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Remarks on the Scattering of X-Rays by Gases and Crystals

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§§1 and 2: Woo's most recent formulas for the separation of the diffusely scattered radiation from polyatomic gases and simple crystals into coherent and incoherent radiation are discussed. It is shown that Woo's formulas for the total scattered radiation reduces to the author's respective classical formulas when $\alpha(=h/mc\lambda)$ is made zero. This removes the objection made by the author in a previous note. It is shown that the incoherent scattered radiation depends upon the root mean square of the E's while the coherent radiation depends upon the arithmetic mean of the E's, thus giving a mathematical distinction between the incoherent and coherent radiation even in the classical theory. §3: Evidence is presented in favor of the true atom form factor f of an atom in a crystal (sylvine) being a function of the temperature of the crystal. The average electron distribution about the center of an atom in a crystal must be a function of the violence of the thermal agitation of the atom. At 0°K the electron distribution in an atom of sylvine is more diffuse than in an atom of argon. As the temperature rises above 0°K the electron distribution becomes less diffuse and finally becomes like that of argon at about room temperature. §4: It is shown that the $S_g=(S+F^2/Z)_c$ relation can be replaced by a relation between experimental quantities alone—otherwise, an empirical relation. §5: A digression on the philosophy of physics in which it is noted that the empirical relation of §4 contains no vestige of the Thomson or any other theory of x-rays. This supports the view that physical laws express relations between pointer readings. §6: The classical theory for the diffuse scattering of x-rays by a crystal consisting of atoms of several kinds is worked out and a formula obtained. By the use of Woo's method, the formulas for the coherent and incoherent radiation are also obtained. The restrictions upon these formulas are discussed.

§1. Polyatomic Gases

THE following papers on the scattering of x-rays by gases and crystals have appeared in the Physical Review during recent months: Paper I by Jauncey,[1] Paper II by Woo,[2] Paper III by Jauncey[3] and Paper IV by Woo.[4] In this section the author wishes to comment on Paper IV by Woo. In Paper I, Jauncey discusses the classical theory of the scattering of x-rays from polyatomic gases whose molecules consist of n atoms of one kind and arrives at the formula[5]

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[1] G. E. M. Jauncey, Phys. Rev. **38**, 194 (1931).

[2] Y. H. Woo, Phys. Rev. **39**, 555 (1932).

[3] G. E. M. Jauncey, Phys. Rev. **39**, 561 (1932).

[4] Y. H. Woo, Phys. Rev. **41**, 21 (1932).

[5] For definition of S *see*, G. E. M. Jauncey and P. S. Williams, Phys. Rev. **41**, 127 (1932).

$$S_{\text{class}} = 1 + (Z+1)f'^2/Z^2 + (f^2/nZ)\sum_{r=1}^{n}{}' \sum_{s=1}^{n}{}'(\sin kl_{rs})/kl_{rs} \tag{1}$$

where

$$k = (4\pi \sin \tfrac{1}{2}\phi)/\lambda \tag{2}$$

and

$$f'^2 = f^2 - \left(Z \sum_{r=1}^{Z} E_r^2 - f^2\right)/(Z-1). \tag{3}$$

In Eqs. (1) and (3) f is the true atom form factor for each atom in the molecule of the gas and l_{rs} is the distance between the rth and sth atoms of a molecule. The quantities E_r are defined in a paper by Jauncey[6] on the diffuse scattering of x-rays by solids. In Paper II Woo takes account of the Compton effect and separates the scattered radiation into coherent and incoherent parts. The result of Woo's separation is to replace Eq. (1) above by

$$S = S_{\text{incoh.}}/(1 + \alpha \text{ vers } \phi)^3 + S_{\text{coh.}} \tag{4}$$

where α is the Compton quantity $h/mc\lambda$. In Paper II Woo gives

$$S_{\text{incoh.}} = 1 - f'^2/Z^2 \tag{5}$$

and

$$S_{\text{coh.}} = (f'^2/nZ)\sum_{r=1}^{n}{}' \sum_{s=1}^{n}{}'(\sin kl_{rs})/kl_{rs} \tag{6}$$

for polyatomic gases whose molecules consist of n atoms of one kind. In Paper III the author objected to Woo's formula for $S_{\text{coh.}}$ because the author believes that a formula which takes account of the separation into coherent and incoherent scattered radiation must reduce to the classical formula when α is put equal to zero. In other words, the right side of Eq. (1) must equal $S_{\text{incoh.}}+S_{\text{coh.}}$, or, as we may write it,

$$S_{\text{class.}} = S_{\text{incoh.}} + S_{\text{coh.}}. \tag{7}$$

This is not the case when Woo's formulas as given in Eqs. (5) and (6) are used.

