

6.1. Intensity of diffracted intensities

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6.1.1. X-ray scattering

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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 xOy containing the incident and diffracted beams (Fig. 6.1.1.1), the amplitude of the scattered wave at a distance r is

$$r_e/r, \quad (6.1.1.1)$$

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 xOy , the amplitude of the scattered wave is

$$\frac{r_e}{r} \cos 2\theta. \quad (6.1.1.2)$$

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

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

The corresponding intensity of scattering per unit solid angle is

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

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

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

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

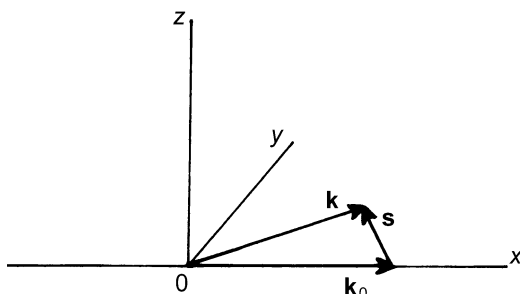


Fig. 6.1.1.1. Scattering by an electron. \mathbf{k}_0 and \mathbf{k} are the incident and scattered wavevectors, respectively.

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

$$\mathbf{S} = 2\pi\mathbf{s}. \quad (6.1.1.6)$$

The total amplitude for coherent scattering from the j th electron is

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

The intensity of coherent scattering is

$$I_{\text{coh}} = I_e f_j^2. \quad (6.1.1.8)$$

The intensity of Compton scattering from that electron is

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

For an atom with atomic number Z ,

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

and

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

where the correction term

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

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 $0 < (\sin \theta)/\lambda < 6.0 \text{ \AA}^{-1}$. The values for hydrogen are calculated from the analytical solution to the Schrödinger equation and are effectively zero for $(\sin \theta)/\lambda > 1.5 \text{ \AA}^{-1}$. 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 (1968a) (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 $0 < (\sin \theta)/\lambda < 2.0 \text{ \AA}^{-1}$, but these have been extended to 6 \AA^{-1} by Fox, O'Keefe & Tabernor (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

6.1. INTENSITY OF DIFFRACTED INTENSITIES

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 Z Method ($\sin \theta / \lambda$) (\AA^{-1})	H 1 E	He 2 RHF	Li 3 RHF	Be 4 RHF	B 5 RHF	C 6 RHF	N 7 RHF	O 8 RHF	F 9 RHF	Ne 10 RHF
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

6. INTERPRETATION OF DIFFRACTED INTENSITIES

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

Element Z Method ($\sin \theta$)/ λ (\AA^{-1})	Na 11 RHF	Mg 12 RHF	Al 13 RHF	Si 14 RHF	P 15 RHF	S 16 RHF	Cl 17 RHF	Ar 18 RHF	K 19 RHF	Ca 20 RHF
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

6.1. INTENSITY OF DIFFRACTED INTENSITIES

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

Element Z Method ($\sin \theta$)/ λ (\AA^{-1})	Sc 21 RHF	Ti 22 RHF	V 23 RHF	Cr 24 RHF	Mn 25 RHF	Fe 26 RHF	Co 27 RHF	Ni 28 RHF	Cu 29 RHF	Zn 30 RHF
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

6. INTERPRETATION OF DIFFRACTED INTENSITIES

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

Element Z Method ($\sin \theta$)/ λ (\AA^{-1})	Ga 31 RHF	Ge 32 RHF	As 33 RHF	Se 34 RHF	Br 35 RHF	Kr 36 RHF	Rb 37 RHF	Sr 38 RHF	Y 39 *RHF	Zr 40 *RHF
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

6.1. INTENSITY OF DIFFRACTED INTENSITIES

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

Element Z Method ($\sin \theta$)/ λ (\AA^{-1})	Nb 41 *RHF	Mo 42 RHF	Tc 43 *RHF	Ru 44 *RHF	Rh 45 *RHF	Pd 46 *RHF	Ag 47 RHF	Cd 48 RHF	In 49 RHF	Sn 50 RHF
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

