# X-ray Incoherent Scattering Functions for Non-Spherical Charge Distributions: N, N⁻, O⁻, O, O⁺, O⁺², O⁺³, F, F⁻, Si⁺⁴, Si⁺³, Si, and Ge

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The atomic incoherent scattering functions of N, N⁻, O⁻, O, O⁺, O⁺², O⁺³, F, F⁻, Si⁺⁴, Si⁺³, Si, and Ge have been calculated according to the Waller–Hartree theory as extended in a previous paper to include the effects of the inherent non-sphericity of the atomic charge distributions. Hartree–Fock wave functions were used in all the computations. The results obtained show large deviations from the previously reported values of James & Brindley. These differences arise mainly from the inclusion in the present calculations of all the exchange integrals in the Waller–Hartree expression.

## 1

The few experimental determinations of the X-ray incoherent scattering intensities available to date (Laval, 1939, 1942; Curien & Deroche, 1956; Walker, 1956) have illustrated the inadequacy of those theoretical expressions for calculating Compton scattering which neglected the contribution due to exchange effects. Recently Keating & Vineyard (1956) and Freeman (1959a) have shown that the Waller & Hartree (1929) theory gives values in good agreement with experiment if accurate Hartree–Fock wave functions are employed in the calculations. Furthermore, calculations of this type for neon, copper, and zinc (Freeman, 1959b) showed very large deviations from previous calculations (Compton & Allison, 1935) in which exchange effects were neglected. Similar results were also obtained very recently (Milberg & Brailsford, 1958) for boron, oxygen, and carbon by these methods. These developments have stimulated the present effort at calculating accurate incoherent scattering functions for atoms for which Hartree–Fock wave functions are available. Further results in this series will be published as they become available.

For many atoms, their electronic charge density is not spherically symmetric and so the scattering depends on the orientation of the scattering vector. In a previous paper (Freeman, 1959c), the Waller–Hartree theory for the incoherent scattering from atoms was extended to include the effects of this inherent nonsphericity of the atomic charge distributions by a general formalism which depends on the use of the matrix elements of a unitary representation of the group of three-dimensional rotations. Applica-

tion was made to derive the angular dependence of the one-electron scattering matrix elements from atoms with *s*, *p*, and *d* electrons. By a proper averaging over all orientations of the scattering vector 'mean' scattering formulae resulted which apply for predicting the scattering from monatomic gases. Using these mean scattering formulae the Compton incoherent scattering intensities have been calculated for atomic nitrogen, oxygen, fluorine, silicon and germanium in varying degrees of ionization. For each ion those Hartree–Fock wave functions were employed which were originally calculated for that electronic state alone.* As in the earlier work referred to above, the present results show large deviations from those of previous calculations in which exchange was neglected. These results are discussed and comparison is made with other theoretical calculations and some recent experimental data.

## 2

Following the notation of a previous paper (Freeman, 1959c), which is an extension of that introduced by Keating & Vineyard (1956), the formulae for the scattering function for the various atoms and ions are given below for the configuration and ground state listed.

(1) N: $1s^2 2s^2 2p^3$, ⁴S.
$$\mathscr{F}(\mathrm{N}) = 2f_{1s}^2 + 2f_{2s}^2 + 3f_{2p}^2 + 4f_{1s,2s}^2 + 6f_{1s,2p}^2 + 6f_{2s,2p}^2 + 6f_{2p,2p}^2 .$$

(2) N⁻: $1s^2 2s^2 2p^4$, ³P.
$$\mathscr{F}(\mathrm{N}^-) = 2f_{1s}^2 + 2f_{2s}^2 + 4f_{2p}^2 + 4f_{1s,2s}^2 + 8f_{1s,2p}^2 + 8f_{2s,2p}^2 + \tfrac{31}{35}f_{2p,2p}^2 .$$

(3) O⁺³: $1s^2 2s^2 2p$, ²P.
$$\mathscr{F}(\mathrm{O}^{+3}) = 2f_{1s}^2 + 2f_{2s}^2 + f_{2p}^2 + 4f_{1s,2s}^2 + 2f_{1s,2p}^2 + 2f_{2s,2p}^2 + \tfrac{1}{5}f_{2p,2p}^2 .$$

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* For example, for the oxygen atom and its ions, Hartree, Hartree & Swirles (1939) calculated SCF wave functions for each system. In the calculations reported here, incoherent scattering intensities were separately calculated for each ion from its wave functions.

(4) $O^{+2}$: $1s^2 2s^2 2p^2$, $^3P$.

$$\mathscr{F}(O^{+2}) = 2f_{1s}^2 + 2f_{2s}^2 + 2f_{2p}^2 + 4f_{1s,\,2s}^2 + 4f_{1s,\,2p}^2$$
$$+ 4f_{2s,\,2p}^2 + \tfrac{11}{5}f_{2p,\,2p}^2 \,.$$

(5) $O^+$: $1s^2 2s^2 2p^3$, $^4S$ .*

$$\mathscr{F}(O^+) = \mathscr{F}(N) \,.$$

(6) $O$: $1s^2 2s^2 2p^4$, $^3P$.

$$\mathscr{F}(O) = \mathscr{F}(N^-) \,.$$

(7) $O^-$: $1s^2 2s^2 2p^5$, $^2P$.

$$\mathscr{F}(O^-) = 2f_{1s}^2 + 2f_{2s}^2 + 5f_{2p}^2 + 4f_{1s,\,2s}^2 + 10f_{1s,\,2p}^2$$
$$+ 10f_{2s,\,2p}^2 + \tfrac{41}{5}f_{2p,\,2p}^2 \,.$$

(8) $F$: $1s^2 2s^2 2p^5$, $^2P$.

$$\mathscr{F}(F) = \mathscr{F}(O^-) \,.$$

(9) $F^-$: $1s^2 2s^2 2p^6$, $^1S$ .

$$\mathscr{F}(F^-) = 2f_{1s}^2 + 2f_{2s}^2 + 6f_{2p}^2 + 4f_{1s,\,2s}^2 + 12f_{1s,\,2p}^2$$
$$+ 12f_{2s,\,2p}^2 + 12f_{2p,\,2p}^2 \,.$$

(10) $Si^{+4}$: $1s^2 2s^2 2p^6$, $^1S$ .

$$\mathscr{F}(Si^4) = \mathscr{F}(F^-) \,.$$

(11) $Si^{+3}$: $1s^2 2s^2 2p^6 3s$, $^3S$ .

$$\mathscr{F}(Si^{+3}) = \mathscr{F}(Si^{+4}) + f_{3s}^2 + 2f_{1s,\,3s}^2 + 2f_{2s,\,3s}^2 + 6f_{2p,\,3s}^2 \,.$$

(12) $Si$: $1s^2 2s^2 2p^6 3s^2 3p^2$, $^3P$.

$$\mathscr{F}(Si) = \mathscr{F}(Si^{+4}) + 2f_{3s}^2 + 2f_{3p}^2 + 4f_{1s,\,3s}^2 + 4f_{2s,\,3s}^2$$
$$+ 12f_{2p,\,3s}^2 + 4[f_{1s,\,3p}^2 + f_{2s,\,3p}^2 + f_{3s,\,3p}^2]$$
$$+ 4f_{2p,\,3p}^2(0) + 8f_{2p,\,3p}^2(2) + \tfrac{11}{5}f_{3p,\,3p}^2 \,.$$

(13) $Ge$: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^2$, $^3P$.

