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Crystallographic data for certain alkaloids. IV.

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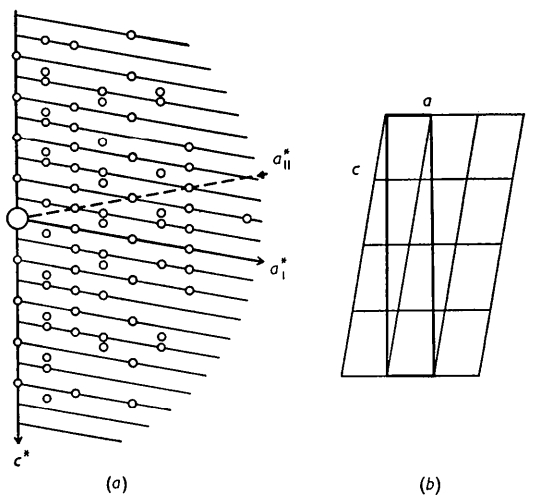
Arecoline hydrobromide, $C_8H_{13}NO_2.HBr$

Crystals grown from solution in hot ethanol were very small prisms of too poor a quality for a useful optical examination. The Laue symmetry appeared to be *mmm*, but oscillation and Weissenberg photographs showed systematic peculiarities in the diffraction pattern which are not readily interpreted in terms of the orthorhombic crystal system. A diagram of the observed *h*0*l* reciprocal-lattice plane is shown in Fig. 1(*a*). The crystals are considered to belong to the monoclinic system and to be twinned polysynthetically with *b** and *c** in common and two orientations of *a**. The unit-cell dimensions (accurate to within about 1%) are then:



(*a*) (*b*)

Fig. 1. (*a*) Observed *h*0*l* reflexions with reciprocal-lattice axes marked for normal twinning. (*b*) Monoclinic and pseudo-orthorhombic unit cells.

$$a = 9{\cdot}90,\ b = 7{\cdot}40,\ c = 14{\cdot}1\ \text{Å};\ \beta = 100 \pm 1°$$

with 4 molecules per unit cell. Density: calculated 1·54 g.cm.$^{-3}$; observed 1·5±0·1 g.cm.$^{-3}$.

Reflexions 0*k*0 are present only when $k = 2n$. Not all the *h*0*l* reflexions can be indexed unambiguously because of the seemingly exact overlapping of independent reflexions from the twin components. The absences which can be established all comply, however, with the rule that reflexions *h*0*l* are present only when $h+l = 2n$. Reflexions *hkl* are present in all orders. The probable space group, therefore, is $P2_1/n$.

This appears to be an example of 'twinning by reticular pseudo-merohedry' (Friedel, 1905): a multiple lattice simulates a symmetry higher than that of the lattice. Here the axis [104] is very closely perpendicular to (001), $\cos\beta = -a/4c$, making possible the pseudo-orthorhombic unit-cell base outlined in Fig. 1(*b*).

The twin operation is one of the operations of orthorhombic pseudo-symmetry associated with this quadruple cell but not included in any possible monoclinic symmetry.

Sparteine sulphate pentahydrate, $C_{15}H_{26}N_2.H_2SO_4.5H_2O$

Crystals grown from dilute ethanol were plates with well formed pinacoids {001}. Oscillation and Weissenberg photographs showed the Laue symmetry to be 2/*m* and gave the monoclinic unit-cell dimensions:

$$a = 8{\cdot}03,\ b = 15{\cdot}2,\ c = 8{\cdot}84\ \text{Å};\ \beta = 91°\ 30' \pm 1°.$$

There are 2 molecules per unit cell. Density: calculated 1·30 g.cm.$^{-3}$; observed 1·28 g.cm.$^{-3}$.

Reflexions 0*k*0 are present only when $k = 2n$. All other classes of reflexions are present in all orders so that the space group is either $P2_1$ or $P2_1/m$. Since the compound is optically active, however, $P2_1$ must be chosen. This choice has been confirmed by an investigation of the distribution of intensities among the *h*0*l* and 0*kl* reflexions (Wilson, 1951).

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On the substantialization of sign sequences.

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Woolfson (1954) describes a method for the determination of the signs of the structure factors of a centrosymmetrical crystal. The method depends on a standard set of sixteen sequences of seven signs (7-sequences) such that each of the 128 possible 7-sequences differs from one of the set in at most one sign. In the present note the structure of the set is explained and is extended to a set, *S*, of 2048 15-sequences such that each of the 32,768 possible