

pattern is shown in Fig. 1. A high ridge appeared at $x = \frac{1}{2}$, 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 ρ_{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 re-introduced. 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 ₂ O) ₁	0.000	0.500
O ₆	0.250	0.371	(H ₂ O) 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
402	402
202	202
605	605
802	802
$\bar{1}\bar{2}.0.6$	$\bar{1}\bar{2}.0.6$
$\bar{1}\bar{2}.0.7$	$\bar{1}\bar{2}.0.7$
10.0.1	10.0.1
$\bar{1}\bar{6}.0.3$	$\bar{1}\bar{6}.0.3$
$\bar{4}.0.12$	$\bar{4}.0.12$
10.0.4	201
	405
	$\bar{1}\bar{0}.0.10$

The writers express their deep appreciation to the Research Corporation for the financial grant under which this and other crystal-structure determinations have been carried on at the Alabama Polytechnic Institute. Much gratitude is also extended to Dr Caroline MacGillavry, for guidance at several stages of the analysis.

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The systematic calculation of interplanar spacings or values of $\sin^2 \theta$ with punched cards.* By JERRY DONOHUE. *Gates and Crellin Laboratories of Chemistry, California Institute of Technology, Pasadena 4, California, U.S.A.*

(Received 8 December 1949)

Some applications of punched cards and International Business Machines to the calculations of crystal-structure

* Contribution no. 1355 from the Gates and Crellin Laboratories of Chemistry.

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

necessity to extend the scope of crystal-structure investigations from the use of prism-zone data only to the use of all of the general reflections makes such a method desirable. The method makes use of but two IBM machines, viz. a hand key punch and a tabulator, the latter preferably equipped with progressive totals.

In the orthogonal crystal systems we have the relation

$$\sin^2 \theta_{hkl} = h^2 \lambda^2 / 4a^2 + k^2 \lambda^2 / 4b^2 + l^2 \lambda^2 / 4c^2.$$

If values of $1/d^2$ are desired, the factor $\lambda^2/4$ is omitted from each term. Three small decks of cards are first prepared with the hand punch; these are designated $(2h-1)\sin^2\theta_{100}$, $(2k-1)\sin^2\theta_{010}$ and $(2l-1)\sin^2\theta_{001}$, where h , k and l run from 1 to their respective maximum observed values. Deck 1 is punched 1 in col. 1, $(2h-1)$ in cols. 4-5, and $(2h-1)\sin^2\theta_{100}$ in cols. 10-15; deck 2 is punched 1 in col. 2, $(2k-1)$ in cols. 6-7, and $(2k-1)\sin^2\theta_{010}$ in cols. 10-15; deck 3 is punched 1 in col. 3, $(2l-1)$ in cols. 8-9, and $(2l-1)\sin^2\theta_{001}$ in cols. 10-15. Columns 1, 2, 3, 4-5, 6-7, 8-9 and 10-15 are then wired to add in separate counters. If we now pass deck 1 through the tabulator, and take progressive totals, we obtain directly the values of $\sin^2\theta_{h00}$, since $\sum_{n=1}^h (2n-1) = h^2$. The process is now repeated after adding to the deck the first $(2k-1)\sin^2\theta_{010}$ card. We now obtain values of $\sin^2\theta_{h10}$. The $\sin^2\theta$ values for the planes $h20$, $h30$, ..., $h01$, $h11$, ..., $h02$, $h12$, etc., are then obtained by continuing the process of adding the proper next card after each pass of the deck. In the general case, the totals in the counters will be h , k , l , h^2 , k^2 , l^2 , $\sin^2\theta_{hkl}$. The squares of the Miller indices are printed as a check to insure that the cards in each deck were fed in the proper

order, since the printed indices themselves are simply counts of the number of cards in each deck. By keeping watch on the value of $\sin^2\theta$ for (h_{\max}, k_l) in each group it is possible to remove cards from the back of the

$$(2h-1)\sin^2\theta_{100}$$

deck in order to keep all the values calculated below a pre-determined maximum, this value being unity if data for all planes within the sphere of reflection are desired.