$$\mathscr{F}(Ge) = 2f_{1s}^2 + 2f_{2s}^2 + 6f_{2p}^2 + 2f_{3s}^2 + 6f_{3p}^2$$
$$+ 10f_{3d}^2 + 2f_{4s}^2 + 2f_{4p}^2$$
$$+ 4[f_{1s,\,2s}^2 + f_{1s,\,3s}^2 + f_{1s,\,4s}^2 + f_{2s,\,3s}^2 + f_{2s,\,4s}^2 + f_{3s,\,4s}^2]$$
$$+ 12[f_{1s,\,2p}^2 + f_{2s,\,2p}^2 + f_{3s,\,2p}^2 + f_{4s,\,2p}^2 + f_{1s,\,3p}^2$$
$$+ f_{2s,\,3p}^2 + f_{3s,\,3p}^2 + f_{4s,\,3p}^2]$$
$$+ 4[f_{1s,\,4p}^2 + f_{2s,\,4p}^2 + f_{3s,\,4p}^2 + f_{4s,\,4p}^2]$$
$$+ 12[f_{2p,\,2p}^2(2) + f_{3p,\,3p}^2(2)] + \tfrac{11}{5}f_{4p,\,4p}^2(2)$$
$$+ 12f_{2p,\,3p}^2(0) + 24f_{2p,\,3p}^2(2)$$
$$+ 4f_{2p,\,4p}^2(0) + 8f_{2p,\,4p}^2(2) + 4f_{3p,\,4p}^2(0) + 8f_{3p,\,4p}^2(2)$$
$$+ 20[f_{1s,\,3d}^2 + f_{2s,\,3d}^2 + f_{3s,\,3d}^2 + f_{4s,\,3d}^2]$$
$$+ 24[f_{2p,\,3d}^2(1) + f_{3p,\,3d}^2(1)]$$
$$+ 36[f_{2p,\,3d}^2(3) + f_{3p,\,3d}^2(3)]$$
$$+ 8f_{4p,\,3d}^2(1) + 12f_{4p,\,3d}^2(3)$$
$$+ \tfrac{700}{49}f_{3d,\,3d}^2(2) + \tfrac{1260}{49}f_{3d,\,3d}^2(4) \,.$$

Here

$$\mathscr{F} = \sum_i \sum_j |f_{ij}|^2 \,,$$

and the incoherent scattering intensity (without the Breit–Dirac factor) is given by $I_{\text{inc}} = Z - \mathscr{F}$ where $Z$ = number of electrons in the atom or ion.

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\* $\mathscr{F}(O^+) = \mathscr{F}(N)$ means that the formula for $O^+$ is the same as the formula for $N$. Separate values of the integrals, $f_{ij}$, were of course used in the calculations.

**3**

The $f_{ij}$ integrals were calculated on Whirlwind I, the MIT digital computer using a spherical Bessel function routine written by Wood (1957) with the numerical Hartree–Fock radial wave functions as direct input data.

**4**

In the accompanying Tables are listed, for each atom & ion, the calculated values of $f_{ij}$, $\mathscr{F}$ and $Z - \mathscr{F}$ as a function of $\sin\theta/\lambda$ in Å$^{-1}$ units. For purposes of comparison with earlier calculations, the values of the diagonal terms

$$\sum_i |f_{ii}|^2$$

are also included, since the difference between this quantity and $\mathscr{F}$ gives the magnitude of the exchange contribution. In the Figures, the values of the scattering intensities are compared with the earlier results (if available) of James & Brindley (Compton & Allison, 1935), hereafter referred to as J&B.
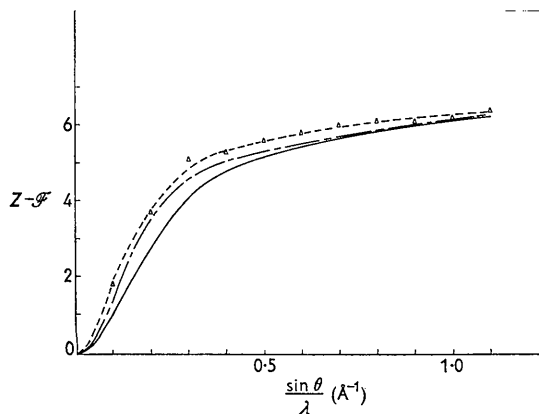


Fig. 1. Incoherent scattering function for nitrogen. The — △ — represent the J&B values, the long dashed curve is our result without exchange and the solid curve is our result calculated according to the complete Waller–Hartree theory.

The numerical results for N and N$^-$ are listed in Table 1 using the SCF wave functions calculated by Hartree & Hartree (1948). The incoherent scattering intensities are plotted in Fig. 1 and compared with the earlier results of James & Brindley. The differences between our values and those of J&B are large, especially for small and intermediate values of $\sin\theta/\lambda$. For N these amount to 70 % of our values at $\sin\theta/\lambda = 0\cdot1$ and 25 % at $\sin\theta/\lambda = 0\cdot3$.

For O$^-$, O, O$^+$, O$^{+2}$, and O$^{+3}$ the results obtained from the SCF wave functions of Hartree, Hartree & Swirles (1939) are given in Table 2 and plotted in Fig. 2 (which also includes the J&B data for O). For O$^+$, O$^{+2}$ and O$^{+3}$, the exchange terms of O were used in order to simplify the computations. Here too the differences between our values and those of J&B are large, being

Table 1. *X-ray incoherent scattering function for nitrogen*

N

| sin $\theta/\lambda$ | $f_{1s}$ | $f_{2s}$ | $f_{2p}$ | $f_{2p,2p}$ | $f_{1s,2s}$ | $f_{1s,2p}$ | $f_{2s,2p}$ | $\Sigma|f_{tt}|^2$ | $\mathscr{F}$ | $7-\mathscr{F}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 0·0 | 1·0000 | 1·0000 | 1·0000 | 0·0000 | 0·0000 | 0·0000 | 0·0000 | 7·000 | 7·000 | 0·000 |
| 0·1 | 0·9947 | 0·8551 | 0·8331 | 0·0627 | −0·0071 | 0·0294 | −0·2573 | 5·547 | 5·950 | 1·050 |
| 0·2 | 0·9790 | 0·5457 | 0·5140 | 0·1574 | 0·0087 | 0·0543 | −0·3426 | 3·454 | 4·176 | 2·824 |
| 0·3 | 0·9540 | 0·2677 | 0·2633 | 0·1909 | 0·0301 | 0·0721 | −0·2887 | 2·390 | 2·925 | 4·075 |
| 0·4 | 0·9209 | 0·0964 | 0·1200 | 0·1740 | 0·0522 | 0·0821 | −0·1954 | 1·940 | 2·220 | 4·780 |
| 0·5 | 0·8811 | 0·0151 | 0·0488 | 0·1396 | 0·0714 | 0·0860 | −0·1153 | 1·679 | 1·823 | 5·177 |
| 0·6 | 0·8363 | −0·0134 | 0·0159 | 0·1053 | 0·0859 | 0·0861 | −0·0600 | 1·467 | 1·562 | 5·438 |
| 0·7 | 0·7878 | −0·0165 | 0·0017 | 0·0775 | 0·0962 | 0·0839 | −0·0260 | 1·278 | 1·361 | 5·639 |
| 0·9 | 0·6851 | −0·0020 | −0·0056 | 0·0410 | 0·1080 | 0·0749 | +0·0039 | 0·949 | 1·030 | 5·970 |
| 1·1 | 0·5831 | 0·0104 | −0·0053 | 0·0221 | 0·1097 | 0·0600 | +0·0110 | 0·683 | 0·753 | 6·247 |

