A MASS SPECTROMETRIC STUDY OF THE STRUCTURE OF FETIDINE

Z. F. Ismailov and S. Yu. Yunusov

Khimiya Prirodnykh Soedinenii, Vol. 6, No. 1, p. 142, 1970

UDC 547.944/945+543.51

We have studied the chemical properties of fetidine and have established its structure, I. The substance belongs to the dimeric benzyltetrahydroisoquinoline-aporphine alkaloids [1].

Under the conditions of mass spectrometry, fetidine behaves, on the one hand, as a benzyltetrahydroquinoline derivative and, on the other hand, as an aporphine derivative. As a result of instantaneous β -rupture in the benzyltetrahydroisoquinoline part of the molecule, the molecular ion is not recorded and an ion-radical with m/e 476 is formed (1.5% of the intensity of the maximum peak, fragment a). The spectrum of the alkaloid has a peak of M⁺⁺ with m/e 341 (3%). The peak of maximum intensity corresponds to fragment b with m/e 206 (100%). Fragment b, by losing a methyl radical, gives the ion-radical c with m/e 191 (10%). The transition b \rightarrow c is shown by the presence of a metastable peak with m* = 191²/206 = 177. The cleavage of the ether bridging link of fragment a leads to the splitting out of a dimethoxybenzyl radical and the appearance of ion d with m/e 327 (5%). Subsequently the ion d with an aporphine structure, decomposes with the formation of fragment e with m/e 284 (3%). For a \rightarrow d m* = 327²/476 = 224.

Thus, the features of the mass spectrometric fragmentation of fetidine confirm the structure I proposed for it.



REFERENCE

1. Z. F. Ismailov and S. Yu. Yunusov, KhPS [Chemistry of Natural Compounds], 2, 43, 1966.

19 September 1969

Institute of the Chemistry of Plant Substances, AS UzSSR