ALKALOIDS OF Nitraria komarovii.

XIV. DEOXYPEGANINE N-OXIDE

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Continuing an investigation of the alkaloids from the epigeal part of the plant Nitraria komarovii Iljin et Lava [1], gathered in May, 1987, by column chromatography of the benzene fraction of the total bases we have isolated a new base (I) with mp 243-244°C (ethanol–acetone), composition $C_{11}H_{12}N_2O$, $[\alpha]_D \pm 0°$.

The mass spectrum of (I) contained the peaks of ions with m/z 188(5), 187(10), 172(45), 171(100), 155(20), 144(30), 143(44), 131(35), 129(65), 116(81), 104(34), 102(35), 89(91), 85(46).

In the UV spectrum of (I), taken in ethanol, the following absorption maxima were observed: λ_{max} (nm) 214, 217, 223, and 285 (log ε 4.04, 4.10, 3.98, and 3.51).

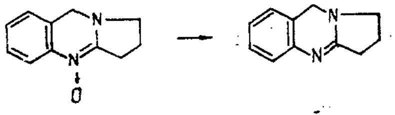
The IR spectrum of (I) exhibited absorption bands at (cm^{-1}) 790, 1195, 1255, 1315, 1360, 1430, 1465, 1505, 1585, 1630, 1680, 2770, 2840, 3030, and 3350-3500.

The molecular composition of the alkaloid was 1 oxygen atom greater than that of deoxypeganine; in other respects their mass-spectral fragmentations were similar. The presence of the $(M - 16)^+$ and $(M - 17)^+$ ions in the mass spectrum of the new base (I) and its ready solubility in water showed its N-oxide nature.

Reduction with zinc in hydrochloric acid gave a substance with mp 86-87°C that was identified by its IR and NMR spectra, and also by a mixed melting point, as deoxypeganine (II) [2].

The PMR spectrum of base (I) taken in $CDCl_3$ revealed the following signals (δ, ppm): 2.22 (m, 2H, H-10), 3.17 (t, 2H, H-9), 3.66 (t, 2H, H-11), 4.71 (s, 2H, H-4); while four aromatic protons resonated at 6.88-7.28 ppm in the form of a multiplet.

The following signals (δ, ppm) appeared in the PMR spectrum of deoxypeganine, taken in $CDCl_3$: 1.98 (m, 2H, H-10), 2.58 (t, 2H, H-9), 3.22 (t, 2H, H-11), and 4.45 (s, 2H, H-4), while the aromatic protons resonated at 6.68-7.05 in the form of a multiplet.



I

II

The downfield displacement (by ~0.2 ppm) of the signals of the aliphatic and aromatic protons as compared with deoxypeganine showed that the base was the N-oxide of deoxypeganine at N-1. N-Oxides have not previously been found among the quinazoline alkaloids, although their presence has been shown indirect [3].

LITERATURE CITED

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