+1)}{2^m\Gamma(a+m+1)}(x-1)^m \\ &= \binom{n+a}{n}{}_2F_1\left(-n, n+a+b+1; a+1; \frac{1-x}{2}\right) \\ &\qquad a \geq -1, b \geq a \end{aligned}$$

and

$$t = \frac{[(2S/\gamma)^2 - 1]}{[(2S/\gamma)^2 + 1]}. \quad (6.1.1.29)$$

Further details are given by Stewart (1980*a*).

In the case of Slater-type orbitals, a simpler form of the radial term may be obtained *via* the recurrence relations (Avery & Watson, 1977)

$$(S^2+\alpha^2)f_{\mu+1,\nu} + (\mu+\nu)(\mu-\nu-1)f_{\mu-1,\nu} = 2\nu\alpha f_{\mu\nu}$$
$$Sf_{\mu,\nu-1} + (\mu-\nu-1)f_{\mu-1,\nu} = \alpha f_{\mu\nu}.$$

Thus, for the lower-order Slater-type functions, we obtain the values listed in Table 6.1.1.9.

Atomic wavefunctions, in the form of sets of orbital contributions using Slater-type functions, are tabulated by Clementi & Roetti (1974). Basis sets for Gaussian orbitals are described by Veillard (1968), Roos & Siegbahn (1970), Huzinaga (1971), van Duijneveldt (1971), Dunning & Jeffrey-Hay (1977), and by McLean & Chandler (1979, 1980). The application of these basis sets to molecular calculations is reviewed by Ahlrichs & Taylor (1981).

6.1.1.5. *The temperature factor*

The atoms in a solid vibrate about their equilibrium positions, with an amplitude that increases with temperature. As a result of this vibration, the amplitude for coherent scattering is modulated by the Fourier transform of the probability distribution for the vibrating atom, known as the temperature factor. The reduction in the intensity of the coherent scattering is accompanied by thermal diffuse scattering, for which the phase relationship between the incident and diffracted beams is altered by the thermal wave, or phonon.

Table 6.1.1.7. *Indices allowed by the site symmetry for the real form of the spherical harmonics $Y_{lmp(\theta,\varphi)}$; λ, μ and j are integers such that $l, m \geq 0$; $(-)^n$ implies $p = -$ for n odd and $p = +$ for n even*

Site symmetry	Coordinate axes	Indices
$\bar{1}$	Any	All (l, m, p)
$\bar{1}$	Any	$(2\lambda, m, p)$
2	$2 \parallel x$	$(l, m, (-)^{l-m})$
	$2 \parallel y$	$(l, m, (-)^l)$
	$2 \parallel z$	$(l, 2\mu, p)$
m	$m \perp x$	$(l, m, (-)^m)$
	$m \perp y$	$(l, m, +)$
	$m \perp z$	$(l, l-2j, p)$
$2/m$	$2 \parallel x, m \perp x$	$(2\lambda, m, (-)^m)$
	$2 \parallel y, m \perp y$	$(2\lambda, m, +)$
	$2 \parallel z, m \perp z$	$(2\lambda, 2\mu, p)$
222	$2 \parallel z, 2 \parallel y$	$(l, 2\mu, (-)^l)$
$mm2$	$2 \parallel x, m \perp z$	$(l, l-2j, +)$
	$2 \parallel y, m \perp z$	$(l, l-2j, (-)^l)$
	$2 \parallel z, m \perp y$	$(l, 2\mu, +)$
mmm	$m \perp z, m \perp y, m \perp z$	$(2\lambda, 2\mu, +)$
$\bar{4}$	$\bar{4} \parallel z$	$(l, 4\mu, p)$
$\bar{4}$	$\bar{4} \parallel z$	$(l, 2l-4j, p)$
$4/m$	$4 \parallel z, m \perp z$	$(2\lambda, 4\mu, p)$
422	$4 \parallel z, 2 \parallel y$	$(l, 4\mu, (-)^l)$
$4mm$	$4 \parallel z, m \perp y$	$(l, 4\mu, +)$
$\bar{4}2m$	$\bar{4} \parallel z, 2 \parallel x$	$(l, 2l-4j, (-)^l)$
	$\bar{4} \parallel z, m \perp y$	$(l, 2l-4j, +)$
$4/mmm$	$4 \parallel z, m \perp z, m \perp x$	$(2\lambda, 4\mu, +)$
$\bar{3}$	$\bar{3} \parallel z$	$(l, 3\mu, p)$
$\bar{3}$	$\bar{3} \parallel z$	$(2\lambda, 3\mu, p)$
32	$3 \parallel z, 2 \parallel y$	$(l, 3\mu, (-)^l)$
	$3 \parallel z, 2 \parallel x$	$(l, 3\mu, (-)^{l-m})$
$3m$	$3 \parallel z, m \perp y$	$(l, 3\mu, +)$
	$\bar{3} \parallel z, m \perp x$	$(l, 3\mu, (-)^m)$
$\bar{3}m$	$\bar{3} \parallel z, m \perp y$	$(2\lambda, 3\mu, +)$
	$\bar{3} \parallel z, m \perp x$	$(2\lambda, 3\mu, (-)^m)$
$\bar{6}$	$\bar{6} \parallel z$	$(l, 6\mu, p)$
$\bar{6}$	$\bar{6} \parallel z$	$(m+2j, 3\mu, p)$
$6/m$	$6 \parallel z, m \perp z$	$(2\lambda, 6\mu, p)$
622	$6 \parallel z, 2 \parallel y$	$(l, 6\mu, (-)^l)$
$6mm$	$6 \parallel z, m \perp y$	$(l, 6\mu, +)$
$\bar{6}m2$	$\bar{6} \parallel z, m \perp y$	$(m+2j, 3\mu, +)$
	$\bar{6} \parallel z, m \perp x$	$(m+2j, 3\mu, (-)^l)$
$6/mmm$	$6 \parallel z, m \perp z, m \perp y$	$(2\lambda, 6\mu, +)$

The first term in an expansion of the probability density $\rho(\mathbf{u})$ for displacement $\mathbf{u}$ about an equilibrium position at the origin is

$$\rho_o(\mathbf{u}) = \frac{\det \boldsymbol{\sigma}_\mathbf{u}^{-1/2}}{8\pi^3}\exp(-\tfrac{1}{2}\mathbf{u}^T \cdot \boldsymbol{\sigma}_\mathbf{u}^{-1} \cdot \mathbf{u}), \quad (6.1.1.30)$$

where $\boldsymbol{\sigma}_\mathbf{u}$ is the dispersion matrix describing the second moments of the displacements about the mean position. The corresponding expression for the temperature factor is

$$T_o(\mathbf{S}) = \exp(-\tfrac{1}{2}\mathbf{S}^T \cdot \boldsymbol{\sigma}_\mathbf{u} \cdot \mathbf{S}), \quad (6.1.1.31)$$

which is the Fourier transform of $\rho_o(\mathbf{u})$.