Before considering Woo's Paper IV, the author wishes to introduce a new symbol f''. The true atom form factor f is defined by[6]

$$f = \sum_{r=1}^{Z} E_r \tag{8}$$

or, in other words, f/Z is the arithmetic mean of the E's. The new quantity f'' is to be defined by

$$f''^2 = Z\sum_{r=1}^{Z} E_r^2 \tag{9}$$

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[6] G. E. M. Jauncey, Phys. Rev. **37**, 1193 (1931).

or, in other words, f''/Z is the root mean square of the E's. Eq. (3) now becomes

$$(Z-1)f'^2 = Zf^2 - f''^2 \tag{10}$$

and Eq. (1) may be written in the form

$$S_{\text{class.}} = 1 - f''^2/Z^2 + (f^2/Z)\left\{1 + (1/n)\sum_{r=1}^{n}{}' \sum_{s=1}^{n}{}'(\sin kl_{rs})/kl_{rs}\right\}. \tag{11}$$

From the point of view of the classical theory the author has no preference as between Eq. (1) and Eq. (11). The only difference is one of symbols.

In Paper IV Woo replies to the objections raised by the author in Paper III and arrives at Eq. (4) together with the defining equations

$$S_{\text{incoh.}} = 1 - f''^2/Z^2 \tag{12}$$

and

$$S_{\text{coh.}} = (f^2/Z)\left\{1 + (1/n)\sum_{r=1}^{n}{}' \sum_{s=1}^{n}{}'(\sin kl_{rs})/kl_{rs}\right\} \tag{13}$$

which replace Eqs. (5) and (6). It is seen that these formulas for $S_{\text{incoh.}}$ and $S_{\text{coh.}}$ satisfy Eq. (7) and so the author's objections are removed. Eq. (13) takes the special forms

$$S_{\text{coh.}} = (f^2/Z)\{1 + (\sin kl)/kl\} \tag{14}$$

for a diatomic gas and

$$S_{\text{coh.}} = (f^2/Z)\{1 + (3 \sin kl)/kl\} \tag{15}$$

for a gas each of whose molecules consist of similar atoms with their centers at the corners of a regular tetrahedron. The quantity l is the distance between two atoms in the same molecule. If there are thermal vibrations of the atoms in the molecules of a gas, then, comparing with the author's Paper I, it is seen that $(\sin kl)/kl$ in Eqs. (14) and (15) is replaced by

$$\{(\sin kl_0)/kl_0\}\exp(-ky^2/4)$$

where y is the most probable change in the separation of any pair of atoms in a molecule from the mean separation l_0.

§2. SIMPLE CRYSTALS

The classical theory of the diffuse scattering of x-rays by simple cubic crystals consisting of atoms of one kind has been worked out by Jauncey and Harvey.[7] This theory leads to the formula

$$S_{\text{class.}} = 1 - f''^2/Z^2 + (f^2 - F^2)/Z \tag{16}$$

in virtue of Eq. (10). The quantity F is the atom form factor as referred to a lattice point, but not to the center of the atom. In Paper IV Woo separates

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[7] G. E. M. Jauncey and G. G. Harvey, Phys. Rev. **37**, 1203 (1931).

the diffusely scattered radiation from a crystal into two parts according to Eq. (4), where $S_{\text{incoh.}}$ is given by Eq. (12) and

$$S_{\text{coh.}} = (f^2 - F^2)/Z. \tag{17}$$

It is seen that the right sides of Eqs. (12), (16), and (17) satisfy Eq. (7).