If the tabulator does not have progressive totals, the same method may be used, but in this case each value of $\sin^2\theta$ to be computed requires a separate pass of the deck through the machine, and the handling of cards is considerably increased.

This method may be extended for use in the hexagonal and monoclinic systems, in which

$$\sin^2\theta = \frac{\lambda^2 h^2}{4a^2} \sin^2\beta + \frac{\lambda^2 k^2}{4b^2} + \frac{\lambda^2 l^2}{4c^2} \sin^2\beta - \frac{\lambda^2 hl \cos\beta}{2ac \sin^2\beta}.$$

The procedure with the first three terms is identical with that outlined above; the last term requires the punching of an additional deck with values of $A_i \lambda^2 \cos\beta / 2ac \sin^2\beta$, the values of A_i being chosen so that combinations of them will form all observed (hkl) combinations. By proper wiring, values of $\sin^2\theta$ for (hkl) and $(\bar{h}\bar{k}\bar{l})$ may be obtained simultaneously.

We have used this method in the calculation of complete $\sin^2\theta_{hkl}$ values for four different crystals. As an illustration of the saving of time effected, a recent calculation of the complete set of over 3000 values inside the Cu $K\alpha$ sphere of reflection for an orthorhombic cell which has $a=11$, $b=13$ and $c=16$ A. took about 4 hr.

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Errata in Lonsdale's Structure Factor Tables. By K. LONSDALE. *Chemistry Department, University College, Gower Street, London W.C.1, England*

(Received 18 November 1949)

In rearranging the structure factor tables for Volume 1 of the new *International Tables*, I have found the following errata, which should be noted by those who are now using the existing *Structure Factor Tables*. I should be most grateful for information of other corrections, if any.

p. 15. Pc , $l=2n$:

$$" \alpha(\bar{h}kl) = -\alpha(h\bar{k}l) = \alpha(hkl) "$$

should read $" \alpha(\bar{h}kl) = -\alpha(h\bar{k}l) \neq \alpha(hkl) "$.

Pc , $l=2n+1$:

$$" \alpha(\bar{h}kl) = -\alpha(h\bar{k}l) "$$

should read $" \alpha(\bar{h}kl) = \pi - \alpha(h\bar{k}l) "$.

p. 16. Cc , $l=2n+1$:

$$" \alpha(\bar{h}kl) = -\alpha(h\bar{k}l) "$$

should read $" \alpha(\bar{h}kl) = \pi - \alpha(h\bar{k}l) "$.

p. 20. Pmc , $l=2n+1$:

$$" \alpha(hkl) = \dots = \pi - \alpha(h\bar{k}l) "$$

should read $" \alpha(hkl) = \dots = \pi - \alpha(hkl) "$.

p. 26. Abm , $k=2n+1$:

Delete "or $k=0$ ".

Ama , $h=2n+1$:

Delete " $h=0$ or".

p. 27. Fdd :

Add } at end of formulae for A and B .

p. 29. Ima , $h=2n+1$:

Delete " $h=0$ or".

p. 64. $I\bar{4}c2$, bottom of page:

Delete " $A'=0$ if $h=\pm k$ ".

p. 80. $I42$, last set of coordinates:

" $y x \bar{z}$ " should read " $\bar{y} x z$ ".

p. 94. $R\bar{3}$, $h-k+l=3n$:

Add] at end of line.

p. 105. Second line:

Add } at end of line.

p. 115. $C\bar{6}c2$, $l=2n+1$:

$$" \alpha(\bar{h}kl) = \pi - \alpha(hkl) "$$

should read $" \alpha(\bar{h}kl) = \pi - \alpha(h\bar{k}l) "$.

p. 121. $C6_12$, $l=6n+1$:

$$" B = 2\{\cos[\sin - \sin] + \sin[\sin - \sin] + \sin[\sin - \sin]\} "$$

should read

$$" B = 2\{\cos[\sin - \sin] + \cos[\sin - \sin] + \cos[\sin - \sin]\} "$$