

DEOXYPEGANIDINE - A NEW ALKALOID

FROM *Peganum harmala*

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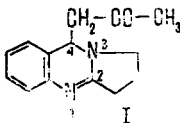
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From the mother liquors of the alkaloids described previously [1-3] we have obtained an optically inactive amorphous base with mp 69-70°C (petroleum ether), mol. wt. 228 (mass spectrometrically), picrate with mp 176°C, perchlorate with mp 166-167°C, nitrate with mp 155-157°C. UV spectrum: $\lambda_{\text{max}}^{\text{ethanol}}$ 218, 224 (inflection), 292 nm (log ϵ 4.13, 4.09, 3.88). The IR spectrum has the intense band of a carbonyl group at 1710 cm^{-1} and also bands at 1490, 1593, and 1628 cm^{-1} which are characteristic for quinazoline bases [4]. The presence of a carbonyl group was confirmed by the preparation of the oxime with mp 177-179°C. In the mass spectrum of the alkaloid, like those of deoxypeganine and peganol [1,3], the strongest peak is that of the ion with m/e 171, and ions with m/e 143, 116, and 89 are also recorded. In the mass spectra of peganine and peganidine [2], the maximum peak is that of the ion with m/e 187. Consequently, the alkaloid is based on a 2,3-trimethylene-3,4-dihydroquinazoline system. The results of a comparison of the IR, mass, mass, and NMR spectra of the base isolated with those of peganidine permitted the conclusion that the alkaloid differs from the latter by the absence of a hydroxy group. The base is a new one and we have called it deoxypeganidine. On passing from peganidine to deoxypeganidine under the conditions given previously [1], we obtained a mixture of substances the separation of which on a column of alumina yielded a compound which was identified chromatographically and by a mixed melting point of the picrates as deoxyvazicine.

When deoxypeganidine was oxidized with potassium permanganate in acetone solution, deoxyvazicine was obtained and identified.

The NMR spectrum of deoxypeganidine (in CDCl_3), like the NMR spectrum of peganidine, lacks a two-proton singlet in the 4.47-ppm region (δ scale) and, therefore, the substituting group is present in position 4. This is confirmed by a one-proton triplet at 5.14 ppm relating to the hydrogen atom at C-4. In the 6.9-7.2-ppm region there are the signals of four aromatic protons, at 1.85-3.7 ppm the multiplets of four methylene groups, and at 1.95 ppm the three-proton singlet of a CH_3 group.

Thus deoxypeganidine has the following structure.



LITERATURE CITED

1. Kh. N. Khashimov, M. V. Telezhenetskaya, and S. Yu. Yunusov, *Khim. Prirodn. Soedin.*, 456 (1969).
2. Kh. N. Khashimov, M. V. Telezhenetskaya, and S. Yu. Yunusov, *Khim. Prirodn. Soedin.*, 599 (1969).
3. M. V. Telezhenetskaya, Kh. N. Khashimov, and S. Yu. Yunusov, *Khim. Prirodn. Soedin.*, 849 (1971).
4. M. Ikram, M. Ehsanul Huq, and S. A. Warst, *Pakist. J. Sci. and Ind. Res.*, 8, 76 (1965).

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