From Eqs. (12), (13), (16), it is seen that through f the coherent portion of the scattered radiation depends upon the arithmetic mean of the E's and that through f'' the incoherent portion depends upon the root mean square of the E's. This seems to give a mathematical distinction between the coherent and incoherent radiation even in the classical theory because the distinction between f'' and f remains even if $\alpha(=h/mc\lambda)$ is zero.

§3. TEMPERATURE AND THE TRUE ATOM FORM FACTOR

In his formulas for the scattering of x-rays by crystals, the author has preferred to write F for the atom form factor as referred to a lattice point, but not to the atom center, instead of in the manner fe^{-M}, where f is the true atom form factor (which is due to the electron distribution relative to the center of the atom) and e^{-M} is the Debye[8] or Waller[9] temperature factor. In the derivation of the classical formulas for the scattering of x-rays by a solid and by a crystal, Jauncey[6,7] notes two different orders of velocity—the velocity of an electron in an atom relative to the center of the atom and the velocity of thermal agitation of the center of an atom about the lattice point with which the atom is associated. The atom may be likened to a planet with an electron atmosphere. The electrons of the atmosphere will pass through all their configurations many times while the atom as a whole is performing one vibration about its lattice point. The effective atom form factor F of an atom in a crystal is made up of two factors—f the true atom form factor and H the temperature factor. The second factor H is due to the changing configurations of the centers of the atoms relative to their respective lattice points, caused by the thermal motions of the atoms in the crystal. The author has made no special assumptions[6] concerning the form of H. Since values of $F(=fH)$ are determined experimentally by measurements of the integrated reflection from crystals, it is only necessary for Eqs. (16) and (17) to include F but not to include the form of H. The form of H is not as yet accurately known. According to James and Brindley,[10] H is fairly well given for sylvine by Waller's formula[9] at low temperatures but is not given by this formula at high temperatures.

In the Debye-Waller formula

$$F = fe^{-M} \tag{18}$$

it is postulated that the true atom form factor f is not affected by the heat motions of the atoms, or, in other words, that the electron distribution in an atom is independent of the violence of the thermal agitation of the atom

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[8] P. Debye, Ann. d. Physik **43,** 49 (1914).

[9] I. Waller, Zeits. f. Physik **17,** 398 (1923).

[10] R. W. James and G. W. Brindley, Proc. Roy. Soc. **A121,** 155 (1928).

amongst the surrounding atoms. If we think of an atom in a crystal as being held to a lattice point by a quasi-elastic force, the atom will be acted upon by no force when at a lattice point and may be considered when at this point as being undistorted. However, if the atom is displaced from its lattice point, some amount of distortion in the electron distribution of the atom will occur. The f value for the atom will be the result of an average electron distribution for the electron configurations of the atom about its own center taken over many (comparatively slow) thermal vibrations of the atom about its lattice point. As the temperature rises the average electron distribution will become more and more distorted, if we measure the distortion as a departure from the electron distribution when the atoms are all at rest at their lattice points. There is no actual attractive force on a given atom towards its lattice point, but this apparent force is due to the forces of the neighboring atoms upon the given atom. As the thermal vibrations of the atoms become more violent, the atoms approach each other more closely and the electron atmospheres of the atoms become more distorted. It seems therefore that the average electron distribution about the center of an atom in a lattice should be a function of the temperature. Accordingly, the true atom form factor f should be a function of the temperature. The situation is somewhat the same as the case in the kinetic theory of gases where the quantity b in van der Waal's equation has been found to be a function of the temperature.[11] As the temperature rises and the impacts between molecules become more violent, the molecules penetrate each other more and more and so the distortion of the molecules due to impacts increases with the temperature.

