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A Study of the Compton Scattering of X-rays. II.
Li, Li$^+$, Be, Na, Na$^+$, Al$^+$, Al^{+3}, K$^+$, Cl$^-$, Ca, Ca$^+$ and Ca^{+2}

BY A. J. FREEMAN

Materials Research Laboratory, Ordnance Materials Research Office, Watertown, Massachusetts
and
Solid State and Molecular Theory Group Massachusetts Institute of Technology, Cambridge, Massachusetts, U.S.A.

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Following the methods of a previous paper, the Compton incoherent scattering functions for Li, Li$^+$, Be, Na, Na$^+$, Al$^+$, Al^{+3}, K$^+$, Cl$^-$, Ca, Ca$^+$ and Ca^{+2} have been calculated using Hartree–Fock self-consistent-field wave functions. As was found earlier, the exchange terms in the Waller–Hartree expression are of considerable importance for obtaining accurate values of the incoherent scattering intensities. Comparison is made with earlier calculations and with the experiments of Laval on KCl, and Cribier on CaF$_2$.

1

This paper represents a continuation of an investigation aimed at determining highly accurate Compton incoherent scattering functions for those atoms for which Hartree–Fock self-consistent-field wave functions are known. In earlier publications we reported results found for aluminum (Freeman, 1959*a*), Ne, Cu$^+$, Cu and Zn^{+2} (Freeman, 1959*b*) and N, N$^-$, O$^-$, O, O$^+$, O^{+2}, O^{+3}, F, F$^-$, Si^{+4}, Si^{+3}, Si and Ge (Freeman, 1959*c*). In this work, and in the work of Keating & Vineyard (1956) on carbon, and Milberg & Brailsford (1958) on boron, carbon and oxygen, it was found that (*a*) inclusion of the exchange terms in the Waller & Hartree (1929) expression resulted in marked decreases from previously available data (Compton & Allison, 1935) and (*b*) these values were in good agreement with the available experimental results.

Using the methods outlined earlier (Freeman, 1959*b*) for determining the necessary matrix elements, incoherent scattering intensities have been calculated for some other atoms and ions (as listed in the title) using numerical Hartree-Fock wave functions.* For each of these the wave functions used were those calculated for the appropriate electronic ground state. The results are given below.

2

The formulae for the scattering functions for the atoms and ions discussed in this paper are given below for the configuration and ground state listed. The notation used follows that given earlier (Freeman, 1959*b*).

1) Li$^+$: $1s^2$, ^1S
$\mathscr{F}(\mathrm{Li}^+)=2f_{1s}^2$
2) Li: $1s^22s$, ^2S
$\mathscr{F}(\mathrm{Li})=2f_{1s}^2+f_{2s}^2+2f_{1s,2s}^2$
3) Be: $1s^22s^2$, ^1S
$\mathscr{F}(\mathrm{Be})=2f_{1s}^2+2f_{2s}^2+4f_{1s,2s}^2$
4) Na$^+$: $1s^22s^22p^6$, ^1S
$\mathscr{F}(\mathrm{Na}^+)=2f_{1s}^2+2f_{2s}^2+6f_{2p}^2+4f_{1s,2s}^2+12f_{1s,2p}^2$
$+12f_{2s,2p}^2+12f_{2p,2p}^2$
5) Na: $1s^22s^22p^63s$, ^2S
$\mathscr{F}(\mathrm{Na})=\mathscr{F}(\mathrm{Na}^+)+f_{3s}^2+2f_{1s,3s}^2+2f_{2s,3s}^2+6f_{2p,3s}^2$
6) Al^{+3}: $1s^22s^22p^6$, ^1S
$\mathscr{F}(\mathrm{Al}^{+3})=\mathscr{F}(\mathrm{Na}^+)$*
7) Al$^+$: $1s^22s^22p^63s^2$, ^1S
$\mathscr{F}(\mathrm{Al}^+)=\mathscr{F}(\mathrm{Al}^{+3})+2f_{3s}^2+4f_{1s,3s}^2+4f_{2s,3s}^2+12f_{2p,3s}^2$
8) K$^+$: $1s^22s^22p^63s^23p^6$, ^1S
$\mathscr{F}(\mathrm{K}^+)=\mathscr{F}(\mathrm{Al}^+)+6f_{3p}^2+12(f_{1s,3p}^2+f_{2s,3p}^2+f_{3s,3p}^2)$
$+12f_{3p,3p}^2+12f_{2p,3p}^2(0)+24f_{2p,3p}^2(2)$
9) Cl$^-$: $1s^22s^22p^63s^23p^6$, ^1S
$\mathscr{F}(\mathrm{Cl}^-)=\mathscr{F}(\mathrm{K}^+)$
10) Ca^{++}: $1s^22s^22p^63s^23p^6$, ^1S
$\mathscr{F}(\mathrm{Ca}^{++})=\mathscr{F}(\mathrm{K}^+)$
11) Ca$^+$: $1s^22s^22p^63s^23p^64s$, ^2S
$\mathscr{F}(\mathrm{Ca}^+)=\mathscr{F}(\mathrm{Ca}^{++})+f_{4s}^2+2(f_{1s,4s}^2+f_{2s,4s}^2+f_{3s,4s}^2)$
$+6(f_{4s,2p}^2+f_{4s,3p}^2)$
12) Ca: $1s^22s^22p^63s^23p^64s^2$, ^1S
$\mathscr{F}(\mathrm{Ca})=\mathscr{F}(\mathrm{Ca}^{++})+2f_{4s}^2+4(f_{1s,4s}^2+f_{2s,4s}^2+f_{3s,4s}^2)$
$+12(f_{4s,2p}^2+f_{4s,3p}^2)$

