

THE X-RAY CRYSTAL STRUCTURE AND STEREOCHEMISTRY OF VERTALINE

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The molecular structure of the alkaloid vertaline (of the Lythaceae group of alkaloids) has been elucidated by X-ray analysis. The results define the constitution and stereochemistry (apart from absolute configuration). Fig. 1. The ring fusion in the quinolizidine ring is *cis*, and the lactone group and the biphenyl ether are linked to the quinolizidine ring in the axial and equatorial positions respectively.

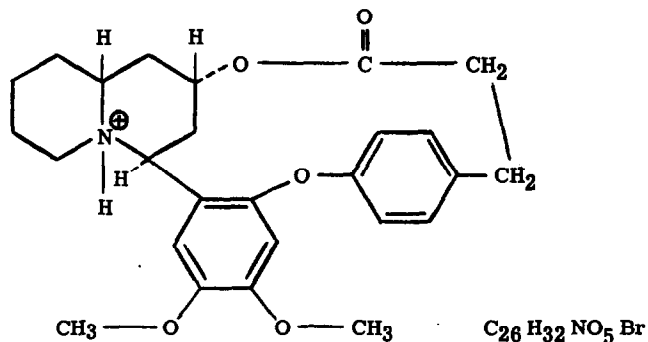


Fig. 1

The X-ray study was carried out on vertaline hydrobromide, crystals of which were supplied by Dr. J. Ferris (1). The crystals belonged to

the orthorhombic system with cell dimensions $a = 7.49\text{\AA}$, $b = 23.47\text{\AA}$, $c = 13.23\text{\AA}$. There are four molecules in the unit cell, and the space group is $P2_12_12_1$. Three dimensional data were collected about the b axis on the Super-Pace automated diffractometer using filtered Molybdenum radiation from which 1484 independent observed reflections were obtained.

The coordinates of the bromide ion were found from a three dimensional Patterson map. The first Fourier synthesis calculated using the bromide phases was uninterpretable. A three dimensional Patterson superposition map was calculated from the four equivalent positions of the bromide ion, and peaks common to both the Fourier map and the superposition were assumed to be true. The atom positions corresponding to these were included in subsequent phasing calculations. The structure was fully determined from the third three dimensional Fourier synthesis. All atom positions were used in subsequent refinement cycles. At present the average discrepancy between the measured and calculated structure amplitudes is 20%. Further refinement is proceeding. Superimposed contour sections illustrating the latest three dimensional electron distribution over the molecule are shown in Fig. 2.

The final structure is consistent with the chemical information supplied by Dr. J. Ferris (private communication).

References

1. J. P. Ferris, J. Org. Chem. 27, 2985 (1962).

Acknowledgments

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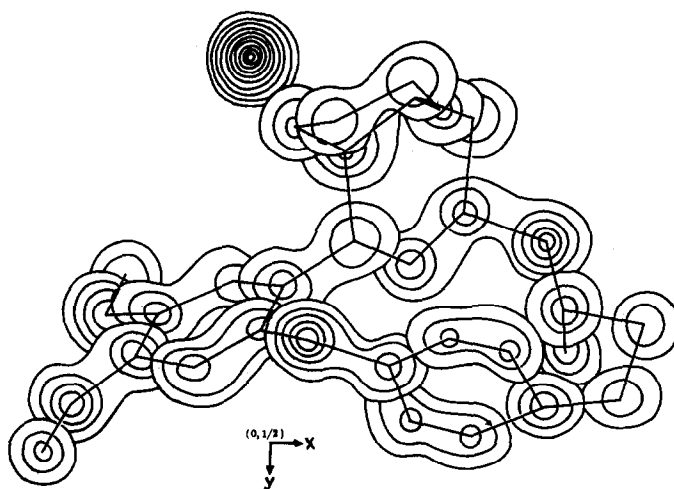


FIG. 2. THE LATEST THREE DIMENSIONAL ELECTRON-DENSITY DISTRIBUTION FOR VERTICALINE HYDROBROMIDE SHOWN BY MEANS OF SUPERIMPOSED CONTOUR SECTIONS PARALLEL TO (001)