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The unit-cell dimensions and space group of rauwolscane.

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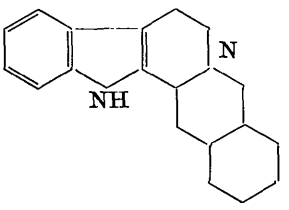
Rauwolscine (Chatterjee, 1953) $C_{21}H_{26}O_3N_2$, m.p. 232° C., is the only alkaloid of *Rauwolfia Canescence* Linn of the Bengal variety. It has been isolated from an alcoholic percolate of the air-dried leaves. Rauwolscine crystallizes from alcohol in thick colourless plates. On applying the Huang–Minlon variant of the Wolff–Kishner reduction, Rauwolscine yields a hydrocarbon rauwolscane, $C_{19}H_{24}N_2$, m.p. 156–157° C.:



This was purified through its hydrochloride. The substance crystallizes from methanol in stout white rods. After several recrystallizations from the same solvent, chromatic purification, and drying over P_2O_5 at 85° C. at a pressure of 0·01 mm. Hg, the pure substance was obtained.

Single crystals suitable for X-ray investigation were prepared by slow evaporation of a solution in acetone at a low temperature. Rauwolscane was found to crystallize in transparent quadrangular plates with one molecule of acetone of crystallization. The reflexion spots recorded in all photographs taken with transparent single crystals begin to disappear, and diffraction lines as in powder photographs are observed, as soon as the crystal loses its acetone of crystallization and transforms into an opaque mass. It may thus be inferred that the acetone of crystallization forms an integral part of the crystalline structure of the substance. Consequently the crystal selected for X-ray investigation was covered with a thin coating of collodion.

Morphological and goniometric studies, carried out by reflection goniometer, showed the crystal to be orthorhombic (Ray, 1955). The crystals were elongated parallel to [100] and were bounded by faces of the forms {100}, {010}, {001} (large), {101} and {011}. The axial ratios calculated from the goniometric measurements were found to agree fairly well with those derived from the X-ray measurements.

Optical properties

Studies under a polarizing microscope, using monochromatic light, showed that rauwolscane is an optically negative orthorhombic crystal. The *a*, *b* and *c* crystallographic directions were found to coincide with the *X*, *Y* and *Z* optical directions respectively:

$$\alpha = 1{\cdot}490, \quad \beta = 1{\cdot}616, \quad \gamma = 1{\cdot}650 .$$

The optic axial angle, measured on the Federov universal stage, is $V_Z = 64°$; and hence $2V_X = 52°$.

Unit-cell dimensions and space group

Oscillation, rotation, and normal and equi-inclination Weissenberg photographs were taken, using copper radiation filtered through a nickel foil of proper thickness. The cell dimensions were found to be

$$a = 7{\cdot}1, \quad b = 12{\cdot}2, \quad c = 23{\cdot}4 \text{ Å} .$$

A higher degree of accuracy is not claimed, since no allowance was made for film shrinkage.

The measured density of the sample was 1·13 g.cm.$^{-3}$ and the calculated density, corresponding to four molecules in the unit-cell, was 1·14 g.cm.$^{-3}$.

The reflexions appearing on the *a*-, *b*- and *c*-axis zero-layer Weissenberg photographs and also on the first and second layer photographs on the *a*-axis taken by the equi-inclination method show the following systematic absences:

hkl, 0*kl*, *h*0*l*, *hk*0: none;
*h*00, 0*k*0, 00*l*: when *h*, *k* and *l*, respectively, are odd.

These conditions indicate the space group $P2_12_12_1$, and packing considerations were found to agree with the assumed space group.

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Systematic absences corresponding to false symmetry.

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The presence in a crystal of screw axes or glide planes is accompanied by certain systematic absences in the X-ray reflections. It is recognized that special arrangements of atoms can cause weak reflections which may be mistaken for systematic absences, especially in the cases of screw axes where the number of relevant reflections observed may be quite small.

There exists, furthermore, a kind of special arrange-