In these expressions, $\mathscr{F}=\Sigma_i\Sigma_j|f_{ij}|^2$ and the intensity (omitting the Breit–Dirac factor) is given by

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* References for these Hartree–Fock wave functions are as follows:
Li$^+$ & Li: Fock & Petrashen (1935)
Be: Hartree & Hartree (1935)
Na$^+$ & Na: Hartree & Hartree (1948)
Al^{+3} & Al$^+$: Froese (1957)
K$^+$ & Cl$^-$: Howland (1958)
Ca^{++}, Ca$^+$, Ca: Hartree & Hartree (1938)

* $\mathscr{F}(\mathrm{Al}^{+3})=\mathscr{F}(\mathrm{Na}^+)$ means: the formula for Al^{+3} is the same as the formula for Na$^+$; the integrals are not the same.

Table 1. *Calculation of the X-ray incoherent scattering functions for* Li$^+$, Li *and* Be

	Li						Li$^+$	
$\sin\theta/\lambda$	f_{1s}	f_{2s}	$f_{1s,2s}$	$\Sigma\|f_{ii}\|^2$	$\mathscr{F}$	$3-\mathscr{F}$	$\mathscr{F}$	$2-\mathscr{F}$
0·0	1·0000	1·0000	0·0000	3·000	3·000	0·000	2·000	0·000
0·1	0·9679	0·2803	0·0191	1·952	1·953	1·047	1·874	0·126
0·2	0·8810	−0·0204	0·0554	1·553	1·559	1·441	1·552	0·448
0·3	0·7612	−0·0099	0·0789	1·159	1·171	1·829	1·159	0·841
0·4	0·6322	0·0057	0·0830	0·799	0·813	2·187	0·799	1·201
0·5	0·5112	0·0099	0·0752	0·523	0·534	2·466	0·523	1·477
0·6	0·4067	0·0095	0·0631	0·331	0·339	2·661	0·331	1·669
0·7	0·3209	0·0084	0·0511	0·206	0·211	2·789	0·206	1·794
0·8	0·2526	0·0061	0·0407	0·128	0·131	2·869	0·128	1·872
0·9	0·1992	0·0059	0·0322	0·079	0·081	2·919	0·079	1·921
1·0	0·1578	0·0032	0·0256	0·050	0·051	2·949	0·050	1·950
1·1	0·1258	0·0050	0·0204	0·032	0·033	2·967	0·032	1·968

Be

$\sin\theta/\lambda$	f_{1s}	f_{2s}	$f_{1s,2s}$	$\Sigma\|f_{ii}\|^2$	$\mathscr{F}$	$4-\mathscr{F}$
0·0	1·0000	1·0000	0·0000	4·000	4·000	0·000
0·1	0·9828	0·5494	0·0114	2·535	2·535	1·465
0·2	0·9349	0·0950	0·0385	1·766	1·772	2·228
0·3	0·8623	−0·0163	0·0670	1·488	1·506	2·494
0·4	0·7746	−0·0146	0·0865	1·200	1·230	2·770
0·5	0·6810	0·0001	0·0944	0·928	0·964	3·036
0·6	0·5885	0·0087	0·0929	0·693	0·727	3·273
0·7	0·5024	0·0126	0·0858	0·505	0·535	3·465
0·9	0·3579	0·0115	0·0660	0·256	0·274	3·726
1·1	0·2520	0·0076	0·0478	0·127	0·136	3·864

Table 2. *Calculation of the X-ray incoherent scattering functions for* Na$^+$ *and* Na

Na$^+$

$\sin\theta/\lambda$	f_{1s}	f_{2s}	f_{2p}	$f_{1s,2s}$	$f_{1s,2p}$	$f_{2s,2p}$	$f_{2p,2p}$	$\Sigma\|f_{ii}\|^2$	$\mathscr{F}$	$10-\mathscr{F}$
0·0	1·0000	1·0000	1·0000	0·0000	0·000	0·000	0·000	10·000	10·000	0·000
0·1	0·9980	0·9478	0·9423	0·0023	0·019	−0·162	0·019	9·121	9·440	0·560
0·2	0·9919	0·8087	0·7950	0·0073	0·036	−0·2814	0·078	7·141	8·107	1·893
0·3	0·9820	0·6251	0·6128	0·0151	0·0529	−0·3365	0·134	5·179	6·572	3·428
0·4	0·9684	0·4399	0·4417	0·0253	0·0673	−0·3349	0·170	3·780	5·183	4·817
0·5	0·9512	0·2821	0·3033	0·0370	0·0793	−0·2975	0·1887	2·948	4·091	5·909
0·6	0·9309	0·1628	0·2006	0·0496	0·0887	−0·2444	0·1879	2·451	3·272	6·728
0·7	0·9078	0·0809	0·1285	0·0624	0·0956	−0·1895	0·1754	2·130	2·686	7·314
0·9	0·8547	+0·0010	0·0467	0·0859	0·1017	−0·0986	0·1381	1·703	1·973	8·027
1·1	0·7946	−0·0163	0·0121	0·1041	0·1005	−0·0410	0·1007	1·385	1·570	8·430

