of (*D*) is small, and the general feature of the weights of resonance structures resemble those of diformylhydrazine. The oxygen atom is definitely charged electro-negatively, since the sum of the contribution of (*B*), (*C*), and (*D*), is large. Like diformylhydrazine the skeleton of the molecule excluding the methyl group has '*S*' shape. This is explained by the electrostatic attraction between the electro-positive nitrogen and the electro-negative oxygen atoms. In addition to the conjugation effect, this intramolecular electrostatic interaction will also contribute to the stability of the planar molecule. As already mentioned, Tomiie (1958*b*) discussed more fully about the conjugation effect in diformylhydrazine which can be applied analogously to diacetylhydrazine.

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X-ray Incoherent Scattering Functions for Non-Spherical Charge Distributions. II. Ti^+, V^{+2}, Mn^{+2}, Mn and Fe

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Compton incoherent scattering functions have been calculated for the transition elements, Ti^+, V^{+2}, Mn^{+2}, Mn^+, Mn and Fe using available Hartree–Fock free atom wave functions. The methods reported earlier for including the effects of non-spherical charge distributions on the scattering function have been employed in these calculations as well. In agreement with previous results, large differences are found from the values of James & Brindley, due mainly to the inclusion of all the exchange terms in the Waller–Hartree theory.

1

For many years, the most widely used values of the Compton scattering intensities were those calculated by James & Brindley (1931). These were based, for the most part, on wave functions calculated by the self-consistent field (SCF) method without exchange.

Table 1. *X-ray incoherent scattering function for* Mn^{+2}

$\sin\theta/\lambda$	f_{1s}	f_{2s}	f_{2p}	f_{3s}	f_{3p}	$f_{2p,2p}$	$f_{3p,3p}$	$f_{1s,2p}$	$f_{2s,2p}$
0·0	1·0000	1·0000	1·0000	1·0000	1·0000	0·00	0·000	0·000	0·000
0·1	0·9996	0·9931	0·9945	0·9376	0·9306	0·00	0·027	0·010	−0·049
0·2	0·9985	0·9729	0·9781	0·7720	0·7505	0·008	0·093	0·020	−0·094
0·3	0·9966	0·9402	0·9514	0·5556	0·5247	0·020	0·164	0·031	−0·1370
0·4	0·9940	0·8963	0·9156	0·3438	0·3153	0·034	0·211	0·040	−0·1751
0·5	0·9907	0·8429	0·8719	0·1741	0·1568	0·048	0·2224	0·050	−0·2072
0·6	0·9867	0·7820	0·8219	0·0600	0·0556	0·0673	0·2058	0·059	−0·2330
0·7	0·9819	0·7159	0·7671	−0·0030	0·0024	0·0873	0·1708	0·0686	−0·2519
0·9	0·9705	0·5761	0·6498	−0·0285	−0·0185	0·1255	0·0919	0·0850	−0·2685
1·1	0·9563	0·4387	0·5317	−0·0022	0·0020	0·1579	0·0343	0·0994	−0·2602

$\sin\theta/\lambda$	$f_{3s,2p}$	$f_{1s,3p}$	$f_{2s,3p}$	$f_{3s,3p}$	$f_{2p,3p}$	$f_{2p,3p}$	$f_{1s,2s}$	$f_{1s,3s}$	$f_{2s,3s}$
0·0	0·0000	0·000	0·0000	0·000	0·0000	0·000	0·0000	0·0000	0·0000
0·1	0·0131	0·003	0·0222	−0·186	0·0017	−0·001	0·0708	0·0007	−0·0642
0·2	0·0236	0·006	0·0417	−0·3172	0·0139	−0·007	0·0714	0·0010	−0·0509
0·3	0·0300	0·0092	0·0566	−0·3681	0·0322	−0·013	0·0724	0·0015	−0·0309
0·4	0·0311	0·0120	0·0652	−0·3461	0·0544	−0·021	0·0737	0·0022	−0·0067
0·5	0·0266	0·0147	0·0674	−0·2792	0·0776	−0·028	0·0754	0·0030	+0·0188
0·6	0·0173	0·0175	0·0635	−0·1975	0·0995	−0·033	0·0773	0·0041	0·0428
0·7	0·0043	0·0203	0·0547	−0·1219	0·1183	−0·036	0·0796	0·0053	0·0632
0·9	−0·0267	0·0252	0·0288	−0·0226	0·1422	−0·033	0·0848	0·0082	0·0884
1·1	−0·0555	0·0299	0·0011	+0·0115	0·1469	−0·021	0·0906	0·0117	0·0920

