PEGANIDINE—A NEW BASE FROM PEGANUM HARMALA

Kh. N. Khashimov, M. V. Telezhenetskaya, and S. Yu. Yunusov

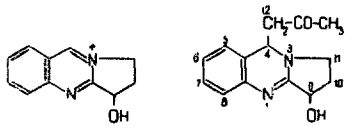
Khimiya Prirodnykh Soedinenii, Vol. 5, No. 6, pp. 599–600, 1969

UDC 547.944/945

From the total alkaloids of the epigeal part of Peganum harmala, in addition to the bases described previously [1], we have isolated a substance with mp 189–190° C $[\alpha]_D$ ±0° (c 1.66; chloroform). On the basis of its elementary analysis and molecular weight (mass spectrum) its composition is $C_{14}H_{16}O_2N_2$. The UV spectrum of the base is similar to that of peganine: λ_{max} 226, 297 mμ (log ε 4.04, 3.96) and the IR spectrum is also very similar to that of peganine, but differs from it. The base is a new one and we have called it peganidine.

The similarity of the UV and IR spectra of peganidine and peganine, and also the isolation of peganidine as a base accompanying peganine, made it possible to assume that these two alkaloids are based on the same heterocyclic skeleton. This is confirmed by the results of a comparative study of the mass and NMR spectra of peganine and peganidine. The ion $(M - 1)^+$ with m/e 187 (fragment a) gives a characteristic peak in the mass spectrum of peganine [2].

The mass spectrum of peganidine has the peak of the molecular ion M^+ with m/e 244, while the strongest peak has m/e 187 and there are also peaks with m/e 169, 159, 131, 104, and 77, which are characteristic for the mass spectrum of peganine. Consequently peganidine is a 4-substituted peganine. In the mass spectrometry of peganidine, fragment a is formed from the molecular ion by the cleavage of an α-bond with the loss of 57 mass units.



Fragment a

I

Information on the nature of the substituent at $C_{(4)}$ is given by the NMR and IR spectra of peganidine. A 3-proton singlet at δ 1.86 is due to a CH_3—CO group, the presence of which is confirmed by absorption bands at 2870, 1350, and 1700 cm^{-1}. The presence of a C=O group was confirmed by the preparation of peganidine oxime with mp 85–87° C and peganidine semicarbazone with mp 204–206° C, mol. wt. 301 (mass spectrum). The acetyl group appears in the mass spectrum of peganidine in the form of a peak with m/e 43. Thus, the substituent at $C_{(4)}$ is the CH_3—CO—CH_2— group, and the structure of peganidine is expressed by formula I. The absence of a well-defined two-proton singlet at δ 4.47 due to the methylene group at $C_{(4)}$ of peganine shows that the substituting group in peganidine is attached at this position.

REFERENCES

1. Kh. N. Khashimov, M. V. Telezhenetskaya, and S. Yu. Yunusov, KhPS [Chemistry of Natural Compounds], 5, 456, 1969.

2. A. K. Bhatnagar and S. P. Popli, Indian J. Chem., 4, No. 6, 291, 1966.

8 May 1969

Institute of the Chemistry of Plant Substances, AS UzSSR