Table 6.1.1.8. *Cubic harmonics $K_{lj}(\theta, \varphi)$ for cubic site symmetries*

$K_{lj}(\theta, \varphi)$	N_{l^2j}	Site symmetry				
		23	$m3$	432	$\bar{4}3m$	$m3m$
$K_0 = Y_{00+} = 1$	4π	×	×	×	×	×
$K_3 = Y_{32-}$	$\frac{240\pi}{7}$	×			×	
$K_4 = Y_{40+} + \frac{1}{168} Y_{44+}$	$\frac{16\pi}{21}$	×	×	×	×	×
$K_{6,1} = Y_{60+} - \frac{1}{360} Y_{64+}$	$\frac{32\pi}{13}$	×	×	×	×	×
$K_{6,2} = Y_{62+} - \frac{1}{792} Y_{66+}$	$\frac{512\pi}{13} \cdot \frac{105}{11}$	×	×			
$K_7 = Y_{72-} + \frac{1}{1560} Y_{76-}$	$\frac{256\pi}{15} \cdot \frac{567}{13}$	×			×	
$K_8 = Y_{80+} + \frac{1}{5940}(Y_{84+} + \frac{1}{672} Y_{88+})$	$\frac{256\pi}{17 \cdot 33}$	×	×	×	×	×
$K_{9,1} = Y_{92-} - \frac{1}{2520} Y_{96-}$	$\frac{512\pi}{19} \cdot 165$	×			×	
$K_{9,2} = Y_{94-} - \frac{1}{4080} Y_{98-}$	$\frac{2048\pi}{19} \cdot \frac{243 \cdot 5005}{17}$	×		×		
$K_{10,1} = Y_{10,0+} - \frac{1}{5460}(Y_{10,4} + \frac{1}{4320} Y_{10,8+})$	$\frac{512\pi}{21} \cdot \frac{3}{65}$	×	×	×	×	×
$K_{10,2} = Y_{10,2+} + \frac{1}{43680}(Y_{10,6+} + \frac{1}{456} Y_{10,10+})$	$\frac{2048\pi}{21} \cdot \frac{4455}{247}$	×	×			

The mean-square displacement of the atom from its mean position in the direction of the vector $\mathbf{v}$ is given by

$$\langle \mathbf{u}^2 \rangle_{\mathbf{v}} = \mathbf{v}^T \mathbf{g}^T \boldsymbol{\sigma}_{\mathbf{u}} \mathbf{g} \mathbf{v} / (\mathbf{v}^T \mathbf{g} \mathbf{v}), \tag{6.1.1.32}$$

where g_{ij} is the covariant metric tensor with the scalar products of the unit-cell vectors $\mathbf{a}_i \cdot \mathbf{a}_j$ as components.

The thermal motion for atoms in crystals is often displayed as surfaces of constant probability density. The surface for the thermal displacement $\mathbf{u}$ is defined by

$$\mathbf{u}^T \boldsymbol{\sigma}_{\mathbf{u}}^{-1} \mathbf{u} = C^2. \tag{6.1.1.33}$$

The square of the distance from the origin to the equiprobability surface in the direction $\mathbf{v}$ is

$$C^2 \mathbf{v}^T \mathbf{g} \mathbf{v} / (\mathbf{v}^T \boldsymbol{\sigma}_{\mathbf{u}}^{-1} \mathbf{v}). \tag{6.1.1.34}$$

This is equal to (6.1.1.32) for C unity only if $\mathbf{v}$ coincides with a principal axis of the vibration ellipsoid.

The probability that a displacement falls within the ellipsoid defined by C is

$$(2/\pi)^{1/2} \int_0^C q^2 \exp(-q^2/2)\, \mathrm{d}q. \tag{6.1.1.35}$$

6.1.1.6. *The generalized temperature factor*

The Gaussian model of the probability density function (p.d.f.) $\rho_o(\mathbf{u})$ for atomic thermal motion defined in (6.1.1.30) is adequate in many cases. Where anharmonicity or curvilinear motion is important, however, more elaborate models are needed.

In the classical (high-temperature) regime, the generalized temperature factor is given by the Fourier transform of the one-particle p.d.f:

$$\rho(\mathbf{u}) = N^{-1} \exp[-V(\mathbf{u})/kT], \tag{6.1.1.36}$$

where

$$N = \int \exp[-V(\mathbf{u})/kT]\, \mathrm{d}\mathbf{u}. \tag{6.1.1.37}$$

In the cases where the potential function $V(\mathbf{u})$ is a close approximation to the Gaussian (harmonic) potential, series expansions based on a perturbation treatment of the anharmonic terms provide a satisfactory representation of the temperature factors. That is, if the deviations from the Gaussian shape are small, approximations obtained by adding higher-order corrections to the Gaussian model are satisfactory.

In an arbitrary coordinate system, the number of significant high-order tensor coefficients for the correction is large. It may be helpful to choose coordinates parallel to the principal axes for the harmonic approximation so that

$$V(\mathbf{u})/kT = 1/2 \sum_{i=1}^{3} (B_i u_i)^2, \tag{6.1.1.38}$$

in which case (6.1.1.36) may be written as

$$\rho_o(\mathbf{u}) = \frac{1}{N_0} \exp\left[-1/2 \sum_i (B_i u_i)^2 \right], \tag{6.1.1.39}$$

where

$$N_0 = \frac{B_1 B_2 B_3}{8\pi^3}. \tag{6.1.1.40}$$

The harmonic temperature factor is

$$T_o(\mathbf{S}) = \exp\left[-1/2 \sum_i (b_i S_i)^2 \right], \tag{6.1.1.41}$$

where b_i and B_i are related by the reciprocity condition

$$b_i B_i = 1. \tag{6.1.1.42}$$

Table 6.1.1.9. $f_{nl}(\alpha, S) = \int_0^\infty r^n \exp(-\alpha r) j_l(Sr)\, dr$

n \ l	1	2	3	4
0	$\frac{1}{(S^2+\alpha^2)}$	$\frac{2\alpha}{(S^2+\alpha^2)^2}$	$\frac{2(3\alpha^2-S^2)}{(S^2+\alpha^2)^3}$	$\frac{24\alpha(\alpha^2-S^2)}{(S^2+\alpha^2)^4}$
1		$\frac{2S}{(S^2+\alpha^2)^2}$	$\frac{8S\alpha}{(S^2+\alpha^2)^3}$	$\frac{8S(5\alpha^2-S^2)}{(S^2+\alpha^2)^4}$
2			$\frac{8S^2}{(S^2+\alpha^2)^3}$	$\frac{48S^2\alpha}{(S^2+\alpha^2)^4}$
3				$\frac{48S^3}{(S^2+\alpha^2)^4}$