Na

$\sin\theta/\lambda$	f_{3s}	$f_{1s,3s}$	$f_{2s,3s}$	$f_{3s,2p}$	$\Sigma\|f_{ii}\|^2$	$\mathscr{F}$	$11-\mathscr{F}$
0·0	1·0000	+0·000	+0·0000	+0·0000	11·000	11·000	0·000
0·1	+0·2166	0·000	0·0210	+0·0366	9·168	9·496	1·504
0·2	−0·0327	0·0007	0·0568	+0·0234	7·142	8·117	2·883
0·3	−0·0052	0·0018	0·0727	−0·0099	5·179	6·583	4·417
0·4	+0·0070	0·0032	0·0657	−0·0317	3·780	5·198	5·802
0·5	0·0086	0·0048	0·0482	−0·0384	2·948	4·105	6·895
0·6	0·0054	0·0066	0·0304	−0·0360	2·451	3·282	7·718
0·7	0·0038	0·0085	0·0164	−0·0295	2·130	2·692	8·308
0·9	0·0010	0·0120	+0·0015	−0·0164	1·703	1·975	9·025
1·1	0·0021	0·0148	−0·0023	−0·0072	1·385	1·571	9·429

$I_{\text{inc.}} = Z - \mathscr{F}$. Z is the number of electrons in the atom or ion.

3

The calculated values of f_{ij}, $\mathscr{F}$, and $Z-\mathscr{F}$ are listed in the Tables, for each atom and ion, as a function of $\sin\theta/\lambda$ in Å^{-1} units. In order to bring out the importance of the exchange contribution the values of the diagonal terms $\Sigma_i|f_{ii}|^2$ are also included. For Al^{+3} and Al$^+$, we list only $\Sigma_i|f_{ii}|^2$ and $\mathscr{F}$ since the f_{ij} used in the calculations were those reported earlier for aluminum (Freeman, 1959*a*). In the Figures, graphical comparison is made with the values of the scattering intensities obtained earlier by James & Brindley (1931), referred to as J&B in what follows.

For Li$^+$, Li, and Be the difference between our values

Table 3. *X-ray incoherent scattering functions for* Al^+ *and* Al^{+3}

Al^+

$\sin\theta/\lambda$	$\Sigma\vert f_{ii}\vert^2$	$\mathcal{F}$	$12-\mathcal{F}$
0·0	12·00	12·00	0·00
0·1	10·21	10·43	1·57
0·2	8·19	8·90	3·10
0·3	6·55	7·76	4·24
0·4	5·08	6·58	5·42
0·5	3·96	5·49	6·51
0·6	3·20	4·56	7·44
0·7	2·70	3·79	8·21
0·9	2·11	2·71	9·29
1·1	1·74	2·08	9·92

Al^{+3}

$\sin\theta/\lambda$	$\Sigma\vert f_{ii}\vert$	$\mathcal{F}$	$10-\mathcal{F}$
0·0	10·00	10·00	0·00
0·1	9·49	9·69	0·31
0·2	8·17	8·85	1·15
0·3	6·55	7·72	2·28
0·4	5·08	6·53	3·47
0·5	3·96	5·43	4·57
0·6	3·20	4·49	5·51
0·7	2·70	3·73	6·27
0·9	2·11	2·68	7·32
1·1	1·74	2·06	7·94

and those of J&B is small. This is expected since there are few exchange terms for these elements of low atomic number. With increasing atomic number the contribution of the exchange terms becomes much more important, and this is shown in the large differences between our values and those of J&B. To illustrate these large differences we have plotted in Figs. 4 and 5 our results for K^+ and Cl^- calculated with and without the exchange terms in the Waller–Hartree expression. As is shown in these Figures,

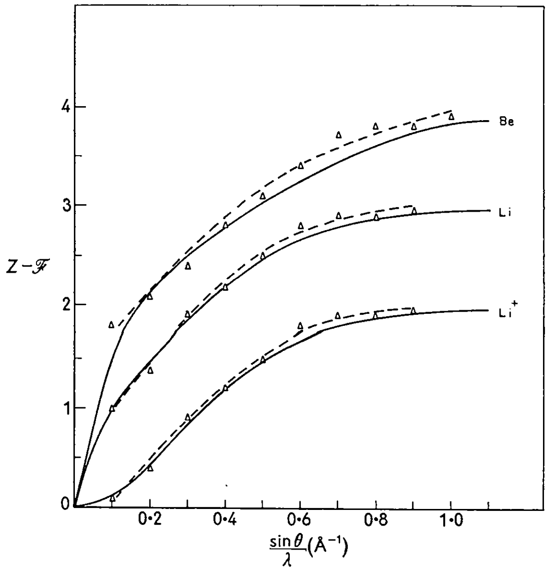

Fig. 1. Incoherent scattering functions for Li^+, Li and Be: the solid curves are our data and ---- △ ---- denotes the J&B values.

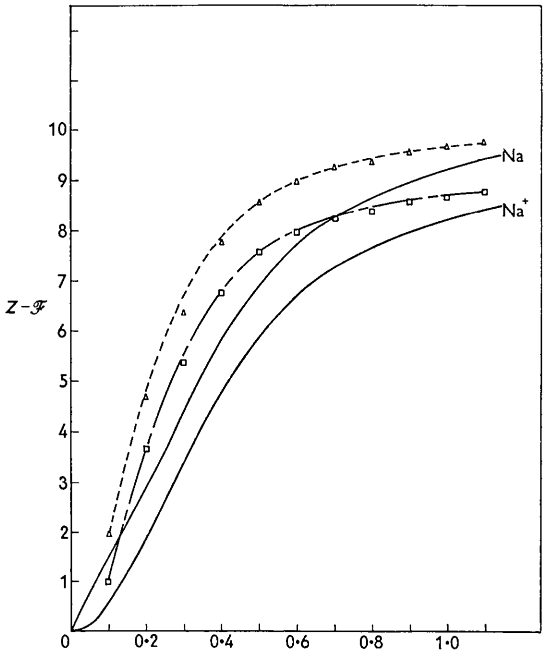

Fig. 2. Incoherent scattering functions for Na^+ and Na: The solid curves are our data, ---- △ ---- denotes the J&B values for Na and ——□—— denotes the J&B values for Na^+.

