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HFS Atomic Scattering Factors*

By H. P. Hanson
The University of Texas, Austin 12, *Texas, U.S.A.*

F. Herman
Lockheed Missiles and Space Company, Sunnyvale, California, U.S.A.

J. D. Lea
The University of Texas, Austin 12, *Texas, U.S.A.*

and S. Skillman
RCA Laboratories, Princeton, N.J., U.S.A.

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Atomic scattering factors calculated from carefully computed Hartree–Fock–Slater wave functions are presented for the neutral elements from $Z=2$ to $Z=100$ over a range of $\sin\theta/\lambda$ values up to 6·0. Because of the nature of the wave functions used and because of the range and density of the parameters for which the calculations have been made, this compilation should represent the most complete and most accurate f values available.

Introduction

The need for good values of the atomic scattering factors in crystallographic studies has long been appreciated. With the introduction of new refined measurement techniques and with the efforts to solve more difficult and more subtle crystal structure problems, this need is now being felt even more acutely. It is generally conceded that the best values of the atomic scattering factors are those obtained from the most sophisticated and presumably most realistic atomic models. In particular, the Hartree–Fock (HF) values have found particular favor although the difficulty of obtaining true HF wave functions has precluded the compilation of form factors for anything but a limited number of elements. A simplification of the basic HF problem which was introduced by Slater (1951) provides one with a computationally tractable problem. The resulting Hartree–Fock–Slater (HFS) wave functions are very good approximations to those obtained by HF; whatever differences exist lie mainly in the same direction as the effect produced by further physical refinements of the HF problem.

Self consistent wave functions have been calculated by Herman & Skillman (1962) for all ground state neutral atoms from $Z=2$ to $Z=103$ using the HFS approach. These values represent the most complete atomic wave functions available both from the point of view of numerical accuracy and of atomic number. For this reason it was felt that a calculation of atomic scattering factors from these wave functions would be of interest and importance.

Discussion

The calculations of the atomic scattering factors were made from the HFS wave functions by incorporating the assumption of spherical symmetry into the expression,

$$f=\sum_j\int|\psi_j|^2\exp\,(i\varkappa\mathbf{s}\,.\,\mathbf{r}_j)d\tau_j\;, \tag{1}$$

obtaining

$$f=\sum_j\int_0^\infty U_j(r)\,\frac{\sin sr}{sr}\,dr \tag{2}$$

using a common notation.

The integration was carried out in a straightforward fashion by means of Simpson's rule. The r coordinate is expressed in terms of the Thomas–Fermi parameter,

$$r=\left(\frac{3}{32\pi^2}\right)^{\frac{2}{3}}\frac{h^2}{2me^2}\,\frac{1}{Z^{\frac{1}{3}}}\,x=\frac{0{\cdot}88534138}{Z^{\frac{1}{3}}}\,x$$

and the integration is performed over x when it has been expressed in units of the first Bohr radius. The x mesh is common to all atoms and is that utilized in the original HFS wave function calculations. It is constructed as follows: The first 41 values of x from 0·00 to 0·10 are given a constant spacing of 0·0025. The next 41 values of x range from an x of 0·10 to an x of 0·30 inclusive with a constant spacing of 0·005. The process of doubling is continued from one block of 41 mesh points until 441 values of x are involved. After expressing all distances in terms of the Bohr radius, the integration was performed with a suitable modification of Simpson's rule to accout for the non-constant intervals. To check the accuracy of the wave

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Table 1. *Atomic scattering factors for elements* $Z=1$ *to* $Z=100$ *as a function of* $\sin\theta/\lambda$

	H	He	Li	Be	B	C	N	O	F	Ne
.00	1.000	2.000	3.000	4.000	5.000	6.000	7.000	8.000	9.000	10.00
.05	.947	1.955	2.722	3.712	4.727	5.757	6.784	7.805	8.823	9.84
.10	.811	1.831	2.242	3.085	4.080	5.141	6.211	7.276	8.332	9.38
.15	.641	1.652	1.927	2.495	3.367	4.383	5.453	6.538	7.625	8.71
.20	.481	1.447	1.760	2.097	2.771	3.662	4.667	5.728	6.814	7.91
.25	.350	1.241	1.644	1.860	2.337	3.063	3.954	4.944	5.991	7.07
.30	.251	1.049	1.533	1.717	2.041	2.601	3.355	4.243	5.218	6.25
.35	.180	.879	1.418	1.618	1.844	2.261	2.875	3.645	4.528	5.49
.40	.130	.734	1.300	1.536	1.710	2.017	2.504	3.153	3.933	4.81
.45	.095	.612	1.181	1.457	1.615	1.844	2.223	2.759	3.433	4.22
.50	.071	.511	1.067	1.378	1.540	1.719	2.012	2.448	3.021	3.71
.55	.053	.428	.960	1.298	1.475	1.626	1.854	2.205	2.686	3.29
.60	.040	.359	.860	1.216	1.413	1.553	1.736	2.017	2.416	2.93
.65	.031	.303	.768	1.134	1.351	1.491	1.644	1.871	2.200	2.64
.70	.024	.256	.685	1.054	1.289	1.436	1.571	1.757	2.028	2.40
.75	.019	.217	.611	.977	1.227	1.383	1.510	1.666	1.891	2.20
.80	.015	.185	.544	.902	1.164	1.332	1.457	1.592	1.780	2.04
.85	.012	.158	.485	.832	1.101	1.281	1.408	1.531	1.690	1.91
.90	.010	.136	.432	.766	1.039	1.229	1.361	1.477	1.616	1.80
.95		.117	.386	.705	.979	1.178	1.317	1.430	1.553	1.72
1.00		.101	.344	.647	.920	1.127	1.273	1.386	1.499	1.64
1.05		.088	.308	.595	.864	1.076	1.229	1.344	1.451	1.58
1.10		.076	.275	.546	.810	1.026	1.185	1.304	1.408	1.52
1.15		.066	.247	.501	.759	.977	1.142	1.265	1.368	1.47
1.20		.058	.222	.460	.711	.929	1.099	1.227	1.330	1.43
1.25		.051	.199	.423	.665	.882	1.056	1.189	1.294	1.39
1.30		.045	.179	.388	.622	.837	1.014	1.151	1.259	1.35
1.35		.040	.162	.357	.581	.794	.973	1.114	1.224	1.32
1.40		.035	.146	.328	.543	.752	.932	1.077	1.191	1.28
1.50		.028	.120	.278	.474	.674	.854	1.004	1.124	1.22
1.60		.022	.099	.237	.414	.603	.781	.934	1.059	1.16
1.70		.018	.082	.202	.362	.539	.712	.866	.995	1.10
1.80		.015	.069	.173	.317	.482	.648	.801	.933	1.04
1.90		.012	.058	.148	.278	.431	.590	.740	.873	.99
2.00		.010	.049	.128	.244	.386	.536	.682	.816	.93
2.20			.036	.096	.190	.309	.443	.579	.709	.83
2.40			.026	.073	.149	.249	.366	.490	.614	.73
2.60			.020	.057	.118	.202	.303	.415	.530	.64
2.80			.015	.044	.094	.164	.252	.352	.457	.56
3.00			.012	.035	.076	.135	.210	.299	.395	.49
3.20			.009	.028	.061	.111	.176	.254	.341	.43
3.40				.023	.050	.092	.148	.217	.295	.38
3.60				.018	.042	.077	.126	.186	.256	.33
3.80				.015	.035	.065	.107	.160	.222	.29
4.00				.013	.029	.055	.091	.138	.193	.26
4.20				.011	.024	.047	.078	.119	.169	.23
4.40				.009	.021	.040	.067	.103	.148	.20
4.60					.018	.034	.058	.090	.130	.18
4.80					.015	.029	.051	.079	.114	.16
5.00					.013	.026	.044	.069	.101	.14
5.20					.012	.022	.039	.061	.089	.12
5.40					.010	.019	.034	.054	.079	.11
5.60						.017	.030	.048	.071	.10
5.80						.015	.027	.042	.063	.09
6.00						.013	.023	.038	.056	.08

