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A graphical method of indexing powder photographs of cubic substances and of determining unit-cell dimensions.

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This note describes a graphical method by means of which it is possible to determine, without any calculation, both the unit-cell dimension and the indices of the reflexions of cubic substances, when the positions of the diffraction lines on the powder photographs are known.

For the cubic system $\sin^2\theta = (h^2+k^2+l^2)\,\lambda^2/4a^2$, while, for a cylindrical camera, the Bragg angle in degrees is given by $\theta = 90L/\pi R$. Here a represents the cell edge, L the distance between corresponding diffraction lines on opposite sides of the undiffracted X-ray beam, and R the diameter of the camera.

By plotting L as a function of a for a given value of $(h^2+k^2+l^2)$, we obtain a smooth curve, which gives for this particular choice of indices the relation between the position of the corresponding diffraction line on the photograph and the cell dimension. Doing so for many values of $(h^2+k^2+l^2)$, we obtain a chart consisting of a large number of curves, from which we can read, conversely, the indices and the unit-cell dimension of the substance under investigation.

The reading of such a graph is carried out very simply by tracing on a strip of paper the measured values of L and by shifting this strip parallel to the L axis across the chart until all marks coincide with the curves. Then for each reflexion the indices are known, while the intersection of the strip with the a axis gives the cell dimension.

Table 1 gives some unit-cell dimensions measured in this way on a graph of 60 × 30 cm. For these readings none of the usual corrections for the line positions has been made.

Table 1. *Results of measurements of cell dimensions*

	a(A.)	
	Graphical	Experimental
Cu	3·66	3·68
Al	4·05	4·04
Ni	3·50	3·52
NaCl	5·60	5·63
KI	7·05	7·05
CaF_2	5·45	5·45
$CaTiO_3$	3·85	3·84

In using this method for measurements of cell dimensions, diffraction lines with a Bragg angle up to about 45° are especially suitable. The accuracy obtainable is about 0·5 % of the measured value, and this method therefore cannot be used for very accurate unit-cell determinations.

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The crystal structure of α-D-glucose.

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In a series of papers published between 1931 and 1935, E. G. Cox and his co-workers gave details of the space groups and unit-cell dimensions of a large number of sugars and sugar derivatives. On the basis of this work, it was suggested that the pyranose ring comprised a nearly planar group of five carbon atoms with one oxygen atom out of the plane (Cox, Goodwin & Wagstaff, 1935). Later work on glucosamine hydrobromide (Cox & Jeffrey, 1939) and sucrose sodium bromide dihydrate (Beevers & Cochran, 1947), however, proved the ring to be of the Sachse *trans* form. No other detailed structure determinations in the sugar series have been reported.

We have made a complete determination of the crystal structure of α-D-glucose. This work, though not yet sufficiently accurate for precise details of the bonding to be given, confirms the above findings relating to the *trans* configuration of the pyranose ring.

Crystal data

The crystals were grown from methanol solution at 18° C., the largest being about 2 mm. in length. Class, orthorhombic bisphenoidal; space group, $P2_12_12_1$; unit-cell dimensions,

$$a = 10\cdot36 \pm 0\cdot02,\ b = 14\cdot84 \pm 0\cdot03,\ c = 4\cdot93 \pm 0\cdot05\ \text{A.};$$

density, found 1·563 g.cm.$^{-3}$, calculated on the basis of 4 molecules of $C_6H_{12}O_6$ per unit cell 1·579 g.cm.$^{-3}$. The unit-cell measurements agree well with those of Hengstenberg & Mark (1930), and of Sponsler & Dore (1931). Sets of Weissenberg and oscillation photographs were taken about the three principal crystallographic axes, and the three Patterson projections and several sections at various z-levels were calculated. A correct interpretation of the projections led to the assignment of approximate x and y co-ordinates which were refined by successive Fourier syntheses. The z parameters were obtained very approximately from packing considerations and were refined by least-squares methods (Hughes, 1941), Fourier refinement being difficult owing to the very poor resolution in the ($h0l$) and ($0kl$) projections.