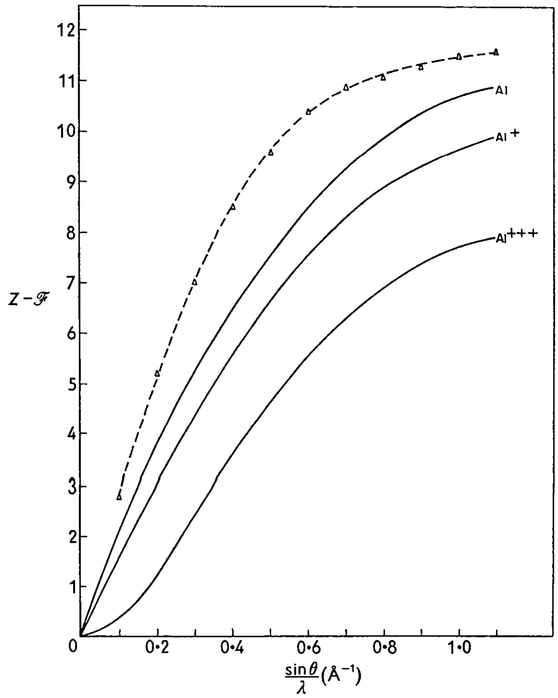

Fig. 3. Incoherent scattering functions for Al, Al^+, Al^{+3}: The solid curves are our data compared with J&B values for aluminum, denoted by ---- △ ----, the Al values were taken from an earlier publication (Freeman, 1959*a*).

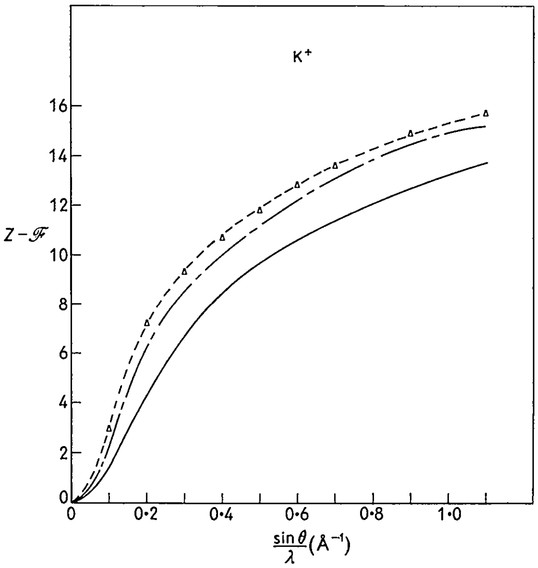

Fig. 4. Incoherent scattering function for K$^+$: The solid curve is our data calculated from the complete Waller–Hartree expression, the long dashed curve is our data with the exchange terms omitted, and ---- △ ---- denotes the J&B values for K$^+$.

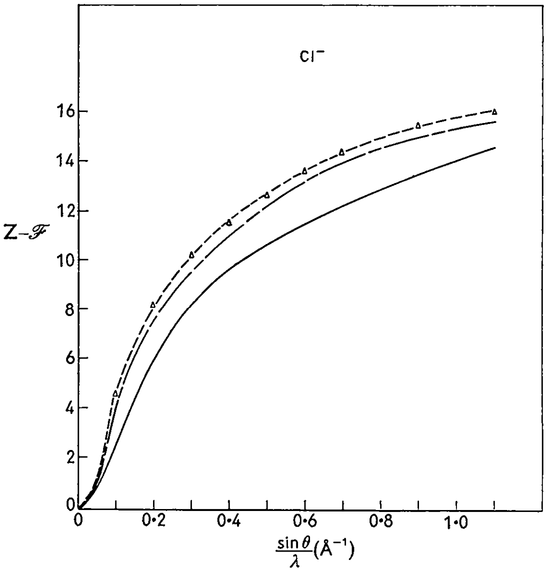

Fig. 5. Incoherent scattering function for Cl$^-$: The solid curve is our data calculated from the complete Waller–Hartree theory, the long dashed curve is our data with the exchange terms omitted, and ---- △ ---- denotes the J&B values for Cl$^-$.

these exchange terms account for almost all the deviations from the J&B data. The remaining source of disagreement arises from some other approximations in the J&B procedures. These were discussed earlier (Freeman, 1959*b*). These comparisons are most clearly shown in Table 7 where we have listed both the absolute and percentage differences of the J&B values from our data. The large differences tabulated for K$^+$, Cl$^-$, and Ca^{++} were also found earlier (Freeman, 1959*c*) for the higher atomic number elements, pointing up the inadequacy of those calculations in which exchange is neglected.