N⁻

| sin $\theta/\lambda$ | $f_{1s}$ | $f_{2s}$ | $f_{2p}$ | $f_{2p,2p}(2)$ | $f_{1s,2s}$ | $f_{1s,2p}$ | $f_{2s,2p}$ | $\Sigma|f_{tt}|^2$ | $\mathscr{F}$ | $8-\mathscr{F}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 0·0 | 1·0000 | 1·0000 | 1·0000 | 0·000 | 0·0000 | 0·000 | 0·0000 | 8·000 | 8·000 | 0·000 |
| 0·1 | 0·9948 | 0·8425 | 0·7534 | 0·086 | 0·0044 | 0·023 | −0·2646 | 5·715 | 6·279 | 1·721 |
| 0·2 | 0·9796 | 0·5219 | 0·4070 | 0·1655 | 0·0152 | 0·0430 | −0·3224 | 3·296 | 4·144 | 3·856 |
| 0·3 | 0·9550 | 0·2494 | 0·1942 | 0·1693 | 0·0310 | 0·0591 | −0·2548 | 2·277 | 2·828 | 5·172 |
| 0·4 | 0·9222 | 0·0878 | 0·0861 | 0·1417 | 0·0491 | 0·0700 | −0·1662 | 1·871 | 2·141 | 5·859 |
| 0·5 | 0·8825 | +0·0128 | 0·0346 | 0·1090 | 0·0668 | 0·0756 | −0·0962 | 1·636 | 1·774 | 6·226 |
| 0·6 | 0·8375 | −0·0128 | 0·0111 | 0·0806 | 0·0822 | 0·0769 | −0·0494 | 1·444 | 1·538 | 6·462 |
| 0·7 | 0·7888 | −0·0153 | +0·0011 | 0·0586 | 0·0941 | 0·0748 | −0·0212 | 1·266 | 1·350 | 6·650 |
| 0·9 | 0·6860 | −0·0017 | −0·0042 | 0·0309 | 0·1065 | 0·0646 | +0·0035 | 0·947 | 1·026 | 6·974 |
| 1·1 | 0·5841 | +0·0099 | −0·0045 | 0·0172 | 0·1058 | 0·0516 | +0·0093 | 0·685 | 0·752 | 7·248 |

of the same percentage amount as was found for nitrogen. Fig. 2 also shows the variation of the scattering with degree of ionization. For large sin $\theta/\lambda$ the curves approach $Z$, the number of electrons in the ion. This was expected from the familiar result for atomic scattering factors that the contribution from the outer electrons in an atom to the form factor is negligible at large sin $\theta/\lambda$. For low sin $\theta/\lambda$ the difference between the curves is not just that due to the difference in $Z$ since the contribution from the outer electrons is appreciable in this region.

The results for O agree with the values of the incoherent scattering intensity also obtained by Milberg & Brailsford (1958). Any small differences in results probably arise from the different interpolation and smoothing procedures used.
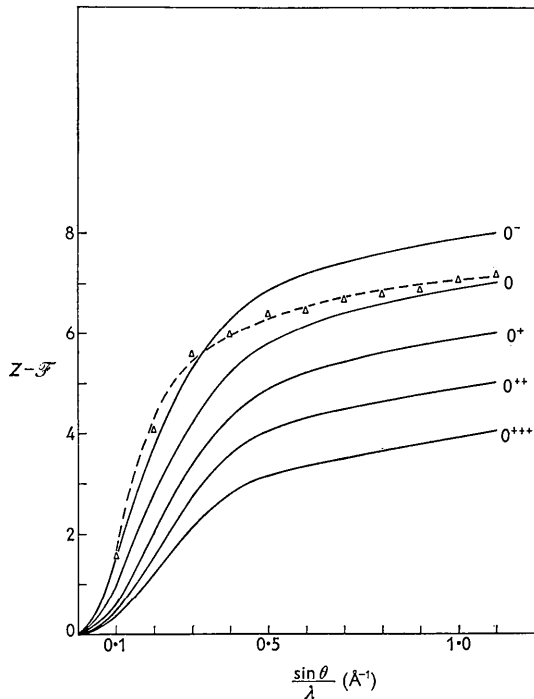


Fig. 2. The incoherent scattering functions for O⁻, O, O⁺, O⁺² and O⁺³ calculated according to the complete Waller–Hartree theory. The −−△−−− denote the J&B values for O.
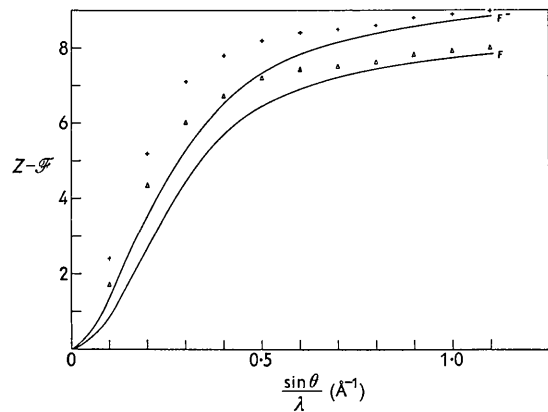


Fig. 3. The incoherent scattering functions for F and F⁻ calculated according to the complete Waller–Hartree theory. The +'s denote the J&B values for F⁻ and the △'s denote the J&B values for F.

Our results for F and F⁻ are summarized in Table 3 and displayed in Fig. 3 (along with the J&B data). Again we see the large deviations from the J&B values, showing the importance of exchange effects. Here these percentage deviations are seen to be somewhat

### Table 2. *X-ray incoherent scattering function for oxygen*

O⁻

| $\sin \theta/\lambda$ | $f_{1s}$ | $f_{2s}$ | $f_{2p}$ | $f_{1s,2s}$ | $f_{1s,2p}$ | $f_{2s,2p}$ | $f_{2p,2p}$ | $\Sigma|f_{ii}|^2$ | $\mathscr{F}$ | $9-\mathscr{F}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 0·0 | 1·0000 | 1·0000 | 1·0000 | 0·0000 | 0·0000 | 0·0000 | 0·0000 | 9·000 | 9·000 | 0·000 |
| 0·1 | 0·9961 | 0·8821 | 0·8160 | 0·0030 | 0·0210 | −0·2369 | 0·0674 | 6·904 | 7·469 | 1·531 |
| 0·2 | 0·9845 | 0·6177 | 0·5103 | 0·0117 | 0·0403 | −0·3254 | 0·1490 | 4·185 | 5·259 | 3·741 |
| 0·3 | 0·9656 | 0·3554 | 0·2851 | 0·0247 | 0·0565 | −0·2940 | 0·1737 | 2·771 | 3·670 | 5·330 |
| 0·4 | 0·9402 | 0·1686 | 0·1500 | 0·0403 | 0·0688 | −0·2201 | 0·1621 | 2·153 | 2·692 | 6·310 |
| 0·5 | 0·9090 | 0·0601 | 0·0749 | 0·0566 | 0·0768 | −0·1477 | 0·1366 | 1·840 | 2·130 | 6·870 |
| 0·6 | 0·8730 | 0·0073 | 0·0347 | 0·0720 | 0·0808 | −0·0910 | 0·1093 | 1·628 | 1·797 | 7·203 |
| 0·7 | 0·8332 | −0·0126 | 0·0137 | 0·0854 | 0·0816 | −0·0514 | 0·0853 | 1·450 | 1·572 | 7·428 |
| 0·9 | 0·7465 | −0·0113 | −0·0017 | 0·1036 | 0·0759 | −0·0090 | 0·0500 | 1·135 | 1·237 | 7·763 |
| 1·1 | 0·6564 | +0·0020 | −0·0045 | 0·1101 | 0·0651 | +0·0310 | 0·0294 | 0·869 | 0·970 | 8·030 |