Jauncey and Harvey[12] have shown that the relation

$$S_{\text{gas}} = (S + F^2/Z)_{\text{cryst}}. \tag{19}$$

holds very well for argon and sylvine at room temperature. On the other hand Jauncey and Williams[5] have found that the $(S+F^2/Z)$ values for sodium fluoride at room temperatures are consistently lower than the S values for neon. Now from Eqs. (4), (12), and (17) it follows that for a crystal

$$S + F^2/Z = (1 - f''^2/Z^2)/(1 + \alpha \operatorname{vers} \phi)^3 + f^2/Z \tag{20}$$

so that, if f and f'' are not functions of the temperature, $(S+F^2/Z)$ should be independent of the temperature. Jauncey and Harvey[13] have measured the S values for sylvine at temperatures of 90°K and 300°K and, using James and Brindley's F values[10] for sylvine at these two temperatures, have found that the $(S+F^2/Z)$ values at 90°K are distinctly less than those at 300°K. According to Eq. (20) the implication of this is that either or both f and f'' are functions of the temperature. If for simplicity we for the present assume $f''=f$ (as is the case if all the E's are equal[14]), then, since $(S+F^2/Z)$ is less at

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[11] See K. F. Herzfeld, Handb. d. Physik. XXII, p. 399.

[12] G. E. M. Jauncey and G. G. Harvey, Phys. Rev. **38**, 1071 (1931).

[13] G. E. M. Jauncey and G. G. Harvey, Phys. Rev. **38**, 1925 (1931).

[14] G. E. M. Jauncey, Phys. Rev. **38**, 1 (1931).

90°K than at 300°K, f is less at 90°K than at 300°K. This means that the average electron distribution in an atom of sylvine departs more and more from the electron distribution in an argon atom as the temperature falls below room temperature. It is just a matter of good fortune that at room temperature the average electron distribution in an atom of sylvine is the same as that in an atom of argon. In the case of sodium fluoride it is probable that room temperature is too low a temperature for the electron distribution in an atom of this crystal to be the same as that for neon. It therefore appears that at temperatures approaching absolute zero, the f values for a crystal (such as KCl or NaF) are less than those for the corresponding gas (argon or neon). Consequently, the electron distribution in an atom of a crystal at absolute zero is more diffuse than in the atom of the corresponding gas. As the temperature rises above absolute zero, the atoms of the crystal vibrate amongst one another with increasing violence with the result that the average electron distribution about the center of each atom becomes less diffuse and finally at high temperatures becomes like the average electron distribution about the center of an atom of the corresponding gas.

It should be remembered that the atoms in crystals like NaF and KCl are ionized. It might be expected that on this account the electron distributions in the atoms of the respective crystals at absolute zero would differ from the electron distributions in the atoms of the corresponding gases.

§4. An Empirical Relation

In a recent report Wollan[15] quotes the author as stating that the relation

$$S_{\text{gas}} = (S + F^2/Z)_{\text{cryst.}} \tag{21}$$

represents a relation which could have been established empirically without the aid of theory. As Dr. Wollan learned of this in private conversation with the author it seems worth while to discuss the statement in greater detail.

For simplicity we shall assume that the scattering occurs without change of wave-length as is pretty nearly the case for argon and sylvine. Crowther's formula[16] for the intensity of x-rays scattered in a direction ϕ from a slab of material whose thickness is t is

$$I_\phi = (AIt/R^2 \cos \tfrac{1}{2}\phi)\cdot s \tag{22}$$

where I is the intensity per unit area of the rays transmitted through the slab when held in the Crowther position, A is the area of the ionization chamber window, R is the distance of the window from the slab, and s is the linear spatial scattering coefficient per unit solid angle in the direction ϕ. The quantity s in Eq. (22) is thus measured and defined in terms of experimental quantities and may therefore itself be considered an experimental quantity. Having found s by means of Eq. (22) we divide by ρ the density of the scattering material and obtain s/ρ which we shall call the mass spatial scattering

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[15] E. O. Wollan, Rev. Mod. Phys. **4**, 205 (1932).

[16] J. A. Crowther, Proc. Roy. Soc. **A86**, 478 (1912).

coefficient per unit solid angle in the direction ϕ. The quantity s/ρ has been determined for argon by Wollan[17] and for sylvine by Harvey.[18] Referring to the paper by Jauncey and Williams,[5] we see that the relation between S the scattering factor per electron and s/ρ the mass spatial scattering coefficient is

$$S = \frac{s/\rho}{(NZ/W)\cdot(e^4/m^2c^4)\cdot(1+\cos^2\phi)/2} \tag{23}$$

where N is Avogadro's number, Z is the number of electrons in an atom of the scatterer, W is its atomic weight, and e, m and c have their usual significance.