4

Although there have been very few experimental determinations of the Compton incoherent intensity to date, such data is in fact available for some of the atoms listed in this paper. In particular comparison

Table 4. *Calculation of the X-ray incoherent scattering function for* K$^+$

K$^+$

$\sin\theta/\lambda$	f_{1s}	f_{2s}	f_{2p}	f_{3s}	f_{3p}	$f_{2p,2p}$	$f_{3p,3p}$	$f_{1s,2p}$	$f_{2s,2p}$	$f_{3s,2p}$
0·0	1·0000	1·0000	1·0000	1·0000	1·0000	0·000	0·0000	0·0000	0·0000	0·0000
0·1	0·9994	0·9870	0·9889	0·8700	0·8382	0·013	0·0630	0·0128	−0·077	0·0197
0·2	0·9974	0·9494	0·9568	0·5704	0·4960	0·015	0·1700	0·0256	−0·1528	0·0322
0·3	0·9942	0·8898	0·9059	0·2710	0·2017	0·030	0·2207	0·0385	−0·2177	0·0346
0·4	0·9896	0·8130	0·8401	+0·0742	+0·0403	0·061	0·1973	0·0506	−0·2707	0·0256
0·5	0·9838	0·7242	0·7640	−0·0141	−0·0170	0·0886	0·1406	0·0620	−0·3093	+0·0087
0·6	0·9768	0·6290	0·6821	−0·0322	−0·0212	0·1147	0·0833	0·0724	−0·3336	−0·0125
0·7	0·9686	0·5328	0·5984	−0·0190	−0·0075	0·1390	0·0411	0·0821	−0·3440	−0·0339
0·9	0·9490	0·3532	0·4396	+0·0174	+0·0184	0·1784	+0·0020	0·0970	−0·3308	−0·0662
1·1	0·9252	0·2082	0·3053	+0·0297	+0·0262	0·1987	−0·0040	0·1133	−0·2868	−0·0779

$\sin\theta/\lambda$	$f_{1s,3p}$	$f_{2s,3p}$	$f_{3s,3p}$	$f_{2p,3p}(0)$	$f_{2p,3p}(2)$	$f_{1s,2s}$	$f_{1s,3s}$	$f_{2s,3s}$	$\Sigma\lvert f_{ii}\rvert^2$	$\mathcal{F}$	$18-\mathcal{F}$
0·0	0·0000	0·0000	0·0000	0·0000	0·0000	0·0000	0·0000	0·0000	18·00	18·00	0·00
0·1	0·0035	0·0215	−0·2605	0·0079	−0·008	0·0006	0·0002	0·0081	15·59	16·50	1·50
0·2	0·0066	0·0367	−0·3655	0·0291	−0·0099	0·0024	0·0006	0·0303	11·76	13·70	4·30
0·3	0·0100	0·0423	−0·3132	0·0578	−0·0206	0·0053	0·0014	0·0604	9·47	11·34	6·66
0·4	0·0132	0·0374	−0·1968	0·0868	−0·0286	0·0094	0·0025	0·0913	8·05	9·59	8·41
0·5	0·0159	0·0242	−0·0921	0·1104	−0·0318	0·0144	0·0039	0·1165	6·82	8·35	9·65
0·6	0·0191	+0·0062	−0·0267	0·1256	−0·0302	0·0203	0·0055	0·1323	5·74	7·43	10·57
0·7	0·0218	−0·0128	+0·0042	0·1316	−0·0236	0·0269	0·0074	0·1375	4·85	6·67	11·33
0·9	0·0267	−0·0437	0·0100	0·1217	−0·0029	0·0419	0·0116	0·1217	3·59	5·35	12·65
1·1	0·0305	−0·0579	−0·0042	0·0965	+0·0181	0·0581	0·0164	0·0875	2·84	4·27	13·73

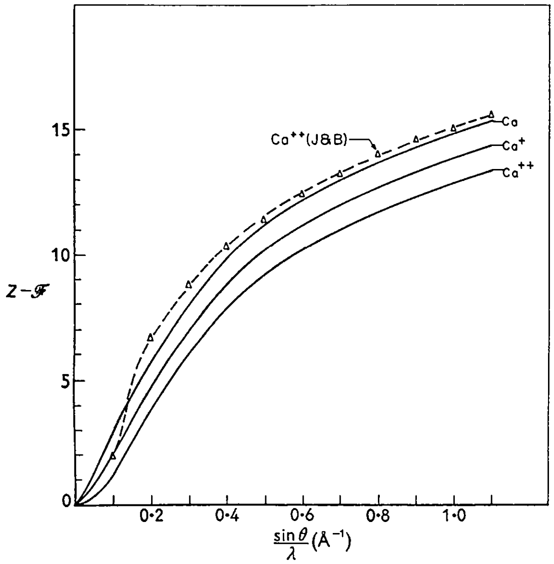

Fig. 6. Incoherent scattering functions for Ca^{++}, Ca$^+$ and Ca: The solid curves are our data and ---- △ ---- denotes the J&B values for Ca^{++}.

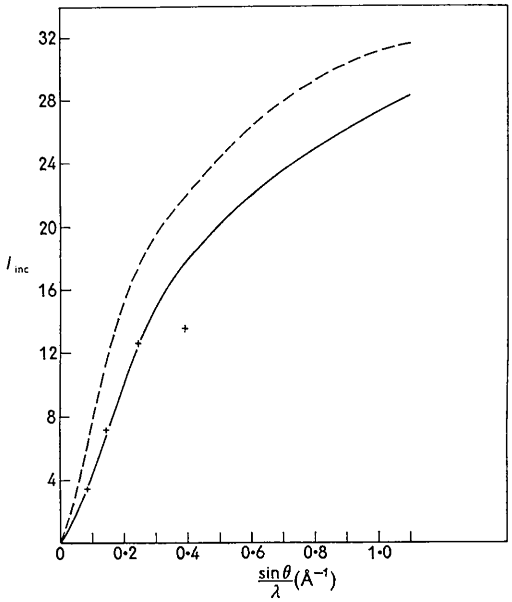

Fig. 7. Incoherent scattering intensity for KCl. The solid curve is our data and the dashed curve represents the values of J&B. The crosses are the experimental values of Laval. (The theoretical curves are plotted without the Breit–Dirac factor.)

can be made with Laval's (1942) measurements on KCl and Cribier's (1958) measurements on CaF_2.

