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X-ray scattering factors computed from numerical Hartree–Fock wave functions

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X-ray scattering factors for neutral atoms from He to Lw and for most of the chemically significant ions through Lu^{3+} have been computed from numerical Hartree–Fock wave functions. The results are given in the form of coefficients for an analytic function.

During the last few years extensive calculations of X-ray scattering factors have been published for several different atomic models. In order of increasing sophistication these have been the Thomas–Fermi–Dirac model by Thomas & Umeda (1957); the Hartree model by Cromer, Larson & Waber (1964); the Hartree–Fock–Slater (HFS) model by Hanson, Herman, Lea & Skillman (1964) and by Hanson & Pohler (1966); and the Dirac–Slater (DS) model, the relativistic equivalent of the HFS model, by Cromer &

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Table 1. *Coefficients and maximum errors, over the range* $0 \le \sin\theta/\lambda \le 1{\cdot}50$, *for analytic approximations of Hartree–Fock scattering factors*

ATOM	A(1)	B(1)	A(2)	B(2)	A(3)	B(3)	A(4)	B(4)	C	EMAX	EMIN
HE	0.76844	10.9071	0.72694	4.30779	0.27631	1.33127	0.21572	25.6848	0.01249	0.242	-0.669
LI	0.99279	4.33979	0.87402	1.26006	0.84240	98.7088	0.23101	212.088	0.05988	0.402	-1.185
LI+1	6.08475	0.00498	0.86773	1.53730	0.80588	4.28524	0.17720	9.81413	-5.93560	0.085	-0.036
BE	2.22744	0.04965	1.55249	42.9165	1.40060	1.66379	0.58290	100.361	-1.76339	0.355	-0.180
BE+2	5.69034	-0.01336	1.19706	0.39000	1.03057	1.97441	0.20150	4.90642	-6.11950	0.013	-0.029
B	2.03876	23.0888	1.41491	0.97848	1.11609	59.8985	0.73273	0.08538	-0.30409	0.082	-0.191
C	1.93019	12.7188	1.87812	28.6498	1.57415	0.59645	0.37108	65.0337	0.24637	0.027	-0.026
N	12.7913	0.02064	3.28546	10.7018	1.76483	30.7773	0.54709	1.48044	-11.3926	0.465	-0.210
O	2.95648	13.8964	2.45240	5.91765	1.50510	0.34537	0.78135	34.0811	0.30413	0.025	-0.046
O -1	3.22563	18.4991	3.01717	6.65680	1.42553	0.40589	0.90525	61.1889	0.42362	0.101	-0.192
F	3.30393	11.2651	3.01753	4.66504	1.35754	0.33760	0.83645	27.9898	0.48398	0.031	-0.062
F -1	3.63220	5.27756	3.51057	14.7353	1.26064	0.44226	0.94071	47.3437	0.65340	0.102	-0.208
NE	3.71272	3.91091	3.52631	9.63126	1.19237	0.40483	0.83080	23.9546	0.73728	0.031	-0.062
NA	5.26400	4.02579	2.17549	10.4796	1.36690	0.84222	1.08859	133.617	1.09912	0.119	-0.255
NA+1	3.99479	3.11047	3.37245	7.14318	1.13877	0.40692	0.65118	15.7319	0.84267	0.010	-0.020
MG	5.59229	4.41142	2.68206	1.36549	1.72235	93.4885	0.73055	32.5281	1.26883	0.281	-0.643
MG+2	4.30491	2.55961	3.14719	5.60660	1.12859	0.41574	0.49034	11.4840	0.92893	0.003	-0.006
AL	5.35047	3.48665	2.92451	1.20535	2.27309	42.6051	1.16531	107.170	1.28489	0.113	-0.265
AL+3	4.17448	1.93816	3.38760	4.14553	1.20296	0.22875	0.52814	8.28524	0.70679	0.004	-0.002
SI	5.79411	2.57104	3.22390	34.1775	2.42795	0.86937	1.32149	85.3410	1.23139	0.020	-0.020
SI+4	4.43918	1.64167	3.20345	3.43757	1.19453	0.21490	0.41653	6.65365	0.74630	0.002	-0.001
P	6.92073	1.83778	4.14396	27.0198	2.01697	0.21318	1.53860	67.1086	0.37870	0.112	-0.056
S	7.18742	1.43280	5.88671	0.02865	5.15858	22.1101	1.64403	55.4651	-3.87732	0.092	-0.164