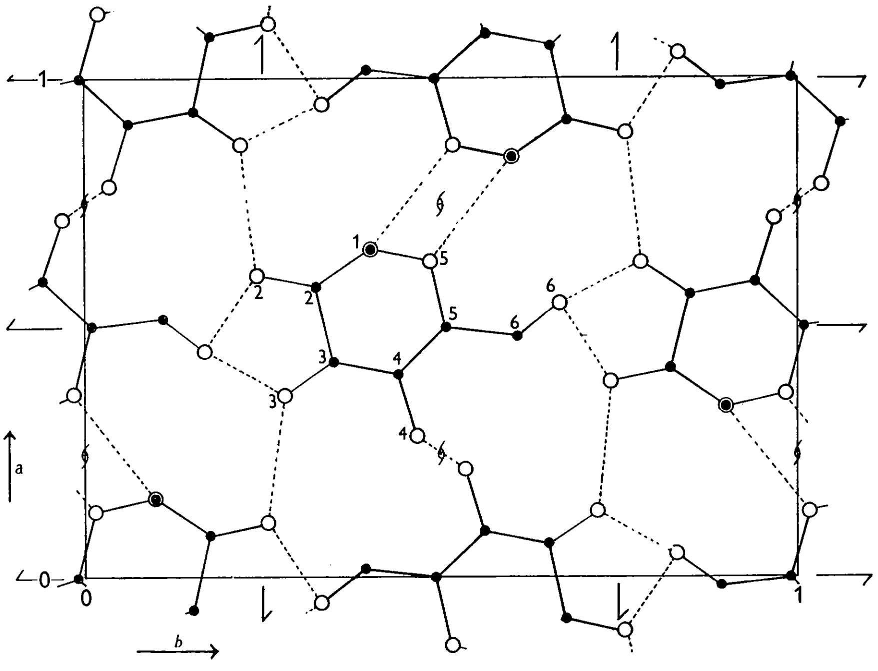

Fig. 1. Projection of completed unit cell down the c axis. Hydrogen bonds are shown as broken lines.

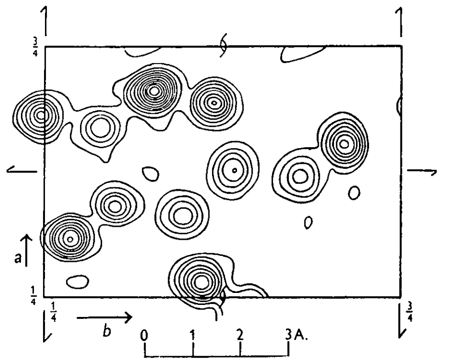

Fig. 2. Fourier projection down the c axis.

The 36 parameters defining the structure are as follows (in 120ths of the cell edges):

	x	y	z		x	y	z
O_1	19	12	79	C_1	19	12	111
O_2	13	31	110	C_2	10	21	5
O_3	104	26	20	C_3	112	18	0
O_4	94	4	8	C_4	109	7	12
O_5	16	2	3	C_5	0	119	118
O_6	6	100	114	C_6	118	107	9

The value of $R=\Sigma||F_{\text{obs.}}|-|F_{\text{calc.}}||/\Sigma|F_{\text{obs.}}|$ is less than 0·30 for each zone.

Description of the structure

Fig. 1 shows a projection of the structure down the c axis, and Fig. 2 an electron-density map calculated for this zone. Contours are drawn at intervals of 2 e.A.$^{-2}$, the zero contour being omitted. Hydrogen bonds between neighbouring molecules are shown as broken lines. Though the accuracy of the structure determination at this stage does not warrant attaching much significance to the bond lengths, the dimensions of the molecule are, on the whole, very similar to those found by Beevers & Cochran (1947). In the present case, however, the C_6–O_6 bond lies more nearly in the plane of the ring, allowing the molecule to take up the flattest possible configuration. The *cis* configuration of hydroxyl groups (1) and (2), which is well established on chemical grounds, is given direct confirmation. The molecules are held together by a very complete cross-linking system of hydrogen bonds, four oxygen atoms of each molecule being each directly attached to two oxygen atoms of the other molecules. In addition, there appear to be bonds between the ring oxygen atoms (5) and hydroxyl groups (1) of neighbouring molecules.

The structure is being refined further by the method of least squares, and it is hoped to publish the results of this work at a later date.

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