For KCl the comparison with our theoretical values is shown in Fig. 7 where we have also included the J&B values as listed in Compton & Allison (1935) for K$^+$ and Cl$^-$. (The Breit–Dirac factor was omitted from the two theoretical curves in Fig. 7 as it would have little effect at the low $\sin\theta/\lambda$ values at which the experiments were carried out.) It is evident that the J&B values are in poor agreement with Laval's (1942) data, the error being between 45–75 %, whereas (except for the highest experimental point) our present calculations agree extremely well with the experimental results.

The inconsistency of Laval's data at $\sin\theta/\lambda = 0{\cdot}4$ is hard to explain since Laval has given no estimate of his experimental error. The excellent agreement of our values with the rest of his data may be somewhat fortuitous, considering the difficulty of obtaining precise experimental values of the incoherent intensity. Also to be considered is the somewhat less favorable

Table 5. *Calculation of the X-ray incoherent scattering function for* Cl$^-$

Cl$^-$

$\sin\theta/\lambda$	f_{1s}	f_{2s}	f_{2p}	f_{3s}	f_{3p}	$f_{2p,2p}$	$f_{3p,3p}$	$f_{1s,2p}$	$f_{2s,2p}$	$f_{3s,2p}$
0·0	1·0000	1·0000	1·0000	1·0000	1·0000	0·000	0·0000	0·0000	0·0000	0·0000
0·1	0·9992	0·9832	0·9851	0·8022	0·6990	0·017	0·1104	0·014	−0·0904	0·0218
0·2	0·9968	0·9342	0·9421	0·4160	0·2705	0·018	0·2017	0·0284	−0·1739	0·0343
0·3	0·9926	0·8584	0·8755	+0·1251	+0·0508	0·045	0·1802	0·0419	−0·2439	0·0322
0·4	0·9870	0·7630	0·7919	−0·0048	−0·0152	0·0781	0·1160	0·0547	−0·2962	+0·0173
0·5	0·9796	0·6562	0·6983	−0·0312	−0·0175	0·1087	0·0601	0·0669	−0·3294	−0·0052
0·6	0·9710	0·5464	0·6017	−0·0168	−0·0037	0·1387	0·0235	0·0779	−0·3440	−0·0288
0·7	0·9608	0·4398	0·5076	+0·0036	+0·0088	0·1626	+0·0050	0·0880	−0·3423	−0·0482
0·9	0·9364	0·2564	0·3415	0·0239	0·0180	0·1937	−0·0030	0·1046	−0·3038	−0·0689
1·1	0·9074	0·1251	0·2153	0·0213	0·0157	0·1999	−0·0001	0·1164	−0·2408	−0·0679

$\sin\theta/\lambda$	$f_{1s,3p}$	$f_{2s,3p}$	$f_{3s,3p}$	$f_{2p,3p}(0)$	$f_{2p,3p}(2)$	$f_{1s,2s}$	$f_{1s,3s}$	$f_{2s,3s}$	$\Sigma\lvert f_{ii}\rvert^2$	$\mathscr{F}$	$18-\mathscr{F}$
0·0	0·0000	0·0000	0·0000	0·0000	0·0000	0·0000	0·0000	0·0000	18·00	18·00	0·00
0·1	0·0028	0·0184	−0·3010	0·0092	−0·0008	0·0007	0·0002	0·0099	14·12	15·32	2·68
0·2	0·0059	0·0305	−0·3301	0·0329	−0·0125	0·0030	0·0007	0·0359	10·34	12·06	5·94
0·3	0·0090	0·0305	−0·2078	0·0620	−0·0212	0·0066	0·0016	0·0689	8·50	9·86	8·14
0·4	0·0118	0·0208	−0·0891	0·0874	−0·0256	0·0115	0·0029	0·0988	7·11	8·45	9·55
0·5	0·0142	+0·0045	−0·0208	0·1036	−0·0244	0·0176	0·0044	0·1185	5·90	7·46	10·54
0·6	0·0166	−0·0135	+0·0062	0·1094	−0·0188	0·0247	0·0062	0·1254	4·89	6·62	11·38
0·7	0·0191	−0·0291	0·0107	0·1065	−0·0093	0·0326	0·0082	0·1208	4·10	5·84	12·16
0·9	0·0232	−0·0471	−0·0010	0·0852	+0·0114	0·0500	0·0128	0·0901	3·04	4·50	13·50
1·1	0·0260	−0·0488	−0·0100	0·0588	+0·0264	0·0681	0·0177	0·0528	2·44	3·48	14·52

Table 6. *Calculation of the X-ray incoherent scattering function for* Ca^{++}, Ca^{+} *and* Ca