$\sin\theta/\lambda$	f_{3d}	$f_{3d,3d}(2)$	$f_{3d,3d}(4)$	$f_{2p,3d}(1)$	$f_{3p,3d}(1)$	$f_{2p,3d}(3)$	$f_{3p,3d}(3)$	$f_{1s,3d}$	$f_{2s,3d}$
0·0	1·0000	0·000	0·000	0·0000	0·0000	0·00	0·000	0·000	0·000
0·1	0·8990	0·039	0·001	0·0303	−0·1930	0·00	−0·02	0·000	−0·002
0·2	0·6660	0·1195	0·010	0·0583	−0·3136	0·002	−0·020	0·000	−0·009
0·3	0·4244	0·1778	0·041	0·0816	−0·3402	0·003	−0·065	0·000	−0·019
0·4	0·2412	0·1971	0·0612	0·0991	−0·2982	0·007	−0·1038	0·0003	−0·0304
0·5	0·1230	0·1857	0·0810	0·1103	−0·2262	0·011	−0·1293	0·0005	−0·0428
0·6	0·0538	0·1604	0·0923	0·1155	−0·1526	0·0164	−0·1399	0·0007	−0·0537
0·7	0·0161	0·1303	0·0948	0·1155	−0·0910	0·0225	−0·1345	0·0011	−0·0632
0·9	−0·0109	0·0787	0·0851	0·1044	−0·0139	0·0336	−0·1031	0·0018	−0·0744
1·1	−0·0132	0·0452	0·0718	0·0854	+0·0165	0·0416	−0·0683	0·0025	−0·0752

$\sin\theta/\lambda$	$f_{3s,3d}$	$\Sigma\|f_{ii}\|^2$	$\mathscr{F}$	$23-\mathscr{F}$
0·0	0·0000	23·00	23·00	0·00
0·1	0·0276	20·92	21·88	1·12
0·2	0·0924	16·63	19·32	3·68
0·3	0·1579	12·93	16·68	6·32
0·4	0·1969	10·61	14·34	8·66
0·5	0·2030	9·18	12·34	10·66
0·6	0·1835	8·12	10·68	12·32
0·7	0·1503	7·16	9·30	13·70
0·9	0·0789	5·51	7·28	15·72
1·1	0·0267	4·31	5·89	17·11

Since few such calculations were available at that time, James & Brindley relied on interpolation procedures to calculate incoherent scattering functions for other elements for which SCF wave functions were not known. Aside from this, the major approximation in their work was the neglect of the exchange terms, f_{ij}, in the Waller–Hartree (1929) expression for the intensity in electron units (e.u.)

$$I\text{ e.u.} = Z-\Sigma_i|f_{ii}|^2-\sum_{j\neq i}\sum|f_{ij}|^2 = Z-\mathscr{F}\,, \qquad (1)$$

where

$$f_{ij} = \int \psi_i^*(\mathbf{r})\exp\left[i\mathbf{k}.\mathbf{r}\right]\psi_j(\mathbf{r})dv \qquad (2)$$

and the ψ_j are the one-electron atomic wave functions and $\mathbf{k}$ denotes the scattering vector. Furthermore they replaced the exponential factor in equation (2) by the first term of the series expansion of the exponential, $\sin kr/kr$, and neglected all higher terms.

In recent years, there has been a determined effort to improve the old James & Brindley data, stimulated by their increasing importance in studies involving the diffuse scattering of X-rays. Using Hartree–Fock wave functions and the complete expression for I e.u. in equation (1), Keating & Vineyard (1956) have calculated an incoherent scattering function for carbon, and Milberg & Brailsford (1958) did the same for boron, carbon and oxygen. Meanwhile the author, in a series of papers (Freeman, 1959*a*, *b*, *c* and 1960) of which this is the last, has calculated incoherent scattering functions for a large number of atoms and ions for which accurate Hartree–Fock wave functions are known. These calculations showed large deviations

