Short Communications

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The unit cell and space group of sodium acetate trihydrate, $NaC_2H_3O_2.3H_2O$.

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Sodium acetate trihydrate crystals, which appear generally in the form of long but very thin needles, belong to the monoclinic system. The lattice parameters were given with a limited accuracy ($a=12{\cdot}4$, $b=10{\cdot}5$, $c=10{\cdot}3$ Å; $\beta=112{\cdot}1°$, $Z=8$) by Padmanabhan (1952) who stated its space group to be either *Cm* or *C*2/*m*. Working on the determination of the structure of $NaC_2H_3O_2 . 3H_2O$, we found that its space group differs from that given by Padmanabhan.

For our investigations small stubby, well-shaped single crystals were used. These crystals were obtained from an almost saturated aqueous solution by cooling it slowly and rubbing the wall of the glass container with a metal rod. If the mother liquor is carefully diluted with water, some of the small stubby crystals assume an almost perfectly spherical form. These crystals were quite suitable for X-ray diffraction work. Unfortunately the crystals spontaneously disintegrated in the open air; therefore they had to be covered with a suitable protecting lacquer immediately on removal from the mother liquor.

The unit-cell dimensions determined from Buerger precession photographs around *b* and *c* axes with Cu $K\alpha$ radiation ($\lambda=1{\cdot}542$ Å), are:

$$a=12{\cdot}321\pm0{\cdot}01 \text{ Å} \qquad b=10{\cdot}425\pm0{\cdot}01 \text{ Å}$$
$$c=10{\cdot}380\pm0{\cdot}01 \text{ Å} \qquad \beta=111{\cdot}71\pm0{\cdot}15° .$$

From these the axial ratios are:

$$a:b:c=1{\cdot}1818:1:0{\cdot}9957,$$

which are in good agreement with those obtained optically (Groth, 1909).

$$a:b:c=1{\cdot}1809:1:0{\cdot}9963 \quad \beta=111°42' .$$

The unit cell contains 8 molecules from which $D_x=1{\cdot}458$ g.cm^{-3} ($D_m=1{\cdot}456$ g.cm^{-3}; Schröder, 1881).

The single-crystal photographs indicate the following conditions for systematic absences of reflexions:

hkl present only for	$h+k=2n$
*h*0*l*	($h=2n$), $l=2n$
0*k*0	($k=2n$) .

These indicate the space group to be either *Cc* or *C*2/*c*.

For the determination of the presence or absence of the centre of symmetry an $N(z)$ statistical test (Howells, Phillips & Rogers, 1950) was made of 75 *hk*0 reflexions, obtained by an integrating Weissenberg goniometer, using the multiple-film technique. The intensities measured with a Zeiss fast photometer were corrected for all factors and were put on an absolute scale by Wilson's method. The intensity distribution curve obviously showed the (001) projection to be centrosymmetric. From this the correct space group is *C*2/*c* (C_{2h}^6), which is also in a good agreement with previous findings that sodium acetate trihydrate belongs to the monoclinic-prismatic crystal class.

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Anomalous dispersion effect in the structure of barium titanate.

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In the structure analysis of barium titanate (Evans, 1961), it was found that the study was indeterminate in that values of the discrepancy index as low as 0·037 were obtained for different sets of structural and thermal parameters. The difficulty was attributed to the strong interaction between some of these parameters in X-ray diffraction and this aspect has been further discussed (Geller, 1961; Megaw, 1962). In view of the interest in this structure analysis, it was felt appropriate to report the effect of the imaginary part of the anomalous scattering, which was neglected in the study.

About 356 reflexions of the type *h*0*l* were measured by Evans to obtain on averaging 99 non-equivalent structure amplitudes, of which 16 were omitted owing to serious extinction. The intensities were fairly strong even at the highest angles where $\sin\theta/\lambda$ was about 1·41 for the Mo $K\alpha$ radiation used in the experiment.