Ca^{++}

$\sin\theta/\lambda$	f_{1s}	f_{2s}	f_{2p}	f_{3s}	f_{3p}	$f_{1s,2s}$	$f_{1s,2p}$	$f_{2s,2p}$	$f_{2p,2p}$	$f_{1s,3s}$
0·0	1·0000	1·0000	1·0000	1·0000	1·0000	0·0000	0·0000	0·0000	0·000	0·0000
0·1	0·9994	0·9886	0·9903	0·8921	0·8717	0·0008	0·0124	−0·0738	0·000	0·0000
0·2	0·9976	0·9551	0·9621	0·6304	0·5773	0·0025	0·0249	−0·1439	0·02	0·0005
0·3	0·9947	0·9019	0·9172	0·3440	0·2854	0·0051	0·0371	−0·2063	0·034	0·0013
0·4	0·9906	0·8326	0·8585	0·1291	0·0924	0·0088	0·0486	−0·2585	0·056	0·0023
0·5	0·9853	0·7514	0·7898	0·0118	0·0017	0·0134	0·0599	−0·2986	0·080	0·0036
0·6	0·9790	0·6633	0·7145	−0·0294	−0·0229	0·0188	0·0704	−0·3260	0·1043	0·0051
0·7	0·9716	0·5724	0·6364	−0·0280	−0·0167	0·0250	0·0803	−0·3409	0·1284	0·0069
0·9	0·9538	0·3979	0·4837	+0·0085	+0·0127	0·0389	0·0977	−0·3380	0·1692	0·0110
1·1	0·9321	0·2501	0·3492	+0·0293	+0·0272	0·0542	0·1113	−0·3035	0·1936	0·0157

$\sin\theta/\lambda$	$f_{2s,3s}$	$f_{3s,2p}$	$f_{1s,3p}$	$f_{2s,3p}$	$f_{3s,3p}$	$f_{3p,3p}$	$f_{2p,3p}(0)$	$f_{2p,3p}(2)$	$\Sigma\|f_{it}\|^2$	$\mathscr{F}$	$18-\mathscr{F}$
0·0	0·0000	0·0000	0·0000	0·0000	0·0000	0·0000	0·0000	0·000	18·00	18·00	0·00
0·1	0·0077	0·0180	0·0035	0·0219	−0·2405	0·0493	0·0073	−0·007	16·02	16·79	1·21
0·2	0·0281	0·0307	0·0068	0·0385	−0·3618	0·1495	0·0268	−0·012	12·44	14·31	3·69
0·3	0·0565	0·0345	0·0101	0·0464	−0·3432	0·2157	0·0539	−0·019	9·95	11·99	6·01
0·4	0·0869	0·0285	0·0134	0·0442	−0·2455	0·2176	0·0829	−0·029	8·46	10·18	7·82
0·5	0·1136	0·0141	0·0165	0·0335	−0·1379	0·1747	0·1083	−0·033	7·26	8·84	9·16
0·6	0·1324	−0·0053	0·0195	0·0170	−0·0571	0·1186	0·1268	−0·034	6·16	7·84	10·16
0·7	0·1418	−0·0261	0·0224	−0·0069	−0·0103	0·0692	0·1370	−0·029	5·23	7·05	10·95
0·9	0·1342	−0·0613	0·0275	−0·0365	+0·0133	0·0119	0·1350	−0·0111	3·89	5·74	12·26
1·1	0·1041	−0·0792	0·0318	−0·0570	+0·0020	−0·0038	0·1136	+0·0106	3·05	4·64	13·36

Ca^{+}

$\sin\theta/\lambda$	f_{4s}	$f_{1s,4s}$	$f_{2s,4s}$	$f_{3s,4s}$	$f_{4s,2p}$	$f_{4s,3p}$	$\|f_{it}\|^2$	$\mathscr{F}$	$19-\mathscr{F}$
0·0	1·0000	0·0000	0·0000	0·0000	0·0000	0·0000	19·00	19·00	0·00
0·1	+0·2815	0·0001	0·0013	0·0464	0·0042	0·0610	16·10	16·89	2·11
0·2	−0·0495	0·0002	0·0060	0·1077	0·0075	0·0119	12·44	14·33	4·67
0·3	+0·0083	0·0004	0·0127	0·1022	0·0089	−0·0526	9·95	12·03	6·97
0·4	0·0219	0·0007	0·0204	0·0560	0·0080	−0·0660	8·46	10·22	8·78
0·5	0·0107	0·0010	0·0278	+0·0155	0·0050	−0·0470	7·26	8·85	10·15
0·6	+0·0007	0·0014	0·0335	−0·0044	+0·0004	−0·0235	6·16	7·85	11·15
0·7	−0·0025	0·0019	0·0369	−0·0086	−0·0051	−0·0071	5·23	7·05	11·95
0·9	−0·0015	0·0030	0·0364	+0·0002	−0·0151	+0·0036	3·89	5·75	13·25
1·1	−0·0019	0·0043	0·0291	0·0074	−0·0208	+0·0014	3·05	4·65	14·35

