The structure factors were calculated according to the expression given above without the introduction of a temperature factor, and with the assumption of either the chair or the boat form of the C_6F_{12} molecule with the distances $r_{CC} = 1{\cdot}50$ A. and $r_{CF} = 1{\cdot}35$ A. The structure was assumed to be the face-centered cubic packing of rotating molecules with $a_0 = 10{\cdot}00$ kX. reported by Christoffers *et al.* (1947). The values of the structure factor found experimentally by these authors are compared with the calculated values in Table 2. All sets of values are reduced to a scale with $F_{111} = 10{\cdot}0$.

Table 2. *Comparison of calculated and observed structure factors*

hkl	$F_{\text{calc.}}$ (chair)	$F_{\text{calc.}}$ (boat)	$F_{\text{obs.}}$
111	+10·0	+10·0	10·0
200	+ 5·2	+ 5·3	5·5
220	− 2·9	− 2·7	4·5
222	− 2·9	− 2·9	7·7
311	− 3·3	− 3·2	5·5
331	− 0·4	− 0·2	1·4
333	+ 0·5	+ 0·5	3·2
400	− 1·4	− 1·2	3·9
420	− 0·1	0·0	2·0
422	+ 0·4	+ 0·5	0·0
440	+ 0·2	+ 0·1	1·7

The decline of the observed structure factors is seen to be much slower than the decline of the calculated structure factors. There was apparently no appreciable difficulty due to absorption, since the size of the sample was about 30 % smaller than the optimum size. It is reasonable to conclude that we are dealing with highly hindered rotation of the molecules or with orientational disorder. This conclusion is corroborated by the point raised by Christoffers *et al.* (1947) that the fluorine atoms of adjacent molecules would approach each other with a minimum distance much smaller than twice the van der Waals radius of fluorine, if the molecules rotated freely. Values of the minimum distance of approach of fluorine atoms calculated by the present authors are 1·78 A. for the boat form and 1·68 A. for the chair form of the C_6F_{12} molecule, although the value of the van der Waals radius of fluorine is 1·35 A., according to Pauling (1945, p. 176).

Further study of the hindered rotator without a fixed axis could be carried out by calculation of the scattering powers of assumed models of the hindered rotator, or by preparation of electron-density maps of the crystal. An attempt was made to find the orientations of maximum probability for the molecules of C_6F_{12} by a three-dimensional Fourier summation. However, the signs of some of the terms could not be fixed because of difficulties with non-convergence, and no conclusions could be drawn.

Appreciation is expressed to Prof. Robert H. Cameron for discussions with respect to the mathematical derivation, and to the donors of the Minnesota Mining and Manufacturing Co. Fellowship in Chemistry to M. V. King for the year 1947–8.

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Short Communications

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A rapid approximate method for correcting low-angle scattering measurements for the influence of the finite height of the X-ray beam.

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(*Received* 7 *July* 1949 *and in revised form* 21 *October* 1949)

Application of the method of Fournet & Guinier (1947) for correcting low-angle scattering measurements for the influence of the finite height of the X-ray beam is limited to materials for which the intensity of low-angle scattering decreases to virtually zero at a small angle. An alternative method of correction described by Shull & Roess (1947) requires that the observed intensity curve be represented by the sum of a number of Gaussian curves, and this is not always possible. The approximate method described below can be applied very rapidly to a low-angle scattering curve of any form.

Any point A on the equator A_1A_2 (Fig. 1) receives diffracted radiation from each point of the specimen P_1P_2. The intensity recorded at A therefore represents the mean value of the intensity diffracted over a finite range of angle. The approximation made consists in assuming that within this range the variation of intensity with angle of diffraction is linear. That is, the intensity measured at A is that corresponding to the mean angle of diffraction of the radiation received at A.

In Fig. 1, H_3H_2 represents the impact on the film of the direct beam passing through the upper half of the specimen P_3P_2. The minimum true angle of diffraction of radiation received at A is equal to the measured angle of diffraction. This is given by

$$\gamma = AH_3/P_3H_3 = a/d,$$

where a ($=AH_3$) is the distance measured along the equator from the centre of the film, and d ($=P_3H_3$) is the distance between specimen and film.

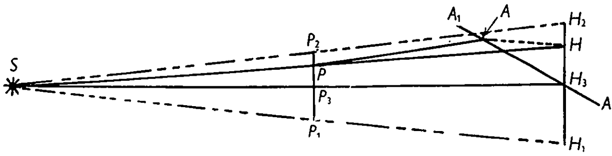

Fig. 1. Perspective representation of experimental arrangement. S, source; P_1P_2, specimen; A_1A_2, equator of film.

