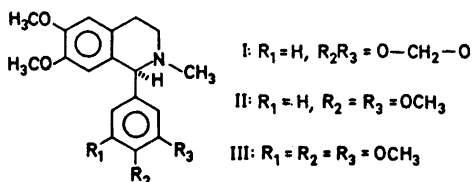


Studies on Orchidaceae Alkaloids

XXXIV.* The Absolute Configuration of Cryptostyline I, II, and III, three 1-Phenyl-1,2,3,4-tetrahydroisokinolines from *Cryptostylis fulva* Schlr.KURT LEANDER,^a BJÖRN LÜNING^a and LEIF WESTIN^b^aDepartment of Organic Chemistry, University of Stockholm, Sandåsgatan 2, S-113 27 Stockholm, Sweden and ^bInstitute of Inorganic and Physical Chemistry, University of Stockholm, S-104 05 Stockholm, Sweden

The occurrence of three optically active 1-phenyl-1,2,3,4-tetrahydroisokinolines in *Cryptostylis fulva* Schlr. has been reported.² Two papers have appeared dealing with the absolute configuration of these alkaloids. Kametani *et al.*³ compared the CD curve of cryptostyline III with that of 1*R*-phenyl-2-methyl-6-methoxy-1,2,3,4-tetrahydroisokinoline, and concluded that the alkaloid has the *R*-configuration. Brossi and Teitel⁴ have recently determined the absolute configuration of cryptostyline I,



II, and III by CD and an X-ray investigation of the hydrobromide of the enantiomer of cryptostyline II. Their studies indicated that the alkaloids have the *S*-configuration.

In this communication an X-ray diffraction investigation of the methiodide of cryptostyline I (IV) is reported.

* For number XXXIII of this series, see Ref. 1.

The crystal structure of IV was determined by the X-ray single crystal technique using an automatic Siemens diffractometer. The methiodide² (IV) crystallises from ethanol in the orthorhombic space group $P2_12_12_1$ with four molecules per asymmetric unit. The cell dimensions are $a = 18.093 \pm 1$ Å, $b = 11.940 \pm 1$ Å, and $c = 9.227 \pm 1$ Å. The absolute configuration of IV was established by studying the anomalous dispersion effect of $CuK\alpha$ radiation by the iodine atoms, including an examination of the Bijvoet pairs. The difference in the *R*-values for the two enantiomers was 2%. This analysis indicates that the cryptostyline has the *S*-configuration. This assignment is in accordance with that of Brossi and Teitel⁴ but in conflict with that of Kametani *et al.*³ Full details of the X-ray diffraction investigation has been published.⁵

It appears from the work on cherylline^{6,7} and the cryptostyline⁴ that a β -(*S*)-configuration is connected with two negative Cotton effects at ≈ 290 nm and 210 nm, respectively. This is also consistent with the results from studies on some lignans⁸ (4-aryltetralins) where, however, only the long wavelength band was recorded.

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