Table 2. *X-ray incoherent scattering function for* Mn$^+$

$\sin\theta/\lambda$	f_{3d}	$f_{3d,3d}(2)$	$f_{3d,3d}(4)$	$f_{2p,3d}(1)$	$f_{3p,3d}(1)$	$f_{2p,3d}(3)$	$f_{3p,3d}(3)$
0·0	1·0000	0·000	0·000	0·000	0·0000	0·000	0·000
0·1	0·8645	0·053	0·002	0·028	−0·1910	0·000	−0·009
0·2	0·5923	0·136	0·017	0·0533	−0·3049	0·001	−0·027
0·3	0·3539	0·1795	0·031	0·0746	−0·3236	0·002	−0·066
0·4	0·1937	0·1816	0·068	0·0905	−0·2779	0·007	−0·1023
0·5	0·0968	0·1624	0·0769	0·1007	−0·2077	0·012	−0·1251
0·6	0·0417	0·1356	0·0856	0·1053	−0·1386	0·0168	−0·1318
0·7	+0·0121	0·1087	0·0844	0·1053	−0·0819	0·0199	−0·1252
0·9	−0·0093	0·0649	0·0722	0·0949	−0·0121	0·0308	−0·0941
1·1	−0·0109	0·0364	0·0559	0·0775	+0·0150	0·0372	−0·0592

$\sin\theta/\lambda$	$f_{1s,3d}$	$f_{2s,3d}$	$f_{3s,3d}$	$\Sigma_i \lvert f_{ii}\rvert^2$	$\mathscr{F}$	$24-\mathscr{F}$
0·0	0·000	0·000	0·000	24·00	24·00	0·00
0·1	0·000	−0·002	0·025	21·37	22·41	1·59
0·2	0·000	−0·008	0·0921	16·55	19·43	4·57
0·3	0·000	−0·0176	0·1541	12·79	16·72	7·28
0·4	0·0004	−0·0280	0·1884	10·53	14·38	9·62
0·5	0·0006	−0·0392	0·1907	9·11	12·33	11·67
0·6	0·0008	−0·0493	0·1702	8·06	10·64	13·36
0·7	0·0010	−0·0577	0·1382	7·11	9·26	14·74
0·9	0·0015	−0·0679	0·0715	5·47	7·24	16·76
1·1	0·0021	−0·0685	0·0242	4·27	5·85	18·15

Table 3. *X-ray incoherent scattering function for* Mn

$\sin\theta/\lambda$	f_{3d}	$f_{3d,3d}(2)$	$f_{3d,3d}(4)$	$f_{2p,3d}(1)$	$f_{3p,3d}(1)$	$f_{2p,3d}(3)$	$f_{3p,3d}(3)$	$f_{4s,3d}$	$f_{1s,3d}$	$f_{2s,3d}$
0·0	1·0000	0·000	0·000	0·000	0·000	0·000	0·000	0·000	0·000	0·000
0·1	0·8875	0·046	0·000	0·029	−0·1928	0·000	−0·016	−0·048	0·000	−0·004
0·2	0·6401	0·1242	0·018	0·056	−0·3111	0·001	−0·028	−0·082	0·000	−0·010
0·3	0·3985	0·1796	0·042	0·079	−0·3347	0·002	−0·065	−0·049	0·000	−0·018
0·4	0·2229	0·1923	0·0665	0·0960	−0·2910	0·0060	−0·1037	−0·006	0·0002	−0·0296
0·5	0·1124	0·1774	0·0810	0·1067	−0·2195	0·0102	−0·1282	+0·019	0·0005	−0·0412
0·6	0·0486	0·1512	0·0901	0·1116	−0·1473	0·0158	−0·1360	0·031	0·0008	−0·0521
0·7	0·0141	0·1223	0·0911	0·1116	−0·0874	0·0223	−0·1314	0·030	0·0011	−0·0612
0·9	−0·0103	0·0733	0·0806	0·1007	−0·0131	0·0322	−0·0994	0·019	0·0016	−0·0718
1·1	−0·0122	0·0410	0·0627	0·0823	+0·0160	0·0401	−0·0626	0·007	0·0022	−0·0726

$\sin\theta/\lambda$	$f_{3s,3d}$	f_{4s}	$f_{1s,4s}$	$f_{2s,4s}$	$f_{3s,4s}$	$f_{2p,4s}$	$f_{3p,4s}$	$\Sigma \lvert f_{ii}\rvert^2$	$\mathscr{F}$	$25-\mathscr{F}$
0·0	0·000	1·000	0·0000	0·000	0·0000	0·0000	0·000	25·00	25·00	0·00
0·1	0·028	+0·36	−0·0025	−0·018	−0·0009	0·0024	0·039	21·08	22·08	2·92
0·2	0·0925	−0·026	−0·0025	−0·015	−0·0028	0·0045	0·020	16·47	19·22	5·78
0·3	0·1569	−0·020	−0·0024	−0·012	−0·0056	0·0060	−0·010	12·83	16·56	8·44
0·4	0·1943	+0·0074	−0·0023	−0·0071	−0·0093	0·0066	−0·042	10·56	14·25	10·75
0·5	0·1988	0·013	−0·0021	−0·0022	−0·013	0·0063	−0·052	9·15	12·26	12·74
0·6	0·1787	0·0082	−0·0019	+0·0027	−0·017	0·0050	−0·045	8·09	10·61	14·39
0·7	0·1458	0·0037	−0·0017	+0·0072	−0·020	0·0029	−0·032	7·14	9·26	15·74
0·9	0·0760	−0·0025	−0·0012	+0·013	−0·025	−0·0029	−0·0081	5·50	7·25	17·75
1·1	0·0255	−0·0043	−0·0005	+0·016	−0·025	−0·0088	+0·0019	4·29	5·85	19·15

