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Revised analytic constants for atomic scattering factors.

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Analytic constants for atomic scattering factors for use with Cu $K\alpha$ and Mo $K\alpha$ radiation have been calculated for the elements of atomic numbers 1–100, based on the scattering factors of Hanson, Herman, Lea & Skillman (*Acta Cryst.* (1964) **17**, 1040).

Vand, Eiland & Pepinsky (1957) have shown that the atomic scattering factor f for Cu $K\alpha$ radiation may be expressed as a function of $x=\sin\theta$, for $0\leq\theta\leq 90°$ by the sum of two exponential terms

$$f=A\exp(-ax^2)+B\exp(-bx^2)\,. \qquad (1)$$

It was suggested that a better fit for Mo $K\alpha$ radiation over this range of θ could be obtained by the use of

$$f=A\exp(-ax^2)+B\exp(-bx^2)+C\,. \qquad (2)$$

Forsyth & Wells (1959) modified this in the following ways.

(1) The reciprocal space variable was changed from x to $s=\sin\theta/\lambda$ so that the values of a and b are independent of λ.

(2) The condition $A+B+C=N$, the number of electrons in the atom or ion, was relaxed to allow an improved fit over the more useful range of values of s.

(3) A weight factor $w=\exp\{-(s-0{\cdot}5)^2\}$ was applied to the least-squares curve fitting procedure to obtain the best agreement in the middle of the curve, *i.e.* at $\theta=45°$, where most crystallographic data occurs.

Tables of values of A, a, B, b and C have been published by Forsyth & Wells (1959) for Cu $K\alpha$ radiation, and by Moore (1963) for both Cu $K\alpha$ and Mo $K\alpha$ radiation. The intention of the present authors is to provide new and revised values of these constants using the more recent atomic scattering factor tables of Hanson, Herman, Lea &

