

6. INTERPRETATION OF DIFFRACTED INTENSITIES

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 Z Method ($\sin \theta$)/ λ (\AA^{-1})	H ¹⁻ 1 C	Li ¹⁺ 3 C	Be ²⁺ 4 C	C _{val} 6 HF	O ¹⁻ 8 HF	F ¹⁻ 9 HF	Na ¹⁺ 11 RHF	Mg ²⁺ 12 RHF	Al ³⁺ 13 HF	Si _{val} 14 HF
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		

6.1. INTENSITY OF DIFFRACTED INTENSITIES

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

Element Z Method ($\sin \theta$)/ λ (\AA^{-1})	Si ⁴⁺ 14 HF	Cl ¹⁻ 17 RHF	K ¹⁺ 19 RHF	Ca ²⁺ 20 RHF	Sc ³⁺ 21 HF	Ti ²⁺ 22 HF	Ti ³⁺ 22 HF	Ti ⁴⁺ 22 HF	V ²⁺ 23 RHF	V ³⁺ 23 HF
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	

6. INTERPRETATION OF DIFFRACTED INTENSITIES

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

Element Z Method ($\sin \theta$)/ λ (\AA^{-1})	V ⁵⁺ 23 HF	Cr ²⁺ 24 HF	Cr ³⁺ 24 HF	Mn ²⁺ 25 RHF	Mn ³⁺ 25 HF	Mn ⁴⁺ 25 HF	Fe ²⁺ 26 RHF	Fe ³⁺ 26 RHF	Co ²⁺ 27 RHF	Co ³⁺ 27 HF
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	

6.1. INTENSITY OF DIFFRACTED INTENSITIES

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

Element Z Method ($\sin \theta$)/ λ (\AA^{-1})	Ni ²⁺ 28 RHF	Ni ³⁺ 28 HF	Cu ¹⁺ 29 RHF	Cu ²⁺ 29 HF	Zn ²⁺ 30 RHF	Ga ³⁺ 31 HF	Ge ⁴⁺ 32 HF	Br ¹⁻ 35 RHF	Rb ¹⁺ 37 RHF	Sr ²⁺ 38 RHF
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

6. INTERPRETATION OF DIFFRACTED INTENSITIES

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

Element Z Method ($\sin \theta$)/ λ (\AA^{-1})	Y ³⁺ 39 *DS	Zr ⁴⁺ 40 *DS	Nb ³⁺ 41 *DS	Nb ⁵⁺ 41 *DS	Mo ³⁺ 42 *DS	Mo ⁵⁺ 42 *DS	Mo ⁶⁺ 42 *DS	Ru ³⁺ 44 *DS	Ru ⁴⁺ 44 *DS	Rh ³⁺ 45 *DS
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

6.1. INTENSITY OF DIFFRACTED INTENSITIES

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

Element Z Method ($\sin \theta$)/ λ (\AA^{-1})	Rh ⁴⁺ 45 *DS	Pd ²⁺ 46 *DS	Pd ⁴⁺ 46 *DS	Ag ¹⁺ 47 *DS	Ag ²⁺ 47 *DS	Cd ²⁺ 48 *DS	In ³⁺ 49 *DS	Sn ²⁺ 50 RHF	Sn ⁴⁺ 50 RHF	Sb ³⁺ 51 *DS
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

6. INTERPRETATION OF DIFFRACTED INTENSITIES

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

Element Z Method ($\sin \theta$)/ λ (\AA^{-1})	Sb ⁵⁺ 51 *DS	I ¹⁻ 53 RHF	Cs ¹⁺ 55 RHF	Ba ²⁺ 56 *DS	La ³⁺ 57 *DS	Ce ²⁺ 58 *DS	Ce ⁴⁺ 58 *DS	Pr ³⁺ 59 *DS	Pr ⁴⁺ 59 *DS	Nd ³⁺ 60 *DS
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

6.1. INTENSITY OF DIFFRACTED INTENSITIES

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

Element Z Method ($\sin \theta$)/ λ (\AA^{-1})	Pm ³⁺ 61 *DS	Sm ³⁺ 62 *DS	Eu ²⁺ 63 *DS	Eu ³⁺ 63 *DS	Gd ³⁺ 64 *DS	Tb ³⁺ 65 *DS	Dy ³⁺ 66 *DS	Ho ³⁺ 67 *DS	Er ³⁺ 68 *DS	Tm ³⁺ 69 *DS
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

6. INTERPRETATION OF DIFFRACTED INTENSITIES

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

Element Z Method ($\sin \theta$)/ λ (\AA^{-1})	Yb ²⁺ 70 *DS	Yb ³⁺ 70 *DS	Lu ³⁺ 71 *DS	Hf ⁴⁺ 72 *DS	Ta ⁵⁺ 73 *DS	W ⁶⁺ 74 *DS	Os ⁴⁺ 76 *DS	Ir ³⁺ 77 *DS	Ir ⁴⁺ 77 *DS	Pt ²⁺ 78 *DS
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

6.1. INTENSITY OF DIFFRACTED INTENSITIES

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

Element Z Method ($\sin \theta$)/ λ (\AA^{-1})	Pt ⁴⁺ 78 *DS	Au ¹⁺ 79 *DS	Au ³⁺ 79 *DS	Hg ¹⁺ 80 *DS	Hg ²⁺ 80 *DS	Tl ¹⁺ 81 *DS	Tl ³⁺ 81 *DS	Pb ²⁺ 82 *DS	Pb ⁴⁺ 82 *DS	Bi ³⁺ 83 *DS
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

6. INTERPRETATION OF DIFFRACTED INTENSITIES

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

Element Z Method ($\sin \theta$)/ λ (\AA^{-1})	Bt ⁵⁺ 83 *DS	Ra ²⁺ 88 *DS	Ac ³⁺ 89 *DS	Th ⁴⁺ 90 *DS	U ³⁺ 92 *DS	U ⁴⁺ 92 *DS	U ⁶⁺ 92 *DS	Np ³⁺ 93 *DS	Np ⁴⁺ 93 *DS	Np ⁶⁺ 93 *DS
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

6.1. INTENSITY OF DIFFRACTED INTENSITIES

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

Element Z Method ($\sin \theta$)/ λ (\AA^{-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