

The Atomic Incoherent Scattering Intensities of Boron, Oxygen and Carbon

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The atomic incoherent scattering intensities of boron, oxygen and carbon in their spectroscopic ground states have been computed. Hartree-Fock wave functions were used in evaluating the complete scattering function. The results obtained are found to differ substantially from previously available values.

In X-ray investigations of the structures of non-crystalline materials, reliable values of the incoherent scattering intensity are required. The availability of Hartree-Fock wave functions and automatic computing equipment has permitted the calculation of atomic incoherent scattering intensities using the complete scattering function including off-diagonal elements (Waller & Hartree, 1929). Recently, a calculation of this type has been made for carbon in the valence state by Keating & Vineyard (1956). Their results differed considerably from previously available values (Compton & Allison, 1935) and agreed quite well with experimental values (Laval, 1939). In view of this, the atomic incoherent scattering intensities for boron, oxygen and carbon in their respective ground states have been computed from the complete scattering function.

Omitting the Breit-Dirac correction, the incoherent scattering intensity for an atom, in terms of the Thomson electron, is

$$I_{\text{inc}} = I_{\text{tot}} - I_{\text{coh}}, \quad (1)$$

where

$$\left. \begin{aligned} I_{\text{tot}} &= \int |\psi_n|^2 \left| \sum_j \exp [i\mathbf{k} \cdot \mathbf{r}_j] \right|^2 dv \\ I_{\text{coh}} &= \int |\psi_n|^2 \sum_j \exp [i\mathbf{k} \cdot \mathbf{r}_j] dv \end{aligned} \right\} \quad (2)$$

In equations (2), ψ_n is the wave function for the normal state of the atom, \mathbf{r}_j the position vector of the j th electron in the atom, and \mathbf{k} the conventional scattering vector, so that $k = 4\pi(\sin \theta)/\lambda$. For any atom the results can be written in terms of the scattering function \mathcal{F} , where $I_{\text{inc}} = Z - \mathcal{F}$ and Z is the number of electrons in the atom.

The calculations were carried out using the wave function of the spectroscopic ground state for each of the atoms considered. The form of the scattering function is given below for the configuration and normal atomic state which was used.

Boron: $1s^2 2s^2 2p, {}^2P_{\frac{1}{2}}$.

$$\mathcal{F} = 2f_{1s}^2 + 2f_{2s}^2 + f_{2p}^2 + 4f_{1s2s}^2 + 2f_{1s2p}^2 + 2f_{2s2p}^2. \quad (3)$$

Oxygen: $1s^2 2s^2 2p^4, {}^3P_2$.

$$\mathcal{F} = 2f_{1s}^2 + 2f_{2s}^2 + 4f_{2p}^2 + 4f_{1s2s}^2 + 8f_{1s2p}^2 + 8f_{2s2p}^2 + \frac{31}{5}f_{2p2p}^2 \quad (4)$$

Carbon: $1s^2 2s^2 2p^2, {}^3P_0$.

$$\mathcal{F} = 2f_{1s}^2 + 2f_{2s}^2 + 2f_{2p}^2 + 4f_{1s2s}^2 + 4f_{1s2p}^2 + 4f_{2s2p}^2 + 2f_{2p2p}^2. \quad (5)$$

The terms f_{1s} , etc., are defined in the paper by Keating & Vineyard (1956). The value of \mathcal{F} for oxygen was found to be dependent upon the relative orientation of \mathbf{k} and the axis of the atom. Equation (4) represents the average over all directions of \mathbf{k} . Our calculation for carbon differs from that of Keating and Vineyard who considered the valence state $1s^2 2s^2 2p^3$, term value 5S .

Hartree-Fock one-electron wave functions were employed in the evaluation of the f 's. Those for boron

Table 1. Incoherent scattering intensities of boron, oxygen and carbon. (Breit-Dirac correction omitted)

$(\sin \theta)/\lambda$ (\AA^{-1})	Incoherent scattering intensity		
	Boron	Oxygen	Carbon
0.00	0.000	0.000	0.000
0.05	0.439	0.272	0.355
0.10	1.381	0.966	1.203
0.15	2.234	1.865	2.141
0.20	2.779	2.777	2.914
0.25	3.084	3.594	3.451
0.30	3.264	4.275	3.826
0.35	3.395	4.819	4.068
0.40	3.510	5.243	4.238
0.45	3.621	5.569	4.372
0.50	3.731	5.818	4.486
0.55	3.840	6.014	4.589
0.60	3.945	6.170	4.686
0.65	4.047	6.299	4.780
0.70	4.144	6.408	4.871
0.75	4.235	6.505	4.960
0.80	4.319	6.593	5.044
0.85	4.396	6.674	5.125
0.90	4.467	6.750	5.202
0.95	4.531	6.823	5.274
1.00	4.588	6.894	5.341
1.10	4.684	7.025	5.462
1.20	4.760	7.148	5.564
1.30	4.818	7.259	5.648
1.40	4.862	7.361	5.718
1.50	4.895	7.451	5.774