CL	9.83957	-0.00053	7.53181	1.11119	6.07100	18.0846	1.87128	45.3666	-8.31430	0.131	-0.283
CL-1	18.0842	0.00129	7.47202	1.12976	6.46337	19.3079	2.43918	59.0633	-16.4654	0.109	-0.231
AR	16.8752	-0.01456	8.32256	0.83310	6.91326	14.9177	2.18515	37.2256	-16.2972	0.121	-0.267
K	8.11756	12.6684	7.48062	0.76409	1.07795	211.222	0.97218	37.2727	1.35009	0.416	-0.194
K +1	9.70659	0.59947	7.37245	11.8765	5.67228	-0.08359	1.90688	26.7668	-6.65819	0.091	-0.201
CA	8.60272	10.2636	7.50769	0.62794	1.75117	149.301	0.96216	60.2274	1.17430	0.404	-0.176
CA+2	13.2063	0.39466	11.0586	-0.08204	7.73221	9.62976	1.72057	20.3341	-15.7176	0.058	-0.125
SC	9.06482	8.77431	7.55526	0.53306	2.05017	123.880	1.28745	36.8890	1.03849	0.262	-0.115
SC+3	13.4008	0.29854	8.02730	7.96290	1.65943	-0.28604	1.57936	16.0662	-6.66668	0.034	-0.072
TI	9.54969	7.60579	7.60067	0.45899	2.17223	109.099	1.75438	27.5715	0.91762	0.137	-0.063
TI+3	17.7344	0.22061	8.73816	7.04716	5.25691	-0.15762	1.92134	15.9768	-14.6519	0.011	-0.013
TI+4	19.5114	0.17885	8.23473	6.67018	2.01341	-0.29263	1.52080	12.9464	-13.2803	0.018	-0.037
V	10.0661	6.67721	7.61420	0.40322	2.23551	98.5954	2.23170	22.5720	0.84574	0.048	-0.044
V +2	9.34513	6.49985	7.68833	0.39491	2.94531	15.9868	0.26998	41.0832	0.75143	0.096	-0.042
V +3	9.43141	6.39535	7.74190	0.38335	2.15343	15.1908	0.01686	63.9690	0.65657	0.106	-0.046
V +5	15.6887	0.67900	8.14208	5.40135	2.03081	9.97278	-9.57602	0.94046	1.71430	0.002	-0.002
CR	10.4757	6.01658	7.51402	0.37426	3.50115	19.0654	1.54902	97.4599	0.95226	0.055	-0.050
CR+2	9.54034	5.66078	7.75090	0.34426	3.58274	13.3075	0.50911	32.4224	0.61690	0.048	-0.022
CR+3	9.68090	5.59463	7.81136	0.33439	2.87602	12.8288	0.11357	32.8761	0.51827	0.053	-0.024
MN	11.2519	5.34818	7.36935	0.34373	3.04107	17.4089	2.27703	84.2139	1.05195	0.058	-0.081
MN+2	9.78094	4.98303	7.79153	0.30421	4.18544	11.4399	0.72736	27.7750	0.51454	0.021	-0.010
MN+3	9.84521	4.91797	7.87194	0.29439	3.56531	10.8171	0.32361	24.1281	0.39397	0.025	-0.011
MN+4	9.96253	4.84850	7.97057	0.28330	2.76067	10.4852	0.05445	27.5730	0.25188	0.027	-0.012
FE	11.9185	4.87394	7.04848	0.34023	3.34326	15.9330	2.27228	79.0339	1.40818	0.062	-0.117
FE+2	10.1270	4.44133	7.78007	0.27418	4.71825	10.1451	0.89547	24.8302	0.47888	0.005	-0.003
FE+3	10.0333	4.36007	7.90625	0.26250	4.20562	9.35847	0.55048	20.4105	0.30429	0.010	-0.005
CO	12.6158	4.48994	6.62642	0.35459	3.57722	14.8402	2.25644	74.7352	1.91452	0.071	-0.141
CO+2	10.5942	4.00858	7.67791	0.25410	5.15947	9.21931	1.01440	22.7516	0.55358	0.004	-0.004
CO+3	10.3380	3.90969	7.88173	0.23867	4.76795	8.35583	0.72559	18.3491	0.28667	0.002	-0.001
NI	13.3239	4.17742	6.18746	0.38682	3.74792	14.0123	2.23195	71.1195	2.49899	0.077	-0.156
NI+2	11.1650	3.65944	7.45636	0.24397	5.51106	8.52556	1.09496	21.1647	0.77218	0.005	-0.009
NI+3	10.7806	3.54770	7.75868	0.22314	5.22746	7.64468	0.84711	16.9673	0.38604	0.002	-0.002
CU	13.9352	3.97779	5.84833	0.44555	4.64221	13.3971	1.44753	74.1605	3.11686	0.085	-0.174
CU+1	12.4655	3.54270	6.63111	0.28920	5.76679	9.31140	1.34230	26.9799	1.79285	0.016	-0.033
CU+2	11.8168	3.37484	7.11181	0.24408	5.78135	7.98760	1.14523	19.8970	1.14431	0.006	-0.012
ZN	14.6744	3.71486	5.62816	0.50033	3.92540	12.8862	2.16398	65.4071	3.59838	0.082	-0.172
ZN+2	12.5225	3.13961	6.68507	0.25431	5.98382	7.55544	1.17317	18.8453	1.63497	0.007	-0.013