6. INTERPRETATION OF DIFFRACTED INTENSITIES

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

Element Z Method ($\sin \theta$)/ λ (\AA^{-1})	Sb 51 RHF	Te 52 *RHF	I 53 RHF	Xe 54 RHF	Cs 55 RHF	Ba 56 RHF	La 57 *RHF	Ce 58 *RHF	Pr 59 *RHF	Nd 60 *RHF
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

6.1. INTENSITY OF DIFFRACTED INTENSITIES

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

Element Z Method ($\sin \theta$)/ λ (\AA^{-1})	Pm 61 *RHF	Sm 62 *RHF	Eu 63 RHF	Gd 64 *RHF	Tb 65 *RHF	Dy 66 *RHF	Ho 67 *RHF	Er 68 *RHF	Tm 69 *RHF	Yb 70 *RHF
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

6. INTERPRETATION OF DIFFRACTED INTENSITIES

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

Element Z Method ($\sin \theta$)/ λ (\AA^{-1})	Lu 71 *RHF	Hf 72 *RHF	Ta 73 *RHF	W 74 *RHF	Re 75 *RHF	Os 76 *RHF	Ir 77 *RHF	Pt 78 *RHF	Au 79 RHF	Hg 80 RHF
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

6.1. INTENSITY OF DIFFRACTED INTENSITIES

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

Element Z Method ($\sin \theta / \lambda$) (\AA^{-1})	Tl 81 *RHF	Pb 82 RHF	Bi 83 RHF	Po 84 *RHF	At 85 *RHF	Rn 86 RHF	Fr 87 *RHF	Ra 88 *RHF	Ac 89 *RHF	Th 90 *RHF
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

6. INTERPRETATION OF DIFFRACTED INTENSITIES

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

Element Z Method ($\sin \theta$)/ λ (\AA^{-1})	Pa 91 *RHF	U 92 RHF	Np 93 *RHF	Pu 94 *RHF	Am 95 *RHF	Cm 96 *RHF	Bk 97 *RHF	Cf 98 *RHF
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

6.1. INTENSITY OF DIFFRACTED INTENSITIES

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

(sin θ)/λ (Å ⁻¹)	f	(sin θ)/λ (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 Be²⁺ 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 θ)/λ 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, \dots, x_n is due to Aitken. $f(x|x_0, x_1, \dots, x_k)$ is the polynomial that coincides with the tabulated values at x_0, x_1, \dots, x_k .

$$\begin{aligned}
 f(x|x_0, x_1) &= \frac{1}{x_1 - x_0} \left| \begin{array}{c} f_0 x_0 - x \\ f_1 x_1 - x \end{array} \right| \\
 f(x|x_0, x_1, x_2) &= \frac{1}{x_2 - x_1} \left| \begin{array}{cc} f(x|x_0, x_1) & x_1 - x \\ f(x|x_0, x_2) & x_2 - x \end{array} \right| \\
 f(x|x_0, x_1, x_2, x_3) &= \frac{1}{x_3 - x_2} \left| \begin{array}{cc} f(x|x_0, x_1, x_2) & x_2 - x \\ f(x|x_0, x_1, x_3) & x_3 - x \end{array} \right|.
 \end{aligned}
 \tag{6.1.1.13}$$

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

$$R_n(x) = \pi_n(x)[x_0, x_1, \dots, x_n, x]. \tag{6.1.1.14}$$

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

$$\pi'_n(x_k) = (x_k - x_0)(x_k - x_1)\dots(x_k - x_{k-1}) \times (x_k - x_{k+1})\dots(x_k - x_n)$$

while

$$\begin{aligned}
 [x_0, x_1] &= \frac{f_0 - f_1}{x_0 - x_1} \\
 [x_0, x_1, x_2] &= \frac{[x_0, x_1] - [x_1, x_2]}{x_0 - x_2} \\
 [x_0, x_1, \dots, x_n] &= \sum_{k=0}^n \frac{f_k}{\pi'_n(x_k)}.
 \end{aligned}$$

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

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

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 $0 < (\sin \theta)/\lambda < 2.0 \text{ \AA}^{-1}$. 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 $2.0 \text{ \AA}^{-1} < (\sin \theta)/\lambda < 6.0 \text{ \AA}^{-1}$, 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

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

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 $2.0 < (\sin \theta)/\lambda < 6.0 \text{ \AA}^{-1}$. 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.