THE STRUCTURE OF ISONITRARINE

A. A. Ibragimov, S. Kh. Maekh, and S. Yu. Yunusov

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From the combined ether-soluble alkaloids of Nitraria schoberi L., collected at the beginning of May 1971 in the budding period we have isolated a new alkaloid, isonitrarine, with the composition $C_{20}H_{25}N_3$, mol. wt. 307 (mass spectrometrically). Isonitrarine (I) is a white crystalline substance with mp 209°C. It gives a crystalline perchlorate with mp 236°C (decomp.) and a hydrochloride with mp 239°C. The UV spectrum of (I) has absorption bands – $\lambda_{max}^{ethanol}$ 226, 280-292 nm (log ε 4.46, 3.84) – that are characteristic for tetrahydro-β-carboline bases. The IR spectrum of (I) shows bands at 3400 and 3200 cm^{-1} (NH), 2950 and 2910 cm^{-1} (CH_2), and 755 cm^{-1} (ortho-disubstituted benzene). The NMR spectrum of (I) (CF_3COOH) has two one-proton signals at 8.26 and 7.35 δ probably belonging to the protons of two NH groups, a multiplet of aromatic protons with its center at 6.96 δ, a one-proton signal at 5.0 δ probably due to a proton attached to a tertiary carbon atom of a tetrahydro-β-carboline system, and a number of multiplets of methylene and methyl groups with their centers at 3.2, 1.95, and 1.45 δ.

The mass spectrum of (I) shows the following peaks of ions: m/e: 307 (M^+, 100%), 306, 279, 278, 224 (85%), 223, 197, 196, 195, 184, 183, 182, 171, 170, 169, 156, 144, 83.

The fragmentation is due to a tetramethylene tetrahydro-β-carboline part of the molecule and is characteristic for bases of the yohimbine and heteroyohimbine type.

Consequently, one nitrogen is an indole nitrogen, a second is a quinolizidine nitrogen, and the third is present in the molecule in the form of a secondary amino group.

When nitramidine [1] was hydrogenated with zinc in hydrochloric acid, a mixture of nitrarine and isonitrarine considerably enriched in the latter was formed. When nitrarine was isomerized under the conditions of Adams hydrogenation in ethanol, after 13 h an approximately equal amount of (I) had been formed.

Thus, isonitrarine has the structure of 3-epinitrarine.

LITERATURE CITED

1. A. A. Ibragimov, S. Kh. Maekh, and S. Yu. Yunusov, Khim. Prirodn. Soedin., 275 (1975).

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