Table 1 (*cont.*)

ATOM	A(1)	B(1)	A(2)	B(2)	A(3)	B(3)	A(4)	B(4)	C	EMAX	EMIN
GA	15.3412	3.63868	5.74150	0.65640	3.10733	16.0719	2.52764	70.7609	4.26842	0.117	-0.249
GA+3	12.6920	2.81262	6.69883	0.22789	6.06692	6.36441	1.00660	14.4122	1.53545	0.003	-0.005
GE	15.4378	3.39715	6.00432	0.73097	3.05158	18.9533	2.93572	63.7969	4.56068	0.110	-0.237
AS	15.4043	3.07517	6.13723	0.74113	3.74679	21.0014	3.01390	57.7446	4.69149	0.083	-0.180
SE	15.5372	2.71530	5.98288	0.68962	4.83996	21.0079	2.93549	52.4308	4.70026	0.051	-0.112
BR	15.9934	2.35651	6.02439	19.7393	5.51599	0.58143	2.88716	47.3323	4.57602	0.025	-0.056
BR-1	15.4080	2.43532	6.78083	22.0832	6.00715	0.68621	2.99332	64.9193	4.80234	0.044	-0.098
KR	16.8494	2.01856	7.19790	18.0409	4.92564	0.39741	2.91606	42.5054	4.10864	0.010	-0.018
RB	11.4809	1.08140	9.46904	18.2800	9.16981	2.38825	1.42608	185.293	5.43921	0.099	-0.216
RB+1	17.8943	1.71750	8.59341	0.09258	7.91428	15.4484	2.47499	32.5110	-0.87756	0.006	-0.007
SR	11.6164	1.85574	9.73009	14.6109	8.68081	0.89852	2.60986	139.830	5.34841	0.066	-0.110
SR+2	18.2430	1.51215	8.90811	13.6536	1.69192	27.8238	-32.1118	-0.01488	39.2691	0.020	-0.036
Y	19.0567	1.24615	6.50783	9.68019	4.81524	18.8903	2.84786	121.353	5.76121	0.158	-0.419
Y +3	18.4202	1.34457	9.75213	12.0631	1.05270	25.1684	-33.4755	-0.01023	40.2513	0.030	-0.063
ZR	19.2273	1.15488	10.1378	10.7877	2.48177	120.126	2.42892	33.3722	5.71886	0.095	-0.273
ZR+4	19.1301	1.16051	10.1098	10.4084	0.98896	20.7214	-0.00004	-3.20442	5.77164	0.022	-0.014
NB	19.3496	1.06626	10.8737	10.5977	3.47687	32.6174	1.64516	120.397	5.65073	0.044	-0.127
NB+3	19.1248	1.07235	18.2989	0.00315	11.0121	10.3385	2.04325	25.9292	-12.4799	0.030	-0.064
NB+5	19.0175	1.06028	10.7591	9.36239	1.09900	0.03765	0.48469	20.9764	4.64045	0.029	-0.063
MO	19.3885	0.97877	11.8308	10.0885	3.75919	31.9738	1.46772	117.932	5.55047	0.021	-0.024
MO+3	19.6761	0.95118	18.0893	-0.00669	11.7086	9.61097	2.50624	24.0356	-12.9813	0.026	-0.057
MO+5	19.6054	0.94029	17.9292	-0.00795	11.3451	8.76715	1.04247	19.3690	-12.9217	0.026	-0.057
MO+6	19.4800	0.94043	17.6328	-0.00723	11.0940	8.29745	0.37154	18.9700	-12.5778	0.024	-0.051
TC	19.3597	0.89356	12.8087	9.27497	3.41372	32.3513	1.99926	107.406	5.41556	0.067	-0.042
RU	19.4316	0.82092	13.7309	8.97737	4.26537	28.2621	1.28720	111.501	5.28192	0.110	-0.055
RU+3	20.8024	0.74711	13.2995	8.36626	3.27542	20.6179	2.21026	-0.14664	1.41087	0.018	-0.037
RU+4	41.5821	0.61466	12.9936	7.99801	2.71276	18.1564	-24.2593	0.43857	6.97025	0.017	-0.036
RH	19.4524	0.75019	14.6845	8.42622	4.50240	26.1564	1.24740	107.780	5.11007	0.130	-0.060
RH+3	25.0958	0.61346	14.1510	7.80244	3.64428	19.0932	-12.5768	0.13532	11.6838	0.011	-0.022