Table 1. *Analytic constants for atomic scattering factors for Cu Kα radiation*

At.No.	Element	A	a	B	b	C	c	At.No.	Element	A	a	B	b	C	c
1	H	0.477	9.457	0.498	33.805	0.025	0.139	51	Sb	25.297	4.461	7.034	40.503	18.609	0.095
2	He	1.233	5.072	0.608	19.191	0.160	0.043	52	Te	25.354	4.103	8.097	37.070	18.496	0.077
3	Li	1.543	3.343	1.056	108.770	0.397	0.140	53	I	25.341	3.787	9.195	33.780	18.414	0.069
4	Be	1.178	3.027	1.991	55.354	0.816	0.271	54	Xe	25.246	3.511	10.330	30.774	18.381	0.064
5	B	1.269	7.015	2.408	39.904	1.306	0.288	55	Cs	25.225	3.855	9.721	33.157	19.790	0.224
6	C	2.270	8.657	2.271	33.344	1.448	0.165	56	Ba	25.688	4.489	8.490	42.565	21.531	0.309
7	N	3.335	7.793	2.129	28.117	1.530	0.093	57	La	25.692	4.487	8.968	42.607	22.087	0.285
8	O	4.332	6.627	2.049	23.850	1.614	0.059	58	Ce	27.030	4.518	8.237	41.321	22.449	0.294
9	F	5.281	5.620	2.003	20.459	1.713	0.040	59	Pr	27.778	4.528	8.040	41.299	22.909	0.284
10	Ne	6.196	4.822	1.967	17.737	1.834	0.032	60	Nd	28.515	4.533	7.825	41.220	23.392	0.276
11	Na	7.435	4.947	1.251	100.528	2.301	0.170	61	Pm	29.278	4.518	7.624	41.255	23.838	0.267
12	Mg	7.366	3.857	2.245	70.636	2.375	0.115	62	Sm	30.038	4.482	7.447	41.084	24.259	0.261
13	Al	7.132	3.302	3.145	56.549	2.679	0.211	63	Eu	30.793	4.468	7.210	41.501	24.749	0.253
14	Si	6.784	2.937	4.114	43.918	3.063	0.200	64	Gd	30.999	4.421	7.534	42.320	25.259	0.227
15	P	6.209	2.942	5.001	35.185	3.754	0.180	65	Tb	32.256	4.398	6.827	41.908	25.686	0.234
16	S	5.695	3.244	5.745	29.218	4.530	0.151	66	Dy	32.975	4.335	6.691	41.691	26.106	0.231
17	Cl	5.447	3.838	6.273	25.136	5.256	0.115	67	Ho	33.673	4.306	6.478	42.264	26.626	0.224
18	Ar	5.655	4.462	6.570	22.173	5.759	0.083	68	Er	34.371	4.249	6.329	42.481	27.085	0.216
19	K	9.834	8.423	2.386	67.058	6.691	0.394	69	Tm	35.042	4.191	6.181	42.601	27.567	0.208
20	Ca	10.258	7.498	2.946	84.987	6.754	0.243	70	Yb	35.702	4.143	6.038	42.903	28.058	0.201
21	Sc	10.940	6.976	3.158	74.160	6.861	0.207	71	Lu	35.866	4.049	6.459	43.294	28.501	0.181
22	Ti	11.690	6.526	3.291	65.936	6.979	0.181	72	Hf	35.921	3.962	6.970	41.644	28.957	0.161
23	V	12.499	6.135	3.351	60.411	7.108	0.163	73	Ta	35.939	3.867	7.553	38.722	29.365	0.147
24	Cr	13.701	6.023	2.936	50.029	7.316	0.174	74	W	35.912	3.840	7.981	36.656	29.974	0.137
25	Mn	14.149	5.429	3.418	51.808	7.391	0.141	75	Re	35.908	3.808	8.424	34.299	30.533	0.132
26	Fe	14.971	5.139	3.421	48.743	7.569	0.130	76	Os	35.959	3.806	8.760	32.482	31.150	0.124
27	Co	15.786	4.866	3.415	46.109	7.763	0.118	77	Ir	36.052	3.839	8.979	31.079	31.846	0.116
28	Ni	16.621	4.599	3.404	43.760	7.940	0.111	78	Pt	35.754	3.736	9.974	25.218	32.155	0.100
29	Cu	17.830	4.554	2.855	38.456	8.277	0.107	79	Au	36.004	3.763	10.144	24.177	32.741	0.093
30	Zn	18.215	4.171	3.338	40.368	8.412	0.103	80	Hg	36.901	3.972	9.201	27.913	33.784	0.103
31	Ga	18.438	3.914	3.779	44.600	8.726	0.128	81	Tl	37.810	4.160	8.308	33.589	34.740	0.122
32	Ge	18.463	3.556	4.627	41.273	8.861	0.118	82	Pb	38.358	4.118	8.435	36.923	35.086	0.114
33	As	18.341	3.245	5.577	36.354	9.040	0.102	83	Bi	38.719	3.962	9.066	37.515	35.117	0.097
34	Se	18.126	2.984	6.569	31.621	9.263	0.091	84	Po	38.951	3.770	9.941	36.472	35.025	0.081
35	Br	17.726	2.846	7.484	28.025	9.753	0.080	85	At	39.134	3.552	10.994	34.574	34.804	0.067
36	Kr	17.319	2.723	8.426	24.917	10.226	0.071	86	Rn	39.234	3.346	12.117	32.491	34.591	0.057
37	Rb	16.909	3.968	6.674	31.706	13.193	0.305	87	Fr	39.070	3.464	11.882	33.714	35.756	0.156
38	Sr	17.749	4.994	5.264	51.400	14.816	0.336	88	Ra	38.968	3.779	11.078	39.170	37.591	0.224
39	Y	17.890	5.006	5.663	49.864	15.307	0.290	89	Ac	38.929	3.774	11.546	40.078	38.200	0.215
40	Zr	18.092	5.059	5.980	47.106	15.808	0.251	90	Th	38.789	3.735	12.204	39.596	38.716	0.202
41	Nb	18.049	4.971	6.660	35.980	16.161	0.217	91	Pa	39.482	3.902	11.612	37.987	39.585	0.209
42	Mo	18.529	5.067	6.750	34.235	16.605	0.192	92	U	39.920	3.956	11.569	37.148	40.195	0.206
43	Tc	19.448	5.232	6.386	39.499	17.066	0.183	93	Np	40.453	4.025	11.396	36.706	40.835	0.203
44	Ru	19.881	5.228	6.647	31.396	17.369	0.156	94	Pu	41.414	4.090	10.931	34.393	41.308	0.206
45	Rh	20.796	5.304	6.403	30.841	17.711	0.144	95	Am	42.137	4.137	10.682	34.221	41.839	0.202
46	Pd	20.579	4.884	7.751	22.800	17.627	0.073	96	Cm	42.571	4.160	10.719	36.117	42.413	0.191
47	Ag	22.769	5.300	5.934	29.356	18.215	0.119	97	Bk	43.365	4.185	10.471	36.021	42.872	0.186
48	Cd	23.898	5.264	5.561	34.979	18.470	0.116	98	Cf	44.202	4.202	10.206	36.037	43.306	0.182
49	In	24.756	5.152	5.462	41.883	18.695	0.131	99	Es	45.086	4.223	9.875	36.476	43.761	0.179
50	Sn	25.126	4.839	6.092	42.986	18.709	0.111	100	Fm	45.970	4.213	9.639	36.458	44.118	0.174

