

A STUDY OF THE ALKALOIDS OF NITRARIA SCHOBERI.
THE STRUCTURE OF NITRARINE.

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A new alkaloid nitrarine [1], $C_{20}H_{25}N_3$, mp 231–232°C (decomp.), $[\alpha]_D^{20} \pm 0^\circ$ has been isolated from Nitraria Schoberi L. (family Zygapylaceae). In descending paper chromatography in the 1-butanol–acetic acid–water (3:1:4) system it has R_f 0.66. In thin-layer chromatography on a fixed layer of silica gel and gypsum (9:1) in the chloroform–methanol–1-butanol–acetic acid system (9:1:1:0.5) it has R_f 0.22.

Nitrarine gives a crystalline dipicrate with mp 207–208°C, dihydrochloride with mp 246–247°C and methiodide with mp 269–270°C. It contains no C–CH₃ or N–CH₃ groups. UV spectrum of I: λ_{max} 228, 278–280 m μ (log ϵ 4.60, 3.98), which is characteristic for β -carboline bases [1].

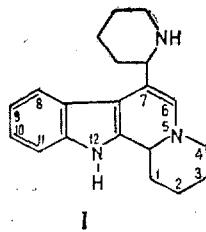
The IR spectrum of I has a strong absorption band at 750 cm^{-1} , which is characteristic for a 1,2-disubstituted benzene ring; absorption bands in the 3300 and 3480 cm^{-1} regions indicate the presence of two NH groups in the molecule.

The mass spectrum of I taken on a MKh-1303 mass spectrometer at an energy of the ionizing electrons of 34 eV and a temperature of 225° C has the peaks of the following ions: $(M^+, m/e 307)$, $(M - 1, m/e 306)$, $\cdot CH_2(CH_2)_3-NH=CH_2, m/e 85$; $-^+NH=CH_2$ with $m/e 70$, $CH_2-NH-CH_2$ with $m/e 43$, and $CH_2=N=CH_2$ with $m/e 42$, which are connected with the fragmentation of a monosubstituted piperidine part of the molecule. An intense peak with $m/e 84$ belongs to the ion formed by cleavage of the C-C bond between a monosubstituted piperidine nucleus and a β -carboline system. By further fragmentation, the ion with $m/e 84$ gives the ions $\cdot CH_2-CH_2-NH=CH_2$ with $m/e 57$, $CH_2=CH-N=CH_2$ with $m/e 56$, and $CH_3-NH=CH_2$ with $m/e 44$.

The splitting off of the ion with m/e 84 from the molecular ion leads to an ion with m/e 223, which is an indolo-tetrahydroquinolizidine derivative from which cleavage between the C_4 carbon and $N_{(5)}$ forms an ion with m/e 169 and an ion with m/e 168- β -carboline derivatives.

The mass spectrum of I also has peaks of medium intensity with m/e 182, 156, 144, 143, and 130, which are formed by fragmentation of the ion with m/e 223.

We propose the following most probable structural formula (I) for nitrarine.



REFERENCE

1. A. W. Sangster and K. L. Stuart, *Chem. Rev.*, 65-69, 1965.

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