Ca

$\sin\theta/\lambda$	f_{4s}	$f_{1s,4s}$	$f_{2s,4s}$	$f_{3s,4s}$	$f_{4s,2p}$	$f_{4s,3p}$	$\|f_{it}\|^2$	$\mathscr{F}$	$20-\mathscr{F}$
0·0	1·000	0·000	0·000	0·000	0·000	0·000	20·00	20·00	0·00
0·1	+0·1983	0·000	0·0009	0·0417	0·0037	0·0526	16·10	16·91	3·09
0·2	−0·0396	0·0001	0·0049	0·0936	0·0065	+0·0086	12·44	14·35	5·65
0·3	+0·0087	0·0003	0·0107	0·0873	0·0076	−0·0462	9·95	12·05	7·95
0·4	0·0160	0·0006	0·0173	0·0473	0·0069	−0·0565	8·46	10·23	9·77
0·5	0·0076	0·0009	0·0236	+0·0129	0·0043	−0·0398	7·26	8·86	11·14
0·6	+0·0002	0·0012	0·0285	−0·0040	+0·0003	−0·0199	6·16	7·85	12·15
0·7	−0·0026	0·0016	0·0313	−0·0073	−0·0043	−0·0060	5·23	7·05	12·95
0·9	−0·0006	0·0026	0·0309	+0·0002	−0·0128	+0·0030	3·89	5·75	14·25
1·1	−0·0029	0·0037	0·0247	0·0063	−0·0177	+0·0012	3·05	4·65	15·35

Table 7. *Absolute and percentage deviations of the J&B values from our data*

	Na^{+}		Na		K^{+}		Cl^{-}		Ca^{++}	
$\sin\theta/\lambda$	Diff.	% Diff.	Diff.	% Diff.	Diff.	% Diff.	Diff.	% Diff.	Diff.	% Diff.
0·0	0·0	0	0·0	0	0·0	0	0·0	0	0·0	0
0·1	−0·4	71	−0·5	33	−1·4	93	−1·9	71	−0·8	66
0·2	−1·8	95	−1·8	62	−2·8	64	−2·3	39	−3·0	81
0·3	−2·0	58	−2·0	45	−2·6	39	−2·1	26	−2·8	47
0·4	−2·0	42	−2·0	34	−2·3	27	−2·0	21	−2·5	32
0·5	−1·7	29	−1·7	25	−2·2	23	−2·1	20	−2·2	24
0·6	−1·3	19	−1·3	17	−2·2	21	−2·2	19	−2·2	22
0·7	−1·0	14	−1·0	12	−2·3	20	−2·2	18	−2·3	21
0·9	−0·6	7	−0·6	7	−2·2	17	−2·0	15	−2·3	19
1·1	−0·4	5	−0·4	4	−2·0	15	−1·5	10	−2·2	16

agreement between Laval's (1942) data for aluminum and (*a*) that of Walker (1956) and (*b*) our theoretical values (Freeman, 1959*a*) which were in excellent agreement with Walker's measurements.

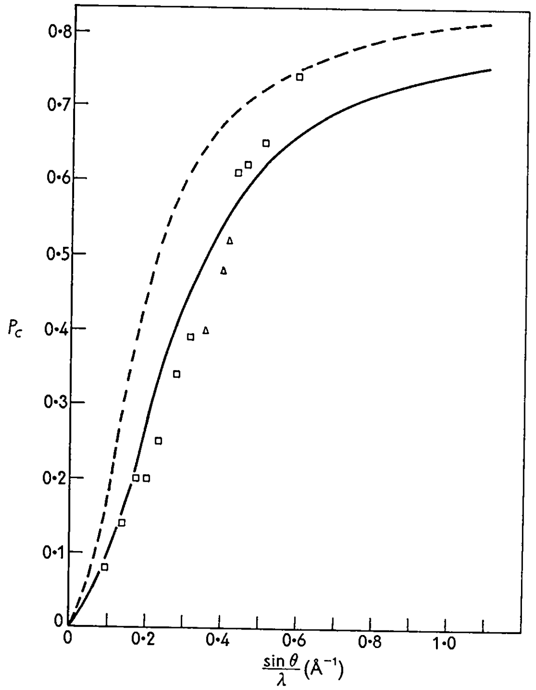

Fig. 8. Incoherent scattering intensity for CaF_2. The squares and triangles are the experimental values of Cribier, the solid curve denotes our values and the dashed curve represents the J&B data.

Our results* for CaF_2 are shown in Fig. 8 along with Cribier's (1958) measured values and the J&B results as tabulated in Compton & Allison for Ca^{++} and F^-. Plotted in Fig. 8 is the incoherent intensity per electron, P_c, as given by the formula

$$P_c = B\left[1 - \frac{\mathscr{F}(Ca^{++}) + 2\mathscr{F}(F^-)}{Z_{Ca^{++}} + 2Z_{F^-}}\right]$$

with B the Breit–Dirac factor. The agreement between our values and experiment is seen to be good over almost the entire range in $\sin\theta/\lambda$. Difficulties in the experimental procedures (which includes some theoretical calculations of the thermal diffuse scattering as well) preclude an accurate estimate of the experimental error, but it appears that our data differs by no more than 15% from the experimental values listed, whereas the J&B data differs from this by from 40 to 100% over almost the entire range of measurement. At high angles ($\sin\theta/\lambda > 0{\cdot}5$) our calculated intensity is below the Cribier data, but this is probably due to the difficulty of calculating the thermal diffuse scattering in this region (due to the importance of multi-phonon scattering).

In general, the good agreement shown in Figs. 7 and 8 is consistent with the agreement found in the few other cases for which experimental evidence is available (Keating & Vineyard, 1956; Freeman, 1959*a*, 1959*b*, 1959*c*) and adds further experimental confirmation to the validity of the Waller–Hartree expression.

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Note added in Proof. Dr P. Meriel has kindly provided us with some of his unpublished measurements on NaCl. Again our calculated values show a significant improvement over the J&B values and are in good agreement with the experimental incoherent intensity.

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* The values for F^- were taken from an earlier publication (Freeman, 1959*c*).

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