Skillman (1964). Only the values in the meaningful range $0 \leq \sin\theta \leq 1$, have been used in the calculations. The usual least-squares criterion has been used to estimate the goodness of fit, but, instead of following the normal procedure and solving non-linear equations to find the values of the constants, an optimization method has been used. The least-squares criterion is that we seek to minimize the sum of squares

$$s = \sum_i w_i \{f_i - A \exp(-as_i^2) - B \exp(-bs_i^2) - C\}^2$$

where f_i is the atomic scattering factor corresponding to the value s_i, and $w_i = \exp\{-(s_i - \bar{s})^2\}$, $\bar{s}$ being the value of s for $\theta = 45°$. For Cu $K\alpha$ radiation the range of s is 0 to 0·65 in steps of 0·05 and $\bar{s} = 0{\cdot}5$ and for Mo $K\alpha$ radiation the range of s is 0 to 1·4 in steps of 0·05 and $\bar{s} = 1{\cdot}0$. The minimization has been performed by mean of the direct methods of Powell (1964, 1965) with the previously published values of the constants as a starting point. The first method is general, and can be used to find the minimum value of any function. The second method applies only to a sum of squares but is more efficient in terms of computer time for this special case. Some of the values in the Table were obtained using both methods as a check. The Tables of values of the constants include a measure of the goodness of fit, ε, given by

$$\varepsilon = \frac{S}{\sum_i w_i} \frac{100}{f_0}$$

where $f_0 = A + B + C$. The same measure has been used by previous workers.

All computations were carried out on an ICT 1905 computer at the Loughborough University of Technology Computer Centre.

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Table 2. *Analytical constants for atomic scattering factors for Mo Kα radiation*