6.1.1.6.1. *Gram–Charlier series*

In the Gram–Charlier series expansion (Kuznetsov, Stratonovich & Tikhonov, 1960), the general p.d.f. $\rho(\mathbf{u})$ is approximated by

$$\left[1 - c^j D_j + \frac{c^{jk}}{2!} D_j D_k - \ldots + (-)^p \frac{c^{jk\ldots\zeta}}{p!} D_\alpha D_\beta \ldots D_\zeta\right] \rho_o(\mathbf{u}). \tag{6.1.1.43}$$

The operator $D_\alpha D_\beta \ldots D_\zeta$ is the pth partial (covariant) derivative $\partial^p / \partial u_\alpha \partial u_\beta \ldots \partial u_\zeta$, and $c^{jk\ldots\zeta}$ is a contravariant component of the coefficient tensor. The quasi-moment coefficient tensors are symmetric for all permutations of indices. The first four have three, six, ten, and fifteen unique components for site symmetry 1. The third- and fourth-order terms describe the skewness and the kurtosis of the p.d.f., respectively.

The Gram–Charlier series may be rewritten using general multidimensional Hermite polynomial tensors, defined by

$$\begin{aligned} H_{\alpha\beta\ldots\zeta}(\mathbf{u}) &= (-)^p \exp(\tfrac{1}{2}\sigma_{jk}^{-1} u^j u^k) \\ &\quad \times D_\alpha D_\beta \ldots D_\zeta \exp(-\tfrac{1}{2}\sigma_{jk}^{-1} u^j u^k). \end{aligned} \tag{6.1.1.44}$$

For $w_j = \sigma_{jk}^{-1} u^k$, and with $\sigma_{jk}^{-1} = \sigma_{kj}^{-1}$ and $w_j w_k = w_k w_j$, the first few general Hermite polynomials may be expressed as

$$\begin{aligned} {}^0H(\mathbf{u}) &= 1 \\ {}^1H_j(\mathbf{u}) &= w_j \\ {}^2H_{jk}(\mathbf{u}) &= w_j w_k - \sigma_{jk}^{-1} \\ {}^3H_{jk}(\mathbf{u}) &= w_j w_k w_l - w_j \sigma_{kl}^{-1} - w_k \sigma_{lj}^{-1} - w_l \sigma_{jk}^{-1} \\ &= w_j w_k w_l - 3 w_{(j} \sigma_{kl)}^{-1} \\ {}^4H_{jklm}(\mathbf{u}) &= w_j w_k w_l w_m - 6 w_{(j} w_k \sigma_{lm)}^{-1} + 3 \sigma_{j(k}^{-1} \sigma_{lm)}^{-1}. \end{aligned} \tag{6.1.1.45}$$

Indices in parentheses indicate terms to be averaged over all unique permutations of those indices.

The Gram–Charlier series is then

$$\rho_o(\mathbf{u}) \left[1 + \frac{1}{3!} c^{jkl} H_{jkl}(\mathbf{u}) + \frac{1}{4!} c^{jklm} H_{jklm}(\mathbf{u}) + \ldots\right], \tag{6.1.1.46}$$

in which the mean and the dispersion of $\rho_o(\mathbf{u})$ have been chosen to make c^j and c^{jk} vanish.

The Fourier transform, after truncating at the quartic term, gives an approximation to the generalized temperature factor:

$$T(\mathbf{S}) = T_o(\mathbf{S}) \left[1 + \frac{i^3}{3!} c^{jkl} S_j S_k S_l + \frac{i^4}{4!} c^{jklm} S_j S_k S_l S_m\right], \tag{6.1.1.47}$$

i.e. the Fourier transform of the Hermite polynomial expansion about the Gaussian p.d.f. is a power-series expansion about the Gaussian temperature factor with even-order terms real and odd-order terms imaginary.

Table 6.1.1.10. *Indices nmp allowed by the site symmetry for the functions $H_n(z)\Phi_{mp}(\varphi)$; μ, ν and j are integers such that $m, n \geq 0$; $(-)^n$ implies $p = -$ for n odd and $p = +$ for n even*