We shall now introduce the quantities r the linear reflection coefficient and r/ρ the mass reflection coefficient of a crystal for x-rays. The mass reflection coefficient is given in terms of experimental quantities by

$$r/\rho = (i_\phi \omega \cos \tfrac{1}{2}\phi)/\rho I t \tag{24}$$

where ω is the angular speed at which the crystal is turned through the Bragg reflection position, i_ϕ is the total energy of the reflected x-rays entering the ionization chamber, I is the energy per unit time per unit area penetrating the crystal, and t is the thickness of the slab of crystal.[19] According to the classical theory of reflection of x-rays from a mosaic crystal[19]

$$r/\rho = \tfrac{1}{2}\cdot\frac{\rho N^2}{W^2}\cdot\lambda^3F^2\cdot\frac{e^4}{m^2c^4}\cdot\frac{1+\cos^2\phi}{\sin\phi\cos\frac{1}{2}\phi}. \tag{25}$$

From Eq. (25) we may obtain an expression for F^2/Z. Upon substituting this expression for F^2/Z, and also the right side of Eq. (23) for S_{gas} and for $S_{\text{cryst.}}$ in Eq. (21), we note that the expression $(NZ/W)\cdot(e^4/m^2c^4)\cdot(1+\cos^2\phi)/2$ factors out, leaving us with

$$(s/\rho)_{\text{gas}} = (s/\rho)_{\text{cryst.}} + \frac{W\sin\phi\cos\frac{1}{2}\phi}{\lambda^3\rho N}\cdot(r/\rho)_{\text{cryst.}}. \tag{26}$$

Now in a simple cubic crystal the principal grating space d is given by

$$d^3 = W/\rho N. \tag{27}$$

This equation together with Bragg's law

$$n\lambda = 2d\sin\tfrac{1}{2}\phi \tag{28}$$

gives

$$\lambda^3\rho N/W = (8\sin^3\tfrac{1}{2}\phi)/n^3 \tag{29}$$

so that Eq. (26) reduces to

$$(s/\rho)_{\text{gas}} = (s/\rho)_{\text{cryst.}} + (n^3/4)\cdot\cot^2\tfrac{1}{2}\phi\cdot(r/\rho)_{\text{cryst.}}. \tag{30}$$

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[17] E. O. Wollan, Phys. Rev. **37**, 862 (1931).

[18] G. G. Harvey, Phys. Rev. **38**, 593 (1931).

[19] See A. H. Compton, *X-Rays and Electrons*, pp. 125–127.

This relation contains only experimental quantities. It contains no such quantities as Avogadro's number, the atomic weight and number of the scatterer, the charge and mass of the electron, or the wave-length of the x-rays. In this present paper we have derived Eq. (30) by means of an extension of Thomson's classical theory of the scattering of x-rays. We have made use of such theoretical concepts as the charge and mass of the electron and the wave-length of x-rays, yet in the final equation all quantities connected with these concepts have cancelled out and we are left with a relation between experimental magnitudes such as angles, densities, thickness, distances, electrometer deflections, and speed of rotation of the crystal. Without any knowledge of the theory of the scattering or reflection of x-rays the relation expressed by Eq. (30) could have been established by means of experimental measurements on the diffuse scattering of x-rays from (say) argon and sylvine together with measurements on the reflecting power of the crystal for x-rays. The quantity n of Eq. (30) may be considered as a pure number obtained experimentally by counting. Hence the relation expressed by Eq. (30) may be called an empirical relation. Of course it is understood that the experimenter would use x-rays of the same hardness (perhaps Barkla's characteristic rays from a metal like copper or molybdenum) for the crystal as for the gas.