O

| $\sin \theta/\lambda$ | $f_{1s}$ | $f_{2s}$ | $f_{2p}$ | $f_{1s,2s}$ | $f_{1s,2p}$ | $f_{2s,2p}$ | $f_{2p,2p}$ | $\Sigma|f_{ii}|^2$ | $\mathscr{F}$ | $8-\mathscr{F}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 0·0 | 1·0000 | 1·0000 | 1·0000 | 0·0000 | 0·000 | 0·000 | 0·0000 | 8·000 | 8·000 | 0·000 |
| 0·1 | 0·9961 | 0·8909 | 0·8686 | 0·0031 | 0·024 | −0·229 | 0·0510 | 6·606 | 7·030 | 0·970 |
| 0·2 | 0·9845 | 0·6379 | 0·5963 | 0·0120 | 0·0446 | −0·3346 | 0·1370 | 4·291 | 5·203 | 2·797 |
| 0·3 | 0·9657 | 0·3753 | 0·3528 | 0·0253 | 0·0625 | −0·3183 | 0·1825 | 2·851 | 3·695 | 4·305 |
| 0·4 | 0·9403 | 0·1814 | 0·1911 | 0·0413 | 0·0761 | −0·2464 | 0·1837 | 2·189 | 2·729 | 5·271 |
| 0·5 | 0·9091 | 0·0660 | 0·0968 | 0·0580 | 0·0851 | −0·1686 | 0·1615 | 1·861 | 2·159 | 5·841 |
| 0·6 | 0·8731 | 0·0090 | 0·0452 | 0·0739 | 0·0897 | −0·1053 | 0·1324 | 1·641 | 1·815 | 6·185 |
| 0·7 | 0·8334 | −0·0129 | 0·0182 | 0·0876 | 0·0906 | −0·0599 | 0·1046 | 1·458 | 1·583 | 6·417 |
| 0·9 | 0·7466 | −0·0120 | −0·0021 | 0·1062 | 0·0844 | −0·0108 | 0·0624 | 1·139 | 1·242 | 6·758 |
| 1·1 | 0·6565 | +0·0020 | −0·0057 | 0·1131 | 0·0726 | +0·0073 | 0·0367 | 0·870 | 0·964 | 7·036 |

O⁺

| $\sin \theta/\lambda$ | $f_{1s}$ | $f_{2s}$ | $f_{2p}$ | $f_{1s,2s}$ | $f_{1s,2p}$ | $f_{2s,2p}$ | $f_{2p,2p}$ | $\Sigma|f_{ii}|^2$ | $\mathscr{F}$ | $7-\mathscr{F}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 0·0 | 1·0000 | 1·0000 | 1·0000 | 0·0000 | | | | 7·000 | 7·000 | 0·000 |
| 0·1 | 0·9962 | 0·9012 | 0·8995 | 0·0031 | | | | 6·052 | 6·370 | 0·630 |
| 0·2 | 0·9846 | 0·6639 | 0·6669 | 0·0121 | | | | 4·267 | 4·951 | 2·049 |
| 0·3 | 0·9659 | 0·4048 | 0·4252 | 0·0258 | | | | 2·936 | 3·570 | 3·430 |
| 0·4 | 0·9405 | 0·2030 | 0·2429 | 0·0422 | | | | 2·231 | 2·637 | 4·363 |
| 0·5 | 0·9093 | 0·0775 | 0·1273 | 0·0596 | | Same as O | | 1·871 | 2·099 | 4·901 |
| 0·6 | 0·8734 | 0·0131 | 0·0609 | 0·0761 | | | | 1·642 | 1·780 | 5·220 |
| 0·7 | 0·8337 | −0·0128 | 0·0252 | 0·0904 | | | | 1·457 | 1·561 | 5·439 |
| 0·9 | 0·7470 | −0·0136 | −0·0020 | 0·1101 | | | | 1·139 | 1·231 | 5·769 |
| 1·1 | 0·6569 | +0·0016 | −0·0070 | 0·1174 | | | | 0·871 | 0·958 | 6·042 |

O⁺⁺

| $\sin \theta/\lambda$ | $f_{1s}$ | $f_{2s}$ | $f_{2p}$ | $f_{1s,2s}$ | $f_{1s,2p}$ | $f_{2s,2p}$ | $f_{2p,2p}$ | $\Sigma|f_{ii}|^2$ | $\mathscr{F}$ | $6-\mathscr{F}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 0·0 | 1·000 | 1·0000 | 1·0000 | 0·0000 | | | | 0·000 | 6·000 | 0·000 |
| 0·1 | 0·9961 | 0·9110 | 0·9164 | 0·0037 | | | | 5·329 | 5·540 | 0·460 |
| 0·2 | 0·9846 | 0·9611 | 0·7121 | 0·0130 | | | | 3·949 | 4·406 | 1·594 |
| 0·3 | 0·9659 | 0·4387 | 0·4811 | 0·0272 | | | | 2·787 | 3·211 | 2·789 |
| 0·4 | 0·9406 | 0·2309 | 0·2905 | 0·0443 | | | | 2·119 | 2·393 | 3·607 |
| 0·5 | 0·9095 | 0·0944 | 0·1598 | 0·0623 | | Same as O | | 1·781 | 1·939 | 4·061 |
| 0·6 | 0·8737 | 0·0204 | 0·0800 | 0·0795 | | | | 1·579 | 1·681 | 4·319 |
| 0·7 | 0·8340 | −0·0112 | 0·0350 | 0·0946 | | | | 1·418 | 1·501 | 4·499 |
| 0·9 | 0·7475 | −0·0152 | −0·0008 | 0·1155 | | | | 1·127 | 1·209 | 4·791 |
| 1·1 | 0·6574 | +0·0012 | −0·0080 | 0·1235 | | | | 0·867 | 0·949 | 5·051 |

O⁺³

| $\sin \theta/\lambda$ | $f_{1s}$ | $f_{2s}$ | $f_{2p}$ | $f_{1s,2s}$ | $f_{1s,2p}$ | $f_{2s,2p}$ | $f_{2p,2p}$ | $\Sigma|f_{ii}|^2$ | $\mathscr{F}$ | $5-\mathscr{F}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 0·0 | 1·0000 | 1·0000 | 1·0000 | 0·0000 | | | | 5·000 | 5·000 | 0·000 |
| 0·1 | 0·9962 | 0·9196 | 0·9288 | 0·0031 | | | | 4·539 | 4·645 | 0·355 |
| 0·2 | 0·9847 | 0·7164 | 0·7486 | 0·0128 | | | | 3·530 | 3·759 | 1·241 |
| 0·3 | 0·9660 | 0·4731 | 0·5317 | 0·0273 | | | | 2·603 | 2·816 | 2·184 |
| 0·4 | 0·9408 | 0·2620 | 0·3389 | 0·0450 | | | | 2·029 | 2·170 | 2·830 |
| 0·5 | 0·9098 | 0·1152 | 0·1964 | 0·0638 | | Same as O | | 1·726 | 1·813 | 3·187 |
| 0·6 | 0·8741 | 0·0307 | 0·1035 | 0·0819 | | | | 1·544 | 1·609 | 3·391 |
| 0·7 | 0·8345 | −0·0083 | 0·0482 | 0·0979 | | | | 1·397 | 1·459 | 3·541 |
| 0·9 | 0·7482 | −0·0174 | 0·0016 | 0·1203 | | | | 1·121 | 1·193 | 3·807 |
| 1·1 | 0·6582 | 0·0000 | −0·0087 | 0·1292 | | | | 0·867 | 0·945 | 4·055 |