Site symmetry	Coordinate axes	Indices
$\underline{1}$	Any	All (n, m, p)
$\bar{1}$	Any	$(n, n+2j, p)$
2	$2 \parallel x$	$(n, m, (-)^n)$
	$2 \parallel y$	$(n, m, (-)^{n-m})$
	$2 \parallel z$	$(n, 2\nu, p)$
m	$m \perp x$	$(n, m, (-)^m)$
	$m \perp y$	$(n, m, +)$
	$m \perp z$	$(2\mu, m, p)$
$2/m$	$2 \parallel x, m \perp x$	$(m+2j, m, (-)^m)$
	$2 \parallel y, m \perp y$	$(m+2j, m, +)$
	$2 \parallel z, m \perp z$	$(2\mu, 2\nu, p)$
222	$2 \parallel z, 2 \parallel y$	$(n, 2\nu, (-)^n)$
$mm2$	$2 \parallel x, m \perp z$	$(2\mu, m+)$
	$2 \parallel y, m \perp z$	$(2\mu, m, (-)^m)$
	$2 \parallel z, m \perp y$	$(n, 2\nu, +)$
mmm	$m \perp z, m \perp y, m \perp z$	$(2\mu, 2\nu, +)$
$\underline{4}$	$4 \parallel z$	$(n, 4\nu, p)$
$\bar{4}$	$4 \parallel z$	$(n, 2n+4j, p)$
$4/m$	$4 \parallel z, m \perp z$	$(2\mu, 4\nu, p)$
422	$4 \parallel z, 2 \parallel y$	$(n, 4\nu, (-)^n)$
$4mm$	$4 \parallel z, m \perp y$	$(n, 4\nu, +)$
$\bar{4}2m$	$\bar{4} \parallel z, 2 \parallel x$	$(n, 2n+4j, (-)^n)$
	$\bar{4} \parallel z, m \perp y$	$(n, 2n+4j, +)$
$4/mmm$	$4 \parallel z, m \perp z, m \perp x$	$(2\mu, 4\nu, +)$
$\underline{3}$	$3 \parallel z$	$(n, 3\nu, p)$
$\bar{3}$	$3 \parallel z$	$(m+2j, 3\nu, p)$
32	$3 \parallel z, 2 \parallel y$	$(n, 3\nu, (-)^{n-m})$
	$3 \parallel z, 2 \parallel x$	$(n, 3\nu, (-)^n)$
$3m$	$3 \parallel z, m \perp y$	$(n, 3\nu, +)$
	$3 \parallel z, m \perp x$	$(n, 3\nu, (-)^m)$
$\bar{3}m$	$\bar{3} \parallel z, m \perp y$	$(m+2j, 3\nu, +)$
	$\bar{3} \parallel z, m \perp x$	$(m+2j, 3\nu, (-)^m)$
$\underline{6}$	$6 \parallel z$	$(n, 6\nu, p)$
$\bar{6}$	$\bar{6} \parallel z$	$(2\mu, 3\nu, p)$
$6/m$	$6 \parallel z, m \perp z$	$(2\mu, 6\nu, p)$
622	$6 \parallel z, 2 \parallel y$	$(n, 6\nu, (-)^n)$
$6mm$	$\bar{6} \parallel z, m \perp y$	$(n, 6\nu, +)$
$\bar{6}m2$	$\bar{6} \parallel z, m \perp y$	$(2\mu, 3\nu, +)$
	$\bar{6} \parallel z, m \perp x$	$(2\mu, 3\nu, (-)^m)$
$6/mmm$	$6 \parallel z, m \perp z, m \perp y$	$(2\mu, 6\nu, +)$

Because of the symmetry of the relationship between the Fourier transform of a real function and its inverse, the functional form of the p.d.f. and that of the temperature factor can be interchanged. Exchanging the role of the Hermite polynomials and the power series from the Gram–Charlier expansion has been studied by Scheringer (1985), with the objective of obtaining the one-particle potentials more directly.

6.1.1.6.2. *Fourier-invariant expansions*

When truncated, an expression for a multipole expansion, p.d.f. or temperature factor must retain those terms essential to the accuracy required of the expansion. Some authors (*e.g.*

Table 6.1.1.11. *Indices n_x, n_y, n_z allowed for the basis functions $H_{n_x}(Ax)H_{n_y}(By)H_{n_z}(Cz)$; λ, μ, and ν are non-negative; conditions for other choices of axes are derived by cyclic permutation*

Symmetry	Coordinate axes	Allowed indices
$\underline{1}$	Any	All (n_x, n_y, n_z)
$\bar{1}$	Any	$n_x + n_y + n_z = 2\lambda$
2	$2 \parallel z$	$n_x + n_y = 2\lambda$
m	$m \perp z$	$n_z = 2\nu$
$2/m$	$2 \parallel z, m \perp z$	$n_x + n_y = 2\lambda, n_z = 2\nu$
222	$2 \parallel z, 2 \parallel y$	n_x, n_y, n_z all even or all odd
$mm2$	$2 \parallel z, m \perp y$	$n_x = 2\lambda, n_y = 2\mu$
mmm	$m \perp z, m \perp y, m \perp z$	$n_x = 2\lambda, n_y = 2\mu, n_z = 2\nu$

Stewart, 1980*b*) strongly favour classes of truncated expansion that retain symmetry properties appropriate to particular classes of transformation, such as rotation or Fourier inversion. Others, emphasizing simplicity, retain the minimum set of terms required to preserve the accuracy needed in the expansion. In either case, it is desirable for the expansion to converge rapidly, and to have a form related to physical theory.

In principle, the one-particle potential may be expanded in any complete set of functions. Harmonic oscillator functions simplify simultaneous interpretation of the probability distribution in real and reciprocal space because their form does not change under Fourier inversion (Kurki-Suonio, Merisalo & Peltonen, 1979).

If both anharmonicity and anisotropy are small, the p.d.f. may be expressed as a rapidly converging expansion in spherical polar coordinates u, θ, φ:

$$\rho(\mathbf{u}) = \rho_o(\mathbf{u})\frac{N_0}{N}\left[1 - \sum_{n,l,m,p} a_{nlmp}R_{nl}(Bu)Y_{lmp}(\theta,\varphi)\right] \quad (6.1.1.48)$$

for non-cubic and

$$\rho(\mathbf{u}) = \rho_o(\mathbf{u})\frac{N_0}{N}\left[1 - \sum_{n,l,j} a_{nlj}R_{nl}(Bu)K_{lj}(\theta,\varphi)\right] \quad (6.1.1.49)$$

for cubic site symmetry. The radial term may be written as

$$R_{nl}(x) = x^l L^{l+1/2}_{(n-l)/2}(x^2), \quad (6.1.1.50)$$

where the associated Laguerre polynomial is

$$L^{\alpha}_{k}(t) = \sum_{\nu=0}^{k}\binom{k+\alpha}{k-\alpha}\frac{(-t)^\nu}{\nu!} \quad (6.1.1.51)$$

with

$$\binom{p}{q} = \frac{\Gamma(p+1)}{[\Gamma(q+1)\Gamma(p-q+1)]} \quad (6.1.1.52)$$

and the normalizing factor

$$N = \frac{8\pi^3}{B^3}\left[1 - \sum_{\nu}(-)^\nu\frac{(2\nu+1)!}{2^{2\nu}(\nu!)^2}a_{2\nu 00+}\right]. \quad (6.1.1.53)$$

The real spherical harmonics $Y_{lmp}(\theta,\varphi)$ and the cubic harmonics $K_{lj}(\theta,\varphi)$ are as defined in Subsection 6.1.1.4. As in the case of multipole expansions, the non-zero coefficients in these expressions are limited by the site symmetry. The restrictions on the temperature factor are identical to those for the generalized scattering factor listed in Tables 6.1.1.7 and 6.1.1.8.