§5. Digression on Philosophy

For convenience we shall for the moment speak of Eq. (21) as a theoretical relation because the numerical values of each of the S's and of the F are obtained by dividing an experimental quantity by quantities which are introduced by the Thomson theory as for instance in Eq. (23). We have shown how the theoretical relation Eq. (21) may be replaced by the empirical relation Eq. (30) which contains no vestige of the Thomson theory. In his physical philosophy, the author inclines to the operational viewpoint of Bridgman.[20] Further, the author supports the view that physical laws express relations between pointer readings made on gross (macroscopic) instruments. Eq. (30) is such a relation. The literature of physics abounds in theoretical relations of the type of Eq. (21). Just as it has been possible to replace the theoretical Eq. (21) by the empirical Eq. (30), so the author believes it is possible to replace other theoretical relations of physics by empirical relations among gross physical magnitudes. The author believes that one purpose of theoretical physics is to facillitate the discovery of empirical relations among gross physical magnitudes. Concepts such as the charge and mass of an electron and the wave-length of x-rays are very useful but the author doubts that they represent reality in the world.[21]

§6. Complicated Crystals

The author has discussed the classical theory of the diffuse scattering of x-rays by solids[6] in a paper to be referred to as Paper V. In a second paper

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[20] P. Bridgman, *Logic of Modern Physics.*

[21] G. E. M. Jauncey, *Modern Physics*, pp. 538–540.

the author together with Harvey has applied the theory to the diffuse scattering by simple cubic crystals consisting of atoms of one kind.[7] We shall refer to this second paper as Paper VI.

Following the argument of Paper V we arrive at Eq. (13) of that paper. Up to this point in Paper V the electrons are not aggregated into atoms. If, instead of aggregating the electrons into atoms of one kind as was done in Paper I, we aggregate them into atoms of two kinds, which we shall distinguish by the subscripts 1 and 2, we obtain, in place of Eq. (22) of Paper V,

$$\begin{aligned} S = 1 &+ \frac{\nu_1(Z_1 - 1)f_1'^2/Z_1 + \nu_2(Z_2 - 1)f_2'^2/Z_2}{\nu_1 Z_1 + \nu_2 Z_2} \\ &+ \{1/n(\nu_1 Z_1 + \nu_2 Z_2)\} \sum{}'' \sum{}'' \iint p_r p_s \cos k(z_r - z_s) dz_r dz_s \end{aligned} \tag{31}$$

where ν_1 and ν_2 are the respective numbers of the atoms of kinds 1 and 2 in a molecule of the solid and n is the number of molecules in the scattering speck. Now, distinguishing between the rapidity of the orbital motions of the electrons in the atoms and the comparative slowness of the heat motions of the atoms about their equilibrium centers as is done on pages 1200 and 1201 of Paper V, we obtain, in place of Eq. (31) of Paper V,

$$\begin{aligned} S = 1 &+ \frac{\nu_1(Z_1 - 1)f_1'^2/Z_1 + \nu_2(Z_2 - 1)f_2'/Z_2}{\nu_1 Z_1 + \nu_2 Z_2} \\ &+ \{1/n(\nu_1 Z_1 + \nu_2 Z_2)\} \cdot \{F_1^2 X_{11} + F_1 F_2 X_{12} + F_2^2 X_{22}\} \end{aligned} \tag{32}$$

where the X's are double summations of cosines. The problem is now to determine the X's for a crystal.

Following the argument of Paper VI, Eq. (4) of that paper is replaced by

$$\begin{aligned} I = &\{Z_1 \sum\sum\sum \cos kw_{pqr} + Z_2 \sum\sum\sum \cos kw_{pqr}\}^2 \\ &+ \{Z_1 \sum\sum\sum \sin kw_{pqr} + Z_2 \sum\sum\sum \sin kw_{pqr}\}^2 \end{aligned} \tag{33}$$

where the first triple summation in each set of braces { } refers to atoms of kind 1 and the second triple summation to atoms of kind 2. Let us consider one of the single summations, say, $\Sigma \cos kw_{pqr}$ where the summation is with respect to p, so that we may write it as $\Sigma \cos kw_p$. The quantity w_p is the perpendicular from a point on a lattice line of the crystal upon the reference plane.[6,7] The lattice points on the line are either such that consecutive points are at equal distances from each other or can be separated into sets of points such that in each set consecutive points are at equal distances from each other. One of these alternatives is true even when the axes of the crystal are not rectangular and when the consecutive atoms along a lattice line are not equally spaced. Hence either $\Sigma \cos kw_p$ has a value given by Eq. (7) of Paper VI or can be broken up into a small number of summations each of which has a value given by this equation. Proceeding to the summations with respect to

