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.

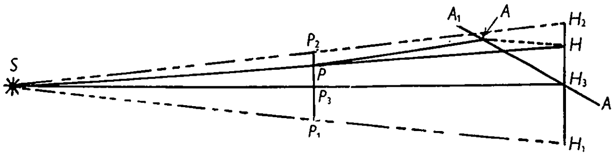

Fig. 1. Perspective representation of experimental arrangement. S, source; P_1P_2, specimen; A_1A_2, equator of film.

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 $$\epsilon_1^2 - \gamma^2 = h_1^2/d^2, \quad (1)$$

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

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

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

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

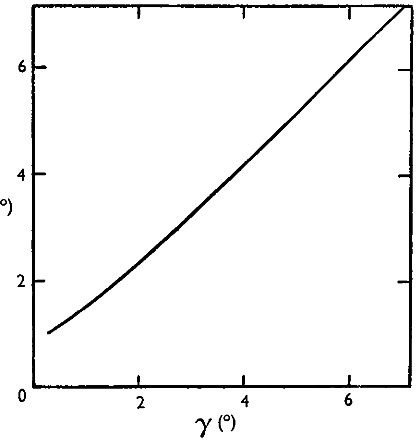

Fig. 2. Relation between $\bar{\epsilon}$ and γ for $h_1/d = 0{\cdot}046$.

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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The structure of the paramolybdate ion.

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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 of the type $3(NH_4)_2O.7MoO_3.4H_2O$ (Sturdivant, 1937; Lindqvist, 1948), all these theories are of course without value. The sole effort to give a description of a paramolybdate ion of the composition $(Mo_7O_{24})^{6-}$ has been made by Anderson (1937; Emeléus & Anderson, 1938). His model is a six-membered ring of MoO_6 octahedra, which are joined by edges. In the middle of this ring there is room for a further MoO_6 octahedron, the whole complex having the formula $(Mo_7O_{24})^{6-}$. This theory was first put forward for the 6-hetero-polyacids and has recently been confirmed by Evans (1948) for $(NH_4)_6TeMo_6O_{24}.7H_2O$ and $K_6TeMo_6O_{24}.7H_2O$. Our X-ray crystallographic structure determination of ammonium paramolybdate, $(NH_4)_6Mo_7O_{24}.4H_2O$, has, however, indicated another configuration for the ion $(Mo_7O_{24})^{6-}$.

The dimensions, already given by Sturdivant (1937), are

$$a=8{\cdot}382,\ b=36{\cdot}125,\ c=10{\cdot}464\ \text{A. and}\ \beta=116^\circ\ 0'.$$

The space group is $P2_1/c$, and there are four formula units in the unit cell. The large monoclinic axis made it impossible to work with a shorter wave-length than Cu $K\alpha$ radiation. The crystal was rotated around the a axis, and Weissenberg photographs were taken of the four available layer lines. After an estimation of all intensities, a complete three-dimensional Patterson synthesis was carried out on the Hägg–Laurent (1946) calculating machine, from which the positions of the molybdenum atoms were determined. A full report of the crystal-structure determination will be given elsewhere. The parameters of the molybdenum atoms are given in Table 1.

Table 1. *Parameters of the molybdenum atoms*

	$x/60$	$y/120$	$z/60$
Mo I	27·0	12·9	22·0
Mo II	19·0	6·1	5·8
Mo III	10·5	23·5	5·2
Mo IV	3·5	16·7	−11·0
Mo V	34·0	23·1	21·2
Mo VI	28·5	16·4	4·5
Mo VII	19·0	8·9	−12·2

A discussion of the possible crystal structures which could be in agreement with these molybdenum positions indicated a structure of the $(Mo_7O_{24})^{6-}$ ion of which Fig. 1 gives an idealized picture. The model could best be described as four MoO_6 octahedra I–IV placed on their edges. I–II and III–IV share edges, I–III and II–IV share corners; thus the four centres of the octahedra (the molybdenum atoms) form a rectangle. On this rectangle three other octahedra, V–VII, are placed on their edges so that these three octahedra share edges with all their neighbours (V with I, III and VI, and so on).

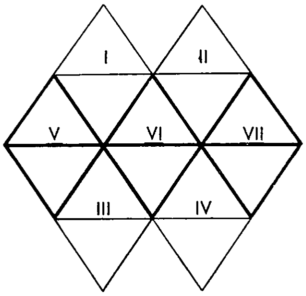

Fig. 1. The structure of the paramolybdate ion $(Mo_7O_{24})^{6-}$. The octahedra which are marked with thin lines are in a lower plane than those which are heavily drawn.

A complete discussion of the chemical consequences of this structure will be given in another paper. It may be noted at this point that the water molecules are not parts of the ion as was previously concluded from dehydration investigations. The paramolybdates, therefore, should not be considered as acid salts but as normal salt hydrates of the hypothetical acid $H_6Mo_7O_{24}$. Possibly some higher molybdates, however, could be formulated as acid salts of $H_6Mo_7O_{24}$. Our investigations on these problems are being continued.

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The crystal structure of di-fructose strontium chloride tri-hydrate.

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In order to determine by X-ray methods the structure of the fructose molecule, a structure determination was undertaken of di-fructose strontium chloride tri-hydrate. This complex was obtained as described by Smith & Tollens (1900). Rotation and Weissenberg photographs were taken with Cu $K\alpha$ radiation of the zero-, first- and second-layer lines about the twofold axis of the crystal. Using these data and external morphology (monoclinic sphenoidal) the space group was determined as C_2^3–$C2$. The lattice constants are:

$$a=16{\cdot}4_0,\ b=8{\cdot}0_8,\ c=11{\cdot}0_5\ \text{A.},\ \beta=128{\cdot}4^\circ.$$

A measured density of $1{\cdot}719\ \text{g.cm.}^{-3}$ led to $Z=2{\cdot}08 \div 2$ molecules of $(C_6H_{12}O_6)_2.SrCl_2.3H_2O$ per cell.

The strontium atoms are fixed by symmetry at $(0, y, 0)$, $(\frac{1}{2}, \frac{1}{2}+y, 0)$, and y can arbitrarily be chosen as zero. The positions of the chlorine atoms were determined from a (010) Patterson to be at $x=0{\cdot}022$, $z=0{\cdot}295$. Mo $K\alpha$ radiation was now used, in order to reduce effects of absorption and to assure convergence of the series. A Fourier synthesis on (010) was carried out on X-RAC, the electronic analogue computer designed and constructed in this laboratory (Pepinsky, 1947). In this first synthesis the phases were taken as determined by the strontium positions, i.e. all positive. The oscilloscope

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