Table 4. *X-ray incoherent scattering function for* Ti$^+$

$\sin\theta/\lambda$	f_{3d}	$f_{3d,3d}(2)$	$f_{3d,3d}(4)$	$f_{2p,3d}(1)$	$f_{3p,3d}(1)$	$f_{2p,3d}(3)$	$f_{3p,3d}(3)$
0·0	1·0000	0·000	0·00	0·0000	0·0000	0·000	0·000
0·1	0·7815	0·081	0·00	0·0192	−0·1830	0·000	−0·016
0·2	0·4261	0·1712	0·036	0·0367	−0·2818	0·001	−0·0314
0·3	0·1950	0·1815	0·074	0·0509	−0·2841	0·0020	−0·0685
0·4	0·0783	0·1521	0·084	0·0611	−0·2299	0·0039	−0·0992
0·5	0·0242	0·1162	0·0851	0·0669	−0·1611	0·0080	−0·1161
0·6	+0·0010	0·0845	0·0764	0·0691	−0·1000	0·0120	−0·1158
0·7	−0·0074	0·0596	0·0685	0·0679	−0·0541	0·0145	−0·1052
0·9	−0·0090	0·0285	0·0479	0·0591	−0·0035	0·0223	−0·0719
1·1	−0·0059	0·0137	0·0315	0·0466	+0·0127	0·0258	−0·0412

$\sin\theta/\lambda$	$f_{1s,3d}$	$f_{2s,3d}$	$f_{3s,3d}$	$\Sigma \lvert f_{ii}\rvert^2$	$\mathscr{F}$	$21-\mathscr{F}$
0·0	0·000	0·000	0·0000	21·00	21·00	0·00
0·1	0·000	−0·001	0·0276	18·72	19·46	1·54
0·2	0·000	−0·0056	0·0900	14·95	16·97	4·03
0·3	0·0001	−0·0122	0·1446	12·02	14·75	6·25
0·4	0·0001	−0·0201	0·1689	10·11	12·75	8·25
0·5	0·0003	−0·0277	0·1628	8·84	11·03	9·97
0·6	0·0004	−0·0343	0·1384	7·85	9·62	11·38
0·7	0·0006	−0·0397	0·1069	6·95	8·48	12·52
0·9	0·0009	−0·0452	0·0499	5·38	6·81	14·19
1·1	0·0012	−0·0443	0·0140	4·23	5·60	15·40

Table 5. *X-ray incoherent scattering function for* V^{+2}

$\sin\theta/\lambda$	f_{3d}	$f_{3d,3d}(2)$	$f_{3d,3d}(4)$	$f_{2p,3d}(1)$	$f_{3p,3d}(1)$	$f_{2p,3d}(3)$	$f_{3p,3d}(3)$
0·0	1·0000	0·000	0·0000	0·000	0·000	0·0000	0·0000
0·1	0·8646	0·049	0·0016	0·024	−0·195	0·0001	−0·0045
0·2	0·5783	0·1440	0·0166	0·0471	−0·3099	0·0008	−0·0287
0·3	0·3201	0·1933	0·0461	0·0657	−0·3256	0·0026	−0·0688
0·4	0·1528	0·1916	0·0740	0·0792	−0·2748	0·0054	−0·1065
0·5	0·0609	0·1636	0·0898	0·0875	−0·2001	0·0094	−0·1287
0·6	0·0156	0·1286	0·0937	0·0908	−0·1289	0·0140	−0·1333
0·7	−0·0046	0·0966	0·0894	0·0898	−0·0727	0·019	−0·1249
0·9	−0·0131	0·0506	0·0705	0·0792	−0·0073	0·0276	−0·0898
1·1	−0·0097	0·0250	0·0502	0·0632	+0·0154	0·0334	−0·0536