	Na	Mg	Al	Si	P	S	Cl	A	K	Ca
.00	11.00	12.00	13.00	14.00	15.00	16.00	17.00	18.00	19.00	20.00
.05	10.60	11.54	12.46	13.47	14.49	15.52	16.54	17.57	18.26	19.16
.10	9.82	10.55	11.32	12.25	13.25	14.29	15.35	16.41	16.86	17.43
.15	9.11	9.60	10.20	10.94	11.81	12.78	13.79	14.84	15.43	15.91
.20	8.44	8.84	9.30	9.85	10.53	11.33	12.23	13.20	13.96	14.50
.25	7.75	8.19	8.58	9.00	9.51	10.14	10.87	11.70	12.52	13.17
.30	7.04	7.57	7.97	8.34	8.73	9.21	9.78	10.45	11.22	11.92
.35	6.34	6.95	7.41	7.78	8.12	8.50	8.94	9.46	10.12	10.90
.40	5.66	6.34	6.87	7.28	7.62	7.94	8.29	8.70	9.23	9.83
.45	5.04	5.75	6.34	6.81	7.17	7.48	7.78	8.11	8.53	9.04
.50	4.48	5.20	5.82	6.34	6.75	7.08	7.36	7.64	7.98	8.39
.55	3.99	4.68	5.33	5.88	6.33	6.69	6.99	7.25	7.53	7.87
.60	3.56	4.22	4.86	5.43	5.92	6.32	6.64	6.91	7.17	7.45
.65	3.19	3.80	4.42	5.00	5.52	5.95	6.31	6.60	6.85	7.10
.70	2.88	3.44	4.02	4.60	5.13	5.59	5.98	6.30	6.56	6.79
.75	2.62	3.12	3.66	4.22	4.75	5.23	5.65	6.00	6.28	6.52
.80	2.40	2.84	3.34	3.87	4.40	4.89	5.32	5.70	6.00	6.26
.85	2.22	2.61	3.06	3.55	4.06	4.55	5.00	5.40	5.73	6.00
.90	2.07	2.40	2.81	3.27	3.76	4.24	4.69	5.11	5.46	5.75
.95	1.94	2.23	2.60	3.02	3.47	3.94	4.40	4.82	5.19	5.50
1.00	1.83	2.09	2.41	2.79	3.22	3.67	4.11	4.54	4.92	5.26
1.05	1.74	1.96	2.25	2.60	2.99	3.41	3.84	4.27	4.66	5.01
1.10	1.67	1.86	2.11	2.42	2.78	3.18	3.59	4.01	4.41	4.77
1.15	1.60	1.77	1.99	2.27	2.60	2.97	3.36	3.77	4.16	4.53
1.20	1.54	1.69	1.89	2.13	2.43	2.76	3.15	3.54	3.92	4.29
1.25	1.50	1.63	1.80	2.02	2.29	2.60	2.95	3.32	3.70	4.07
1.30	1.45	1.57	1.72	1.92	2.16	2.45	2.77	3.13	3.49	3.85
1.35	1.41	1.52	1.65	1.83	2.05	2.31	2.61	2.94	3.29	3.65
1.40	1.37	1.47	1.59	1.75	1.95	2.18	2.46	2.78	3.11	3.45
1.50	1.31	1.40	1.50	1.62	1.78	1.98	2.21	2.48	2.78	3.09
1.60	1.25	1.33	1.42	1.52	1.65	1.81	2.01	2.24	2.50	2.78
1.70	1.19	1.27	1.35	1.44	1.55	1.68	1.84	2.04	2.26	2.51
1.80	1.14	1.22	1.30	1.37	1.46	1.57	1.71	1.87	2.07	2.29
1.90	1.09	1.17	1.24	1.32	1.40	1.49	1.60	1.74	1.90	2.10
2.00	1.03	1.12	1.20	1.27	1.34	1.42	1.51	1.63	1.77	1.93
2.20	.93	1.05	1.11	1.18	1.24	1.31	1.38	1.47	1.57	1.69
2.40	.84	.94	1.02	1.09	1.16	1.22	1.28	1.35	1.43	1.51
2.60	.75	.85	.94	1.02	1.08	1.14	1.20	1.26	1.32	1.39
2.80	.67	.77	.86	.94	1.01	1.07	1.13	1.18	1.24	1.30
3.00	.59	.69	.78	.87	.94	1.01	1.06	1.12	1.17	1.22
3.20	.53	.62	.71	.80	.87	.94	1.00	1.06	1.11	1.16
3.40	.47	.56	.65	.73	.81	.88	.94	1.00	1.05	1.10
3.60	.41	.50	.59	.67	.74	.82	.88	.94	.99	1.04
3.80	.37	.45	.53	.61	.69	.76	.82	.88	.94	.99
4.00	.33	.40	.48	.56	.63	.70	.77	.83	.89	.94
4.20	.29	.36	.43	.51	.58	.65	.72	.79	.84	.89
4.40	.26	.32	.39	.46	.53	.60	.67	.73	.79	.84
4.60	.23	.29	.35	.42	.49	.55	.62	.68	.74	.79
4.80	.21	.26	.32	.38	.45	.51	.57	.64	.69	.75
5.00	.18	.24	.29	.35	.41	.47	.53	.59	.65	.71
5.20	.16	.21	.26	.32	.38	.43	.49	.55	.61	.67
5.40	.15	.19	.24	.29	.34	.40	.46	.51	.57	.63
5.60	.13	.17	.22	.27	.32	.37	.42	.48	.53	.59
5.80	.12	.16	.20	.24	.29	.34	.39	.45	.50	.55
6.00	.11	.14	.18	.22	.27	.31	.36	.41	.47	.52

	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
.00	21.00	22.00	23.00	24.00	25.00	26.00	27.00	28.00	29.00	30.00
.05	20.20	21.24	22.27	23.38	24.33	25.36	26.39	27.41	28.43	23.45
.10	18.52	19.58	20.64	21.93	22.77	23.84	24.90	25.93	27.20	28.06
.15	16.85	17.85	18.88	20.24	20.99	22.05	23.12	24.19	25.56	26.33
.20	15.35	16.27	17.24	18.54	19.26	20.29	21.34	22.40	23.79	24.53
.25	13.96	14.81	15.71	16.87	17.62	18.62	19.63	20.66	21.99	22.75
.30	12.65	13.44	14.28	15.29	16.08	17.02	17.99	18.98	20.20	21.01
.35	11.47	12.19	12.96	13.82	14.63	15.51	16.43	17.38	18.47	19.33
.40	10.43	11.07	11.77	12.51	13.30	14.12	14.98	15.87	16.86	17.73
.45	9.55	10.12	10.73	11.37	12.11	12.86	13.66	14.49	15.36	16.23
.50	8.82	9.31	9.85	10.40	11.07	11.75	12.47	13.23	14.01	14.86
.55	8.24	8.65	9.10	9.56	10.17	10.77	11.42	12.11	12.81	13.61
.60	7.76	8.10	8.49	8.90	9.41	9.94	10.52	11.13	11.76	12.49
.65	7.36	7.66	7.99	8.33	8.77	9.23	9.74	10.28	10.84	11.50
.70	7.03	7.29	7.57	7.87	8.24	8.63	9.07	9.55	10.04	10.64
.75	6.74	6.97	7.22	7.48	7.80	8.13	8.51	8.93	9.36	9.89
.80	6.48	6.70	6.92	7.16	7.42	7.71	8.04	8.41	8.79	9.25
.85	6.24	6.45	6.66	6.87	7.11	7.36	7.64	7.96	8.29	8.70
.90	6.00	6.22	6.42	6.62	6.83	7.06	7.30	7.58	7.87	8.22
.95	5.76	5.99	6.20	6.39	6.59	6.79	7.01	7.25	7.51	7.81
1.00	5.53	5.77	5.98	6.18	6.37	6.56	6.75	6.97	7.20	7.43
1.05	5.30	5.55	5.77	5.97	6.16	6.34	6.53	6.72	6.93	7.16
1.10	5.07	5.33	5.57	5.77	5.96	6.14	6.32	6.50	6.69	6.90
1.15	4.84	5.12	5.36	5.57	5.77	5.95	6.12	6.30	6.47	6.66
1.20	4.62	4.90	5.16	5.38	5.58	5.77	5.94	6.11	6.28	6.45
1.25	4.39	4.69	4.96	5.18	5.40	5.59	5.76	5.93	6.09	6.25
1.30	4.18	4.48	4.75	4.99	5.22	5.41	5.59	5.76	5.92	6.08
1.35	3.97	4.28	4.56	4.80	5.04	5.24	5.42	5.59	5.75	5.91
1.40	3.77	4.08	4.36	4.61	4.85	5.07	5.26	5.43	5.59	5.75
1.50	3.40	3.70	3.99	4.24	4.50	4.72	4.93	5.11	5.28	5.44
1.60	3.07	3.35	3.63	3.89	4.15	4.39	4.60	4.80	4.98	5.15
1.70	2.78	3.04	3.31	3.57	3.83	4.07	4.29	4.49	4.68	4.85
1.80	2.52	2.77	3.02	3.26	3.52	3.76	3.98	4.20	4.39	4.58
1.90	2.30	2.53	2.76	2.99	3.24	3.47	3.69	3.91	4.10	4.30
2.00	2.12	2.32	2.53	2.74	2.98	3.20	3.42	3.64	3.83	4.03
2.20	1.83	1.98	2.15	2.33	2.53	2.73	2.94	3.14	3.33	3.53
2.40	1.62	1.74	1.87	2.02	2.18	2.36	2.53	2.72	2.90	3.08
2.60	1.47	1.56	1.67	1.78	1.92	2.06	2.21	2.37	2.53	2.70
2.80	1.36	1.43	1.52	1.61	1.71	1.83	1.95	2.09	2.23	2.38
3.00	1.28	1.33	1.40	1.48	1.56	1.65	1.75	1.87	1.98	2.11
3.20	1.21	1.26	1.31	1.37	1.44	1.52	1.60	1.69	1.79	1.90
3.40	1.15	1.19	1.24	1.29	1.35	1.41	1.48	1.56	1.64	1.73
3.60	1.09	1.13	1.18	1.23	1.27	1.33	1.38	1.45	1.52	1.59
3.80	1.04	1.08	1.13	1.17	1.21	1.26	1.31	1.36	1.42	1.48
4.00	.99	1.03	1.08	1.12	1.16	1.20	1.24	1.29	1.34	1.39
4.20	.94	.99	1.03	1.07	1.11	1.15	1.19	1.23	1.27	1.32
4.40	.89	.94	.98	1.03	1.07	1.10	1.14	1.18	1.22	1.26
4.60	.85	.90	.94	.98	1.02	1.06	1.10	1.13	1.17	1.21
4.80	.80	.85	.90	.94	.98	1.02	1.06	1.09	1.13	1.16
5.00	.76	.81	.86	.90	.94	.98	1.02	1.05	1.09	1.12
5.20	.72	.77	.82	.86	.90	.94	.98	1.01	1.05	1.08
5.40	.68	.73	.78	.82	.86	.90	.94	.98	1.01	1.04
5.60	.64	.69	.74	.78	.83	.87	.91	.94	.98	1.01
5.80	.60	.65	.70	.75	.79	.83	.87	.91	.94	.98
6.00	.57	.62	.65	.71	.76	.80	.84	.87	.91	.94