RH+4	41.5236	0.52905	13.8272	7.49419	3.07969	16.9498	-25.9694	0.32686	8.53824	0.013	-0.027
PD	19.5123	0.68583	15.3800	7.95714	5.38330	23.1808	0.81015	65.9295	4.91427	0.139	-0.062
PD+2	19.4652	0.68159	15.5805	7.80880	4.04748	20.9573	0.02216	110.020	4.88510	0.145	-0.063
PD+4	51.1288	0.43734	14.6979	7.03139	3.41607	15.8623	-38.2678	0.26589	11.0241	0.009	-0.019
AG	19.5284	0.62387	16.5811	7.39504	4.99150	22.2282	1.21404	100.226	4.68114	0.124	-0.055
AG+1	19.5416	0.62273	16.4239	7.39663	5.12995	20.5530	0.24053	59.0604	4.66470	0.133	-0.059
AG+2	19.5152	0.62050	16.4852	7.30347	4.32525	19.3673	0.02777	92.9184	4.64695	0.136	-0.059
CD	19.5528	0.56604	17.5717	6.79630	4.47374	21.2907	1.98562	85.2777	4.41158	0.104	-0.046
CD+2	19.5901	0.56389	17.3740	6.83082	4.62594	17.8856	0.03770	76.2909	4.37269	0.121	-0.052
IN	19.5872	0.51510	18.7169	6.29430	4.02722	22.7308	2.51452	88.5675	4.14542	0.072	-0.034
IN+3	19.6698	0.50926	18.1942	6.28098	4.09851	15.4189	0.00365	160.227	4.03396	0.105	-0.045
SN	19.6527	0.46604	19.5108	5.76321	3.86895	24.0627	3.14764	78.1533	3.81227	0.051	-0.026
SN+2	19.7166	0.46027	18.9265	5.66448	3.79775	17.7248	1.86248	42.8086	3.69648	0.075	-0.033
SN+4	19.7914	0.45879	18.9162	5.76682	3.64761	13.3733	-0.	-0.	3.64494	0.088	-0.038
SB	20.0755	5.24328	19.7766	0.41858	4.30389	26.0178	3.44952	70.1646	3.38881	0.039	-0.021
SB+3	19.8617	0.41409	19.5199	5.18292	3.73465	16.8529	1.61027	35.1406	3.27356	0.059	-0.026
SB+5	19.9613	0.41262	19.5889	5.30028	3.24333	11.7603	-0.	-0.	3.20701	0.071	-0.031
TE	20.4608	4.74225	20.0336	0.37041	5.38664	27.3458	3.33079	65.0573	2.78462	0.038	-0.018
I	20.7492	4.27091	20.5640	0.31960	6.86158	27.3186	2.97589	61.5375	1.84739	0.045	-0.020
I -1	20.8307	4.29514	20.4454	0.32402	7.52618	29.8990	3.18616	81.4344	2.00513	0.034	-0.017
XE	21.6679	0.26422	21.0085	3.83526	8.43382	26.2297	2.62265	58.4830	0.26635	0.055	-0.024
CS	22.3163	0.23092	21.1792	3.49464	10.7382	25.1864	1.46163	232.829	-0.70709	0.035	-0.035
CS+1	23.9649	0.20448	21.2204	3.43876	9.76727	23.4941	1.61550	49.7057	-2.56728	0.064	-0.029
BA	27.7489	0.15152	21.3777	3.09817	11.0400	20.6774	2.68186	178.819	-6.85854	0.054	-0.026
BA+2	29.2996	0.14047	21.4669	3.08785	10.9209	20.8818	0.80126	46.8842	-8.48753	0.067	-0.031
LA	33.2109	0.11040	21.7181	2.83641	11.6222	19.3886	3.17239	144.438	-12.7404	0.037	-0.035
LA+3	43.6346	0.07854	21.7192	2.78360	11.7264	18.4930	0.32945	49.2222	-23.4085	0.053	-0.029
CE	29.4100	0.12335	22.2428	2.74837	11.9818	18.3794	3.19259	139.603	-8.84560	0.040	-0.039
CE+3	49.1105	0.06535	22.3499	2.67229	11.8399	17.2040	0.67455	38.1904	-28.9739	0.044	-0.022
CE+4	66.7693	0.04464	21.8563	2.53711	12.2486	16.4477	0.09617	64.4675	-46.9691	0.031	-0.032
PR	22.9220	2.78604	22.2518	0.18015	12.2269	17.6663	2.72431	160.915	-1.13930	0.031	-0.029

