STRUCTURE OF RESEDININE

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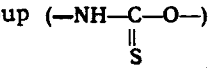
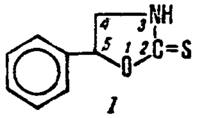
Resedinine (I) [1], according to the results of elementary analysis, has the composition C_9H_9NOS, mp 119-121°C (benzene), $[\alpha]^{20}_{D}$ +70° (c 1.0; CH_3OH). Its UV spectrum showed one absorption maximum at 246 nm (log ε 4.29), and its IR spectrum has absorption bands at 710, 770 cm^{-1} (monosubstituted benzene ring), 1170, 1535 cm^{-1}, characteristic for a thionocarbamate group  $(-NH-\underset{\underset{S}{\|}}{C}-O-)$ [2], and a broad band at 3170-3260 cm^{-1} (NH). The mass spectrum of (I) also confirms the suggested composition, having peaks of ions with 179.0410 (M^+), 136, 123, 118, 107, 104, 91, 77, 51.

The NMR spectrum of (I) ($CDCl_3$, δ scale, JNM 100/100 MHz, HMDS as internal standard) is similar to that of resedine [1] and has signals at 7.34 ppm (5 H, singlet, monosubstituted benzene ring), 8.52 ppm (1 H, singlet, NH), and three one-proton triplets at 3.65, 4.10, and 5.80 ppm due to the protons of vicinal methylene and methine groups.

Resedine does not undergo catalytic hydrogenation and does not contain any $C-CH_3$ groups. On comparing the compositions of residine and resedinine it is easy to see that the latter has a sulfur atom in place of one oxygen atom. A spectroscopic analysis showed the identity of the heterocyclic skeletons of these alkaloids. Since the IR spectrum of resedinine lacks the absorption of an amide carbonyl group it is obvious that resedinine has a thiocarbonyl group in place of an ordinary carbonyl group.

The facts given permit the following structure (I) to be proposed:



I

When compound (I) was reduced with $LiAlH_4$, a liquid base (II) was formed. A study of the IR, mass, and NMR spectra of the diacetyl derivative showed that (II) has the structure of (β-hydroxy-β-phenylethyl)(methyl)amine. This agrees well with the suggested structure (I).

Thus, resedinine (I) has the structure of 5-phenyloxazalidine-2-thione.

LITERATURE CITED

1. M. M. Tadzhibaev, K. L. Lutfullin, V. M. Malikov, and S. Yu. Yunusov, Khim. Prirodn. Soedin., 271 (1976).
2. E. B. Astwood, M. A. Greer, and M. G. Ettlinger, J. Biol. Chem., 181, 121 (1949).

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