	Ga	Ge	As	Se	Br	Kr	Rb	Sr	Y	Zr
.00	31.00	32.00	33.00	34.00	35.00	36.00	37.00	38.00	39.00	40.00
.05	30.34	31.32	32.32	33.32	34.33	35.35	36.02	36.86	37.91	38.94
.10	28.80	29.67	30.61	31.59	32.59	33.61	34.06	34.64	35.58	36.52
.15	27.00	27.72	28.53	29.41	30.33	31.29	31.90	32.38	33.16	34.03
.20	25.18	25.82	26.49	27.23	28.03	28.88	29.63	30.21	30.88	31.63
.25	23.43	24.03	24.63	25.26	25.93	26.64	27.42	28.09	28.72	29.39
.30	21.74	22.37	22.95	23.51	24.09	24.70	25.40	26.10	26.70	27.32
.35	20.11	20.79	21.39	21.95	22.48	23.02	23.64	24.30	24.87	25.44
.40	18.55	19.28	19.93	20.51	21.05	21.55	22.10	22.70	23.24	23.77
.45	17.07	17.84	18.54	19.16	19.72	20.24	20.75	21.29	21.81	22.30
.50	15.69	16.48	17.21	17.88	18.47	19.01	19.52	20.03	20.53	21.01
.55	14.41	15.20	15.95	16.65	17.28	17.86	18.38	18.89	19.38	19.85
.60	13.25	14.01	14.76	15.47	16.14	16.75	17.30	17.81	18.31	18.79
.65	12.21	12.93	13.66	14.37	15.05	15.68	16.26	16.80	17.31	17.80
.70	11.28	11.96	12.65	13.34	14.02	14.67	15.27	15.82	16.36	16.86
.75	10.47	11.09	11.73	12.40	13.06	13.70	14.32	14.89	15.44	15.96
.80	9.76	10.32	10.91	11.53	12.17	12.80	13.41	14.00	14.56	15.10
.85	9.14	9.64	10.18	10.76	11.35	11.96	12.57	13.15	13.72	14.26
.90	8.61	9.05	9.54	10.06	10.62	11.19	11.77	12.35	12.91	13.46
.95	8.16	8.54	8.97	9.45	9.95	10.49	11.04	11.60	12.15	12.70
1.00	7.76	8.10	8.48	8.90	9.36	9.86	10.37	10.91	11.44	11.98
1.05	7.42	7.72	8.05	8.43	8.84	9.29	9.77	10.27	10.78	11.30
1.10	7.13	7.38	7.68	8.01	8.38	8.78	9.22	9.69	10.17	10.67
1.15	6.87	7.09	7.35	7.64	7.97	8.33	8.73	9.16	9.61	10.09
1.20	6.63	6.84	7.07	7.32	7.61	7.94	8.30	8.69	9.10	9.54
1.25	6.43	6.61	6.81	7.04	7.30	7.59	7.91	8.26	8.64	9.05
1.30	6.24	6.41	6.59	6.79	7.02	7.28	7.57	7.88	8.23	8.61
1.35	6.06	6.22	6.39	6.57	6.78	7.00	7.26	7.55	7.86	8.20
1.40	5.90	6.05	6.21	6.38	6.56	6.76	6.99	7.25	7.53	7.84
1.50	5.59	5.74	5.88	6.03	6.18	6.35	6.54	6.74	6.97	7.23
1.60	5.31	5.45	5.59	5.73	5.87	6.01	6.17	6.34	6.52	6.73
1.70	5.03	5.18	5.33	5.45	5.59	5.73	5.86	6.00	6.16	6.33
1.80	4.75	4.92	5.07	5.21	5.34	5.47	5.60	5.72	5.86	6.00
1.90	4.49	4.66	4.82	4.96	5.10	5.23	5.35	5.48	5.60	5.72
2.00	4.22	4.40	4.57	4.73	4.87	5.00	5.13	5.25	5.37	5.49
2.20	3.72	3.91	4.09	4.26	4.42	4.57	4.70	4.83	4.95	5.06
2.40	3.27	3.46	3.64	3.81	3.98	4.14	4.29	4.43	4.56	4.69
2.60	2.87	3.05	3.23	3.40	3.57	3.74	3.89	4.04	4.18	4.31
2.80	2.53	2.70	2.86	3.03	3.19	3.36	3.52	3.67	3.82	3.95
3.00	2.25	2.39	2.54	2.70	2.85	3.01	3.17	3.32	3.47	3.61
3.20	2.02	2.14	2.27	2.41	2.55	2.70	2.85	3.00	3.14	3.26
3.40	1.83	1.94	2.05	2.17	2.30	2.43	2.57	2.71	2.84	2.98
3.60	1.68	1.77	1.86	1.97	2.08	2.20	2.32	2.45	2.58	2.71
3.80	1.55	1.63	1.71	1.80	1.90	2.01	2.11	2.23	2.35	2.47
4.00	1.45	1.52	1.59	1.67	1.75	1.84	1.94	2.04	2.14	2.25
4.20	1.37	1.43	1.49	1.55	1.63	1.70	1.79	1.88	1.97	2.07
4.40	1.30	1.35	1.40	1.46	1.52	1.59	1.66	1.74	1.82	1.91
4.60	1.25	1.29	1.33	1.38	1.44	1.49	1.56	1.62	1.70	1.77
4.80	1.20	1.24	1.28	1.32	1.36	1.41	1.47	1.53	1.59	1.66
5.00	1.15	1.19	1.22	1.26	1.30	1.35	1.39	1.45	1.50	1.56
5.20	1.11	1.15	1.18	1.21	1.25	1.29	1.33	1.38	1.42	1.48
5.40	1.08	1.11	1.14	1.17	1.21	1.24	1.28	1.32	1.36	1.41
5.60	1.04	1.07	1.10	1.13	1.16	1.20	1.23	1.27	1.30	1.34
5.80	1.01	1.04	1.07	1.10	1.13	1.16	1.19	1.22	1.25	1.29
6.00	.97	1.01	1.03	1.06	1.09	1.12	1.15	1.18	1.21	1.24