Waber (1965). A comparison of these four models has been made by Cromer (1965).

Except for relativistic effects (and the rather trivial effect of electron correlation) the best free atom approximation is the Hartree–Fock (HF) model. HF scattering factors for elements through Kr ($Z=36$) have been computed by a number of persons and their results have been tabulated by Ibers in *International Tables for X-ray Crystallography* (1962). Most of these HF scattering factors were calculated from analytic wave functions.

Mann (1967) has recently made extensive calculations of numerical HF wave functions from which we have computed X-ray scattering factors for all neutral atoms through Lw ($Z=103$) and for most of the chemically significant ions through Lu ($Z=71$). These HF scattering factors were computed from $\sin\theta/\lambda=0$ to 1·50 at intervals of 0·01 Å^{-1} and the detailed results have been tabulated elsewhere (Cromer & Mann, 1967). For convenience in use and for brevity in this publication these scattering factors have been fitted to the analytic function

$$f(\sin\theta/\lambda)=\sum_{i=1}^{4} a_i \exp\left[-b_i \sin^2\theta/\lambda^2\right]+c\,.$$

The coefficients along with the maximum and minimum *percentage* deviations of the analytic fit defined as $E=(f_{\mathrm{HF}}-f_{\mathrm{analytic}})\times 100/f_{\mathrm{HF}}$ are listed in Table 1.

There is some duplication of other work here. The lighter elements are included because analytic expressions for HF scattering factors have not, heretofore, been published and

Table 1 (*cont.*)