$\sin\theta/\lambda$	$f_{1s,3d}$	$f_{2s,3d}$	$f_{3s,3d}$	$\Sigma\lvert f_{ii}\rvert^2$	$\mathscr{F}$	$21-\mathscr{F}$
0·0	0·000	0·0000	0·0000	21·00	21·00	0·00
0·1	0·000	−0·0019	0·0288	19·12	19·89	1·11
0·2	0·000	−0·0075	0·0950	15·37	17·52	3·48
0·3	0·0002	−0·0157	0·1581	12·22	15·17	5·83
0·4	0·0003	−0·0253	0·1914	10·20	13·09	7·91
0·5	0·0004	−0·0352	0·1911	8·90	11·31	9·69
0·6	0·0007	−0·0441	0·1673	7·89	9·84	11·16
0·7	0·0008	−0·0513	0·1327	6·98	8·65	12·35
0·9	0·0012	−0·0591	0·0649	5·40	6·90	14·10
1·1	0·0017	−0·0587	0·0198	4·23	5·64	15·36

from the James & Brindley (1931) values in agreement with the available experimental results.

For non-spherical charge distributions, Freeman (1959*d*) has given a formalism for calculating the dependence of the incoherent scattering intensity on the orientation of the scattering vector and has derived practical formulae applicable to the case of the scattering from free atoms distributed at random. The results reported here were calculated according to the procedures given in that paper as applied to the cases considered. The details of the actual computations as well as an explanation of the notation used were given earlier (Freeman, 1959*b*) and so will not be repeated here.

2

For the atoms considered here, the formulae for $\mathscr{F}$ appropriate to the electronic configuration and ground state term value are given below. In order to avoid needless repetition they are expressed in terms of the formula for the contribution to $\mathscr{F}$ of the core electrons ($1s^2 2s^2 2p^6 3s^2 3p^6$) which are common to all the atoms,

$$\begin{aligned}\mathscr{F}(\text{core}) &= 2f_{1s}^2+2f_{2s}^2+6f_{2p}^2+2f_{3s}^2+6f_{3p}^2\\ &\quad+4(f_{1s,\,2s}^2+f_{1s,\,3s}^2+f_{2s,\,3s}^2)\\ &\quad+12(f_{1s,\,2p}^2+f_{2s,\,2p}^2+f_{3s,\,2p}^2+f_{1s,\,3p}^2+f_{2s,\,3p}^2+f_{3s,\,3p}^2)\\ &\quad+12(f_{2p,\,2p}^2(2)+f_{3p,\,3p}^2(2)+f_{2p,\,3p}^2(0)+2f_{2p,\,3p}^2(2))\,.\end{aligned}$$

1) Ti^+: $3d^3$, ^4F

$$\begin{aligned}\mathscr{F}(\text{Ti}^+) &= \mathscr{F}(\text{core})+3f_{3d}^2+\tfrac{155}{49}f_{3d,\,3d}^2(2)+\tfrac{153}{49}f_{3d,\,3d}^2(4)\\ &\quad+6(f_{1s,\,3d}^2+f_{2s,\,3d}^2+f_{3s,\,3d}^2)\\ &\quad+\tfrac{756}{105}(f_{2p,\,3d}^2(1)+f_{3p,\,3d}^2(1))+\tfrac{1134}{105}(f_{2p,\,3d}^2(3)+f_{3p,\,3d}^2(3))\,.\end{aligned}$$

2) V^{+2}: $3d^3$, ^4F

$$\mathscr{F}(\text{V}^{+2})=\mathscr{F}(\text{Ti}^+).^*$$

3) Mn^{+2}: $3d^5$, ^6S

$$\begin{aligned}\mathscr{F}(\text{Mn}^{+2}) &= \mathscr{F}(\text{core})+5f_{3d}^2+\tfrac{350}{49}f_{3d,\,3d}^2(2)+\tfrac{630}{49}f_{3d,\,3d}^2(4)\\ &\quad+10(f_{1s,\,3d}^2+f_{2s,\,3d}^2+f_{3s,\,3d}^2)\\ &\quad+12(f_{2p,\,3d}^2(1)+f_{3p,\,3d}^2(1))+18(f_{2p,\,3d}^2(3)+f_{3p,\,3d}^2(3))\,.\end{aligned}$$

4) Mn^+: $3d^{6}$, ^5D

$$\begin{aligned}\mathscr{F}(\text{Mn}^+) &= \mathscr{F}(\text{core})+6f_{3d}^2+\tfrac{370}{49}f_{3d,\,3d}^2(2)+\tfrac{631}{49}f_{3d,\,3d}^2(4)\\ &\quad+12(f_{1s,\,3d}^2+f_{2s,\,3d}^2+f_{3s,\,3d}^2)\\ &\quad+\tfrac{72}{5}(f_{2p,\,3d}^2(1)+f_{3p,\,3d}^2(1))+\tfrac{108}{5}(f_{2p,\,3d}^2(3)+f_{3p,\,3d}^2(3))\,.\end{aligned}$$

