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THE SCATTERING OF X-RAYS BY POLYATOMIC GASES

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Abstract

Recently Jauncey has shown that the factor F in Compton's formula for the scattering of x-rays by an atom should be the average atomic structure factor F' instead of the true atomic structure factor. Taking this into account, the general expression for the intensity of total scattering of x-rays by polyatomic gases previously deduced by the writer is modified replacing F by F'. The theory is applied to the scattering of x-rays by diatomic gases and the theoretical scattered intensity is actually compared with the absolute measurements made by Wollan on the scattering of Mo $K\alpha$ rays by H_2, N_2 and O_2. The values of F and F' are calculated from the Hartree field. On the whole Wollan's results support the new formula, though the old one represents in each case the general feature of the scattering curve. It is pointed out that, for the scattering by a diatomic gas of like atoms, Jauncey's theory of the scattering of x-rays by polyatomic molecules consisting of atoms of one kind gives results practically identical with those of the present theory, provided the change of wave-length due to the Compton effect is corrected for.

IN A recent paper[1] the writer has developed a general theory of the intensity of total scattering of x-rays by polyatomic gases on the assumption that, in considering the scattering of x-rays by a polyatomic molecule, only the coherent radiation from the different atoms in the molecule will interfere with each other according to the classical wave-principles, whereas the incoherent radiation will be simply added up. The mathematical formulation is based upon the theoretical investigation by A. H. Compton[2] and Raman[3] on the scattering of x-rays by a dynamic atom in which the electrons are regarded as a gas distributed in an enclosure surrounding the nucleus. Compton's formula may be written

$$I_\phi = I_e\left\{F^2 + \frac{Z - F^2/Z}{[1 + \gamma(1 - \cos\phi)]^3}\right\}, \tag{1}$$

where I_ϕ is the intensity scattered to a distance R in a direction ϕ with the incident radiation, I_e is the independent scattering from a single electron as

[1] Y. H. Woo, Proc. Nat. Acad. Sci. **17**, 467 (1931). This paper is referred to later as I.
[2] A. H. Compton, Phys. Rev. **35**, 925 (1930).
[3] C. V. Raman, Indian J. Phys. **3**, 357 (1928).

calculated by J. J. Thomson,[4] F is the atomic structure factor of the scattering atom, $\gamma = h/mc\lambda$, and Z, h, m, c and λ have their usual significance.

Recently Jauncey[5] has pointed out that the factor F in Eq. (1) should be a quantity F' (to be called later the average atomic structure factor) instead of the true atomic structure factor as defined in the theory of the reflection of x-rays by crystals. This comes out from the fact that Compton and Jauncey make different assumptions regarding the probability function that any one electron in the scattering atom shall lie between distances r and $r+dr$ from the nucleus. While Compton[6] assumes that this probability is the same for every electron in the atom, Jauncey[7] postulates that it is different for electrons in the different electron groups. According to Jauncey,[7] the relation between the average atomic structure factor F' and the true atomic structure factor F is expressed by

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

where E_r is the average amplitude of the waves scattered by the r-$^{\text{th}}$ electron in the scattering atom and where the true atomic structure factor F is given by

$$F = \sum_{1}^{Z} E_r. \tag{3}$$

Introducing the modification discussed by Jauncey, Compton's formula (I) becomes

$$I_\phi = I_e \left\{ F'^2 + \frac{Z - F'^2/Z}{[1+\gamma(1-\cos\phi)]^3} \right\}. \tag{4}$$

Thus, according to our fundamental assumption stated above, the intensity scattered at an angle ϕ with the primary beam by a molecule containing atoms $1, \ldots i, \ldots n$ arranged at fixed distances from each other is given by

$$I_{\phi n} = I_e \sum_{1}^{n} \sum_{1}^{n} F_i' F_j' \frac{\sin k s_{ij}}{k s_{ij}} + I_e \sum_{1}^{n} \frac{Z_i - F_i'^2/Z_i}{[1+\gamma(1-\cos\phi)]^3}, \tag{5}$$

where F_i' is the average atomic structure factor for the i^{th} atom, $k = (4\pi/\lambda)\sin\frac{1}{2}\phi$, s_{ij} is the distance of any atom i from any other atom j, and the other notations have the same meaning as those employed in Eq. (1). The expression (5) differs from the formula (2) of I in replacing F by F' as suggested by Eq. (4).

