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# ACTION OF BASES ON AZIRIDINEIMMONIUM THIOCYANATES

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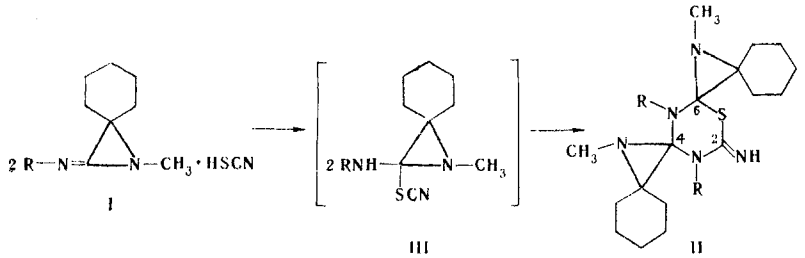
In an attempt to obtain aziridineimines in the free state by decomposition of their thiocyanates I with organic or inorganic bases we observed the condensation of two molecules of the aziridineimine and thiocyanic acid. The thiadiazine structure of the condensation products is in agreement with the results of elementary analysis and data from the IR, PMR, $^{13}C$ NMR, and mass spectra.



Compounds of the II type are formed in quantitative yields even during chromatography of salts I on $Al_2O_3$ (activity II). The unusual ease of the cyclization is evidently a consequence of the increased reactivity of the exocyclic C=N bond of the aziridineimine, which facilitates the possibility of the base-catalyzed formation of hypothetical aziridine III.

IR spectra (KBr) of thiadiazines II: 3370-3470 (NH) and 1610-1625 $cm^{-1}$ (C=N). PMR spectrum of thiadiazine II (R = $C_6H_5CH_2$) ($d_6$-DMSO, 60°C): 1.61 (m, 10H, cyclohexylidene fragments): 1.88, 2.06 (two s, 3H, $CH_3$—N); 4.21, 4.27 (two s, 2H, $CH_2C_6H_5$); 7.12, 7.17 (two s, 5H, $C_6H_5$); 8.53 ppm (broad s, NH). The shift of the signals of the protons of the N—$CH_3$ group to stronger field as compared with aziridineimine is presumably due to shielding of the benzene rings that are drawn close to them in space. $^{13}C$ NMR spectrum of this compound: 170.2 [$C_{(2)}$], 127.9 [$C_{(6)}$], 117.3 [$C_{(4)}$], 68.3 and 63.6 (spiro-C of the cyclohexylidene groups); 140.1, 136.9, 127.3, 127.1, 126.4, and 125.9 ($C_6H_5$); 45.5 and 45.1 ($CH_2$—$C_6H_5$); 35.6, 35.3, 31.4, 31.0, 27.7, 26.9, 24.8, 23.9, 22.3, 22.0, and 21.8 ppm (cyclo-$C_6H_{10}$). Mass spectrum, m/z (relative intensities, %): $M^+$ 516 (17.8), 405 (7.3), 365 (9.4), 286 (100.0), 232 (5.2), 117 (15.7), 111 (13.6), 68 (5.2), 34 (6.3).

The results of thin-layer chromatography and data from the PMR and $^{13}C$ NMR spectra constitute evidence that only one isomeric form of thiadiazine II is obtained in the condensation.

Thiadiazines II are stable under normal conditions and react with difficulty with carboxylic acid chlorides; the reaction with excess $CH_3I$ leads to the formation of a monosubstituted compound.

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