Table 1 (*cont.*)

	Cb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn
.00	41.00	42.00	43.00	44.00	45.00	46.00	47.00	48.00	49.00	50.00
.05	40.04	41.07	42.02	43.12	44.15	45.28	46.19	47.14	48.02	48.96
.10	37.82	38.87	39.69	40.97	42.02	43.35	44.13	44.97	45.69	46.52
.15	35.23	36.22	36.96	38.28	39.32	40.66	41.45	42.20	42.86	43.55
.20	32.64	33.54	34.25	35.46	36.46	37.68	38.52	39.26	39.95	40.56
.25	30.19	30.99	31.71	32.73	33.65	34.70	35.58	36.36	37.09	37.75
.30	27.95	28.66	29.38	30.19	31.02	31.91	32.78	33.59	34.37	35.07
.35	25.97	26.59	27.27	27.93	28.66	29.40	30.23	31.03	31.82	32.56
.40	24.24	24.78	25.42	25.95	26.59	27.21	27.96	28.72	29.50	30.25
.45	22.74	23.23	23.79	24.25	24.80	25.33	25.99	26.69	27.41	28.14
.50	21.43	21.88	22.39	22.80	23.27	23.73	24.30	24.92	25.58	26.25
.55	20.28	20.70	21.16	21.54	21.97	22.37	22.86	23.40	23.98	24.59
.60	19.23	19.65	20.07	20.44	20.84	21.21	21.64	22.10	22.60	23.14
.65	18.26	18.68	19.09	19.47	19.84	20.20	20.57	20.98	21.42	21.89
.70	17.34	17.78	18.18	18.57	18.94	19.29	19.64	20.01	20.39	20.80
.75	16.47	16.92	17.33	17.74	18.11	18.47	18.80	19.14	19.49	19.65
.80	15.62	16.09	16.52	16.95	17.33	17.70	18.03	18.36	18.68	19.01
.85	14.80	15.29	15.74	16.18	16.58	16.97	17.31	17.63	17.95	18.26
.90	14.00	14.51	14.98	15.44	15.86	16.26	16.62	16.95	17.26	17.57
.95	13.24	13.76	14.24	14.71	15.15	15.57	15.94	16.29	16.61	16.92
1.00	12.51	13.03	13.52	14.01	14.46	14.89	15.29	15.65	15.99	16.30
1.05	11.82	12.33	12.83	13.32	13.79	14.23	14.64	15.02	15.39	15.70
1.10	11.17	11.67	12.17	12.66	13.13	13.59	14.01	14.41	14.78	15.12
1.15	10.56	11.05	11.54	12.02	12.50	12.96	13.39	13.81	14.19	14.55
1.20	10.00	10.47	10.94	11.42	11.89	12.35	12.79	13.21	13.61	13.99
1.25	9.48	9.92	10.38	10.84	11.30	11.76	12.21	12.64	13.05	13.45
1.30	9.00	9.42	9.86	10.30	10.75	11.20	11.64	12.08	12.49	12.89
1.35	8.57	8.96	9.37	9.80	10.23	10.67	11.10	11.53	11.95	12.36
1.40	8.18	8.54	8.93	9.33	9.74	10.16	10.59	11.01	11.43	11.84
1.50	7.51	7.81	8.14	8.49	8.86	9.25	9.64	10.05	10.45	10.85
1.60	6.96	7.22	7.49	7.79	8.12	8.46	8.82	9.19	9.56	9.95
1.70	6.52	6.73	6.96	7.21	7.49	7.79	8.10	8.43	8.78	9.13
1.80	6.16	6.33	6.53	6.74	6.97	7.22	7.49	7.78	8.09	8.41
1.90	5.86	6.01	6.17	6.34	6.54	6.75	6.98	7.23	7.50	7.79
2.00	5.60	5.73	5.87	6.02	6.18	6.36	6.56	6.77	7.00	7.25
2.20	5.17	5.28	5.39	5.50	5.63	5.76	5.90	6.05	6.22	6.41
2.40	4.79	4.90	5.00	5.10	5.20	5.31	5.42	5.54	5.66	5.80
2.60	4.43	4.54	4.65	4.75	4.85	4.95	5.04	5.14	5.24	5.35
2.80	4.08	4.20	4.32	4.43	4.53	4.62	4.72	4.81	4.90	4.99
3.00	3.74	3.87	4.00	4.11	4.22	4.32	4.42	4.51	4.60	4.69
3.20	3.42	3.55	3.68	3.80	3.91	4.02	4.13	4.22	4.32	4.41
3.40	3.12	3.25	3.38	3.50	3.62	3.73	3.84	3.95	4.05	4.14
3.60	2.84	2.97	3.09	3.22	3.34	3.45	3.57	3.68	3.78	3.88
3.80	2.59	2.71	2.83	2.95	3.07	3.19	3.30	3.41	3.52	3.63
4.00	2.36	2.48	2.59	2.71	2.82	2.94	3.05	3.16	3.27	3.38
4.20	2.17	2.27	2.38	2.49	2.60	2.71	2.82	2.93	3.04	3.14
4.40	2.00	2.09	2.19	2.29	2.39	2.50	2.60	2.71	2.81	2.92
4.60	1.85	1.94	2.03	2.12	2.21	2.31	2.41	2.51	2.61	2.71
4.80	1.73	1.80	1.88	1.97	2.05	2.14	2.23	2.33	2.42	2.52
5.00	1.62	1.69	1.76	1.83	1.91	1.99	2.08	2.16	2.25	2.34
5.20	1.53	1.59	1.65	1.72	1.79	1.86	1.94	2.02	2.10	2.18
5.40	1.45	1.51	1.56	1.62	1.68	1.75	1.82	1.89	1.96	2.04
5.60	1.39	1.43	1.48	1.54	1.59	1.65	1.71	1.78	1.85	1.92
5.80	1.33	1.37	1.42	1.46	1.51	1.56	1.62	1.68	1.74	1.81
6.00	1.28	1.32	1.36	1.40	1.44	1.49	1.54	1.59	1.65	1.70

