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The Complete Incoherent Scattering Function for Carbon†

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(Received 16 April 1956)

The frequent use of organic substances to put X-ray intensities on an absolute basis gives special importance to the calculation of the incoherent scattering from carbon. Calculations by Berghuis *et al.* for the coherent scattering showed appreciable divergences from older work, and we were motivated to extend the calculations to the incoherent scattering.

The wave functions of Jucys computed by the Hartree-Fock method with exchange were used in computing the complete incoherent scattering function for the configuration $1s^2 2s 2p^3$ and term value 5S . The calculations show that the incoherent scattering at small and intermediate values of $(\sin \theta)/\lambda$ is appreciably less than previously predicted and more in agreement with the values found experimentally by Laval.

The frequent use of organic substances to put X-ray intensities on an absolute basis gives special importance to the calculation of the incoherent scattering from carbon. Berghuis *et al.* (1955) have recently calculated the atomic scattering factor for carbon, using the wave functions of Jucys (1947), which had been computed by the Hartree-Fock method with exchange. These calculations for the coherent scattering showed appreciable divergences from the older data, and we were thus motivated to extend the calculations to the incoherent scattering. Jucys' wave functions, which appear to be the best now available for carbon, were used.

The incoherent scattering in electron units can be written as $B^{-3}[Z - \mathcal{F}]$ (James, 1948, chap. 9).‡ B is the Breit-Dirac recoil correction factor, Z is the atomic number of the atom, and \mathcal{F} , the incoherent scattering function, is given by

$$\mathcal{F} = \sum_{j, k=1}^Z |f_{jk}|^2 \quad (1)$$

(James, 1948, chap. 3).

Here

$$f_{jk} = \int \psi_j^*(\mathbf{r}) \alpha_j^* e^{i\mathbf{k} \cdot \mathbf{r}} \psi_k(\mathbf{r}) \alpha_k dv, \quad (2)$$

where $\psi_j(\mathbf{r})$ is the spatial part of the j th one-electron wave function, α_j is the corresponding spin function, and \mathbf{k} is the difference between incoming and outgoing wave vectors ($k = 4\pi \sin \theta / \lambda$). We have calculated

\mathcal{F} for the configuration $1s^2 2s 2p^3$, and term value 5S . Because the wave functions of this configuration transform orthogonally on axis rotation, \mathcal{F} is independent of the orientation of \mathbf{k} . Furthermore, the hybridized atomic orbitals leading to tetrahedral bonding, as in diamond and the saturated hydrocarbons, are also formed by an orthogonal transformation on this configuration (Eyring, Walter & Kimball, 1944). Thus \mathcal{F} is also a correct zero-order approximation for carbon in these covalent compounds.

For this configuration and term, \mathcal{F} reduces to the form

$$\mathcal{F} = 2f_{1s}^2 + f_{2s}^2 + 3f_{2p}^2 + 2f_{1s2s}^2 + 6f_{1s2p}^2 + 6f_{2s2p}^2 + 6f_{2p2p}^2, \quad (3)$$

where

$$\left. \begin{aligned} f_{1s} &= \int_0^\infty R_{1s}(r) j_0(kr) R_{1s}(r) r^2 dr, \\ f_{2s} &= \int_0^\infty R_{2s}(r) j_0(kr) R_{2s}(r) r^2 dr, \\ f_{2p} &= \int_0^\infty R_{2p}(r) j_0(kr) R_{2p}(r) r^2 dr, \\ f_{1s2s} &= \int_0^\infty R_{1s}(r) j_0(kr) R_{2s}(r) r^2 dr, \\ f_{1s2p} &= \int_0^\infty R_{1s}(r) j_1(kr) R_{2p}(r) r^2 dr, \\ f_{2s2p} &= \int_0^\infty R_{2s}(r) j_1(kr) R_{2p}(r) r^2 dr, \\ f_{2p2p} &= \int_0^\infty R_{2p}(r) j_2(kr) R_{2p}(r) r^2 dr. \end{aligned} \right\} \quad (4)$$

† Under the auspices of the U.S. Atomic Energy Commission.

‡ The inverse second power would appear if numbers of quanta were being counted.