ATOM	A(1)	B(1)	A(2)	B(2)	A(3)	B(3)	A(4)	B(4)	C	EMAX	EMIN
PR+3	49.4655	0.06197	22.9705	2.57634	11.8015	16.0371	1.12179	32.3673	-29.3586	0.030	-0.015
PR+4	62.6752	0.04586	22.4952	2.45900	12.4946	15.5713	0.20294	46.5889	-42.8667	0.023	-0.024
ND	23.4069	2.71587	19.7073	0.20950	12.5016	16.9122	2.72850	156.556	1.64038	0.033	-0.047
ND+3	49.4292	0.05936	23.6116	2.48611	11.6190	14.9366	1.68986	28.4515	-29.3493	0.021	-0.011
PM	23.8480	2.65746	17.5535	0.24780	12.7324	16.2463	2.72975	152.682	4.12018	0.035	-0.064
PM+3	49.2699	0.05709	24.2700	2.40059	11.3481	13.9124	2.32869	25.6906	-29.2165	0.017	-0.008
SM	24.2242	2.60993	15.9132	0.29475	12.9238	15.6554	2.72836	149.221	6.19355	0.040	-0.080
SM+3	36.3271	0.07823	24.8502	2.33602	11.3426	13.1872	2.62300	24.3996	-16.1429	0.004	-0.004
EU	24.5148	2.57255	14.8058	0.34930	13.0799	15.1280	2.72477	146.103	7.85731	0.046	-0.094
EU+2	25.6516	2.36073	23.9387	0.13260	10.5738	12.6495	4.05853	25.0026	-3.22358	0.003	-0.004
EU+3	33.2862	0.08350	25.5041	2.26275	11.1494	12.3883	3.13496	22.8351	-13.0748	0.002	-0.002
GD	24.4004	2.47491	14.0308	0.40238	13.1754	14.4670	3.24472	119.738	9.12488	0.052	-0.106
GD+3	29.0290	0.09521	26.1387	2.19696	11.0510	11.7141	3.52244	21.6929	-8.74150	0.002	-0.002
TB	24.3736	2.46637	13.8649	0.47517	13.2510	14.0424	3.24435	117.446	10.2420	0.057	-0.116
TB+3	26.7821	2.13333	25.9463	0.10597	10.9724	11.0974	3.88172	20.7042	-5.58307	0.002	-0.003
DY	24.6193	2.52208	14.2735	0.54556	13.3567	13.8487	2.70316	138.385	11.0290	0.059	-0.122
DY+3	27.3805	2.07832	22.2062	0.12643	10.9975	10.5960	4.10030	19.9671	-1.68516	0.003	-0.005
HO	24.3162	2.52724	14.9012	0.61572	13.3895	13.5041	2.69309	136.246	11.6817	0.061	-0.128
HO+3	27.9956	2.02324	19.9560	0.14275	11.0106	10.1165	4.33205	19.2589	0.70499	0.003	-0.005
ER	23.8201	2.54419	15.8796	0.68445	13.3938	13.1932	2.68190	134.282	12.2062	0.063	-0.133
ER+3	28.5315	1.97796	17.4316	0.17182	11.1113	9.73821	4.43156	18.7294	3.49325	0.003	-0.006
TM	23.1386	2.57320	17.1707	0.74948	13.3703	12.9126	2.66981	132.468	12.6322	0.064	-0.136
TM+3	29.0215	1.93707	15.6168	0.20467	11.2288	9.40342	4.49403	18.2607	5.63812	0.004	-0.008
YB	22.3028	2.61393	18.7202	0.80868	13.3200	12.6590	2.65701	130.783	12.9818	0.064	-0.138
YB+2	29.1313	1.99979	13.5855	0.32335	11.4132	9.59277	4.69659	20.3507	9.17182	0.007	-0.015
YB+3	29.4761	1.89879	14.4357	0.23793	11.3446	9.09408	4.54681	17.8206	7.19600	0.004	-0.008
LU	21.1866	0.88654	20.1760	2.68610	13.0532	12.2746	3.21190	107.128	13.3489	0.067	-0.145
LU+3	29.8480	1.86596	13.6268	0.27623	11.4750	8.82479	4.56009	17.4364	8.48923	0.004	-0.009
HF	24.6725	0.97400	17.2295	2.89038	12.8069	12.2897	3.55970	93.4381	13.7049	0.074	-0.161
TA	28.1757	1.04034	14.4288	3.20784	12.6412	12.5054	3.74436	85.0183	13.9824	0.080	-0.178
W	31.0935	1.07885	12.5273	12.8331	12.3769	3.63298	3.79138	79.7647	14.1842	0.084	-0.191
RE	33.2961	1.09315	12.3497	13.2559	11.2819	4.16736	3.72367	76.6562	14.3239	0.086	-0.199
OS	34.8667	1.08840	11.9524	13.8042	11.1851	4.79179	3.56436	75.1399	14.4097	0.085	-0.201
IR	35.9454	1.06924	11.9980	5.43443	11.2501	14.4983	3.34312	74.7918	14.4449	0.079	-0.192
PT	36.8102	1.04422	13.0747	6.07340	11.3323	15.7018	2.31421	73.8375	14.4526	0.072	-0.178
AU	37.3027	1.00810	14.9306	6.52550	10.3425	16.5100	2.01229	76.9117	14.3992	0.059	-0.150
HG	37.5186	0.96455	17.0353	6.65786	8.51121	16.8438	2.63340	76.7228	14.2911	0.044	-0.113
TL	37.6947	0.92263	19.7195	6.78248	6.38290	19.2435	3.00960	85.9267	14.1800	0.034	-0.092
PB	37.7383	0.87755	21.3394	6.58964	5.17527	21.2437	3.71604	78.8094	14.0203	0.023	-0.063
BI	37.7143	0.83222	22.4542	6.27051	4.84549	24.4693	4.14816	72.1558	13.8301	0.013	-0.037
PO	37.6297	0.78640	23.1323	5.86644	5.59203	27.8678	4.04218	68.1617	13.5991	0.008	-0.012
AT	37.4971	0.74012	23.5635	5.42694	7.15953	29.8350	3.45924	66.3564	13.3183	0.011	-0.006
RN	37.3308	0.69354	23.8933	4.98696	9.02222	30.0338	2.77349	65.5799	12.9796	0.032	-0.015
FR	37.1902	0.65303	24.1306	4.61305	11.5026	29.2597	1.47980	257.965	12.6868	0.031	-0.017
RA	36.9820	0.60394	24.2495	4.17857	11.8719	24.3782	2.72428	200.024	12.1642	0.053	-0.024
AC	36.8705	0.56458	24.7131	3.88776	12.3889	23.1506	3.26501	161.726	11.7484	0.050	-0.023
TH	36.7754	0.52510	25.2506	3.61658	13.0681	22.3410	3.63791	139.164	11.2497	0.046	-0.024
PA	37.1457	0.52020	25.2998	3.66300	13.7846	20.6539	3.29611	150.973	11.4561	0.024	-0.023
U	37.2808	0.50239	25.6563	3.58562	14.3501	19.6342	3.30732	146.633	11.3864	0.026	-0.024
NP	37.3968	0.48676	26.0671	3.52325	14.8366	18.7419	3.31586	142.798	11.3632	0.027	-0.026
PU	37.6407	0.47976	26.5603	3.57178	15.4492	17.9814	2.79814	165.232	11.5358	0.022	-0.022
AM	37.6909	0.46617	27.1436	3.52195	15.7842	17.3069	2.79600	161.931	11.5685	0.023	-0.029
CM	37.5543	0.44932	27.6657	3.38713	15.8858	16.6498	3.32758	133.547	11.5431	0.031	-0.037
BK	37.5273	0.43930	28.3202	3.35014	16.1181	16.1000	3.32793	131.027	11.6823	0.031	-0.045
CF	37.6111	0.43255	29.2465	3.39285	16.4566	15.6791	2.78216	153.766	11.8853	0.027	-0.051
ES	37.4979	0.42353	30.0495	3.35234	16.5881	15.2381	2.77596	151.474	12.0698	0.029	-0.056
FM	37.3380	0.41562	30.8936	3.31193	16.6818	14.8362	2.76929	149.344	12.2983	0.031	-0.061
MD	37.1301	0.40883	31.7721	3.27132	16.7422	14.4683	2.76232	147.353	12.5741	0.033	-0.065
NO	36.8731	0.40324	32.6784	3.23045	16.7732	14.1302	2.75513	145.481	12.9008	0.034	-0.068
LW	36.3813	0.40165	33.1999	3.13608	16.6469	13.7255	3.31406	119.377	13.4313	0.037	-0.073

