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Short Communications

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Preliminary single-crystal X-ray and optical study of nor-harman, $C_{11}H_8N_2$.

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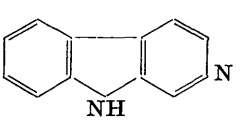
Introduction

Very few complete structure determinations of the heterogeneous ring compounds containing more than one benzene nucleus have been reported. The author has undertaken a systematic investigation of some ring compounds the complete determination of whose structure will give very valuable data for the study of *Rauwolfia* alkaloids. The preliminary crystal data of the compounds rauwolscane, $C_{19}H_{24}N_2$, and harmine, $C_{12}H_{13}N_2O$, have been reported (Ray, 1956, 1957), and the present paper reports the results of X-ray and optical measurements carried out with single crystals of nor-harman. A complete structure determination of this simple compound by the Fourier-synthesis method has been taken up and the results will be published in due course.

Experimental

Nor-harman, $C_{11}H_8N_2$, a colourless substance melting at 198–9° C., is of particular interest because it is the simplest of the series of the heterogeneous compounds mentioned above, having the structural formula



The crystals used in this investigation were from materials very kindly supplied by Dr Schlittler of the Ciba Pharmaceutical Products, New Jersey. The compound subsequently synthesized here by Dr (Mrs) A. Chatterjee and Dr P. Bagchi gave identical results. The substance was crystallized from a solution containing a mixture of alcohol and acetone. Thin plates and rod-like crystals, which are seldom well-formed, are usually obtained. The crystals exhibit the forms {011} and {110}; the faces {110} though present are not well developed.

Morphological and goniometric studies showed the crystal to be orthorhombic and gave

$$a:b:c = 0{\cdot}5982:1:1{\cdot}494 .$$

The axial ratios calculated from the X-ray results were found to agree fairly well with those derived goniometrically.

Studies under a polarizing microscope showed that Nor-harman is optically positive. The refractive indices along the three principal directions are

$$\alpha = 1{\cdot}758, \quad \beta = 1{\cdot}759, \quad \gamma = 1{\cdot}806 .$$

Single-crystal rotation and Weissenberg diagrams were obtained along the three crystallographic directions with a very small crystal, using copper radiation filtered through nickel foil of proper thickness. Rotation as well as Weissenberg diagrams gave

$$a = 5{\cdot}9, \quad b = 9{\cdot}8, \quad c = 14{\cdot}6 \text{ Å} .$$

A higher degree of accuracy is not claimed as no allowance has been made for the film shrinkage etc.

Complete sets of $h00$, $0k0$, $00l$, $h0l$, $0kl$, $hk0$ and hkl data were recorded on Weissenberg photographs. The planes $h00$, $0k0$ and $00l$ are absent when h, k and l, respectively, are odd. No other systematic absences were found. These conditions indicate the space group $P2_12_12_1$–D_2^4 with four molecules of nor-harman in the unit cell. The density of the crystal, determined by flotation, was 1·32 g.cm.$^{-3}$, and the calculated density, corresponding to four molecules of nor-harman in the unit cell, is 1·319 g.cm.$^{-3}$.

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