Tetrahedron Letters No. 7, pp. 24-26, 1960. Pergamon Press Ltd. Printed in Great Britain.

AN X-RAY STUDY OF THE CONFIGURATION OF CEVINE

W. T. Eeles

Viriamu Jones Laboratory, University College, Cardiff

(Received 7 March 1960)

THE structure and configuration of cevine have been the subject of extensive study. Milestones in their elucidation were the deduction of the form of the skeleton,[1] and the assignment of the hydroxyl groups.[2] Recently

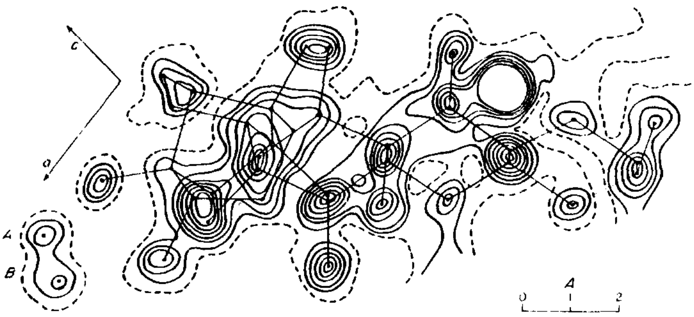


FIG.1. Electron-density map of cevine hydroiodide [010] projection, space group $P2_1$, $\underline{a} = 7{\cdot}7$, $\underline{b} = 10{\cdot}8$, $\underline{c} = 17{\cdot}4$A, $\beta = 97^{\circ}$. Two molecules per unit cell.

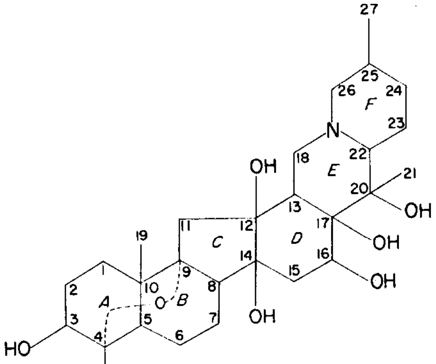
---

[1] W.A. Jacobs and S.W. Pelletier, J. Org. Chem. 18, 765 (1953).

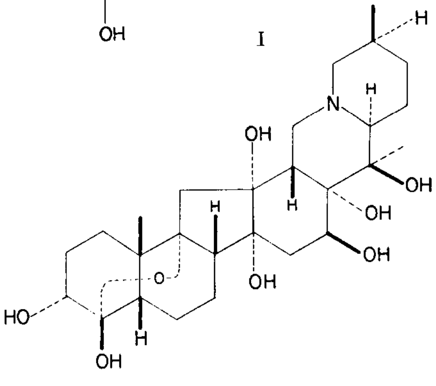
[2] D.H.R. Barton, O. Jeger, V. Prelog and R.B. Woodward, Experientia 10, 81 (1954).

comprehensive evidence of the relative configuration of the various centres of asymmetry has been published.[3]

The author has been engaged in the study of various cevine derivatives by X-ray crystallographic methods, and has independently arrived at the configuration given in ref. 3. The evidence for this is presented in Fig.1 which shows a projected electron-density map of cevine hydroiodide. Hydrogen atoms are beyond the limits of resolution but the other constituents show up clearly. In addition to the cevine molecule and its associated iodine atom



I



II

---

[3] S.M. Kupchan, W.S. Johnson and S. Rajagopalan, Tetrahedron 7, 47 (1959).

there are two molecules of water of crystallization, A and B. Though some of the carbon and oxygen atoms are not individually resolved, their positions can be inferred with the aid of plausible wire models of the cevine molecule. The models which were used were based on the formula I (formula XXXI of ref. 2), and the only one which satisfies the X-ray data has the configuration II. This is identical with that given in ref. 3.

With the exception of the configuration at C_{20} the X-ray data constitutes conclusive evidence of all the stereochemical features of cevine. Little need be said here about the A-B-C system except that the hydroxyl at C_3 is equatorial and all three rings are somewhat distorted, C being non-planar. The rings E,D and F are a system of trans-fused 'chairs' with C_{27} and the hydroxyls at C_{12},C_{14},C_{16} and C_{17} in axial dispositions. The arrangement of the methyl and hydroxyl groups at C_{20} which is favoured is that shown in II; but the distinction between the two possibilities rests on the actual heights of peaks and these are not sufficiently accurate to preclude the alternative arrangement.

This investigation is continuing and it is hoped that full crystallographic details will be publishable elsewhere in the near future. The author wishes to acknowledge his indebtedness to Professor A.J.C. Wilson and his staff for advice and help with the computations, and to Professor D.H.R. Barton for providing specimens.