From the Fourier invariance of harmonic oscillator functions,

$$T(\mathbf{S}) = \frac{N_0}{N}\exp(-b^2S^2/2) \times\left[1 - \sum_{n,l,m,p} a_{nlmp}i^nR_{nl}(bS)Y_{lmp}(\theta_S,\varphi_S)\right] \quad (6.1.1.54)$$

and

$$T(\mathbf{S}) = \frac{N_0}{N}\exp(-b^2S^2/2) \times\left[1 - \sum_{n,l,j} a_{nlj}i^nR_{nl}(bS)K_{lj}(\theta_S,\varphi_S)\right] \quad (6.1.1.55)$$

for non-cubic and cubic site symmetries, respectively. θ_S and φ_S are polar coordinates in reciprocal space.

With an appropriate choice of origin, the first-order (110+) and (111±) terms vanish. The isotropic harmonic (200+) and constant (000+) terms have been removed from the summation. If coordinate axes are chosen coincident with the principal axes for the harmonic approximation, (221±) and (222−) vanish. (220+) indicates the prolateness and (222+) the non-axiality in the harmonic approximation (Kurki-Suonio, 1977). Terms with $n \geq 2$ describe the anharmonicity.

The approximations in (6.1.1.48) to (6.1.1.55) fail if the anisotropy, indicated by the size of the (220+) and (222+) terms, or the anharmonicity is large. If the anharmonicity and non-axiality are small, one can invoke Fourier-invariant expansions in cylindrical polar coordinates u_r, u_z, φ:

$$\rho(\mathbf{u}) = \rho_o(\mathbf{u})\frac{N_0}{N} \times\left[1 - \sum_{n_z,n,m,p} b_{n_znmp}H_{n_z}(B_zu_z)\mathbf{P}_{nm}(B_ru_r)\Phi_{mp}(\varphi)\right] \quad (6.1.1.56)$$

and

$$T(S) = \frac{N_0}{N}\exp[-\tfrac{1}{2}(b_r^2S_r^2 + b_z^2S_z^2)] \times\left[1 - \sum_{n_z,n,m,p} b_{n_znmp}H_{n_z}(b_zS_z)\mathbf{P}_{nm}(b_rS_r)\Phi_{mp}(\varphi_S)\right], \quad (6.1.1.57)$$

where S_r, S_z, φ_S are cylindrical coordinates for S.

$$\mathbf{P}_{nm}(x) = x^mL^m_{(n-m)/2}(x^2), \quad \Phi_{m\pm}(\varphi) = \begin{matrix}\cos m\varphi \\ \sin m\varphi\end{matrix} \quad (6.1.1.58)$$

and

$$N = \frac{8\pi^3}{B_r^2B_z}\left[1 - \sum_{\mu\nu}(-)^\nu\frac{(2\mu)!}{\mu!}b_{2\mu 2\nu 0+}\right]. \quad (6.1.1.59)$$

The indices allowed for the site symmetrical basis are as indicated in Table 6.1.1.10.

Again, the first-order (100+) and (011±) terms vanish with the appropriate choice of origin. For coordinate axes coinciding with the principal axes of the harmonic approximation, (111±) and (022−) vanish. (020+), (200+), and (000+) have been removed from the summation.

Equations (6.1.1.56) and (6.1.1.57) apply accurately to non-cubic symmetries with rotation axes higher than twofold where non-axiality vanishes. Where non-axiality is large, it is preferable to use the Cartesian Fourier invariant expansion

$$\rho(\mathbf{u}) = \frac{N_0}{N}\exp\left[-1/2\sum_i B_i^2 u_1^2\right] \times \left[1 - \sum_{n_x,n_y,n_z} c_{n_x n_y, n_z} H_{n_x}(B_x u_x) H_{n_y}(B_y u_y) H_{n_z}(B_z u_z)\right] \tag{6.1.1.60}$$

and

$$T(\mathbf{S}) = \frac{N_0}{N}\exp\left[-1/2\sum_i b_i^2 u_1^2\right] \times \left[1 - \sum_{n_x,n_y,n_z} c_{n_x n_y, n_z} H_{n_x}(b_x u_x) H_{n_y}(b_y u_y) H_{n_z}(b_z u_z)\right], \tag{6.1.1.61}$$

where

$$N = \frac{8\pi^3}{B_x B_y B_z}\left[1 - \sum_{\lambda\mu\nu}\frac{(2\lambda)!(2\mu)!(2\nu)!}{\lambda!\mu!\nu!} c_{2\lambda 2\mu 2\nu}\right]. \tag{6.1.1.62}$$

The indices allowed under the site symmetry are listed in Table 6.1.1.11.

The first-order terms vanish with suitable choice of origin. (110), (101), and (011) vanish if the coordinates coincide with the principal axes for the harmonic approximation, and (200), (020), (002), and (000) are removed from the summation. Only anharmonic terms remain.

6.1.1.6.3. *Cumulant expansion*

In a cumulant expansion (Johnson & Levy, 1974), the entire series is expressed in exponential form. The cumulant expansion about $\mathbf{S} = 0$ for the generalized temperature factor is

$$T(\mathbf{S}) = \exp\left[1 + i\kappa^j S_j + \frac{i^2}{2!}\kappa^{jk} S_j S_k + \frac{i^3}{3!}\kappa^{jkl} S_j S_k S_l + \frac{i^4}{4!}\kappa^{jklm} S_j S_k S_l S_m + \ldots\right], \tag{6.1.1.63}$$

where the coefficient tensor $\kappa^{\alpha\beta\ldots\zeta}$, a symmetric tensor of order p, is the pth-order cumulant. The inverse Fourier transform is the Edgeworth expansion around the Gaussian p.d.f. Cumulants can be expressed in terms of moments and *vice versa*. The pth moment $\mu^{\alpha\beta\ldots\zeta}$ (if it exists) of a general p.d.f., $\rho(\mathbf{x})$, is a symmetric tensor defined as

$$\mu^{\alpha\beta\ldots\zeta}(\mathbf{x}) = \int_{-\infty}^{\infty} x^\alpha x^\beta \ldots x^\zeta \rho(\mathbf{x})\,\mathrm{d}\mathbf{x}. \tag{6.1.1.64}$$