	Sb	Te	I	Xe	Cs	Ba	La	Ce	Pr	Nd
.00	51.00	52.00	53.00	54.00	55.00	56.00	57.00	58.00	59.00	60.00
.05	49.97	50.96	51.96	52.97	53.60	54.43	55.45	56.48	57.51	58.53
.10	47.41	48.35	49.31	50.29	50.77	51.30	52.20	53.40	54.45	55.51
.15	44.30	45.11	45.96	46.85	47.53	48.04	48.76	50.13	51.18	52.24
.20	41.23	41.90	42.61	43.36	44.14	44.79	45.42	46.83	47.86	48.91
.25	38.36	38.96	39.58	40.21	40.94	41.66	42.26	43.59	44.59	45.61
.30	35.71	36.31	36.88	37.45	38.09	38.78	39.36	40.57	41.51	42.48
.35	33.25	33.88	34.46	35.01	35.59	36.21	36.78	37.86	38.73	39.62
.40	30.96	31.62	32.24	32.81	33.36	33.93	34.49	35.44	36.24	37.07
.45	28.85	29.54	30.18	30.78	31.34	31.89	32.45	33.28	34.01	34.77
.50	26.94	27.62	28.27	28.90	29.48	30.03	30.58	31.31	31.99	32.70
.55	25.23	25.87	26.52	27.15	27.74	28.30	28.87	29.51	30.14	30.80
.60	23.71	24.31	24.92	25.54	26.13	26.70	27.26	27.83	28.42	29.04
.65	22.39	22.93	23.49	24.07	24.65	25.21	25.77	26.28	26.83	27.41
.70	21.24	21.72	22.23	22.76	23.30	23.84	24.39	24.84	25.36	25.90
.75	20.24	20.66	21.11	21.59	22.09	22.60	23.12	23.53	24.02	24.51
.80	19.36	19.73	20.13	20.56	21.01	21.48	21.96	22.34	22.79	23.25
.85	18.58	18.91	19.27	19.65	20.05	20.48	20.92	21.27	21.68	22.10
.90	17.87	18.18	18.50	18.84	19.20	19.59	19.99	20.31	20.69	21.07
.95	17.21	17.51	17.81	18.11	18.44	18.79	19.15	19.45	19.80	20.15
1.00	16.60	16.89	17.17	17.46	17.76	18.08	18.41	18.69	19.00	19.32
1.05	16.01	16.30	16.58	16.86	17.14	17.43	17.73	18.00	18.29	18.58
1.10	15.44	15.74	16.02	16.30	16.57	16.84	17.12	17.38	17.65	17.92
1.15	14.88	15.19	15.49	15.76	16.03	16.30	16.56	16.81	17.06	17.32
1.20	14.34	14.66	14.96	15.25	15.52	15.78	16.04	16.28	16.53	16.77
1.25	13.80	14.14	14.45	14.75	15.02	15.29	15.55	15.79	16.02	16.26
1.30	13.27	13.62	13.95	14.26	14.54	14.82	15.08	15.32	15.55	15.78
1.35	12.74	13.11	13.45	13.77	14.07	14.35	14.62	14.86	15.10	15.33
1.40	12.23	12.60	12.96	13.29	13.60	13.90	14.17	14.42	14.66	14.89
1.50	11.25	11.63	12.00	12.35	12.69	13.00	13.30	13.56	13.81	14.06
1.60	10.33	10.71	11.09	11.45	11.80	12.13	12.45	12.72	12.99	13.24
1.70	9.50	9.86	10.23	10.59	10.94	11.29	11.62	11.90	12.18	12.45
1.80	8.75	9.09	9.44	9.79	10.14	10.48	10.81	11.10	11.39	11.68
1.90	8.09	8.40	8.73	9.06	9.39	9.72	10.05	10.34	10.64	10.92
2.00	7.52	7.80	8.09	8.40	8.71	9.02	9.34	9.63	9.92	10.21
2.20	6.61	6.82	7.05	7.30	7.56	7.82	8.10	8.36	8.63	8.90
2.40	5.95	6.11	6.28	6.47	6.67	6.89	7.11	7.33	7.56	7.80
2.60	5.46	5.58	5.71	5.86	6.01	6.17	6.35	6.53	6.72	6.92
2.80	5.09	5.18	5.29	5.40	5.51	5.64	5.78	5.92	6.07	6.23
3.00	4.77	4.86	4.95	5.04	5.13	5.23	5.34	5.46	5.58	5.71
3.20	4.49	4.58	4.66	4.74	4.83	4.91	5.00	5.10	5.19	5.30
3.40	4.23	4.32	4.40	4.48	4.56	4.64	4.72	4.80	4.88	4.97
3.60	3.98	4.07	4.15	4.24	4.32	4.39	4.47	4.55	4.62	4.70
3.80	3.73	3.82	3.91	4.00	4.08	4.16	4.24	4.32	4.39	4.46
4.00	3.48	3.58	3.68	3.77	3.86	3.94	4.02	4.10	4.17	4.25
4.20	3.25	3.35	3.45	3.54	3.63	3.72	3.80	3.89	3.96	4.04
4.40	3.02	3.12	3.22	3.32	3.42	3.51	3.59	3.68	3.76	3.84
4.60	2.81	2.91	3.01	3.11	3.20	3.30	3.39	3.47	3.56	3.64
4.80	2.62	2.71	2.81	2.91	3.00	3.10	3.19	3.27	3.36	3.44
5.00	2.44	2.53	2.62	2.72	2.81	2.90	2.99	3.08	3.17	3.25
5.20	2.27	2.36	2.45	2.54	2.63	2.72	2.81	2.90	2.98	3.07
5.40	2.12	2.21	2.29	2.38	2.46	2.55	2.64	2.72	2.80	2.89
5.60	1.99	2.07	2.15	2.23	2.31	2.39	2.47	2.56	2.64	2.72
5.80	1.87	1.94	2.01	2.09	2.17	2.25	2.33	2.40	2.48	2.56
6.00	1.77	1.83	1.90	1.97	2.04	2.11	2.19	2.25	2.34	2.41

	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb
.00	61.00	62.00	63.00	64.00	65.00	66.00	67.00	68.00	69.00	70.00
.05	59.56	60.58	61.60	62.62	63.65	64.67	65.68	66.70	67.72	68.74
.10	56.56	57.61	58.66	59.59	60.76	61.81	62.85	63.90	64.95	65.99
.15	53.30	54.37	55.43	56.22	57.56	58.63	59.69	60.75	61.92	62.88
.20	49.97	51.03	52.09	52.82	54.23	55.30	56.37	57.44	58.52	59.58
.25	46.63	47.67	48.72	49.44	50.82	51.89	52.95	54.02	55.10	56.16
.30	43.46	44.45	45.46	46.20	47.50	48.53	49.57	50.62	51.68	52.73
.35	40.54	41.48	42.43	43.17	44.38	45.37	46.37	47.38	48.41	49.42
.40	37.92	38.79	39.68	40.41	41.52	42.45	43.40	44.37	45.36	46.33
.45	35.56	36.37	37.20	37.91	38.91	39.80	40.69	41.61	42.55	43.47
.50	33.43	34.18	34.95	35.64	36.55	37.38	38.22	39.08	39.97	40.84
.55	31.47	32.17	32.89	33.56	34.38	35.16	35.95	36.76	37.59	38.42
.60	29.67	30.32	30.99	31.65	32.39	33.11	33.85	34.61	35.40	36.17
.65	28.00	28.60	29.23	29.87	30.54	31.21	31.91	32.62	33.36	34.09
.70	26.45	27.02	27.60	28.22	28.82	29.45	30.10	30.77	31.47	32.16
.75	25.02	25.55	26.10	26.69	27.23	27.82	28.43	29.06	29.71	30.36
.80	23.72	24.21	24.71	25.27	25.77	26.32	26.89	27.47	28.08	28.68
.85	22.54	22.99	23.45	23.98	24.43	24.94	25.46	26.01	26.57	27.14
.90	21.47	21.88	22.31	22.80	23.21	23.68	24.16	24.67	25.19	25.72
.95	20.51	20.89	21.28	21.73	22.10	22.53	22.98	23.44	23.93	24.41
1.00	19.66	20.00	20.36	20.76	21.10	21.50	21.91	22.33	22.78	23.23
1.05	18.89	19.20	19.53	19.89	20.21	20.57	20.94	21.33	21.74	22.15
1.10	18.20	18.49	18.78	19.12	19.41	19.74	20.08	20.43	20.80	21.18
1.15	17.58	17.85	18.12	18.42	18.69	18.99	19.30	19.62	19.96	20.30
1.20	17.01	17.26	17.52	17.79	18.04	18.31	18.60	18.89	19.20	19.51
1.25	16.49	16.73	16.97	17.22	17.45	17.71	17.97	18.23	18.51	18.80
1.30	16.01	16.24	16.46	16.70	16.92	17.15	17.39	17.64	17.90	18.16
1.35	15.55	15.77	15.99	16.21	16.43	16.65	16.87	17.10	17.34	17.58
1.40	15.12	15.34	15.55	15.76	15.97	16.18	16.39	16.61	16.83	17.05
1.50	14.29	14.51	14.72	14.93	15.13	15.33	15.53	15.73	15.93	16.13
1.60	13.49	13.72	13.94	14.16	14.36	14.56	14.76	14.94	15.13	15.32
1.70	12.71	12.96	13.19	13.42	13.63	13.83	14.03	14.22	14.41	14.59
1.80	11.95	12.20	12.45	12.70	12.91	13.13	13.33	13.53	13.72	13.91
1.90	11.20	11.47	11.73	11.99	12.21	12.44	12.65	12.86	13.06	13.25
2.00	10.49	10.76	11.02	11.29	11.52	11.76	11.99	12.20	12.41	12.61
2.20	9.17	9.44	9.70	9.97	10.21	10.46	10.70	10.93	11.15	11.37
2.40	8.05	8.29	8.54	8.79	9.02	9.27	9.50	9.74	9.97	10.19
2.60	7.13	7.34	7.55	7.78	8.00	8.22	8.44	8.67	8.89	9.11
2.80	6.40	6.58	6.76	6.95	7.14	7.34	7.54	7.74	7.94	8.15
3.00	5.84	5.98	6.13	6.29	6.45	6.62	6.79	6.97	7.15	7.33
3.20	5.41	5.52	5.64	5.77	5.90	6.04	6.19	6.34	6.49	6.65
3.40	5.06	5.16	5.26	5.36	5.47	5.58	5.71	5.83	5.96	6.10
3.60	4.78	4.86	4.95	5.03	5.13	5.22	5.32	5.43	5.53	5.65
3.80	4.54	4.61	4.69	4.76	4.84	4.93	5.01	5.10	5.19	5.29
4.00	4.32	4.39	4.46	4.53	4.60	4.68	4.75	4.85	4.91	4.99
4.20	4.11	4.18	4.25	4.32	4.39	4.46	4.53	4.60	4.67	4.74
4.40	3.91	3.98	4.05	4.12	4.19	4.26	4.32	4.39	4.46	4.52
4.60	3.71	3.79	3.86	3.93	4.00	4.07	4.13	4.20	4.25	4.33
4.80	3.52	3.60	3.67	3.75	3.82	3.89	3.95	4.02	4.08	4.15
5.00	3.33	3.41	3.49	3.56	3.64	3.71	3.78	3.84	3.91	3.97
5.20	3.15	3.23	3.31	3.38	3.46	3.53	3.60	3.67	3.74	3.80
5.40	2.97	3.05	3.13	3.21	3.29	3.36	3.43	3.50	3.57	3.64
5.60	2.80	2.88	2.96	3.04	3.12	3.19	3.26	3.34	3.41	3.47
5.80	2.64	2.72	2.80	2.88	2.95	3.03	3.10	3.17	3.25	3.32
6.00	2.49	2.57	2.64	2.72	2.80	2.87	2.94	3.02	3.09	3.16

