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Ethanolamine hydrogen *d*-tartrate: optical properties and X-ray diffraction data.*

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Ethanolamine hydrogen *d*-tartrate, $C_6H_{13}NO_7$, may be crystallized from an aqueous solution containing the appropriate proportions of ethanolamine and *d*-tartaric acid.

The crystals, which are piezoelectric, belong to the monoclinic sphenoidal class and have the appearance shown in Fig. 1 (*a*), the sphenoids {011} and {1$\bar{1}$0} defining

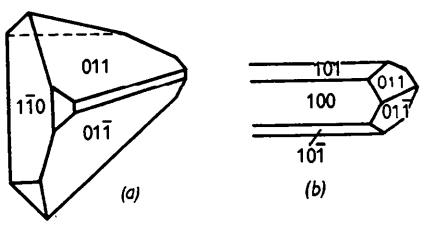

Fig. 1. Crystal habit.

the general shape of the crystals. When grown rapidly from a highly supersaturated solution, however, needles with pronounced pinacoids {100}, {101} and {10$\bar{1}$} are formed (Fig. 1 (*b*)).

The principal X-ray diffraction data and optical properties of these crystals are given below and in Table 1.

$C_6H_{13}NO_7$. Molecular weight = 211·2.

Density (18° C.) = 5·51 g.cm.$^{-3}$.

Table 1. *Principal 'powder' lines.*

(Intensities visually estimated; *d* not corrected for absorption).

d (Å)	Intensity	*d* (Å)	Intensity
7·64	*w*	3·34	*s*
5·92	*s*	3·22	*m–s*
5·75	*w*	3·12	*w*
5·59	*w*	2·96	*w*
5·34	*m*	2·86	*w–m*
4·65	*m*	2·81	*w–m*
4·40	*m*	2·67	*m*
3·90	*m*	2·63	*w*
3·81	*vs*	2·40	*w–m*
3·73	*m*	2·38	*m*
3·56	*w*	2·11	*w–m*
3·46	*m*		

(*w* = weak; *m* = medium; *s* = strong; *vs* = very strong)

Dimensions (±0·03 Å) of selected monoclinic structure cell:

$a = 8{\cdot}83$, $b = 7{\cdot}51$, $c = 7{\cdot}60$ Å; $\beta = 92°$.

Molecules per unit cell = 8 (calculated density = 5·57 g.cm.$^{-3}$).

Probable space group: $P2_1$–C_2^2: $0l0$ halved.

Cleavage: 001 (excellent).

Biaxial negative: optical axial angle ($2V$) approximately 19½° at 18° C. (sodium light).

Refractive indices (±0·001); sodium light; 18° C.:

$\gamma = 1{\cdot}551$ parallel to *b*.
$\beta = 1{\cdot}549$ parallel to *a* (to within ½°).
$\alpha = 1{\cdot}485$.

Dispersion: too weak for positive description.

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A simple mechanical structure-factor computing aid.

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A calculating analogue machine has been constructed which has proved useful in structure-factor calculations. It calculates simultaneously eleven values

$$C_n = \cos 2\pi(nu+m), \quad n = 0, 1, 2, \ldots, 10,$$

for any value of $0 \leqq u \leqq 1$ and $0 \leqq m \leqq 1$.

These two variables are fed into the machine by means of two hand-wheels. In order to reach a three-digit accuracy of setting, each variable is displayed on a pair of dials geared in a 1:10 ratio, the first dial reading the first digit, the second dial the second and third digits. The machine essentially consists of a 0:1:2:...:10 gear-box, in which the rotation *u* of the first hand-wheel is multiplied by *n* by a train of gears (see Fig. 1). The rotation *m* is then added to each product, for example by means of a differential. The sum $nu+m$ is then displayed as the angular displacement of the pointers on the eleven

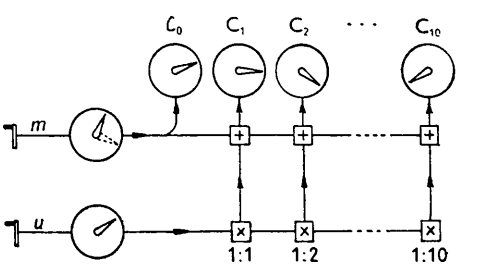

Fig. 1. Principle of the machine.

