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).

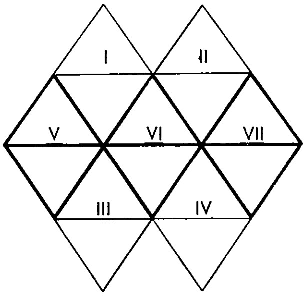

Fig. 1. The structure of the paramolybdate ion $(Mo_7O_{24})^{6-}$. The octahedra which are marked with thin lines are in a lower plane than those which are heavily drawn.

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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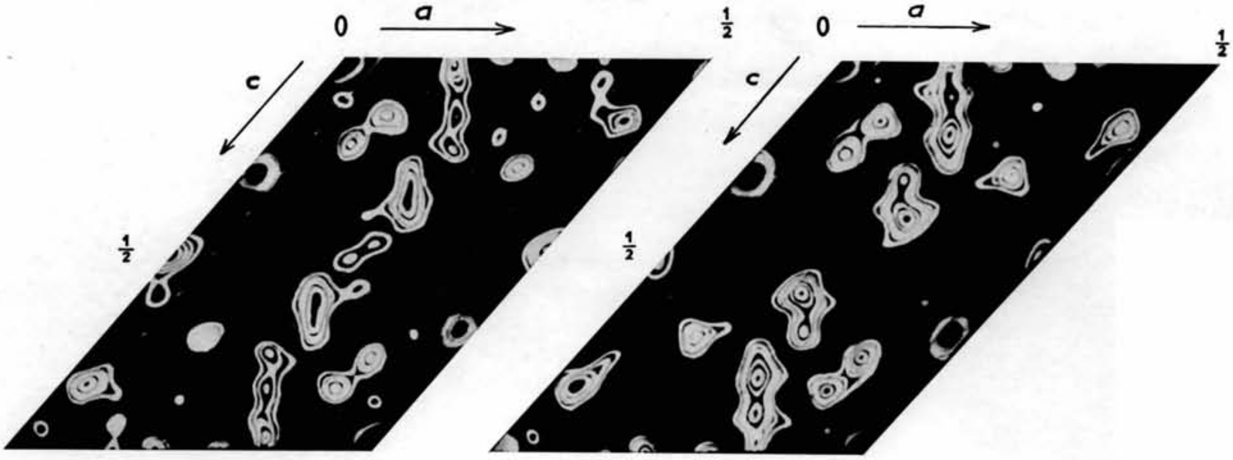

Fig. 1. Fig. 2.

Fig. 1. X-RAC oscilloscope pattern of Fourier synthesis on (010) with all phases positive.

Fig. 2. X-RAC oscilloscope pattern of Fourier synthesis on (010) with revised phases.

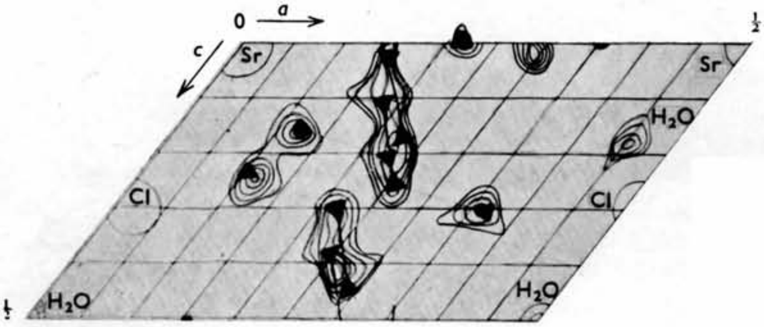

Fig. 3. Projection of model on to Fourier map.

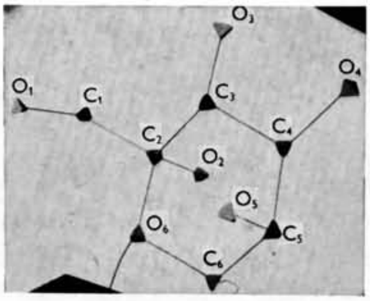

Fig. 4. Model of molecule.

pattern is shown in Fig. 1. A high ridge appeared at $x=\frac{1}{4}$, which was taken to be due to the unresolved fructose residue.