Now let us apply the above theory to the scattering of x-rays by a diatomic gas consisting of two like atoms. Since there is only one value of F' or F, we have for the scattering per electron

[4] J. J. Thomson, "Conduction of Electricity through Gases," 2nd Edition, p. 325.

[5] G. E. M. Jauncey, Phys. Rev. **37**, 1193 (1931). Cf. also G. Herzog, Zeits. f. Physik **69**, 207 (1931).

[6] A. H. Compton, reference 2, p. 930.

[7] G. E. M. Jauncey, reference 5, p. 1201.

$$S = \frac{I_{\phi 2}}{2ZI_e} = \left(1 + \frac{\sin ks}{ks}\right)\frac{A^2}{Z} + \frac{1 - A^2/Z^2}{[1 + \gamma(1 - \cos\phi)]^3}, \quad (6)$$

where s is the distance between the two atoms in the scattering molecule, A is equal to F' according to Eq. (5) and is equal to F if Eq. (2) of I is followed.

Wollan[8] has recently reported experiments on the absolute measurements of the intensity of the scattering of Mo $K\alpha$ rays by H_2, N_2 and O_2. In order to compare Eq. (6) with Wollan's results, it is necessary to calculate the values of F and F' for the atoms in the scattering molecule. From the tables given by James and Brindley[9] or by the interpolation method designed by these authors,[9] we can easily find the contribution of a single electron of each of the electron groups in any of the three atoms H, N and O to its F. That is, we can find the values of the E_r's calculated according to the Hartree method. Thus the average atomic structure factor F' and the true atomic structure factor F can be evaluated according to Eqs. (2) and (3) without difficulty. For the case of hydrogen, F' is equal to F. For oxygen and nitrogen, we group the electrons into groups as shown in Table I and denote each group by the

TABLE I.

	Z	K (1 0)	L (2 0)	(2 1)
O	8	2	2	6
N	7	2	2	5

TABLE II. *Values of F and F'.*

ϕ	$\frac{\sin \frac{1}{2}\phi}{\lambda}$	H $F=F'$	N F	N F'	O F	O F'
10°	0.123	0.72	5.53	5.52	6.75	6.74
15°	0.184	0.53	4.35	4.30	5.57	5.55
20°	0.245	0.36	3.53	3.44	4.74	4.69
25°	0.306	0.25	2.88	2.71	3.88	3.80
30°	0.365	0.16	2.43	2.18	3.22	3.07
40°	0.482	0.08	1.88	1.51	2.35	2.09
50°	0.596	0.04	1.67	1.27	1.88	1.50
60°	0.704	0.03	1.56	1.19	1.65	1.25
70°	0.808	0.02	1.46	1.11	1.56	1.18
80°	0.905	0.01	1.35	1.03	1.47	1.11
90°	0.996	0.00	1.26	0.96	1.39	1.05

quantum numbers (nl) in the usual way. The values of F' and F for H, N and O so obtained are tabulated in Table II. It will be noticed that for comparatively large values of $\sin \phi/2/\lambda$ the difference F—F' becomes quite appreciable. This is in agreement with the conclusion recently drawn by Jauncey.[10] In view of the fact, however, that the values of E_r employed in the present calculation are estimated from the Hartree field,[11] the values of F and F'

