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THE STRUCTURE OF LEDECORINE

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UDC 547.943

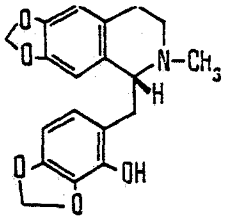
Continuing the separation of the combined alkaloids of *Corydalis ledebouriana* [1], we have isolated a new base with mp 199-200°C (methanol), $[\alpha]_D$ −112° (c 0.42; CH_3OH) which we have called ledecorine (I). The UV spectrum [$\lambda_{max}^{ethanol}$ 240 infl., 295 nm (log ε 3.88, 3.74)] is similar to that of corydalisol [2]. The IR spectrum of the base shows absorption bands at (cm^{-1}) 935 and 1040 (methylenedioxy group), 1590 and 1620 (aromatic ring), and 3430 (hydroxy group). The mass spectrum of the base lacks the peak of the molecular ion and has the peaks of ions with m/e 190 (100%), 175, 160, and 149.

In the NMR spectrum of ledecorine at 4.20 ppm (J = 6 Hz) there is a triplet characteristic for the C_1 proton of a benzyltetrahydroisoquinoline alkaloid. Signals are also observed in the form of a three-proton singlet at 2.55 ppm ($N-CH_3$), one-proton singlets at 5.86 and 5.88 ppm (CH_2O_2), a two-proton singlet at 6.01 ppm (CH_2O_2), one-proton singlets at 6.23 and 6.54 ppm (para aromatic protons), and one-proton doublets at 6.27 and 6.58 ppm (J = 8 Hz, orthoaromatic protons). Methylene protons are represented by signals at 2.60-3.20 ppm.

The facts given permit ledecorine to be assigned to the benzyltetrahydroisoquinoline alkaloids. The methylation of ledecorine with diazomethane gave the O-methyl ether (II).

When the protons of the methoxy group in O-methylledecorine were irradiated with a strong radiofrequency field, no nuclear Overhauser effect with the aromatic protons was observed. Consequently, there are no aromatic protons adjacent to the hydroxy group in ledecorine. The presence in the mass spectra of (I) and (II) of an ion with m/e 190 and of the signals of para and ortho aromatic protons in the NMR spectrum, and also the results of the NOE measurements show that one of the methylenedioxy groups is present in ring A at C_6 and C_7, and the second methylenedioxy group and the hydroxy group are present in ring C at C_4', C_3', and C_2', respectively.

In the ORD spectrum of ledecorine there are two negative Cotton effects which show the R configuration of the asymmetric center [3]. According to the results obtained, ledecorine has the following structure:



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X-RAY STRUCTURAL INVESTIGATION OF THE ALKALOID SOPHORIDINE

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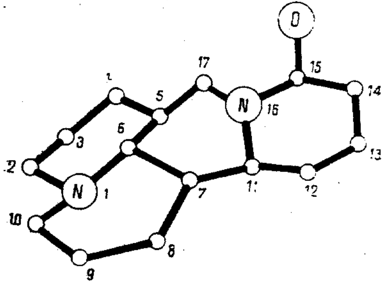
Information on the spatial structure of sophoridine up to 1975 was ambiguous and only investigations by the INDOR method and by PMR spectroscopy at 300 MHz [1] made it possible to reduce this ambiguity. It was shown that sophoridine has a conformation with two rings in the boat form (rings B and C). However, the IR spectra of sophoridine in the liquid and solid phases proved to be different [2] and, in view of the lability of the conformation of this alkaloid found in a study of chemical reactions in solutions, it could be assumed that the spatial structure of sophoridine in the crystalline state was different from that in solutions. In order to determine the conformational state of the sophoridine molecule in crystals we have made an x-ray structural investigation of this compound.

Single crystals of sophoridine obtained by crystallization from petroleum ether have an acicular form. The parameters of the monoclinic cell measured on precession x-ray diagrams and refined on a "Sinteks $P2_1$" diffractometer were as follows: $a = 5.458(1)$, $b = 10.640(2)$, $c = 11.989(2)$ Å, $Y = 99.7(3)°$, $V = 686.2$ Å^3, mol. wt. = 258, $d_{calc} = 1.19$ g/cm^3, $Z = 2$, space group $P2_1$. The intensities of 920 reflections were measured by $\theta/2\theta$ scanning in CuK$_\alpha$ radiation (graphite monochromator) up to $2\theta \leq 110°$ on the above-mentioned diffractometer; 802 reflections with $I \geq 2\sigma$ were used in the calculations.

A model of the structure was found by using the "Roentgen-75" system of programs [3] and was refined by the method of least squares in the anisotropic approximation to $R = 0.090$ by a program of the "Kristall" group [4]. The geometry of the molecule is shown in Fig. 1.



Ring A has the chair form with the same departure of the C(3) and C(6) apical atoms from the C(1) C(2) C(4) C(5) plane of ±0.68 Å, i.e., less than for the ideal cyclohexane C_6 chair of ±0.73 Å [5]. Rings B and C have the $^{1,8}B$ and $^{5,11}B$ unsymmetrical boat conformations with different bends of the apices. The deviations of the angles in these rings from the plane of the "bottom" of the boat are 0.68 Å and 0.60 Å for the N(1) and C(5) and for the C(8) and C(11) atoms, respectively. The conformation of ring D is close to the half-chair conformation; the C(12) and C(13) atoms deviate in opposite directions by 0.60 and 0.13 Å from the plane of the other atoms of the ring. Thus, the conformation of ring D of sophoridine in the crystal differs from the conformation of this ring in solution [1].

The A/B, A/C, and C/D ring linkages are trans and the B/C linkage is cis. The coordination of the N(1) nitrogen is pyramidal. Because of conjugation in the lactam fragment of the

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