Table 1. Calculation of the incoherent scattering functions

$(\sin \theta)/\lambda$	f_{1s}	f_{2s}	f_{2p}	f_{1s2s}	f_{1s2p}	f_{2s2p}	f_{2p2p}	\mathcal{F}
0.0	1.000	1.000	0.999	0.0000	0.0000	0.0000	0.0000	6.000
0.1	0.993	0.816	0.779	0.0028 ₄	0.0337 ₉	-0.2830 ₇	0.0624 ₃	4.970
0.2	0.972	0.452	0.405	0.0180 ₂	0.0555 ₃	-0.3394 ₃	0.1759 ₆	3.489
0.3	0.938	0.170	0.164	0.0390 ₅	0.0721 ₈	-0.2442 ₄	0.1857 ₃	2.468
0.4	0.895	0.031	0.054	0.0614 ₃	0.0814 ₉	-0.1371 ₀	0.1824 ₉	1.973
0.5	0.843	-0.015	0.012	0.0811 ₆	0.0839 ₂	-0.0636 ₂	0.1055 ₃	1.568
0.6	0.786	-0.018	-0.002	0.0959 ₃	0.0812 ₁	-0.0226 ₁	0.0717 ₉	1.328
0.7	0.725	-0.009	-0.006	0.1051 ₁	0.0751 ₀	-0.0019 ₅	0.0479 ₈	1.121
0.8	0.665	0.001	-0.006	0.1090 ₆	0.0672 ₀	0.0072 ₁	0.0320 ₁	0.942
0.9	0.604	0.009	-0.005	0.1087 ₅	0.0587 ₄	0.0104 ₂	0.0216 ₃	0.777
1.0	0.547	0.014	-0.004	0.1052 ₃	0.0505 ₂	0.0109 ₂	0.0149 ₂	0.638
1.1	0.492	0.017	-0.003	0.0996 ₄	0.0430 ₃	0.0101 ₅	0.0114 ₂	0.516
1.2	0.442	0.018	-0.002	0.0927 ₂	0.0364 ₃	0.0089 ₁	0.0072 ₇	0.417
1.3	0.395	0.018	-0.002	0.0852 ₃	0.0307 ₄	0.0076 ₇	0.0054 ₂	0.333

Here j_n is the n th-order spherical Bessel function, and $R_{1s}(r)$, $R_{2s}(r)$, etc., are the radial factors in the one-electron wave functions.

The first three f 's of (4) were kindly supplied by Dr MacGillavry from the work of Berghuis *et al.* The remaining four f 's were expressed as integrals of products of circular functions and Jucys' radial wave functions, and a harmonic analysis was then carried out by numerical integration, using an interval of 0.03945 atomic units.

Table 1 gives the f 's and the incoherent scattering function. The first three f 's of equation (3) can be considered as diagonal terms and the remaining four as non-diagonal terms of a scattering matrix. In older work (Compton & Allison, 1935) the non-diagonal terms were neglected. The incoherent scattering, $Z - \mathcal{F}$,

without the Breit-Dirac correction, is plotted in Fig. 1 as given by Compton & Allison (dashed line), as computed from Jucys' wave functions but including the diagonal terms only (broken line), and as computed from Jucys' wave functions including diagonal and non-diagonal terms (solid line).

It is evident that the inclusion of the non-diagonal terms, which are often ignored, appreciably reduces the incoherent scattering at small and intermediate values of $(\sin \theta)/\lambda$. For $(\sin \theta)/\lambda = 0.6$, the approximate limit for Cu $K\alpha$ radiation, the present calculations predict an incoherent scattering 7% less than that given by Compton & Allison.

Measurements of the diffuse scattering from diamond (Laval, 1939) have shown discrepancies from the values given by Compton & Allison in the same direction as our calculations, though of somewhat larger magnitude.

The authors wish to thank Mr Stuart S. Rideout, Dysart A. Ravenhall, and Miss Betty Oppenheim for programming this problem for the B. N. L. Computer. They are also indebted to Dr MacGillavry for making the results of her computations available to us.

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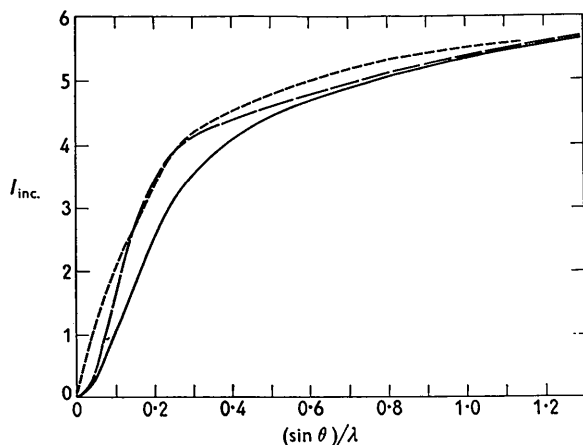


Fig. 1. The incoherent scattering from carbon (without the Breit-Dirac correction).

Dashed line: from Compton & Allison.

Broken line: from present calculations with diagonal terms only.

Full line: from present calculations with non-diagonal and diagonal terms.