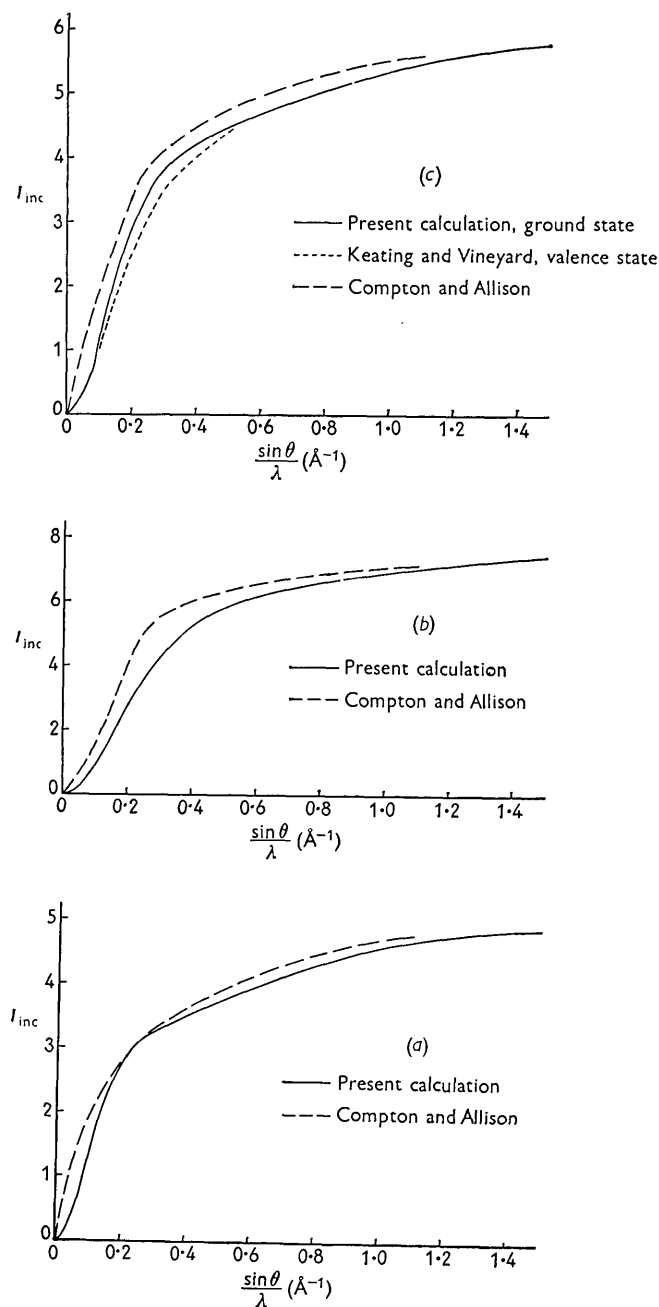


Fig. 1. Atomic incoherent scattering intensity of (a) boron, (b) oxygen and (c) carbon. (Breit-Dirac correction omitted).

were obtained from Glembotskii, Kibartas & Iutsis (1956), for oxygen from Hartree, Hartree & Swirles (1939), and for carbon from Jucys (1939). The calculations were carried out with the aid of an IBM 650 digital computer.

The calculated atomic incoherent scattering intensities are listed in Table 1 as a function of $(\sin \theta)/\lambda$. In Figs. 1a, b and c the present results for boron, oxygen and carbon, respectively, are compared with the previously available values and, in the case of carbon, with the valence state results of Keating & Vineyard (1956). It can be seen from the figures that the results of the present calculations differ considerably from the values given by Compton & Allison (1935). That the present values are, in general, the lower is to be expected from the inclusion of off-diagonal elements in the calculation. The new and old values differ by about 30% to 40% at $(\sin \theta)/\lambda = 0.1 \text{ \AA}^{-1}$ and about 5% to 6% at $(\sin \theta)/\lambda = 0.6 \text{ \AA}^{-1}$. The present ground state values and Keating & Vineyard's valence state values differ noticeably only in the range of $(\sin \theta)/\lambda$ from 0.1 \AA^{-1} to 0.5 \AA^{-1} .

The authors have learned from Dr Arthur J. Freeman of Watertown Arsenal that he has computed the incoherent scattering intensities for a large number of atoms, including oxygen. We have had the opportunity of comparing our results for oxygen with Dr Freeman's and find that, although calculated for somewhat different states, they agree to well within usable accuracy. We should like to thank Messrs. James Seward and Duncan Preece of this laboratory for programming the computations for the IBM 650.

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