5) Mn: $3d^5 4s^2$, ^6S

$$\begin{aligned}\mathscr{F}(\text{Mn}) &= \mathscr{F}(\text{Mn}^{+2})+2f_{4s}^2+4[f_{1s,\,4s}^2+f_{2s,\,4s}^2+f_{3s,\,4s}^2]\\ &\quad+10f_{4s,\,3d}^2+12[f_{2p,\,4s}^2+f_{3p,\,4s}^2]\,.\end{aligned}$$

6) Fe: $3d^6 4s^2$, ^5D

$$\begin{aligned}\mathscr{F}(\text{Fe}) &= \mathscr{F}(\text{Mn}^+)+2f_{4s}^2+4(f_{1s,\,4s}^2+f_{2s,\,4s}^2+f_{3s,\,4s}^2)\\ &\quad+12(f_{2p,\,4s}^2+f_{3p,\,4s}^2)+12f_{4s,\,3d}^2\,.\end{aligned}$$

3

In the calculations for Mn^{+2} we used the wave functions of Hartree (1954). For Ti^+, V^{+2}, Mn^+ and Mn, Hartree (1956) used the core functions of Mn^{+2} to calculate approximate wave functions for the outer electrons of these ions. In our work, we used these approximate wave functions because they were the best ones available at the time these calculations were begun.† For Fe, we used the wave functions of Wood & Pratt (1957) as calculated by the unrestricted Hartree–Fock method in which Slater's average exchange potential formulation was used to simplify the variational problem. Only the wave functions of α

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[*] The notation $\mathscr{F}(\text{V}^{+2})=\mathscr{F}(\text{Ti}^+)$ means that the *formula* for $\mathscr{F}$ for V^{+2} is the same as the *formula* for Ti^+, although the numerical values of the f_{ij} integrals may be different.

[†] Since that time Worsley (1958) has published the first really accurate Hartree-Fock calculation for a transition metal (V^{+2}) and more recently Watson (1959) has calculated analytic Hartree–Fock wave functions for the entire iron transition group, including atoms in many stages of ionization.

Table 6. *X-ray incoherent scattering function for* Fe

$\sin\theta/\lambda$	f_{1s}	f_{2s}	f_{3s}	f_{4s}	f_{2p}	f_{3p}	f_{3d}	$f_{2p,2p}(2)$	$f_{3p,3p}(2)$
0·0	1·0000	1·0000	1·0000	1·0000	1·0000	1·0000	1·0000	0·000	0·000
0·1	0·9992	0·9943	0·9463	0·5388	0·9949	0·9415	0·9104	0·002	0·008
0·2	0·9983	0·9760	0·8014	0·0462	0·9803	0·7856	0·7027	0·005	0·084
0·3	0·9967	0·9457	0·6051	−0·0371	0·9563	0·5806	0·4805	0·0089	0·1478
0·4	0·9950	0·9059	0·4030	−0·0018	0·9241	0·3780	0·3006	0·0283	0·2006
0·5	0·9925	0·8566	0·2299	+0·0199	0·8847	0·2124	0·1737	0·0420	0·2237
0·6	0·9891	0·8004	0·1030	0·0206	0·8391	0·0963	0·0914	0·0620	0·2180
0·7	0·9858	0·7385	+0·0236	0·0130	0·7889	+0·0265	+0·0412	0·0768	0·1915
0·9	0·9766	0·6061	−0·0283	+0·0003	0·6796	−0·0181	−0·0032	0·1175	0·1180
1·1	0·9658	0·4733	−0·0110	−0·0021	0·5672	−0·0051	−0·0133	0·1491	0·0538