[8] E. O. Wollan, Phys. Rev. **37**, 862 (1931); Proc. Nat. Acad. Sci. **17**, 475 (1931).
[9] James and Brindley, Phil. Mag. **12**, 81 (1931).
[10] G. E. M. Jauncey, Phys. Rev. **38**, 1 (1931).
[11] Cf. James and Brindley, reference 9.

given here are perhaps more accurate than those obtained by the simple method devised by Jauncey.[10]

Using the values of F and F' tabulated in Table II, a calculation is made of the scattering of Mo $K\alpha$ rays by H_2, N_2 and O_2 according to Eq. (6). The values of s are taken to be equal to 1.10A, 1.21A and 1.10A for H_2, O_2 and N_2 respectively.[12] The theoretical values of the scattering per electron S together with the experimental results observed by Wollan[13] are given in Table III. In order to see the variation of S with the scattering angle ϕ, these results are

TABLE III. *Values of the scattering per electron.*

ϕ	H_2		N_2			O_2		
	S $(F=F')$	S obs.	S $(A=F)$	S $(A=F')$	S obs.	S $(A=F)$	S $(A=F')$	S obs.
10°	1.31	—	7.32	7.29	6.90	8.93	8.92	8.05
15°	1.11	1.27	3.90	3.84	—	4.89	4.86	4.90
20°	0.99	1.10	2.40	2.34	2.45	3.05	3.00	2.96
25°	0.98	1.03	1.76	1.67	—	2.24	2.19	2.00
30°	0.98	1.00	1.55	1.45	1.35	1.96	1.88	1.72
40°	0.98	0.98	1.44	1.27	1.25	1.67	1.52	1.43
50°	0.97	0.97	1.35	1.18	1.15	1.37	1.23	1.15
60°	0.95	0.95	1.24	1.12	1.05	1.22	1.10	1.04
70°	0.94	0.93	1.18	1.07	1.03	1.20	1.09	1.02
80°	0.92	0.92	1.15	1.05	1.01	1.17	1.07	1.01
90°	0.91	0.91	1.12	1.03	0.96	1.12	1.03	0.96

plotted in Figs. 1 and 2. The curve I assumes $A=F$ and the curve I' $A=F'$. The circles show the observed values. It is seen that on the whole Wollan's experiments support Eq. (6) for the case $A=F'$, though Eq. (6) with $A=F$ represents in each case the general feature of the scattering curve.

In this connection it may be mentioned that Wollan[14] has previously made a comparison of his own data with Eq. (6) for the case $A=F$. He estimated the F values from the atomic field of Thomas[15] and Fermi.[16] The agreement between theory and experiment is in general not quite satisfactory. This is perhaps well explained by the consideration just given above. Assuming $A=F$, the writer[17] has also compared Eq. (6) with the experiments reported by Barrett[18] on the scattering of x-rays of various wave-lengths by diatomic gases. In some cases the agreement seems to be all right. However, since Barrett's measurements give relative values of the scattering per electron, but not absolute values, there may remain some arbitrariness in fitting the observed data with the calculated results. So far as the writer is aware, the experiments of Wollan seem to be the only ones which give absolute val-

[12] These values of s are calulated according to Rasetti's measurements of the moment of inertia, cf. Phys. Rev. **34,** 367 (1930)

[13] E. O. Wollan, reference 8.

[14] E. O. Wollan, Proc. Nat. Acad. Sci. **17,** 475 (1931).

[15] L. H. Thomas, Proc. Camb. Phil. Soc. **23,** 542 (1927).

[16] E. Fermi, Zeits. f. Physik **48,** 73 (1928).

[17] Y. H. Woo, Proc. Nat. Acad. Sci. **17,** 467 and 470 (1931).

[18] C. S. Barrett, Proc. Nat. Acad. Sci. **14,** 20 (1928); Phys. Rev. **34,** 22 (1928).