	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg
.00	71.00	72.00	73.00	74.00	75.00	76.00	77.00	78.00	79.00	80.00
.05	69.74	70.76	71.78	72.80	73.91	74.83	75.85	76.94	77.96	78.90
.10	66.91	67.88	68.88	69.89	70.91	71.93	72.97	74.21	75.25	76.07
.15	63.67	64.52	65.43	66.36	67.32	68.31	69.30	70.60	71.63	72.36
.20	60.32	61.08	61.89	62.73	63.61	64.51	65.44	66.63	67.61	68.34
.25	56.90	57.64	58.38	59.15	59.95	60.77	61.61	62.63	63.54	64.29
.30	53.50	54.24	54.96	55.69	56.42	57.17	57.94	58.78	59.60	60.38
.35	50.23	50.98	51.70	52.40	53.09	53.79	54.50	55.19	55.94	56.72
.40	47.14	47.90	48.62	49.31	49.98	50.65	51.31	51.91	52.59	53.34
.45	44.28	45.04	45.76	46.44	47.11	47.75	48.38	48.94	49.57	50.27
.50	41.63	42.39	43.11	43.79	44.45	45.09	45.70	46.25	46.84	47.50
.55	39.19	39.93	40.65	41.34	42.00	42.65	43.24	43.79	44.36	44.98
.60	36.93	37.66	38.37	39.06	39.73	40.36	40.97	41.54	42.10	42.69
.65	34.82	35.55	36.25	36.94	37.60	38.24	38.86	39.45	40.01	40.58
.70	32.86	33.57	34.27	34.95	35.62	36.26	36.88	37.49	38.06	38.62
.75	31.04	31.72	32.41	33.08	33.75	34.39	35.02	35.64	36.23	36.78
.80	29.34	30.00	30.67	31.33	31.99	32.63	33.26	33.89	34.48	35.05
.85	27.76	28.39	29.04	29.68	30.33	30.97	31.59	32.23	32.83	33.40
.90	26.30	26.90	27.52	28.14	28.77	29.40	30.02	30.65	31.25	31.82
.95	24.96	25.53	26.11	26.71	27.31	27.92	28.53	29.15	29.75	30.32
1.00	23.73	24.26	24.81	25.38	25.95	26.54	27.13	27.73	28.32	28.89
1.05	22.62	23.11	23.62	24.15	24.69	25.25	25.81	26.39	26.97	27.54
1.10	21.60	22.06	22.53	23.02	23.53	24.05	24.59	25.14	25.70	26.25
1.15	20.69	21.10	21.53	21.99	22.46	22.95	23.46	23.98	24.51	25.05
1.20	19.86	20.24	20.63	21.05	21.48	21.94	22.41	22.90	23.40	23.92
1.25	19.12	19.46	19.82	20.20	20.60	21.02	21.45	21.91	22.38	22.86
1.30	18.45	18.76	19.08	19.43	19.79	20.17	20.58	20.99	21.43	21.89
1.35	17.84	18.12	18.42	18.73	19.06	19.41	19.78	20.16	20.57	20.99
1.40	17.29	17.55	17.81	18.10	18.40	18.71	19.05	19.40	19.77	20.17
1.50	16.33	16.55	16.77	17.00	17.25	17.51	17.79	18.08	18.39	18.72
1.60	15.50	15.69	15.89	16.09	16.30	16.52	16.75	16.99	17.24	17.52
1.70	14.77	14.94	15.12	15.30	15.49	15.68	15.87	16.08	16.29	15.52
1.80	14.09	14.26	14.43	14.60	14.78	14.95	15.12	15.30	15.48	15.68
1.90	13.44	13.62	13.79	13.96	14.13	14.29	14.46	14.62	14.79	14.96
2.00	12.81	13.00	13.18	13.36	13.53	13.69	13.85	14.01	14.17	14.32
2.20	11.59	11.80	12.00	12.19	12.38	12.56	12.73	12.89	13.05	13.21
2.40	10.42	10.64	10.86	11.07	11.28	11.47	11.66	11.84	12.02	12.19
2.60	9.33	9.56	9.78	10.00	10.22	10.42	10.63	10.83	11.02	11.20
2.80	8.36	8.58	8.79	9.01	9.22	9.44	9.64	9.85	10.05	10.25
3.00	7.52	7.72	7.92	8.12	8.32	8.53	8.73	8.94	9.14	9.34
3.20	6.82	6.99	7.17	7.35	7.53	7.72	7.91	8.11	8.30	8.49
3.40	6.24	6.38	6.54	6.70	6.86	7.03	7.20	7.38	7.56	7.74
3.60	5.77	5.89	6.02	6.16	6.30	6.44	6.59	6.75	6.91	7.07
3.80	5.39	5.49	5.60	5.71	5.83	5.96	6.09	6.22	6.36	6.51
4.00	5.07	5.16	5.25	5.35	5.45	5.56	5.67	5.78	5.90	6.03
4.20	4.81	4.89	4.97	5.05	5.14	5.23	5.32	5.42	5.52	5.63
4.40	4.59	4.66	4.73	4.80	4.87	4.95	5.03	5.11	5.20	5.29
4.60	4.39	4.45	4.52	4.58	4.65	4.72	4.79	4.86	4.93	5.01
4.80	4.21	4.27	4.33	4.39	4.45	4.51	4.58	4.64	4.71	4.78
5.00	4.03	4.09	4.15	4.21	4.27	4.33	4.39	4.45	4.51	4.57
5.20	3.87	3.93	3.99	4.05	4.10	4.16	4.22	4.27	4.33	4.39
5.40	3.70	3.76	3.83	3.88	3.94	4.00	4.06	4.11	4.17	4.22
5.60	3.54	3.61	3.67	3.73	3.79	3.85	3.90	3.96	4.01	4.06
5.80	3.38	3.45	3.51	3.57	3.64	3.69	3.75	3.81	3.86	3.92
6.00	3.23	3.30	3.36	3.42	3.49	3.55	3.61	3.66	3.72	3.77

Table 1 (*cont.*)