it is convenient to have a complete tabulation of HF scattering factors in one place. Also, because we used numerical wave functions, many of these results should be more accurate than previous calculations, although the differences between these scattering factors and those computed from analytic wave functions are not large (about 0·02 electron at most).

The importance of relativistic effects can be judged by inspecting Fig. 7 in Cromer (1965) where the HFS and DS scattering factors are compared. These scattering factors are essentially identical up to $Z \sim 40$ and do not differ greatly until $Z > \sim 55$. Thus, HF scattering factors are probably the best to use for atoms lighter than Cs ($Z = 55$). For heavier elements, HF scattering factors are too small because of the neglect of the relativistic contraction of the atom, and it is now believed that the DS scattering factors (Cromer & Waber, 1965) are in error by being too large. Kohn & Sham (1965) and Cowan, Larson, Liberman. Mann & Waber (1966) have given evidence that the Slater (1951) $\varrho^{1/3}$ exchange coefficient should be $\frac{2}{3}$ as great as that given by Slater. This change in coefficient has the effect of lowering the exchange energy, expanding the atom and, therefore, decreasing the scattering factor. Thus, scattering factors calculated from a relativistic HF model should lie between the HF and DS scattering factors for the heavier elements. Until relativistic HF scattering factors are available, however, the HF or DS scattering factors should be about equally useful for heavy elements.