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

F⁻

| $\sin\theta/\lambda$ | $f_{1s}$ | $f_{2s}$ | $f_{2p}$ | $f_{1s,2s}$ | $f_{1s,2p}$ | $f_{2s,2p}$ | $f_{2p,2p}$ | $\Sigma|f_{ii}|^2$ | $\mathscr{F}$ | $10-\mathscr{F}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 0·0 | 1·0000 | 1·0000 | 1·0000 | 0·0000 | 0·0000 | 0·0000 | 0·0000 | 10·000 | 10·000 | 0·000 |
| 0·1 | 0·9969 | 0·9085 | 0·8595 | 0·0025 | 0·0195 | −0·2131 | 0·0527 | 8·105 | 8·654 | 1·346 |
| 0·2 | 0·9878 | 0·6896 | 0·5949 | 0·0097 | 0·0378 | −0·3177 | 0·1310 | 5·232 | 6·460 | 3·540 |
| 0·3 | 0·9730 | 0·4482 | 0·3710 | 0·0207 | 0·0536 | −0·3164 | 0·1696 | 3·467 | 4·704 | 5·296 |
| 0·4 | 0·9528 | 0·2524 | 0·2191 | 0·0341 | 0·0665 | −0·2618 | 0·1721 | 2·586 | 3·466 | 6·534 |
| 0·5 | 0·9277 | 0·1204 | 0·1244 | 0·0487 | 0·0758 | −0·1947 | 0·1561 | 2·137 | 2·670 | 7·330 |
| 0·6 | 0·8984 | 0·0430 | 0·0676 | 0·0633 | 0·0818 | −0·1345 | 0·1334 | 1·860 | 2·173 | 7·827 |
| 0·7 | 0·8656 | 0·0036 | 0·0345 | 0·0768 | 0·0848 | −0·0871 | 0·1101 | 1·651 | 1·852 | 8·148 |
| 0·9 | 0·7924 | −0·0153 | 0·0052 | 0·0979 | 0·0835 | −0·0283 | 0·0713 | 1·318 | 1·450 | 8·550 |
| 1·1 | 0·7136 | −0·0059 | −0·0029 | 0·1097 | 0·0758 | 0·0200 | 0·0446 | 1·042 | 1·163 | 8·837 |

F

| $\sin\theta/\lambda$ | $f_{1s}$ | $f_{2s}$ | $f_{2p}$ | $f_{1s,2s}$ | $f_{1s,2p}$ | $f_{2s,2p}$ | $f_{2p,2p}$ | $\Sigma|f_{ii}|^2$ | $\mathscr{F}$ | $9-\mathscr{F}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 0·0 | 1·0000 | 1·0000 | 1·0000 | 0·0000 | | | | 9·000 | 9·000 | 0·000 |
| 0·1 | 0·9969 | 0·9148 | 0·8939 | −0·0026 | | | | 7·680 | 8·139 | 0·861 |
| 0·2 | 0·9879 | 0·7064 | 0·6605 | −0·0099 | | | | 5·272 | 6·294 | 2·706 |
| 0·3 | 0·9730 | 0·4680 | 0·4323 | −0·0210 | | | | 3·502 | 4·536 | 4·464 |
| 0·4 | 0·9528 | 0·2680 | 0·2636 | −0·0348 | | | | 2·549 | 3·282 | 5·718 |
| 0·5 | 0·9277 | 0·1296 | 0·1527 | −0·0497 | | Same as F⁻ | | 2·071 | 2·518 | 6·482 |
| 0·6 | 0·8984 | 0·0470 | 0·0842 | −0·0646 | | | | 1·800 | 2·066 | 6·934 |
| 0·7 | 0·8656 | 0·0047 | 0·0434 | −0·0784 | | | | 1·607 | 1·779 | 7·221 |
| 0·9 | 0·7924 | −0·0159 | 0·0068 | −0·1002 | | | | 1·298 | 1·416 | 7·584 |
| 1·1 | 0·7136 | −0·0064 | −0·0037 | −0·1123 | | | | 1·035 | 1·146 | 7·854 |

Table 4. *X-ray incoherent scattering function for silicon*

Si⁺⁴

| $\sin\theta/\lambda$ | $f_{1s}$ | $f_{2s}$ | $f_{2p}$ | $f_{2p,2p}$ | $f_{1s,2s}$ | $f_{1s,2p}$ | $f_{2s,2p}$ | $\Sigma|f_{ii}|^2$ | $\mathscr{F}$ | $10-\mathscr{F}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 0·0 | 1·0000 | 1·0000 | 1·0000 | 0·00 | 0·0000 | 0·000 | 0·000 | 10·000 | 10·000 | 0·000 |
| 0·1 | 0·9988 | 0·9727 | 0·9746 | 0·02 | 0·0016 | 0·017 | −0·116 | 9·591 | 9·757 | 0·243 |
| 0·2 | 0·9951 | 0·8958 | 0·9029 | 0·037 | 0·0048 | 0·032 | −0·217 | 8·493 | 9·070 | 0·930 |
| 0·3 | 0·9890 | 0·7816 | 0·7979 | 0·075 | 0·0100 | 0·048 | −0·2907 | 7·065 | 8·107 | 1·893 |
| 0·4 | 0·9806 | 0·6470 | 0·6755 | 0·116 | 0·0170 | 0·0618 | −0·3331 | 5·660 | 7·039 | 2·961 |
| 0·5 | 0·9699 | 0·5084 | 0·5508 | 0·152 | 0·0254 | 0·0748 | −0·3454 | 4·496 | 5·997 | 4·003 |
| 0·6 | 0·9571 | 0·3791 | 0·4346 | 0·177 | 0·0349 | 0·0858 | −0·3331 | 3·628 | 5·054 | 4·946 |
| 0·7 | 0·9424 | 0·2671 | 0·3335 | 0·192 | 0·0452 | 0·0955 | −0·3041 | 3·029 | 4·256 | 5·744 |
| 0·9 | 0·9075 | 0·1072 | 0·1827 | 0·1951 | 0·0665 | 0·1093 | −0·2237 | 2·328 | 3·088 | 6·912 |
| 1·1 | 0·8666 | 0·0233 | 0·0914 | 0·1743 | 0·0867 | 0·1163 | −0·1443 | 1·918 | 2·360 | 7·640 |