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output dials. In order to read cosines directly, the dials are graduated unevenly in cosine of the angle from $+1{\cdot}00$ to $-1{\cdot}00$. To prevent mistakes of sign, the negative half of each dial is painted red, the positive half blue. One of the output dials is shown in Fig. 2. In the present

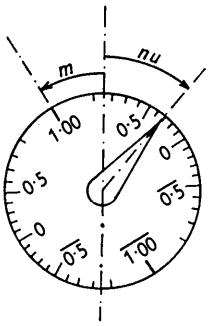

Fig. 2. One of the dials, reading $\cos 2\pi(nu+m)$.

machine, mechanical differentials are eliminated by imparting to all the output dials a rotation $-m$ and to the output pointers a rotation nu, so that each pointer is displaced $nu+m$ from the zero of its dial.

If the calculation of a structure factor

$$F(hkl) = \sum_{i}^{N} f_i \cos 2\pi(hx_i+ky_i+lz_i)$$

is required, for example, for eleven values of h in the interval $H \leqq h \leqq H+10$, the machine is set

$$u = x_i,\ m = Hx_i+ky_i+lz_i\ .$$

(For special reflexions, the procedure is simplified by substituting zero for Miller indices concerned.)

The nth dial then indicates the result for $h = n+H$. Eleven consecutive cosines relating to one atom only can thus be read off at one setting of the machine. This procedure is repeated N times for separate atoms $i = 1, 2, \ldots, N$, the cosines are written down, multiplied by f_i and summed as usual by hand or on an adding machine (the multiplication and summation may be reversed for groups of atoms having the same f_i).

By taking, say, $H = 0, 10, 20, \ldots$, any range of Miller indices can be covered, so that the range of the machine is unlimited. As there are eleven output dials, structure factors such as $h = 10, 20, \ldots$, are computed twice, which is useful for checking purposes.

If sines are required instead of cosines, $m-\frac{1}{4}$ instead of m can be set into the machine. This setting of the m dials can be assisted by extra pointers painted red which are displaced by $+\frac{1}{4}$ from the cosine pointers. Similarly, any phase angles can be set by adding them to m, if required.

The machine can also be used for structure-factor calculation expressed as products of sines and cosines and for other purposes; it proved especially convenient for calculations involving combination of Fourier transforms. Using the machine, the calculation of structure factors is speeded up several times compared with the long-hand method and is very reliable.

I wish to thank Prof. J. Monteath Robertson for his great interest.

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Crystallographic data of β-chondrosamine hydrochloride.

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During the last few years it has been found that chondrosamine (2-aminogalactose) is a constituent of blood group substances (Aminoff & Morgan, 1948), submaxillary mucin, gangliosides (Blix, Svennerholm & Werner, 1950) and serum glycoproteins (Werner, 1951; Odin & Werner, 1952). In most of these compounds chondrosamine occurs together with glucosamine from which it is separable only with difficulty. The best means for the identification of chondrosamine have been found to be the X-ray diffraction patterns of the hydrochlorides. The characteristic spacings of the powder diagrams of α- and β-chondrosamine hydrochloride have been reported earlier (Werner, 1952).

The crystal structure, however, is still unknown, presumably because of the difficulty of preparing crystals large enough for single-crystal measurements. This has now been accomplished in our laboratory with one of the anomers, β-chondrosamine hydrochloride.

The preliminary results of studies on those crystals are reported here.

The crystals of β-chondrosamine hydrochloride, $C_6H_{13}O_5N.HCl$, (mol.wt. 215·6) were found to be orthorhombic, with the unit cell dimensions:

$$a = 9{\cdot}40,\quad b = 9{\cdot}85,\quad c = 19{\cdot}85\ \text{Å}\ .$$

Using Cu $K\alpha$ radiation, oscillation and Weissenberg photographs about the three axes and the diagonal [110] showed absent ($h00$) reflexions for h odd and absent ($0k0$) for k odd. The ($00l$) were also absent for l odd, except (005) which was registered though very weak. This establishes the space group as D_2^3–$P2_12_12$.

The density, measured by the flotation method, was found to be 1·55 g.cm.$^{-3}$, which requires 8 molecules in the cell (calculated density = 1·56 g.cm.$^{-3}$).

The crystals are fragile, thin, needle-shaped prisms bounded by {110}.

The spacings calculated from the reflexions on the powder diagram reported earlier (Werner, 1952) agree perfectly with those found on the Weissenberg photographs.

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