TETRAMETHYLENETETRAHYDRO-β-CARBOLINE FROM Nitraria schoberi

B. M. Pakhritdinov, N. Yu. Novgorodova, M. Normatov, and S. Yu. Yunusov

UDC 547.944/945

TABLE 1.

Substance	M+ 226	(M−1) 225	m/e 197	m/e 184	m/e 170	m/e 169	m/e 156
	%						
Base with mp 149—150°	85	100	24	8	24	30	10
Tetramethylenetetrahydro-β-carboline	55	100	33	10	25	25	10

Continuing a study of the alkaloids of the plant Nitraria schoberi L. (family Zygophyllaceae) [1], we have isolated a white crystalline base with the composition $C_{15}H_{18}N_2$, mp 149-150°C (petroleum ether), $[\alpha]_D^{20}$ −82.9° (c 0.44; C_2H_5OH).

The UV spectrum – $\lambda_{max}^{ethanol}$ 228, 284, 292 nm (log ε 4.43, 3.50, 3.43) – is characteristic for the alkaloid tetramethylene-tetrahydro-β-carboline [2, 3].

The IR spectrum has absorption bands at 3280 cm^{-1} (NH) and 750 cm^{-1} (ortho-disubstituted benzene nucleus). The base contains no C−CH_3, N−CH_3, or O−CH_3 groups.

In the NMR spectrum (taken on a JNM-4H-100/100 MHz instrument in deuterochloroform) at δ 7.76 ppm, there is a well-defined one-proton singlet due to the N−H of the indole part of the molecule. A multiplet at δ 7.06 ppm (4H) is due to the aromatic protons of a benzene ring.

In the high-field region there are multiplets at δ 2.93 and 1.66 ppm which are assigned to methylene and methine protons.

In the mass spectrum of the base (MKh-1303 instrument at 100°C with an ionizing energy of 40 eV) there is the peak of the molecular ion with m/e 226 (85%) (confirming the composition of the base); the splitting out of one hydrogen from C-3 leads to the formation of an ammonium ion with m/e 225 (100%). The peaks of ions with m/e 170 and 169 are characteristic for alkaloids derived from 1,2,3,4-tetrahydro-β-carboline [4]. The spectrum also has peaks of ions with m/e 184 and 156 which are formed from the molecular ion by retrodiene degradation [4]. An ion with m/e 197 arises by the expulsion of ethylene from M-1. A comparison of the fragmentation of the base with mp 149-150°C and that of tetramethylenetetrahydro-β-carboline shows that the two substances have the same structure (Table 1).

Thus, a comparison of the properties and the UV and mass spectra of the base isolated and of tetramethylenetetrahydro-β-carboline shows their identity.

LITERATURE CITED

1. M. Normatov and S. Yu. Yunusov, KhPS [Chemistry of Natural Compounds], 139 (1968).
2. J. H. Groves, J. Chem. Soc., 650 (1952).

Institute of the Chemistry of Plant Substances, Academy of Sciences of the Uzbek SSR. Translated from Khimiya Prirodnykh Soedinenii, No. 5, pp. 641-642, September-October, 1970. Original article submitted June 9, 1970.

3. S. R. Johns and J. A. Laberton, Chem. Comm., 13, 421 (1966).
4. L. D. Antonaccio et al., J. Am. Chem. Soc., 84, 2163 (1962).