The relations between the lower-order moments and cumulants are

$$\begin{aligned}
\mu^j &= \kappa^j \\
\mu^{jk} &= \kappa^{jk} + \kappa^j\kappa^k \\
\mu^{jkl} &= \kappa^{jkl} + \kappa^j\kappa^{kl} + \kappa^k\kappa^{lj} + \kappa^l\kappa^{jk} + \kappa^j\kappa^k\kappa^l \\
&= \kappa^{jkl} + 3\kappa^{(j}\kappa^{kl)} + \kappa^j\kappa^k\kappa^l \\
\mu^{jklm} &= \kappa^{jklm} + 3\kappa^{j(k}\kappa^{lm)} + 4\kappa^{(j}\kappa^{klm)} \\
&\quad + 6\kappa^{(j}\kappa^k\kappa^{lm)} + \kappa^j\kappa^k\kappa^l\kappa^m
\end{aligned} \tag{6.1.1.65}$$

and, conversely,

$$\begin{aligned}
\kappa^j &= \mu^j \\
\kappa^{jk} &= \mu^{jk} - \mu^j\mu^k \\
\kappa^{jkl} &= \mu^{jkl} - 3\mu^{(j}\mu^{kl)} + 2\mu^j\mu^k\mu^l \\
\kappa^{jklm} &= \mu^{jklm} - 3\mu^{j(k}\mu^{lm)} - 4\mu^{(j}\mu^{klm)} \\
&\quad + 12\mu^{(j}\mu^k\mu^{lm)} - 6\mu^j\mu^k\mu^l\mu^m.
\end{aligned} \tag{6.1.1.66}$$

In the Gram–Charlier and Fourier-invariant expansions, the Fourier-transform relationship between the p.d.f. and the temperature factor to given order can be made exact. Each cumulant μ^{jkl} contributes to all higher-order quasi-moment terms and *vice versa*. Hence, a given cumulant expansion is to an extent arbitrarily truncated (Kuhs, 1983). Care is required when interpreting the coefficients (Zucker & Schulz, 1982).

On the other hand, the cumulant expansion has the advantage of yielding tractable expressions for the one-particle potential in the quantum regime (Mair, 1980*a*). In that regime, equation (6.1.1.36) for the one-particle potential is invalid, and the expressions relating $V(\mathbf{u})$ to $\rho(\mathbf{u})$ in the Gram–Charlier and Fourier-invariant expansions are cumbersome (Mair & Wilkins, 1976).

Coefficients obtained by applying least-squares methods to structure-factor equations related to the truncated cumulant expansions do not necessarily yield non-negative p.d.f.'s nor are the linear-term coefficients necessarily faithful representations of the mean. Caution must be exercised in interpreting the results.

All the methods are satisfactory in the case of rapidly converging potential series. The methods are equivalent up to λ^2 in the van Hove order parameter (Mair, 1980*b*). Difficulties are encountered with convergence of the series in the case of strong anharmonicity, in which case numerical or alternative analytical models may be necessary. If the anharmonicity is such that the difference between the expansions is significant, it may be preferable to evaluate the Fourier transforms directly, as recommended by Mackenzie & Mair (1985).

6.1.1.6.4. *Curvilinear density functions*

For groups of atoms moving on the surface of a circle or sphere, perturbation expansions in Cartesian coordinates may converge slowly. Methods of representing curvilinear density functions that are multimodal or have large amplitude are described by Press & Hüller (1973).

For atoms constrained to rotate about a single axis,

$$a(\mathbf{u}) = \frac{1}{2\pi\tau}\delta(r-\tau)\delta(z)f(\varphi), \tag{6.1.1.67}$$

where r, z, φ are cylindrical coordinates for the displacement $\mathbf{u}$. Setting

$$f(\varphi) = \sum_{m=0} c_m \exp(im\varphi) + c_m^*(-im\varphi) \tag{6.1.1.68}$$

and

$$\exp(i\mathbf{S}\cdot\mathbf{r}) = \exp(iS_z z)\exp[iS_r r\cos(\varphi_S - \varphi)] \tag{6.1.1.69}$$

and using

$$\exp[iS_r r\cos(\varphi_S-\varphi)] = \sum_{l=0}(2-\delta_{l0})i^l J_l(S_r r)\cos[l(\varphi_S-\varphi)] \tag{6.1.1.70}$$

yields

$$T(\mathbf{S}) = \sum_{l=0} i^l J_l(S_r\tau)[c_l\exp(il\varphi_S) + c_l^*\exp(-il\varphi_S)]. \tag{6.1.1.71}$$

For atoms moving on the surface and a sphere, the density function may be written

$$\rho(\mathbf{u}) = \sum_{l=0}^{\infty} \sum_{j=1}^{2l+1} a_{lj}(u) K_{lj}(\theta, \varphi), \tag{6.1.1.72}$$

where u, θ, φ are spherical polar displacement coordinates and the K_{lj} are cubic harmonics. Thus, for a rigid molecule, the density function for nuclei confined to move on a spherical shell of radius τ is

$$a_{lj}(\mathbf{u}) = c_{lj}\delta(u - \tau)/u^2. \tag{6.1.1.73}$$

Expansion of $\exp(i\mathbf{S}\cdot\mathbf{r})$ in cubic harmonics

$$\exp(i\mathbf{S}\cdot\mathbf{r}) = 4\pi \sum_{l,j} i^l j_l(Sr) K_{lj}(\theta_S, \varphi_S) K_{lj}(\theta, \varphi) \tag{6.1.1.74}$$

leads to

$$T(\mathbf{S}) = 4\pi \sum_{l,j} i^l c_{lj} j_l(S\tau) K_{lj}(\theta_S, \varphi_S). \tag{6.1.1.75}$$

Equations (6.1.1.71) and (6.1.1.75) are useful when the p.d.f.'s (6.1.1.67) and (6.1.1.72) can be approximated by a limited number of significant terms. They are readily adapted to the case of oscillations about axes of symmetry (Press & Hüller, 1973).

6.1.1.6.5. *Model-based curvilinear density functions*

For rotational oscillations, which are the curvilinear coordinate analogues of the p.d.f.'s approximating harmonic rectilinear motion, techniques for evaluating the temperature factor are described by Johnson & Levy (1974).

The p.d.f. for an atom in a group of atoms undergoing large-amplitude rotational oscillation (libration) can sometimes be approximated satisfactory by a standard p.d.f. on the circle or on the sphere. The closest analogues of the rectilinear Gaussian p.d.f. are the Brownian-diffusion p.d.f.'s defined on the closed spaces of the circle and the sphere. For statistical analysis, two other p.d.f.'s, the von Mises 'circular normal' and the Fisher 'spherical normal', are often substituted for the Brownian-diffusion density functions because of their simpler forms.

