

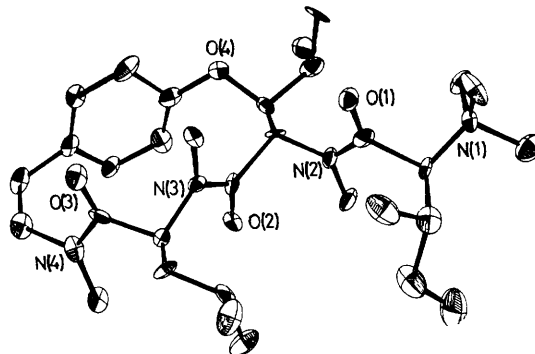
## X-ray Analysis of Tri-*N*-methylfrangulanine Methiodide

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**Summary** The crystal structure of a peptide alkaloid derivative, tri-*N*-methylfrangulanine methiodide, is reported.

FRANGULANINE is a peptide alkaloid,<sup>1</sup> with a 14-membered ring, whose structure has been established chemically.<sup>2</sup> We have now elucidated the crystal structure of a derivative of frangulanine, which was isolated from *Hovenia dulcis* Thunb.<sup>3</sup> (Rhamnaceae). Methylation of frangulanine with methyl iodide gave tri-*N*-methylfrangulanine methiodide, m.p. 242–244°, C<sub>32</sub>H<sub>53</sub>N<sub>4</sub>O<sub>4</sub>I, crystallizing in space group *P*2<sub>1</sub>2<sub>1</sub>2<sub>1</sub> with *a* = 8.826, *b* = 49.950, *c* = 8.296 Å and *Z* = 4. The intensity data were collected using Cu-*K*<sub>α</sub> radiation and an automatic four-circle diffractometer, and 1383 reflections were observed. The structure was solved by the heavy atom method and the current *R* index is 10.1%.



The stereochemistry of the β-hydroxyleucine group was confirmed to be the *erythro* form and a twisted correlation between the benzene ring and the neighbouring double bond was shown.

(Received, 3rd June 1974; Com. 633.)

<sup>1</sup> E. W. Warnhoff, 'Fortschritte der Chemie Organischer Naturstoffe,' Bd. 28, S. 192, Springer, Wien, 1970.

<sup>2</sup> R. Tschesche, H. Last, and H. W. Fehlhaber, *Chem. Ber.*, 1967, **100**, 3937; M. Gonzales Sierra, O. A. Mascaretti, F. J. Oiaz, E. A. Rúveda, Ching-Jer Chang, E. W. Hagaman, and E. Wenkety, *J.C.S. Chem. Comm.*, 1972, 915.

<sup>3</sup> M. Takai, Y. Ogihara, and S. Shibata, *Phytochemistry*, 1973, **12**, 2985.