A deck of cards with the analytic coefficients may be obtained from the authors.

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Extinction in a lithium fluoride sphere.

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Intensity measurements have been made on a sphere of lithium fluoride with Mo $K\alpha$ and Cu $K\alpha$ radiations. The sphere, of radius $2{\cdot}99 \pm 0{\cdot}03 \times 10^{-2}$ cm, was ground from a cleavage fragment of a synthetic crystal obtained from the Harshaw Company. The $\mu_0 R$ value was 0·11 for Mo $K\alpha$ and 0·96 for Cu $K\alpha$.

According to recent theory (Zachariasen, 1967) the observed structure factors, F_σ, are related to the calculated values, F_c, as follows (for unpolarized incident radiation):

$$\begin{aligned} F_\sigma &= CF_c y^{1/2}, \\ y &= (y_1 + K^2 y_K)/(1+K^2), \\ y_K &= (1+2X_K)^{-1/2}, \\ x_K &= r^* K^2 Q_0 \lambda^{-1} \bar{T}, \\ r^* &= r[1+(r/\lambda g)^2]^{-1/2}, \\ \bar{T} &= AdA^*/d\mu_0 . \end{aligned} \tag{1}$$

C is the scale factor while $K=1$ for the normal and $K=|\cos 2\theta|$ for the parallel component of polarization. The other symbols have their usual meanings.

It is sometimes convenient to use a simplified, but approximate form of equation (1), namely

$$\begin{aligned} y &= (1+2x)^{-1/2} \\ x &= r^* Q_0 \lambda^{-1} \bar{T} p_2/p_1 \end{aligned} \tag{2}$$

where

$$p_2/p_1 = (1+\cos^4 2\theta)/(1+\cos^2 2\theta) .$$

The intensities of all reflections with $2\theta < 90°$ were measured with molybdenum radiation, only the reflections ($HK0$) with $2\theta < 120°$ with copper radiation.

The stationary counter-crystal procedure was used with Zr or Ni filter. The counting rate was kept low by attenuating the beam with a set of carefully calibrated Ni foils. A balanced Y–Zr filter was used for background correction for the molybdenum data. In the copper case the background was measured at $2\theta \pm 2°$, and the mean value taken to be the background under the peak.

The intensities varied very little from plane to plane of a given form with an indicated accuracy of one per cent for the mean value. The F_σ values are given in Tables 1 and 2 (adjusted to ultimate C values of unity).

Table 1. *Structure factors.* Mo $K\alpha$

HKL	F_c	$F_c y^{\frac{1}{2}}$	F_σ
111	19·9	18·9	19·0
200	30·0	27·3	27·1
220	21·9	21·0	21·0
311	9·59	9·52	9·31
222	17·0	16·7	16·7
400	13·8	13·6	13·9
331	6·31	6·30	6·18
420	11·5	11·4	11·4
422	9·86	9·81	9·80
511	4·87	4·86	4·95
333	4·87	4·86	5·07
440	7·62	7·60	7·59
531	4·10	4·10	4·09
442	6·83	6·81	6·87
600	6·83	6·81	6·81
620	6·17	6·16	6·14
533	3·59	3·59	3·58
622	5·63	5·62	5·60
444	5·16	5·15	5·06
711	3·22	3·22	3·22
551	3·22	3·22	3·24
640	4·76	4·75	4·69
642	4·41	4·40	4·32
731	2·90	2·90	2·91
553	2·90	2·90	2·87

Table 1 *(cont.)*

Table 2. *Structure factors.* Cu $K\alpha$

HKO	F_c	$F_c y^{\frac{1}{2}}$	F_σ
200	30·0	23·9	23·7
220	21·9	19·4	19·7
400	13·8	13·1	13·3
420	11·5	11·2	11·0

In the interpretation of the data the f curves of Cromer & Waber (1964) for Li^+ and F^- were adopted, and the very small anomalous dispersion corrections were neglected.

The closest agreement between the sets F_σ and $CF_c y^{1/2}$ for the molybdenum data was sought as C, B_{Li}, B_F, and r^*_{Mo} were varied. For $r^*_{Mo} = 2{\cdot}2 \times 10^{-6}$ cm one finds $B_{Li} =$