X-RAC was now applied with great advantage at this point. As is being discussed in a separate report by Pepinsky & MacGillavry (in the Press), one of the criteria which an acceptable computed density function must satisfy is that the function must not perform large excursions into the negative density regions. (Actually $\rho_{\text{calc.}}$ should never become negative, but it may be expected to do so because of inaccuracies in the Fourier coefficient amplitudes and non-convergence of the series.) Another statement of the criterion is that the background should be smooth. This criterion was applied in the following manner. All contour lines were switched out, and the variable contour level was adjusted to the background. The signs of the Fourier coefficients were then reversed one by one. Whenever the function showed larger or more numerous dips, the original positive sign was restored. In a few cases a change of sign noticeably improved the background, and for these the coefficient was set in with negative sign. Then the variable contour line was switched out and the fixed contours were reintroduced. The resulting oscilloscope pattern is reproduced as Fig. 2. This shows definite improvement in resolution; furthermore, some low peaks of the previous pattern have disappeared.

Scale models based on possible structures using standard bond angles and distances were made. These models were projected by a parallel beam of light on to the Fourier map (Fig. 2). It became evident that only the model *β*-D-fructo-pyranose, with the Sachsse *trans*- (chair-shaped) form of the ring, could be made to fit the projection. This agrees with the observation of the rotatory power of the complex when first put into solution (Smith & Tollens, 1900). The superposed shadow is shown in Fig. 3, and the model itself in Fig. 4.

Proof of the structure and the effectiveness of the sign determination were checked for this projection by structure-factor calculations. Trial-and-error computations improved the agreement between observed and calculated factors. Unfortunately, the plane of the fructose ring is nearly perpendicular to the projection plane, allowing good resolution only for four of the hydroxyl groups. Four of the six water molecules are in general positions and are clearly resolved. A peak at $0, y, \frac{1}{2}$ indicates that the positions of the other two water molecules are on this two-fold axis. Computations based on the (010) projection are shown in the following tables. Table 1 gives the x and z atomic parameters. Table 2 lists the negative structure factors as automatically determined on X-RAC, and as calculated from the atomic parameters. All of these factors are small, since the strontium contribution is positive and generally overwhelming. Agreement results for eleven factors. One factor shows up as negative from the X-RAC method and positive from the atomic center calculations, and three show up negative from the latter calculations and positive from X-RAC. A (110) projection, which has least overlapping and from which the parameters of every atom can in principle be determined, is now being carried out.

Table 1. *x and z parameters of atoms*

	x/a	z/c		x/a	z/c
Sr	0	0	C_1	0·230	0·199
Cl	0·022	0·295	C_2	0·262	0·252
O_1	0·124	0·170	C_3	0·194	0·100
O_2	0·369	0·301	C_4	0·221	0·163
O_3	0·191	−0·023	C_5	0·237	0·314
O_4	0·159	0·023	C_6	0·292	0·437
O_5	0·116	0·242	$(H_2O)_1$	0·000	0·500
O_6	0·250	0·371	$(H_2O)_2$	0·451	0·188

Table 2. *Negative structure factors as determined by X-RAC and as calculated from atomic parameters*

Negative *F*'s by X-RAC *hkl*	Negative *F*'s calculated *hkl*
200	200
002	002
$\bar{4}02$	$\bar{4}02$
202	202
$\bar{6}05$	$\bar{6}05$
$\bar{8}02$	$\bar{8}02$
$\overline{12}.0.6$	$\overline{12}.0.6$
$\overline{12}.0.7$	$\overline{12}.0.7$
10.0.1	10.0.1
$\overline{16}.0.3$	$\overline{16}.0.3$
$\bar{4}.0.12$	$\bar{4}.0.12$
10.0.4	201
	405
	$\overline{10}.0.10$

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The systematic calculation of interplanar spacings or values of sin $^2\theta$ with punched cards.*

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Some applications of punched cards and International Business Machines to the calculations of crystal-structure analysis have been the subject of several papers from this and other laboratories. In this communication, an additional application is described: one enabling the rapid calculation of the entire set of values of $1/d_{hkl}$ or $\sin^2\theta_{hkl}$ for all planes within the reflection sphere. The increasing

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