	Tl	Pb	Bi	Po	At	Rn	Fr	Ra	Ac	Th
.00	81.00	82.00	83.00	84.00	85.00	86.00	87.00	88.00	89.00	90.00
.05	79.77	80.72	81.69	82.67	83.67	84.67	85.27	86.08	87.08	88.10
.10	76.77	77.57	78.43	79.33	80.26	81.21	81.69	82.19	83.04	83.94
.15	73.02	73.68	74.39	75.14	75.94	76.77	77.46	77.99	78.64	79.36
.20	69.02	69.65	70.27	70.91	71.57	72.26	73.02	73.68	74.27	74.88
.25	65.03	65.69	66.31	66.90	67.49	68.08	68.78	69.48	70.07	70.64
.30	61.16	61.87	62.53	63.15	63.73	64.29	64.91	65.58	66.16	66.72
.35	57.50	58.25	58.96	59.62	60.24	60.82	61.40	62.01	62.60	63.16
.40	54.10	54.85	55.59	56.28	56.95	57.57	58.16	58.75	59.34	59.91
.45	50.99	51.72	52.44	53.16	53.85	54.51	55.12	55.71	56.32	56.91
.50	48.16	48.85	49.55	50.25	50.94	51.62	52.26	52.87	53.49	54.09
.55	45.60	46.24	46.90	47.56	48.24	48.91	49.56	50.18	50.81	51.43
.60	43.27	43.87	44.48	45.11	45.75	46.40	47.04	47.67	48.29	48.91
.65	41.14	41.70	42.27	42.86	43.46	44.08	44.70	45.31	45.92	46.54
.70	39.16	39.71	40.25	40.81	41.37	41.95	42.54	43.13	43.72	44.31
.75	37.32	37.85	38.38	38.91	39.45	39.99	40.54	41.11	41.67	42.24
.80	35.59	36.12	36.64	37.15	37.66	38.18	38.71	39.24	39.78	40.32
.85	33.95	34.48	35.00	35.50	36.00	36.50	37.01	37.52	38.02	38.54
.90	32.38	32.92	33.44	33.95	34.44	34.93	35.42	35.91	36.40	36.89
.95	30.88	31.43	31.95	32.47	32.96	33.45	33.93	34.40	34.88	35.35
1.00	29.46	30.00	30.54	31.05	31.55	32.04	32.52	32.99	33.45	33.91
1.05	28.10	28.64	29.18	29.70	30.20	30.69	31.17	31.64	32.10	32.56
1.10	26.80	27.35	27.88	28.40	28.91	29.41	29.89	30.36	30.82	31.27
1.15	25.58	26.12	26.65	27.17	27.68	28.17	28.66	29.13	29.59	30.05
1.20	24.44	24.96	25.47	25.99	26.50	26.99	27.48	27.95	28.42	28.87
1.25	23.36	23.86	24.37	24.87	25.37	25.86	26.35	26.82	27.29	27.75
1.30	22.36	22.84	23.32	23.81	24.30	24.79	25.27	25.74	26.21	26.66
1.35	21.43	21.89	22.35	22.82	23.29	23.77	24.24	24.70	25.17	25.62
1.40	20.58	21.00	21.44	21.89	22.34	22.80	23.26	23.72	24.18	24.63
1.50	19.07	19.44	19.82	20.21	20.62	21.04	21.47	21.90	22.33	22.77
1.60	17.81	18.12	18.44	18.79	19.14	19.51	19.90	20.29	20.69	21.09
1.70	16.76	17.02	17.29	17.58	17.88	18.20	18.54	18.88	19.24	19.61
1.80	15.88	16.10	16.33	16.57	16.82	17.09	17.38	17.68	17.99	18.32
1.90	15.13	15.32	15.51	15.71	15.93	16.16	16.40	16.65	16.92	17.20
2.00	14.48	14.64	14.81	14.99	15.17	15.36	15.57	15.78	16.01	16.25
2.20	13.36	13.50	13.65	13.79	13.94	14.09	14.24	14.40	14.57	14.75
2.40	12.35	12.50	12.65	12.79	12.93	13.07	13.20	13.34	13.47	13.61
2.60	11.38	11.55	11.71	11.87	12.01	12.16	12.30	12.43	12.56	12.69
2.80	10.44	10.62	10.80	10.97	11.13	11.29	11.44	11.59	11.73	11.86
3.00	9.53	9.73	9.91	10.10	10.27	10.44	10.61	10.77	10.92	11.07
3.20	8.69	8.88	9.07	9.26	9.44	9.62	9.80	9.97	10.13	10.29
3.40	7.92	8.10	8.29	8.47	8.65	8.84	9.01	9.19	9.36	9.53
3.60	7.24	7.41	7.58	7.76	7.93	8.11	8.28	8.45	8.63	8.80
3.80	6.65	6.81	6.96	7.12	7.28	7.45	7.61	7.78	7.94	8.11
4.00	6.16	6.29	6.43	6.57	6.72	6.86	7.02	7.17	7.33	7.48
4.20	5.74	5.85	5.97	6.10	6.23	6.36	6.49	6.63	6.78	6.92
4.40	5.39	5.49	5.59	5.70	5.81	5.92	6.04	6.17	6.30	6.43
4.60	5.09	5.18	5.27	5.36	5.46	5.56	5.66	5.77	5.88	6.00
4.80	4.85	4.92	5.00	5.08	5.16	5.25	5.34	5.43	5.53	5.63
5.00	4.63	4.70	4.77	4.83	4.91	4.98	5.06	5.14	5.23	5.31
5.20	4.44	4.50	4.56	4.63	4.69	4.76	4.83	4.90	4.97	5.05
5.40	4.28	4.33	4.39	4.44	4.50	4.56	4.62	4.68	4.75	4.82
5.60	4.12	4.17	4.22	4.28	4.33	4.39	4.44	4.50	4.56	4.62
5.80	3.97	4.02	4.07	4.13	4.18	4.23	4.28	4.33	4.39	4.44
6.00	3.83	3.88	3.93	3.98	4.03	4.08	4.13	4.18	4.23	4.28