At.No.	Element	A	a	B	b	C	ε	At.No.	Element	A	a	B	b	C	ε
1	H	0.377	7.388	0.608	29.389	0.012	0.223	51	Sb	20.196	1.424	18.251	11.658	11.513	0.715
2	He	0.835	2.722	1.115	12.729	0.041	0.277	52	Te	21.773	1.638	16.977	13.528	12.359	0.718
3	Li	1.679	2.377	1.134	90.426	0.167	0.642	53	I	23.218	1.784	16.133	15.618	12.946	0.670
4	Be	1.633	1.414	2.095	50.046	0.242	0.295	54	Xe	24.245	1.849	15.889	17.227	13.329	0.593
5	B	1.569	1.035	3.015	29.848	0.353	0.443	55	Cs	24.857	1.848	15.801	17.594	13.566	0.542
6	C	1.447	1.017	3.882	20.031	0.585	0.532	56	Ba	25.494	1.846	15.746	18.211	13.801	0.543
7	N	1.422	1.368	4.601	15.061	0.883	0.541	57	La	26.107	1.834	15.991	19.150	14.001	0.510
8	O	1.804	1.964	5.012	12.513	1.100	0.468	58	Ce	26.735	1.835	16.125	17.281	14.204	0.483
9	F	2.641	2.400	5.064	11.084	1.229	0.364	59	Pr	27.400	1.823	16.295	16.791	14.375	0.461
10	Ne	3.660	2.486	4.977	9.981	1.310	0.280	60	Nd	28.127	1.813	16.407	16.358	14.542	0.439
11	Na	6.801	3.188	2.465	22.456	1.481	0.748	61	Pm	28.861	1.798	16.524	15.915	14.696	0.423
12	Mg	7.563	2.844	2.764	45.474	1.573	0.578	62	Sm	29.617	1.782	16.622	15.488	14.843	0.407
13	Al	7.664	2.344	3.608	43.211	1.616	0.420	63	Eu	30.392	1.762	16.713	15.075	14.976	0.395
14	Si	7.674	1.937	4.582	36.532	1.650	0.293	64	Gd	31.164	1.735	16.827	15.547	15.099	0.401
15	P	7.639	1.608	5.603	29.886	1.667	0.221	65	Tb	32.006	1.720	16.856	14.337	15.223	0.373
16	S	7.589	1.341	6.653	24.414	1.667	0.204	66	Dy	32.823	1.697	16.923	13.977	15.340	0.364
17	Cl	7.537	1.127	7.714	20.255	1.654	0.199	67	Ho	33.650	1.673	16.981	13.636	15.449	0.356
18	Ar	7.471	0.952	8.790	17.009	1.639	0.208	68	Er	34.502	1.648	17.021	13.324	15.557	0.349
19	K	7.340	0.891	9.299	14.781	1.874	0.551	69	Tm	35.366	1.623	17.050	13.020	15.664	0.342
20	Ca	7.102	0.996	9.593	14.179	2.557	0.902	70	Yb	36.194	1.597	17.120	12.721	15.764	0.337
21	Sc	6.951	1.096	10.174	13.296	3.114	0.930	71	Lu	37.092	1.575	17.063	13.186	15.906	0.357
22	Ti	6.980	1.264	10.584	12.665	3.690	0.921	72	Hf	37.816	1.544	17.235	13.561	16.030	0.363
23	V	7.293	1.475	10.792	12.230	4.193	0.895	73	Ta	38.372	1.502	17.641	13.736	16.105	0.359
24	Cr	7.332	1.481	11.669	10.768	4.417	0.699	74	W	38.777	1.456	18.202	13.711	16.171	0.351
25	Mn	9.102	1.983	10.314	12.336	4.965	0.794	75	Re	39.092	1.406	18.879	13.530	16.208	0.338
26	Fe	10.483	2.205	9.724	12.800	5.241	0.729	76	Os	39.295	1.353	19.678	13.192	16.226	0.329
27	Co	11.958	2.349	9.101	13.326	5.452	0.662	77	Ir	39.439	1.302	20.528	12.803	16.253	0.319
28	Ni	13.284	2.404	8.652	13.551	5.616	0.604	78	Pt	39.326	1.226	21.976	12.034	16.069	0.258
29	Cu	13.313	2.226	9.632	10.865	5.657	0.471	79	Au	39.360	1.176	22.964	11.560	16.060	0.250
30	Zn	15.819	2.392	7.919	13.859	5.878	0.498	80	Hg	39.577	1.157	23.347	11.402	16.319	0.297
31	Ga	17.634	2.425	6.942	18.326	6.043	0.504	81	Tl	39.759	1.144	23.626	11.224	16.639	0.353
32	Ge	18.608	2.332	6.957	22.264	6.139	0.447	82	Pb	40.046	1.150	23.686	11.314	17.148	0.413
33	As	19.074	2.175	7.514	23.596	6.184	0.367	83	Bi	40.412	1.171	23.599	11.599	17.788	0.465
34	Se	19.301	2.000	8.321	22.964	6.190	0.290	84	Po	40.872	1.205	23.372	12.117	18.541	0.503
35	Br	19.419	1.832	9.241	21.577	6.179	0.227	85	At	41.414	1.246	23.085	12.842	19.340	0.526
36	Kr	19.475	1.674	10.241	19.939	6.148	0.182	86	Rn	41.986	1.287	22.841	13.710	20.113	0.531
37	Rb	19.589	1.550	10.777	18.459	6.160	0.296	87	Fr	42.352	1.304	22.667	14.020	20.684	0.524
38	Sr	19.804	1.465	11.232	18.026	6.253	0.454	88	Ra	42.774	1.323	22.476	14.481	21.263	0.537
39	Y	19.946	1.382	11.998	17.640	6.338	0.483	89	Ac	43.322	1.355	22.315	15.440	21.926	0.539
40	Zr	19.995	1.300	12.864	16.890	6.424	0.493	90	Th	43.829	1.377	22.329	16.386	22.495	0.528
41	Nb	19.886	1.190	14.149	15.470	6.371	0.402	91	Pa	43.404	1.337	23.502	14.712	22.697	0.503
42	Mo	19.826	1.117	15.136	14.469	6.446	0.401	92	U	43.446	1.331	24.071	14.313	23.102	0.488
43	Tc	19.808	1.097	15.673	13.982	6.794	0.491	93	Np	43.484	1.328	24.613	13.890	23.525	0.475
44	Ru	19.577	1.001	17.108	12.617	6.722	0.392	94	Pu	43.095	1.298	25.758	12.704	23.781	0.445
45	Rh	19.397	0.958	18.082	11.791	6.926	0.393	95	Am	43.159	1.299	26.260	12.342	24.219	0.434
46	Pd	19.172	0.894	19.435	10.925	6.981	0.314	96	Cm	43.728	1.328	26.084	12.692	24.816	0.444
47	Ag	18.903	0.901	19.969	10.363	7.529	0.384	97	Bk	43.880	1.332	26.496	12.343	25.253	0.435
48	Cd	18.687	0.957	20.181	10.132	8.379	0.473	98	Cf	44.083	1.341	26.834	12.032	25.715	0.426
49	In	18.653	1.053	20.022	10.079	9.358	0.572	99	Es	44.339	1.350	27.128	11.735	26.163	0.419
50	Sn	19.091	1.214	19.371	10.539	10.470	0.660	100	Fm	44.621	1.359	27.407	11.450	26.605	0.411