The p.d.f. for Brownian diffusion on a circle, also called the 'wrapped normal' p.d.f. (Feller, 1966; Lévy, 1938), is given by

$$\rho(\theta) = \frac{1}{(2\pi)^{1/2}\sigma} \sum_{n=-\infty}^{\infty} \exp[-(\theta - 2n\pi)^2/2\sigma^2], \tag{6.1.1.76}$$

which may be transformed (Bellman, 1961) into

$$\rho(\theta) = \frac{1}{2\pi} \sum_{m=0}^{\infty} (2 - \delta_{m0}) \exp(-m^2\sigma^2/2) \cos(m\theta). \tag{6.1.1.77}$$

The von Mises p.d.f. (Gumbel, Greenwood & Durand, 1953; Mardin, 1972; von Mises, 1918) is

$$\rho(\theta) = \frac{\exp(k_c \cos\theta)}{2\pi I_o(k_c)} = \frac{1}{2\pi} \sum_{m=0}^{\infty} (2 - \delta_{m0}) \frac{I_m(k_c)}{I_0(k_c)} \cos(m\theta). \tag{6.1.1.78}$$

$I_m(x)$ is the mth-order Bessel function of the first kind with imaginary argument. The parameter σ^2 is the variance; k_c is a measure of concentration such that when k_c is zero the probability density is uniformly distributed over the circle, and when k_c is large the density is concentrated around the modal vector at $\theta = 0$. An approximate relation between σ^2 and k_c can be obtained by equating expressions for the centres of mass of the circular Brownian diffusion and von Mises p.d.f.'s (Stephens, 1963),

$$\exp(-\sigma^2/2) = \frac{I_1(k_c)}{I_0(k_c)}. \tag{6.1.1.79}$$

For small σ^2 (large k_c), we find that

$$\sigma^2 \simeq 1/k_c. \tag{6.1.1.80}$$

Equations (6.1.1.76) to (6.1.1.78) can be generalized to describe multimodal density functions with modes (maxima) arranged symmetrically about the circle. The p.d.f. for the s-modal Brownian-diffusion p.d.f. with one of the s modes at $\theta = \theta_0$ is

$$\begin{aligned}\rho(\theta) &= \frac{1}{\sqrt{2\pi}s\sigma} \sum_{m=-\infty}^{\infty} \exp[-(\theta - \theta_0 - 2\pi m/s)^2/2\sigma^2] \\ &= \frac{1}{2\pi} \sum_{m=0}^{\infty} (2 - \delta_{m0}) \exp[-(ms\sigma)^2/2] \cos[ms(\theta - \theta_0)].\end{aligned} \tag{6.1.1.81}$$

The two-dimensional Fourier transform (Chidambaram & Brown, 1973) of the last equation in terms of the polar coordinates (S, θ) of the reciprocal-space vector $\mathbf{S}$ relative to an origin at the centre of the circle is

$$T(\mathbf{S}) = \sum_{j=0}^{\infty} (2 - \delta_{j0}) i^{js} J_{js}(Sr) \exp[-(js\sigma)^2/2] \cos js\theta_0, \tag{6.1.1.82}$$

where $J_n(x)$ is the Bessel function of the first kind of order n with real argument. Corresponding equations for the von Mises s-modal density function (Atoji, Watanabe & Lipscomb, 1953; King & Lipscomb, 1950; Mardin, 1972) are

$$\begin{aligned}\rho(\theta) &= \frac{1}{2\pi I_o(K_c)} \exp[K_c \cos s(\theta - \theta_0)] \\ &= \frac{1}{2\pi} \sum_{m=0}^{\infty} (2 - \delta_{m0}) \frac{I_m(K_c)}{I_o(K_c)} \cos ms(\theta - \theta_0)\end{aligned} \tag{6.1.1.83}$$

and

$$T(\mathbf{S}) = \sum_{j=0}^{\infty} (2 - \delta_{j0}) i^{js} J_{js}(Sr) \frac{I_j(K_c)}{I_0(K_c)} \cos js\theta_0, \tag{6.1.1.84}$$

where K_c, a measure of concentration over $1/s$th of the circle about θ_0, is substituted for the k_c parameter of the unimodal von Mises density function and K_c is related to k_c approximately by

$$I_1(k_c)/I_0(k_c) = I_s(K_c)/I_0(K_c). \tag{6.1.1.85}$$

For symmetrical Brownian diffusion on a sphere (Furry, 1957; Lévy, 1938; Mardin, 1972; Perrin, 1928), the p.d.f. in terms of the angular displacement θ from the pole is

$$\rho(\theta) = \sum_{n=0}^{\infty} \frac{2n+1}{4\pi} \exp[-n(n+1)V] P_n(\cos\theta) \sin\theta, \tag{6.1.1.86}$$

where $P_n(x)$ is the nth-order Legendre polynomial. The Fisher (1953) 'spherical normal' p.d.f. (Mardin, 1972) is a similar density function given by

$$\begin{aligned}\rho(\theta) &= \frac{k_s}{4\pi \sinh k_s} \exp(k_s \cos\theta) \sin\theta \\ &= \sum_{n=0}^{\infty} \frac{(2n+1)}{4\pi} \frac{I_{n+1/2}(k_s)}{I_{1/2}(k_s)} P_n(\cos\theta) \sin\theta.\end{aligned} \tag{6.1.1.87}$$

The parameters V (variance) and k_s are measures of concentration analogous to those for the circle and may be related (Roberts & Ursell, 1960) by an equation analogous to (6.1.1.79),

$$\exp(-V/2) = \coth k_s - \frac{1}{k_s} = \frac{I_{3/2}(k_s)}{I_{1/2}(k_s)}, \quad (6.1.1.88)$$

the small V approximation being

$$V \simeq 2/k_s. \quad (6.1.1.89)$$

Equations (6.1.1.86) and (6.1.1.87) are generalized to place the mode of the density at (r, θ', φ') by replacing $\cos\theta$ by $\cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\varphi - \varphi')$ and by replacing $P_n(\cos\theta)$ by

$$P(\cos\theta)P_n(\cos\theta') + 2\sum_{m=1}^{n}\frac{(n-m)!}{(n-m)!} \times P_n^m(\cos\theta)P_n^m(\cos\theta')\cos m(\varphi - \varphi').$$

The three-dimensional Fourier transform of the generalized form of (6.1.1.86) in terms of $\mathbf{S}$ in spherical coordinates (S, θ_S, φ_S) is

$$T(\mathbf{S}) = \sum_{q=0}^{\infty} i^q \frac{(2q+1)}{r^2}\exp[-q(q+1)V] \times \sum_{s=0}^{\infty}\frac{4}{2p+1}Y_{qs+}(\theta', \varphi')Y_{qs+}(\theta_S, \varphi_S)j_q(Sr), \quad (6.1.1.90)$$

where r is the radius of the sphere, and j_n is the nth-order spherical Bessel function of the first kind. The real spherical harmonics Y_{lmp} are normalized as in (6.1.1.22).