| | | Si⁺³ | | | | | | | Si | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $\sin\theta/\lambda$ | $f_{3s}$ | $f_{1s,3s}$ | $f_{2s,3s}$ | $f_{2p,3s}$ | $\Sigma|f_{ii}|^2$ | $\mathscr{F}$ | $11-\mathscr{F}$ | $\Sigma|f_{ii}|^2$ | $\mathscr{F}$ | $14-\mathscr{F}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 0·0 | 1·0000 | 0·0000 | 0·0000 | 0·0000 | 11·00 | 11·00 | 0·00 | 14·00 | 14·00 | 0·00 |
| 0·1 | 0·7432 | 0·0002 | 0·0175 | 0·0333 | 10·14 | 10·32 | 0·68 | 10·94 | 11·54 | 2·46 |
| 0·2 | 0·2812 | 0·0010 | 0·0586 | 0·0441 | 8·57 | 9·17 | 1·83 | 8·68 | 9·43 | 4·57 |
| 0·3 | +0·0130 | 0·0024 | 0·1020 | +0·0272 | 7·07 | 8·13 | 2·87 | 7·07 | 8·24 | 5·76 |
| 0·4 | −0·0397 | 0·0042 | 0·1293 | −0·0056 | 5·66 | 7·07 | 3·93 | 5·66 | 7·18 | 6·82 |
| 0·5 | −0·0117 | 0·0065 | 0·1343 | −0·0388 | 4·50 | 6·04 | 4·96 | 4·50 | 6·15 | 7·85 |
| 0·6 | +0·0170 | 0·0092 | 0·1212 | −0·0623 | 3·63 | 5·11 | 5·89 | 3·63 | 5·21 | 8·79 |
| 0·7 | 0·0286 | 0·0121 | 0·0979 | −0·0738 | 3·03 | 4·31 | 6·69 | 3·03 | 4·40 | 9·60 |
| 0·9 | 0·0218 | 0·0183 | 0·0485 | −0·0694 | 2·33 | 3·12 | 7·88 | 2·33 | 3·18 | 10·82 |
| 1·1 | 0·0083 | 0·0244 | 0·0153 | −0·0501 | 1·92 | 2·38 | 8·62 | 1·92 | 2·41 | 11·59 |

larger than were found for nitrogen and oxygen. For F we used the SCF wave functions of Allen* (1957) while for F⁻ those of Froese (1957) were employed. The exchange terms calculated for F⁻ were used in the calculations for F.

For Si⁺³ and Si⁺⁴ we used the wave functions of Hartree, Hartree & Manning (1941). Since no such wave functions are available for Si we used the $3p$

* I am grateful to Dr L. C. Allen for allowing me the use of his unpublished wave functions.

wave function recently calculated for aluminum (Freeman & Hartree, 1957) along with the wave functions for Si⁺³ to make up the neutral atom. (This approximation is not a very drastic one since the $3p$ wave functions for aluminum and silicon should not differ by very much.) See Table 4 and Fig. 4 for a summary of these results. The deviations from the earlier J&B values are large even for intermediate values of $\sin\theta/\lambda$; these deviations amount to 25–30% in the region $0\cdot2 \le \sin\theta/\lambda \le 0\cdot6$.
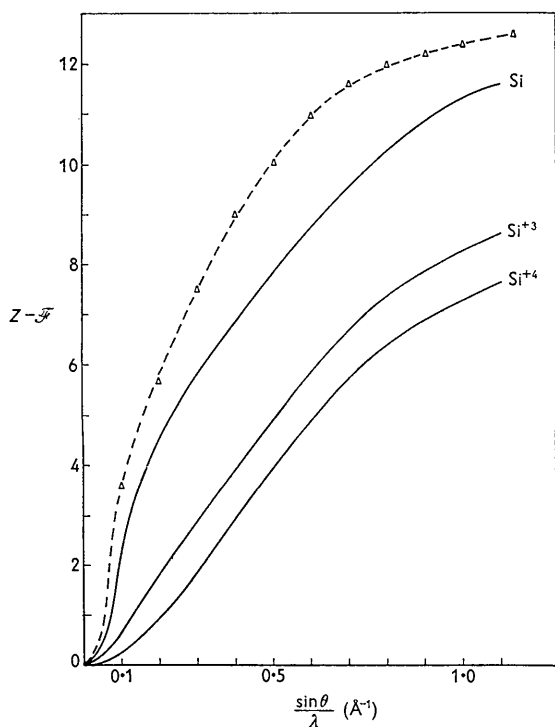
Fig. 4. The incoherent scattering functions for Si, $Si^{+4}$ and $Si^{+3}$ according to the complete Waller–Hartree theory. The $--\triangle---$ denote the J&B values for Si.
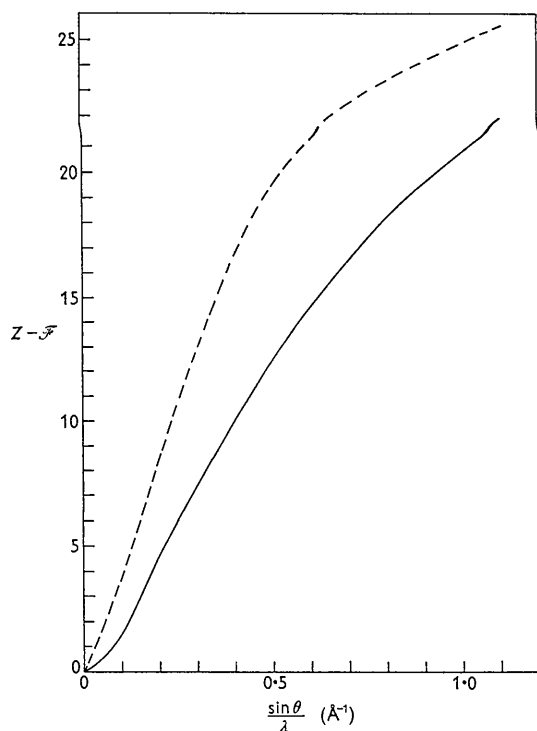


Fig. 5. The incoherent scattering function for Ge. The dashed curve is the result without exchange and the solid curve is our result calculated according to the complete Waller–Hartree expression.

For Ge* the calculations were a good deal more involved since the number of exchange terms rises rapidly with atomic number. (From Table 5 it is seen that there are 34 non-diagonal terms and 13 diagonal terms which enter into the Waller–Hartree expression). While individually the exchange terms are small their sum is quite appreciable. This is seen in Fig. 5 where we have plotted the incoherent scattering function as calculated with and without exchange. The exchange contribution, which amounts to 3·9 electron units (e.u.), or 82% of the calculated intensity at $\sin\theta/\lambda = 0\cdot2$, to 7·0 electron units or 55% of the calculated intensity at $\sin\theta/\lambda = 0\cdot5$, is large over the entire range of $\sin\theta/\lambda$. Even at $\sin\theta/\lambda = 0\cdot9$, this contribution reduces the calculated intensity by 4·5 electron units (or 23% of the calculated value). Similar remarks are appropriate for the entire range of $\sin\theta/\lambda$, as is seen directly from the data given in Table 5. These results are in complete agreement with those found earlier for Cu (Freeman, 1959b).

**5**

No direct experimental determination of the Compton intensity has been made for any of the atoms discussed in this paper. The importance of including exchange terms in the Waller–Hartree expression, however, is indicated in the recent experiments of Learn (1958) on silicon and Cole (1959) on germanium. These workers were investigating lattice vibrations and for this needed an accurate determination of the diffuse X-ray scattering (TDS). Since the TDS is always accompanied by the incoherent Compton scattering, an accurate knowledge of the latter is required if quantitative information is to be obtained from the former. In the case of silicon and germanium the Compton scattering intensity is especially important since it makes up a large part of the total observed scattering. For Ge, Cole found that the incoherent intensity as calculated without the exchange terms† was larger at some angles than the observed total intensity—clearly an unsatisfactory result. (Similar results were obtained using Bewilogua's (1931) calculations, based on the Fermi–Thomas method). Using the values for the incoherent scattering function given in this paper, Cole finds a considerable reduction in the calculated Compton scattering and therefore a more reasonable value for the TDS. In fact this calculated incoherent intensity is about 50% of the total measured intensity. In the case of Si, Learn found similar results to those cited for Ge (the exchange contribution being smaller because of a lower atomic number).