$\sin\theta/\lambda$	$f_{3d,3d}(2)$	$f_{3d,3d}(4)$	$f_{1s,2s}$	$f_{1s,3s}$	$f_{2s,3s}$	$f_{1s,4s}$	$f_{2s,4s}$	$f_{3s,4s}$	$f_{1s,2p}$
0·0	0·000	0·00	0·0000	0·0000	0·0000	0·0000	0·0000	0·0000	0·000
0·1	0·041	0·00	0·0384	0·0133	0·0070	0·0038	0·0008	0·0284	0·008
0·2	0·104	0·01	0·0393	0·0136	0·0182	0·0038	0·0035	0·0772	0·017
0·3	0·1639	0·03	0·0405	0·0139	0·0355	0·0039	0·0079	0·1120	0·025
0·4	0·1896	0·043	0·0421	0·0145	0·0569	0·0041	0·0133	0·1117	0·034
0·5	0·1887	0·068	0·0441	0·0151	0·0801	0·0043	0·0193	0·0847	0·042
0·6	0·1717	0·082	0·0467	0·0159	0·1026	0·0045	0·0254	0·0503	0·049
0·7	0·1478	0·090	0·0497	0·0169	0·1225	0·0048	0·0310	+0·0218	0·057
0·9	0·0989	0·097	0·0563	0·0191	0·1485	0·0054	0·0391	−0·0058	0·071
1·1	0·0610	0·075	0·0644	0·0218	0·1528	0·0061	0·0418	−0·0055	0·083

$\sin\theta/\lambda$	$f_{2s,2p}$	$f_{3s,2p}$	$f_{1s,3p}$	$f_{2s,3p}$	$f_{3s,3p}$	$f_{2p,3p}(0)$	$f_{4s,2p}$	$f_{4s,3p}$	$f_{1s,3d}$	$f_{2s,3d}$
0·0	0·000	0·0000	0·000	0·0000	0·0000	0·0000	0·0000	0·0000	0·000	−0·000
0·1	−0·054	0·0117	0·003	0·0191	−0·1729	0·0047	+0·0030	+0·0403	0·000	−0·001
0·2	−0·106	0·0218	0·005	0·0362	−0·3023	0·0155	0·0055	+0·0393	0·000	−0·008
0·3	−0·1545	0·0285	0·0076	0·0490	−0·3639	0·0320	0·0072	−0·0002	0·0001	−0·017
0·4	−0·2000	0·0306	0·0105	0·0571	−0·3595	0·0524	0·0080	−0·0440	0·0003	−0·030
0·5	−0·2394	0·0275	0·0130	0·0593	−0·3078	0·0746	0·0077	−0·0668	0·0004	−0·0415
0·6	−0·2729	0·0202	0·0155	0·0556	−0·2342	0·0964	0·0062	−0·0666	0·0007	−0·0538
0·7	−0·2997	+0·0088	0·0180	0·0470	−0·1588	0·1160	0·0036	−0·0534	0·0011	−0·0647
0·9	−0·3337	−0·0203	0·0225	0·0194	−0·0458	0·1438	−0·0036	−0·0210	0·0014	−0·0798
1·1	−0·3422	−0·0499	0·0268	−0·0122	+0·0046	0·1536	−0·0119	−0·0016	0·0011	−0·0848

$\sin\theta/\lambda$	$f_{3s,3d}$	$f_{4s,3d}$	$f_{2p,3d}(1)$	$f_{3p,3d}(1)$	$f_{2p,3d}(3)$	$f_{3p,3d}(3)$	$f_{2p,3p}(2)$	$\Sigma_i\|f_{ii}\|^2$	$\mathscr{F}$	$26-\mathscr{F}$
0·0	0·000	0·000	0·000	0·000	0·000	0·000	0·00	26·00	26·00	0·00
0·1	0·022	−0·044	0·029	−0·176	0·000	0·000	0·00	22·59	23·51	2·49
0·2	0·080	−0·0513	0·0574	−0·296	0·004	−0·025	−0·011	17·79	20·53	5·47
0·3	0·143	−0·0682	0·0819	−0·3374	0·007	−0·054	−0·0125	13·88	17·99	8·01
0·4	0·1865	−0·0228	0·1007	−0·3136	0·0059	−0·0913	−0·0185	11·26	15·66	10·34
0·5	0·2023	+0·0149	0·1142	−0·2546	0·0089	−0·1194	−0·0281	9·64	13·66	12·34
0·6	0·1933	0·0355	0·1220	−0·1860	0·0151	−0·1348	−0·0325	8·52	11·98	14·02
0·7	0·1682	0·0418	0·1243	−0·1228	0·0214	−0·1375	−0·0353	7·57	10·56	15·44
0·9	0·1014	0·0323	0·1166	−0·0334	0·0336	−0·1158	−0·0358	5·93	8·47	17·53
1·1	0·0441	0·0164	0·0994	+0·0094	0·0422	−0·0807	−0·0265	4·64	7·00	19·00

spin were used; the inclusion of the β spin wave functions would greatly complicate the already lengthy calculations without substantially changing the results.