The Fourier transform of the generalized form of (6.1.1.87) is identical to (6.1.1.90) except that the term $\exp[-q(q+1)V]$ in (6.1.1.90) is replaced by $I_{q+1/2}(k_s)/I_{1/2}(k_s)$.

The foregoing equations describe isotropic distributions on a sphere. The p.d.f. for general anisotropic Brownian diffusion (or rotation) on a sphere is not available in a convenient form. However, some of the results of Perrin (1934) and Favro (1960) on rotational Brownian motion are applicable to thermal motion. For example, the centre of mass of a p.d.f. resulting from anisotropic diffusion on a sphere is given by equation (6.8) of Favro (1960). The following equation valid in Cartesian coordinates is obtained if the diffusion tensor $\mathbf{D}$ of Favro's equation is replaced by the substitution $\mathbf{L} = 2\mathbf{D}$

$$\langle\mathbf{x}\rangle = \exp[-\tfrac{1}{2}(\mathrm{tr}(\mathbf{L})\mathbf{I} - \mathbf{L})]\mathbf{r} = \mathbf{r} - \tfrac{1}{2}[\mathrm{tr}(\mathbf{L})\mathbf{I} - \mathbf{L}]\mathbf{r} + \tfrac{1}{8}[\mathrm{tr}(\mathbf{L})\mathbf{I} - \mathbf{L}]^2\mathbf{r} - \ldots, \quad (6.1.1.91)$$

where $\mathbf{r}$ is the vector from the centre of the sphere to the mode of the p.d.f. on the sphere and $\langle\mathbf{x}\rangle$ is the vector to the centre of mass. This equation, which is valid for all amplitudes of libration $\mathbf{L}$, can be used to describe the apparent shrinkage effect in molecules undergoing librational motion.

6.1.1.6.6. *The quasi-Gaussian approximation for curvilinear motion*

The p.d.f.'s defined by (6.1.1.77), (6.1.1.78), (6.1.1.86) and (6.1.1.87), and their Fourier transforms given in §6.1.1.6.5 may be considered 'inverted series' since zero-order terms describe uniform distributions. The inverted series converge slowly if the density is concentrated near the mode. If σ^2 in (6.1.1.76) is sufficiently small, the cyclic overlap on the circle becomes unimportant and the summation for $n \neq 0$ can be neglected. In this limiting case, the p.d.f. assumes the same form as a one-dimensional rectilinear Gaussian density function except that the variable is the angle φ. A similar relation must exist between the p.d.f. on the sphere and the two-dimensional Gaussian function. This 'quasi-Gaussian' approximation is the basis for a number of structure-factor equations for atoms with relatively small amplitude components of curvilinear motion (Dawson, 1970; Kay & Behrendt, 1963; Kendall & Stuart, 1963; Maslen, 1968; Pawley & Willis, 1970).

6.1.1.7. *Structure factor*

The amplitude of coherent scattering from the contents of one unit cell in a crystalline material is the structure factor

$$F(\mathbf{S}) = \int \rho(\mathbf{r})\exp(i\mathbf{S}\cdot\mathbf{r})\,\mathrm{d}r, \quad (6.1.1.92)$$

where the integration extends over the unit cell. If there are N atoms in the cell, this may be expressed as

$$F(\mathbf{S}) = \sum_{j=1}^{N} f_j T_j \exp(i\mathbf{S}\cdot\mathbf{r}_j), \quad (6.1.1.93)$$

where $\mathbf{r}_j$ is the mean position and T_j is the temperature factor of the jth atom. In an ideal model of the scattering process in which (6.1.1.93) is exact, f_j is the atomic scattering factor derived from (6.1.1.7). In practice, there are wavelength-dependent changes to the amplitude and phase of the atom's scattering due to dispersion or resonance. To correct for this, each scattering factor may be written

$$f = f^0 + f' + if'', \quad (6.1.1.94)$$

where f^0 is the kinematic scattering factor and f' and f'' are real and imaginary corrections for dispersion.

6.1.1.8. *Reflecting power of a crystal*

The reflecting power of a small crystal of volume ΔV, rotated at angular velocity ω through a Bragg reflection, defined as the ratio of ω times the reflected energy to the incident-beam intensity, is

$$r_e^2\left(\frac{1+\cos^2 2\theta}{2\sin 2\theta}\right)\lambda^3\frac{F(\mathbf{S})^2}{V_C^2}\Delta V, \quad (6.1.1.95)$$

where V_c is the unit-cell volume. This expression, which assumes negligible absorption, shows that the integrated intensity is proportional to the crystal volume. The maximum intensity is proportional to $(\Delta V)^2$, but the angular width of the reflecting region varies inversely as ΔV.

In the kinematic theory of diffraction, it is assumed that the crystal is comprised of small domains of perfect crystals for which the intensities are additive. In that case, (6.1.1.95) applies also to finite crystals.

6.1.2. Magnetic scattering of neutrons (By P. J. Brown)

6.1.2.1. *Glossary of symbols*

m_n	Neutron mass
m_e	Electron mass
γ	Neutron magnetic moment in nuclear magnetons (-1.91)
μ_B	Bohr magneton
μ_N	Nuclear magneton
r_e	Classical electron radius $\mu_B e^2/4\pi m_e$
$\mathbf{P}_i$	Electron momentum operator
$\mathbf{S}_e$	Electron spin operator
$\mathbf{S}_n$	Neutron spin operator
$\mathbf{M}(r)$	Magnetization density operator
$\mathbf{k}$	Scattering vector $(H/2\pi)$
$\hat{\mathbf{k}}$	A unit vector parallel to $\mathbf{k}$
$\mathbf{r}_n$	A lattice vector
$\mathbf{g}$	A reciprocal-lattice vector $(h/2\pi)$
$\boldsymbol{\tau}$	Propagation vector for a magnetic structure

references