I am pleased to acknowledge the help given by Dr John Wood with some of the Whirlwind routines.

Table 5. *Incoherent scattering function for germanium*

Ge

| sin θ/λ | $f_{1s}$ | $f_{2s}$ | $f_{3p}$ | $f_{4s}$ | $f_{2p}$ | $f_{3d}$ | $f_{3s}$ | $f_{4p}$ | $f_{1s,2s}$ | $f_{1s,4s}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 0·0 | 1·0000 | 1·0000 | 1·0000 | 1·0000 | 1·0000 | 1·0000 | 1·0000 | 1·0000 | 0·0000 | 0·0000 |
| 0·1 | 0·9998 | 0·9961 | 0·9666 | 0·6544 | 0·9969 | 0·9640 | 0·9532 | 0·4968 | 0·0002 | 0·0002 |
| 0·2 | 0·9991 | 0·9844 | 0·8726 | 0·1656 | 0·9877 | 0·8639 | 0·8297 | 0·0395 | 0·0009 | 0·0002 |
| 0·3 | 0·9980 | 0·9652 | 0·7349 | −0·0251 | 0·9726 | 0·7198 | 0·6676 | −0·0340 | 0·0019 | 0·0003 |
| 0·4 | 0·9964 | 0·9389 | 0·5757 | −0·0332 | 0·9520 | 0·5572 | 0·5033 | −0·0109 | 0·0034 | 0·0004 |
| 0·5 | 0·9944 | 0·9063 | 0·4166 | −0·0037 | 0·9262 | 0·3994 | 0·3595 | 0·0077 | 0·0053 | 0·0006 |
| 0·6 | 0·9919 | 0·8680 | 0·2745 | 0·0147 | 0·8958 | 0·2625 | 0·2444 | 0·0123 | 0·0076 | 0·0007 |
| 0·7 | 0·9890 | 0·8248 | 0·1594 | 0·0190 | 0·8614 | 0·1545 | 0·1581 | 0·0116 | 0·0103 | 0·0009 |
| 0·9 | 0·9820 | 0·7276 | 0·0184 | 0·0104 | 0·7831 | 0·0259 | 0·0533 | 0·0056 | 0·0166 | 0·0014 |
| 1·1 | 0·9732 | 0·6222 | −0·0273 | 0·0014 | 0·6969 | −0·0161 | 0·0063 | 0·0014 | 0·0242 | 0·0020 |

| sin θ/λ | $f_{1s,3s}$ | $f_{1s,4p}$ | $f_{2s,4s}$ | $f_{2s,3s}$ | $f_{2s,4p}$ | $f_{3s,4s}$ | $f_{1s,3p}$ | $f_{1s,2p}$ | $f_{2s,3p}$ | $f_{2s,2p}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 0·0 | 0·0000 | 0·0000 | 0·0000 | 0·0000 | 0·0000 | 0·0000 | 0·000 | 0·000 | 0·0000 | 0·000 |
| 0·1 | 0·0335 | 0·0004 | 0·0008 | −0·4237 | 0·0028 | −0·1449 | 0·002 | 0·007 | 0·0165 | −0·043 |
| 0·2 | 0·0333 | 0·0009 | 0·0023 | −0·4126 | 0·0056 | −0·0314 | 0·005 | 0·016 | 0·0317 | −0·084 |
| 0·3 | 0·0331 | 0·0014 | 0·0047 | −0·3948 | 0·0081 | 0·0577 | 0·008 | 0·024 | 0·0447 | −0·124 |
| 0·4 | 0·0327 | 0·0019 | 0·0078 | −0·3714 | 0·0100 | 0·0931 | 0·0099 | 0·032 | 0·0545 | −0·162 |
| 0·5 | 0·0323 | 0·0023 | 0·0117 | −0·3434 | 0·0114 | 0·0881 | 0·0122 | 0·041 | 0·0607 | −0·1975 |
| 0·6 | 0·0318 | 0·0028 | 0·0159 | −0·3124 | 0·0121 | 0·0645 | 0·0146 | 0·048 | 0·0630 | −0·2299 |
| 0·7 | 0·0312 | 0·0032 | 0·0203 | −0·2795 | 0·0122 | 0·0374 | 0·0171 | 0·056 | 0·0614 | −0·2583 |
| 0·9 | 0·0297 | 0·0042 | 0·0284 | −0·2130 | 0·0104 | −0·0023 | 0·0216 | 0·071 | 0·0484 | −0·3025 |
| 1·1 | 0·0280 | 0·0050 | 0·0344 | −0·1519 | 0·0066 | −0·0183 | 0·0260 | 0·0841 | 0·0264 | −0·3300 |

Ge

| sin θ/λ | $f_{4s,4p}$ | $f_{3s,4p}$ | $f_{3p,4p}(0)$ | $f_{2p,4p}(0)$ | $f_{4s,3p}$ | $f_{4s,2p}$ | $f_{2p,3p}(0)$ | $f_{3p,3s}$ | $f_{2p,3s}$ | $f_{3d,4p}(3)$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 0·0 | 0·0000 | 0·0000 | 0·0000 | 0·0000 | 0·0000 | 0·0000 | 0·0000 | 0·000 | 0·000 | 0·0000 |
| 0·1 | −0·3484 | +0·0117 | −0·0347 | 0·0004 | 0·0337 | 0·0019 | −0·0273 | −0·137 | 0·010 | 0·0038 |
| 0·2 | −0·2288 | +0·0112 | −0·0570 | 0·0014 | 0·0429 | 0·0037 | −0·0337 | −0·254 | 0·0178 | 0·0189 |
| 0·3 | −0·0578 | −0·0023 | −0·0762 | 0·0031 | 0·0237 | 0·0051 | −0·0438 | −0·3318 | 0·0243 | 0·0326 |
| 0·4 | +0·0066 | −0·0217 | −0·0824 | 0·0055 | −0·0093 | 0·0062 | −0·0566 | −0·3669 | 0·0283 | 0·0340 |
| 0·5 | +0·0119 | −0·0382 | −0·0747 | 0·0083 | −0·0396 | 0·0068 | −0·0713 | −0·3622 | 0·0294 | 0·0250 |
| 0·6 | +0·0028 | −0·0471 | −0·0582 | 0·0114 | −0·0579 | 0·0067 | −0·0866 | −0·3273 | 0·0273 | 0·0119 |
| 0·7 | −0·0056 | −0·0479 | −0·0389 | 0·0146 | −0·0629 | 0·0059 | −0·1015 | −0·2742 | 0·0223 | −0·0006 |
| 0·9 | −0·0088 | −0·0341 | −0·0083 | 0·0208 | −0·0474 | 0·0025 | −0·1266 | −0·1554 | 0·0052 | −0·0167 |
| 1·1 | −0·0050 | −0·0163 | +0·0052 | 0·0256 | −0·0232 | −0·0026 | −0·1415 | −0·0618 | −0·0178 | −0·0214 |