	Pa	U	Np	Pu	Am	Cm	Bk	Cf	E	Fm
.00	91.00	92.00	93.00	94.00	95.00	96.00	97.00	98.00	99.00	100.00
.05	89.13	90.16	91.18	92.22	93.24	94.25	95.27	96.29	97.31	98.33
.10	85.12	86.17	87.21	88.41	89.46	90.36	91.42	92.46	93.50	94.55
.15	80.66	81.69	82.73	84.07	85.12	85.88	86.94	88.00	89.05	90.12
.20	76.16	77.14	78.15	79.48	80.51	81.22	82.26	83.31	84.36	85.42
.25	71.79	72.70	73.63	74.85	75.83	76.55	77.55	78.56	79.59	80.62
.30	67.71	68.53	69.38	70.44	71.35	72.08	73.01	73.97	74.94	75.92
.35	63.98	64.71	65.48	66.38	67.20	67.93	68.79	69.67	70.57	71.49
.40	60.59	61.25	61.94	62.70	63.45	64.15	64.93	65.73	66.56	67.40
.45	57.48	58.09	58.71	59.37	60.04	60.71	61.42	62.15	62.90	63.67
.50	54.60	55.17	55.75	56.32	56.93	57.58	58.22	58.88	59.57	60.27
.55	51.90	52.45	53.00	53.51	54.08	54.70	55.29	55.90	56.52	57.16
.60	49.37	49.90	50.43	50.90	51.44	52.03	52.58	53.15	53.72	54.30
.65	46.99	47.51	48.03	48.48	48.99	49.56	50.08	50.60	51.14	51.68
.70	44.78	45.29	45.79	46.23	46.72	47.27	47.76	48.26	48.76	49.26
.75	42.71	43.21	43.70	44.14	44.62	45.14	45.61	46.08	46.56	47.03
.80	40.80	41.29	41.77	42.21	42.67	43.17	43.63	44.08	44.53	44.98
.85	39.02	39.51	39.98	40.42	40.88	41.35	41.79	42.23	42.66	43.10
.90	37.38	37.86	38.32	38.77	39.21	39.67	40.10	40.52	40.94	41.36
.95	35.85	36.32	36.78	37.23	37.67	38.10	38.53	38.94	39.35	39.76
1.00	34.41	34.87	35.33	35.79	36.22	36.65	37.07	37.48	37.88	38.28
1.05	33.05	33.52	33.97	34.43	34.87	35.28	35.70	36.11	36.51	36.90
1.10	31.77	32.23	32.69	33.15	33.59	34.00	34.41	34.82	35.22	35.61
1.15	30.54	31.00	31.46	31.93	32.37	32.77	33.19	33.60	34.00	34.39
1.20	29.37	29.83	30.29	30.76	31.20	31.61	32.03	32.44	32.84	33.23
1.25	28.23	28.70	29.16	29.63	30.07	30.49	30.91	31.33	31.73	32.13
1.30	27.15	27.61	28.07	28.54	28.99	29.41	29.84	30.26	30.67	31.07
1.35	26.10	26.56	27.02	27.49	27.94	28.36	28.79	29.22	29.63	30.04
1.40	25.09	25.55	26.01	26.47	26.92	27.35	27.78	28.21	28.63	29.04
1.50	23.21	23.65	24.09	24.54	24.99	25.42	25.85	26.28	26.71	27.13
1.60	21.50	21.92	22.34	22.77	23.19	23.62	24.05	24.47	24.90	25.32
1.70	19.98	20.36	20.75	21.15	21.55	21.96	22.37	22.78	23.20	23.61
1.80	18.65	18.99	19.34	19.70	20.07	20.45	20.84	21.23	21.62	22.02
1.90	17.49	17.79	18.10	18.43	18.76	19.11	19.46	19.82	20.19	20.56
2.00	16.50	16.76	17.03	17.31	17.61	17.92	18.24	18.56	18.90	19.24
2.20	14.93	15.12	15.32	15.53	15.75	15.99	16.23	16.49	16.75	17.03
2.40	13.75	13.90	14.05	14.21	14.38	14.55	14.73	14.92	15.13	15.34
2.60	12.81	12.94	13.06	13.19	13.32	13.46	13.60	13.75	13.90	14.06
2.80	11.98	12.11	12.23	12.35	12.46	12.58	12.70	12.82	12.95	13.07
3.00	11.20	11.33	11.46	11.58	11.70	11.82	11.93	12.04	12.15	12.27
3.20	10.44	10.58	10.72	10.85	10.97	11.10	11.22	11.33	11.44	11.55
3.40	9.68	9.84	9.99	10.12	10.26	10.40	10.53	10.65	10.77	10.88
3.60	8.96	9.12	9.27	9.42	9.56	9.71	9.85	9.98	10.11	10.23
3.80	8.27	8.43	8.58	8.73	8.89	9.04	9.18	9.32	9.46	9.59
4.00	7.63	7.79	7.94	8.09	8.24	8.39	8.54	8.68	8.82	8.96
4.20	7.06	7.21	7.35	7.49	7.64	7.79	7.93	8.08	8.22	8.36
4.40	6.56	6.69	6.82	6.96	7.09	7.23	7.37	7.51	7.65	7.78
4.60	6.11	6.23	6.36	6.48	6.60	6.73	6.86	6.99	7.12	7.26
4.80	5.73	5.84	5.95	6.06	6.17	6.29	6.41	6.53	6.65	6.77
5.00	5.40	5.50	5.60	5.69	5.80	5.90	6.01	6.12	6.23	6.34
5.20	5.13	5.21	5.29	5.38	5.47	5.56	5.66	5.76	5.86	5.96
5.40	4.89	4.96	5.03	5.11	5.19	5.27	5.36	5.45	5.54	5.63
5.60	4.68	4.74	4.81	4.88	4.95	5.02	5.10	5.17	5.25	5.34
5.80	4.50	4.55	4.61	4.68	4.74	4.80	4.87	4.94	5.01	5.08
6.00	4.34	4.39	4.44	4.50	4.55	4.61	4.67	4.73	4.80	4.86

functions and the integration technique, the normalization integral,

$$I = \int_0^\infty \sum_i^Z \omega_i P^2(r)\, dr \,,$$

was evaluated, again using a standard notation. The values obtained at the extremes of the data were $I_2 = 2{\cdot}0000004$ and $I_{103} = 103{\cdot}00002$. Thus this aspect of the calculation is numerically accurate to seven significant figures. However, one can see that for very large values of s the mesh at large x is too coarse to take into account the rapid undulations of the $\sin sr$ term of equation 2. However, at the x values where this effect may be felt, the value of the electronic density is so small as to make this effect negligible. This was shown in two ways: (1) The coarseness of the integration mesh was doubled for a range of elements. Differences were observed only in the fourth decimal place. (Only two decimal places for $Z > 10$ are presented here.) (2) The more accurate integration method due to Luke (1954) was used for several elements again with only small differences appearing in the fourth decimal place. The numerical accuracy is then at least one order of magnitude better than the data presented here, but, of course, the physical accuracy does not warrant retention of more digits.

Table 1 presents atomic scattering factors for elements $Z = 1$ to $Z = 100$ to two decimal places and covers a range of $\sin\theta/\lambda$ up to 6·0. These are selected from a set of original data in which f values for $Z = 1$ to $Z = 103$ are given to six significant figures (4 decimal places) for every 0·5 unit of $(4\pi/\lambda)\sin\theta$ up to 6·0 and for every 0·05 unit of $\sin\theta/\lambda$ up to 6·0. This large range is given because these f values are useful in computing electron scattering amplitudes for electron diffraction. The values for hydrogen, obtained from the exact wave function, are included for completeness.

A detailed comparison of these results with f values obtained by other investigators using various other techniques will appear elsewhere. It may be pointed out, however, that in general the results are close to those obtained from the HF wave functions that are available and they merge with them for large s values. As one might anticipate, these results most nearly duplicate those obtained by Freeman & Wood (1959) who used wave functions obtained by slightly more flexible HFS calculations which permitted different potentials to electrons of different spin.

Of fundamental importance, of course, is the question of physical accuracy. The HFS technique yields wave functions, and hence f values, which approximate quite closely those obtained by HF for isolated atoms. The assumption of free electron exchange made by Slater is a better one for condensed matter than for isolated atoms. Thus empirically the HFS f values may be at least as good as the HF in the majority of the experimentally important cases. There are other inherent limitations and defects in these calculations. For example: (1) they do not make allowances for the dispersion effects which occur when λ is in the vicinity of an X-ray absorption edge, (2) they assume spherical symmetry, (3) the wave functions from which the f values are computed are not corrected for spin-orbit effects, and (4) the wave functions are not corrected for relativistic effects.

Conclusions and comments

Despite the intrinsic approximations in these calculations, it is felt that the scattering factors presented here represent a substantial improvement over most values available. They possess the inherent advantages of being relatively complete and of having been obtained in a coherent fashion, the same type of approximation being involved in the calculations for each of the atoms. There are numerous obvious extensions of these calculations. In preparation at present are the following: (1) the scattering amplitudes for electron scattering both within the first Born approximation and in the case where consideration is taken of the phase change, (2) the inelastic scattering factors, (3) X-ray and electron scattering factors for ions, and (4) analytic approximations to the X-ray and electron scattering factors.

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Hartree Scattering Factors for Elements 37 through 98*

By Don T. Cromer, Allen C. Larson and James T. Waber

University of California, Los Alamos Scientific Laboratory, Los Alamos, New Mexico, U.S.A.

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Hartree scattering factors are given for atoms of atomic number 37 through 98 and for several of their ions. The values are listed in tabular form and as analytic functions. Values are also given for two low-lying excited states of cerium. Differences between the Hartree and Thomas–Fermi–Dirac scattering factors are discussed.

Introduction

Atomic scattering factors obtained from Hartree self-consistent-field (SCF) calculations have been available in the past for only a very few atoms and ions above atomic number 36. Boyd, Larson & Waber (1963) have recently completed Hartree SCF calculations for all atoms of the periodic table, many ions, and many excited states. In this paper we present scattering factors for the ground states of elements of atomic number 37 and higher, for several of their ions, and for two excited states of cerium. (For elements of lower atomic number, scattering factors which have been obtained from more accurate wave functions are already available in standard references.)

We have published in a Los Alamos Scientific Laboratory report (Cromer, Larson & Waber, 1963) a set of Hartree SCF scattering factors for all atoms in the periodic table, in a more detailed form than in the present paper. Although this publication duplicates light element work by others, it has the advantage of presenting in a single unit complete information on Hartree SCF scattering factors.

Calculations

Details of the Hartree SCF calculations will be given elsewhere by Boyd, Larson & Waber (1964). The scattering factors were computed from the total radial density functions by straightforward means (James, 1948). Calculations were performed for the most part with an IBM 7090 computer and, in the

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