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

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

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

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

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

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

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

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

With this definition of the spherical harmonics,

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

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

references