Our results are listed in the tables as a function of $\sin\theta/\lambda$ in Å^{-1} units. Values for all the f_{ij} integrals as well as $\mathscr{F}$ and $Z-\mathscr{F}$ are given in order to facilitate an estimate of these quantities for atoms for which no such information is available. Also included is the quantity $\Sigma|f_{ii}|^2$, since $\mathscr{F}-\Sigma_i|f_{ii}|^2$ is the exchange contribution.

The results for Mn^{+2}, Mn^{+} and Mn are illustrated in Fig. 1. Also included is a plot of the exchange contribution for Mn^{+2} as this shows the importance of the exchange terms in equation (1). (No James & Brindley (1931) values are available for these atoms but they generally are higher than our data by at least the exchange contribution.) Similar results were obtained for Ti^{+} and V^{+2} as seen from the tables. Fig. 2 shows a plot of our data for Fe, compared with the values for $Z-\mathscr{F}$ in which the exchange terms were completely neglected. Again we see the importance of these terms, amounting to 50% of the intensity in the region of $\sin\theta/\lambda=0·2$ and 0·3, in agreement with earlier findings, especially for the heavier atoms (Freeman, 1959*a*, *b*, *c* and 1960).

4

No experimental determinations of the incoherent scattering functions have been made for the atoms considered here, and so no comparison can be made with our theoretical values. It has, however, been established in previous work (Keating & Vineyard, 1956; Freeman, 1959*a*, *b*, *c* and 1960) that the cal-

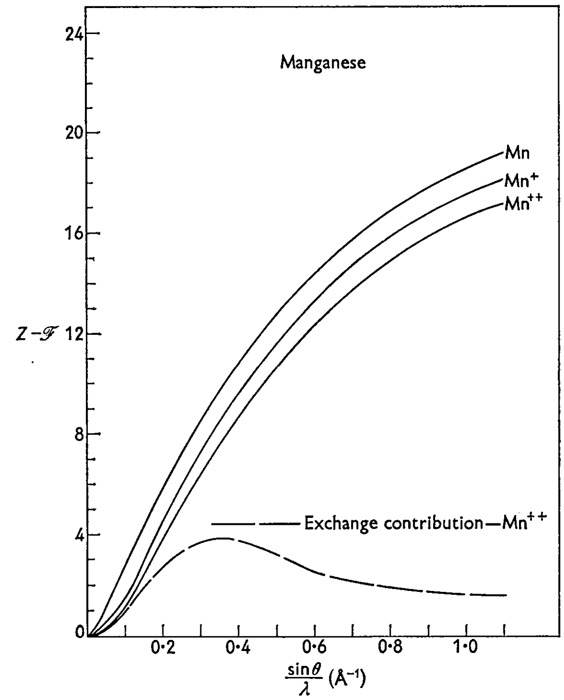

Fig. 1. The incoherent scattering functions for Mn^{+2}, Mn^{+} and Mn; the dashed curve denotes the exchange contribution for Mn^{+2}.

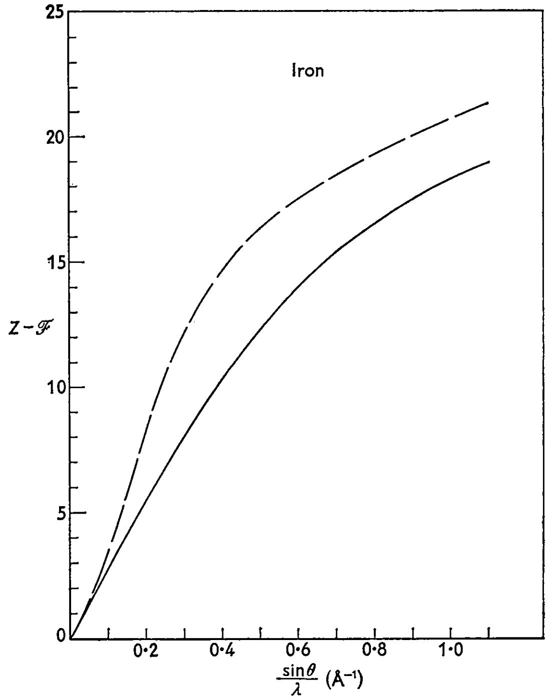

Fig. 2. The incoherent scattering function for Fe; the solid curve is the result including all exchange terms and the dashed curve is the result excluding exchange.

culations as described in this series yield results in good agreement with experiment whereas the earlier more approximate ones do not. For this reason we conclude that the values of the Compton incoherent scattering functions as reported here are the best theoretical values available to date.

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