| sin θ/λ | $f_{3p,3p}(2)$ | $f_{2p,2p}(2)$ | $f_{2p,3p}(2)$ | $f_{3p,3d}(1)$ | $f_{2p,3d}(1)$ | $f_{1s,3d}$ | $f_{2s,3d}$ | $f_{4s,3d}$ | $f_{3s,3d}$ | $f_{3p,3d}(3)$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 0·0 | 0·0000 | 0·0000 | 0·0000 | 0·000 | 0·000 | 0·000 | 0·0000 | 0·0000 | 0·0000 | 0·000 |
| 0·1 | 0·0143 | 0·0012 | −0·0010 | −0·139 | 0·026 | −0·109 | −0·0015 | −0·0212 | 0·0142 | −0·0014 |
| 0·2 | 0·0527 | 0·0048 | −0·0038 | −0·2514 | 0·050 | −0·109 | −0·0059 | −0·0564 | 0·0520 | −0·0101 |
| 0·3 | 0·1042 | 0·0109 | −0·0081 | −0·3195 | 0·0729 | −0·108 | −0·0128 | −0·0674 | 0·1015 | −0·0290 |
| 0·4 | 0·1553 | 0·0190 | −0·0134 | −0·3414 | 0·0925 | −0·107 | −0·0217 | −0·0502 | 0·1491 | −0·0556 |
| 0·5 | 0·1954 | 0·0290 | −0·0192 | −0·3258 | 0·1086 | −0·107 | −0·0319 | −0·0208 | 0·1846 | −0·0843 |
| 0·6 | 0·2184 | 0·0405 | −0·0249 | −0·2857 | 0·1209 | −0·107 | −0·0427 | 0·0066 | 0·2034 | −0·1097 |
| 0·7 | 0·2236 | 0·0533 | −0·0230 | −0·2338 | 0·1292 | −0·106 | −0·0534 | 0·0259 | 0·2054 | −0·1282 |
| 0·9 | 0·1922 | 0·0814 | −0·0364 | −0·1297 | 0·1354 | −0·104 | −0·0724 | 0·0394 | 0·1732 | −0·1407 |
| 1·1 | 0·1347 | 0·1102 | −0·0368 | −0·0518 | 0·1303 | −0·102 | −0·0858 | 0·0330 | 0·1197 | −0·1274 |

| sin θ/λ | $f_{2p,3d}(3)$ | $f_{3p,4p}(2)$ | $f_{2p,4p}(2)$ | $f_{4p,3d}(1)$ | $f_{3d,3d}(2)$ | $f_{3d,3d}(4)$ | $f_{4p,4p}(2)$ | $\Sigma\lvert f_{ii}\rvert^2$ | $\mathscr{F}$ | $32-\mathscr{F}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 0·0 | 0·0000 | 0·000 | 0·000 | 0·0000 | 0·000 | 0·0000 | 0·0000 | 32·00 | 32·00 | 0·00 |
| 0·1 | 0·0001 | 0·044 | 0·000 | 0·0592 | 0·005 | 0·0002 | 0·1710 | 28·07 | 30·41 | 1·59 |
| 0·2 | 0·0004 | 0·089 | −0·001 | 0·0619 | 0·030 | 0·0026 | 0·1987 | 23·39 | 27·25 | 4·75 |
| 0·3 | 0·0014 | 0·1323 | −0·001 | 0·0248 | 0·066 | 0·0103 | 0·0910 | 19·06 | 24·61 | 7·39 |
| 0·4 | 0·0031 | 0·1550 | −0·002 | −0·0146 | 0·108 | 0·0237 | 0·0217 | 15·27 | 21·98 | 10·02 |
| 0·5 | 0·0057 | 0·1530 | −0·003 | −0·0388 | 0·1478 | 0·0404 | −0·0020 | 12·48 | 19·46 | 12·54 |
| 0·6 | 0·0091 | 0·1332 | −0·0042 | −0·0475 | 0·1791 | 0·0573 | −0·0042 | 10·69 | 17·27 | 14·73 |
| 0·7 | 0·0132 | 0·1052 | −0·0053 | −0·0457 | 0·1965 | 0·0720 | −0·0020 | 9·53 | 15·41 | 16·59 |
| 0·9 | 0·0227 | 0·0521 | −0·0070 | −0·0299 | 0·1895 | 0·0900 | +0·0025 | 7·92 | 12·41 | 19·59 |
| 1·1 | 0·0327 | 0·0203 | −0·0073 | −0·0137 | 0·1454 | 0·0936 | +0·0037 | 6·48 | 10·10 | 21·90 |

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# Short Communications

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## Rare earth ion radii in the iron garnets.

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In examination of the rare earth-iron garnets, it has been found that the relative effective CN(12) radii (Geller, 1957) derived from the rare earth perovskites are applicable. (These have not been obtained as yet for any of the rare earth ions smaller than Gd.) The iron garnets of the trivalent ions of Sm, Eu, Gd and Y were carefully prepared in ceramic form by a method described elsewhere (Gilleo & Geller, 1958). The lattice constants of these specimens are listed in Table 1; listed also are those given by Bertaut & Forrat (1957).

Table 1. *Lattice constants of some rare earth-iron garnets*

$a_0$ (Å)

| Dodecahedral ion | Mitchell | See text | Bertaut & Forrat |
|---|---|---|---|
| $Sm^{3+}$ | 12·528 | 12·530 | 12·524 |
| $Eu^{3+}$ | 12·498 | 12·498 | 12·518 |
| $Gd^{3+}$ | 12·474 | 12·471 | 12·479 |
| $Y^{3+}$ | 12·376 | 12·376 | 12·376 |

Although it is possible that the effective sizes of atoms may change differently with the same change in coordination,* it is somewhat less likely to happen for closely related rare earth ions than for such ions as $Fe^{3+}$ and $Al^{3+}$.† Though few, the results obtained by use of the radius differences are gratifying. The relative effective CN(12) radii for the ions in the order of the Table 1 listing

are 1·310, 1·304, 1·299, 1·281 Å. The lattice constant difference per 0·010 Å change in radius is about 0·053 Å. Using $Y_3Fe_2(FeO_4)_3$ (this has been made and measured many times) as standard, the reproduced lattice constants obtained are as shown in the third column of Table 1. The agreement with the measured values of the present work is good and may indicate a larger (than $Eu^{3+}$) ion impurity in the Eu-iron garnet reported by Bertaut & Forrat (1957).

It is now possible to obtain the relative effective CN(12) radii of some of the other trivalent rare earth ions (i.e. those not thus far obtained from the perovskites) from values of garnet lattice constants. Values of $a_0$ obtained for crystals of $Er_3Fe_2(FeO_4)_3$ grown by Nielsen & Dearborn (1958) and of $Lu_3Fe_2(FeO_4)_3$ made in ceramic form are 12·352 and 12·280 Å respectively leading to values 1·276 and 1·262 Å for the relative CN(12) radii of $Er^{3+}$ and $Lu^{3+}$ respectively.

It is noteworthy that similar reasoning led to an exact prediction of the lattice constant of $Mn_3Fe_2Si_3O_{12}$ (Geller & Miller, 1959).

* Rare earth ions have CN(8) in the garnets.

† In $Y_3Fe_2(FeO_4)_3$, the ratio of tetrahedral to octahedral Fe–O distances is 0·94; in $Y_3Al_2(AlO_4)_3$ the analogous Al–O ratio is 0·91.

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