The maximum true angle of diffraction for the point A is given, for a point source, by the angle H_2P_2A. This is

$$\epsilon_1 = AH_2/d.$$

Hence $$\epsilon_1^2 - \gamma^2 = h_1^2/d^2, \tag{1}$$

where $2h_1$ ($=2H_2H_3$) is the height of the direct beam at its point of impact on the film.

For a source of small finite height $2s$, it is easily shown that

$$\epsilon_1^2 - \gamma^2 = (1 + 2ds/d_1h_1)\, h_1^2/d^2, \tag{2}$$

where d_1 ($=SP_3$) is the distance from source to specimen. Here $2h_1$ is the height of the uniform part of the direct beam, excluding the penumbra which results from the finite height of the source. In making the correction it will be assumed that the variation of intensity with angle of diffraction is linear in the range γ to ϵ_1. If the height of the source is appreciable, the range of angle in which it is necessary to make this assumption is increased. However, comparison of equations (1) and (2) shows that, since d and d_1 are normally of the same order of magnitude, the height of the source is not an important factor provided that it is considerably less than the height of the beam.

In Fig. 1, H represents, for a point source, the point of impact on the film of the ray passing through the point P of the specimen. For a source of finite height, H represents the *mean* point of impact of the direct beam passing through P. The (mean) angle of diffraction of radiation received at A from the point P is

$$\epsilon = AH/d.$$

Hence $$\epsilon^2 - \gamma^2 = h^2/d^2 \quad \text{or} \quad \epsilon = (h^2/d^2 + \gamma^2)^{\frac{1}{2}}, \tag{3}$$

where h is the height of H above H_3.

We require to find the relationship between the measured angle, γ, and the mean value, $\bar{\epsilon}$, of the true angle of diffraction ϵ for radiation received at A.

From equation (3)

$$\bar{\epsilon} = \frac{1}{h_1}\int_0^{h_1}\left(\frac{h^2}{d^2} + \gamma^2\right)^{\frac{1}{2}} dh,$$

or $$\bar{\epsilon} = \frac{1}{2}\left(\frac{h_1^2}{d^2} + \gamma^2\right)^{\frac{1}{2}} + \frac{\gamma^2 d}{2h_1}\log_e\left[\frac{1}{\gamma}\left\{\frac{h_1}{d} + \left(\frac{h_1^2}{d^2} + \gamma^2\right)^{\frac{1}{2}}\right\}\right]. \tag{4}$$

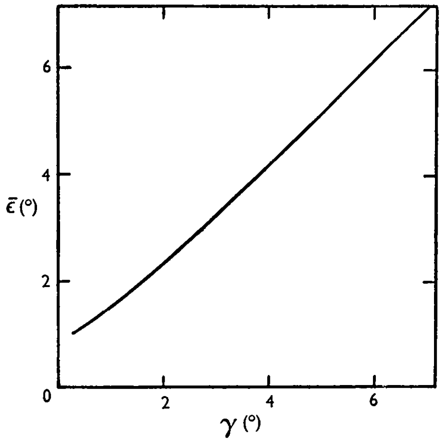

Fig. 2. Relation between $\bar{\epsilon}$ and γ for $h_1/d = 0{\cdot}046$.

It will be noted that the form of the correction given by equation (4) is independent of the height of the source, though the larger the source the larger the approximation involved.

The relationship between $\bar{\epsilon}$ and γ is shown in Fig. 2 for $h_1/d = 0{\cdot}046$. To apply the correction, the curve corresponding to Fig. 2 is calculated once and for all for the value of h_1/d adopted, and this gives at once the angular displacement which must be applied to any point on the measured intensity curve.

It is seen in Fig. 2 that for a given value of h_1/d there is a lower limit to the values of the true angle of diffraction which can be obtained by this method. To extend the measurements to smaller angles it is necessary to use a shorter beam or a longer sample–film distance.

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Acta Cryst. (1950). **3**, 159

The structure of the paramolybdate ion.

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(*Received* 31 *October* 1949)

Most theories of the structure of the paramolybdate ion have been based on a formula including twelve molybdenum atoms in the ion, e.g. $5(NH_4)_2O.12MoO_3.7H_2O$. As the paramolybdates have been shown to have formulae