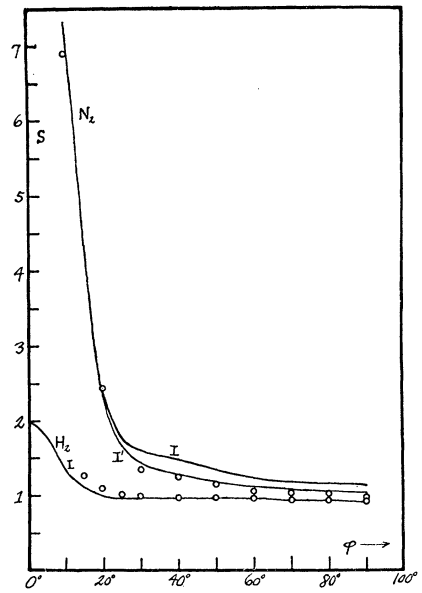

Fig. 1. Curve I, $A = F$; Curve I', $A = F'$; circles, experimental points.

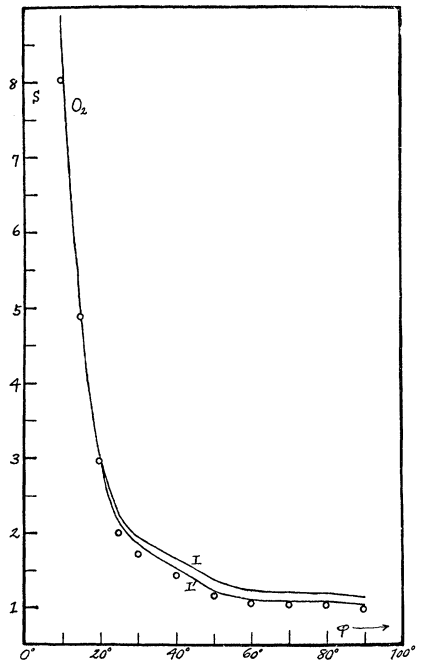

Fig. 2. Curve I, $A = F$; Curve I', $A = F'$; circles, experimental points.

ues. This shows that absolute measurements on the intensity of total scattering of x-rays by polyatomic gases and vapors for different wave-lengths are much desired.

As is well known, the factor $[1+\gamma(1-\cos\phi)]^{-3}$ is introduced to correct for the change of wave-length in the Compton effect for the incoherent part of the intensity of the total scattering. For the case of the scattering of x-rays by monatomic gases, its importance has been emphasized by the writer.[19] Though the maximum scattering angle in Wollan's experiments only amounts to 90°, the significance of this factor is well illustrated by the following example. In Table IV are given the values of the scattering per electron for the

TABLE IV. *Uncorrected values of scattering per electron for* O_2.

	10°	15°	20°	25°	30°	40°	50°	60°	70°	80°	90°
S (uncorrected)	8.92	4.87	3.01	2.20	1.89	1.54	1.26	1.15	1.15	1.14	1.13

scattering of Mo $K\alpha$ by O_2 calculated according to Eq. (6) for $A=F'$ without the correction factor. In comparison with the corresponding corrected and observed values of S listed in Table III, it is evident that the corrected values are in better accord with the experiment. Similar results are obtained for the scattering of Mo $K\alpha$ rays by H_2 and N_2.

Recently Jauncey[20] has also proposed a theory of the scattering of x-rays by a polyatomic molecule consisting of atoms of one kind. When applied to the case of the scattering of x-rays by a diatomic gas of two like atoms, Jauncey's formula may be written

$$S=\frac{F'^2}{Z}+\frac{\sin ks}{ks}\frac{F^2}{Z}+1-\frac{F'^2}{Z^2}, \tag{7}$$

where the effect of the change of wave-length is neglected. When this effect is corrected for, Eq. (7) gives results practically identical with those calculated according so Eq. (6) for the case $A=F'$.

[19] Y. H. Woo, Proc. Nat. Acad. Sci. **16,** 814 (1930) and **17,** 470 (1931).
[20] G. E. M. Jauncey, Phys. Rev. **38,** 194 (1931).