q and r we arrive at a result similar to Eq. (11) of Paper VI. Now, except for particular values of $k\{=(4\pi \sin \frac{1}{2}\phi)/\lambda\}$, the right side of Eq. (11) of Paper VI is of the order unity. As in Paper VI, we divide by the total number of atoms in the speck of scattering matter and find S to be of the order of 10^{-17} if we are dealing with a speck of crystal of linear dimensions, say, 0.1 mm. The order 10^{-17} may be called zero, so that $S=0$ for a speck of crystal consisting of point atoms located exactly and permanently at the lattice points of the crystal. Now, referred to Eq. (32), S must become zero for point atoms located at lattice points—that is, for $f_1'=F_1=Z_1$ and $f_2'=F_2=Z_2$. Hence, substituting these values in the right side of Eq. (32) and rearranging, we obtain

$$(n\nu_1 + X_{11})Z_1^2 + X_{12}Z_1Z_2 + (n\nu_2 + X_{22})Z_2^2 = 0. \tag{34}$$

Since X_{11}, X_{12}, and X_{22} are constants determined only by the geometrical make-up of the crystal and do not depend on Z_1 and Z_2 and since also Eq. (34) holds for any values of Z_1 and Z_2, this equation is an identity. Hence

$$X_{11} = -n\nu_1,\ X_{12} = 0,\ \text{and}\ X_{22} = -n\nu_2. \tag{35}$$

Substituting in Eq. (32) and eliminating f' by means of Eq. (10), we obtain

$$S_{\text{class.}} = \left\{1 - \frac{\nu_1 f_1''^2/Z_1 + \nu_2 f_2''^2/Z_2}{\nu_1 Z_1 + \nu_2 Z_2}\right\} + \left\{\frac{\nu_1(f_1^2 - F_1^2) + \nu_2(f_2^2 - F_2^2)}{\nu_1 Z_1 + \nu_2 Z_2}\right\}. \tag{36}$$

The extension of this formula to the scattering by crystals consisting of more than two kinds of atoms is obvious. Woo's method of taking account of the Compton effect gives Eq. (4) together with

$$S_{\text{incoh.}} = 1 - \left(\sum_r \nu_r f_r''^2/Z_r\right)\Big/\sum_r \nu_r Z_r \tag{37}$$

and

$$S_{\text{coh.}} = \left(\sum_r \nu_r(f_r^2 - F_r^2)\right)\Big/\sum_r \nu_r Z_r \tag{38}$$

where the subscript r refers to the rth type of atom in a molecule of the crystal.

In conclusion it should be noted that the validity of Eq. (36) and also of Eqs. (37) and (38) for the diffuse scattering from a complicated crystal rests upon the validity of the same simplifying assumptions as were made in Paper V in the derivation of Eq. (16) of the present paper for a simple cubic crystal consisting of atoms of one kind. The first simplifying assumption is that expressed by Eq. (14) of Paper V in which it is assumed that the probability function for each electron is symmetrical about a reference plane (see Paper V) through the nucleus. This may not be the case in certain types of crystals. This assumption of symmetry is back of Eq. (26) of Paper V. Then, again, the assumption of symmetry in the thermal vibrations of the atoms of the crystal about their respective lattice points is back of Eq. (29)

of Paper V. In section 3 of the present paper we have seen that the electron distribution about the center of an atom of a crystal is probably a function of the temperature. At absolute zero the probability of an electron in an atom of sylvine being in a volume element dv is not only a function of the distance r of dv from the nucleus but also of the direction of the line joining dv and the nucleus with respect to the axes of the crystal. This will affect the f values for the atoms of the crystal. Above absolute zero it seems from the evidence given in §3 that the function of the direction approaches a constant as the temperature increases, so that at high temperatures the electron distribution about the nucleus of an atom of sylvine is a function of the distance r alone as is the case in an atom of argon.