# A NEW METHOD OF SYNTHESIZING 2,2-SUBSTITUTED 1,3-OXATHIOLANES

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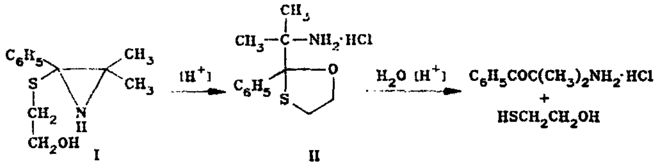
In an investigation of the reactivity of 2-axiridinyl-β-hydroxyethyl sulfide I [1] under conditions of heterolytic cleavage of the aziridine ring, we detected a reaction leading to the formation of a well-known class of sulfur-containing heterocyclic compounds — 2,2-substituted 1,3-oxathiolanes:



The chemical shifts of $^1H$ and $^{13}C$ in the spectra of oxathiolanes II are extremely close to those for 2,2-disubstituted 1,3-oxathiolanes [2], including the two-faced angle between the planes $S-C_{(4)}-C_{(5)}$ and $C_{(4)}-C_{(5)}-O$ (45.8°) that we calculated according to the R-factor method [3]. Mass spectrometric analysis of compound II showed the presence of $[M^+ - HCl]$ 223, corresponding to the gross formula II-HCl. Acid hydrolysis of compound II, resulting in the isolation of the original β-hydroxyethanethiol and 2-amino-2-methyl-1-phenylpropanone-1, provides still more evidence for the structure of the 1,3-oxathiolane II.

2-(2-Amino-2-propyl)-2-phenyl-1,3-oxathiolane hydrochloride (II) was synthesized by exposure of 2.25 g (0.01 mole) 2-(3,3-dimethyl-2-phenyl)aziridinyl-β-hydroxyethyl sulfide (I) [1] in 30 ml of acetone to 0.86 ml of conc. HCl in 5 ml of alcohol for 3 h at 70°C. After recrystallization of the precipitate formed from an alcohol–ether mixture, 1:3, the yield was 2.1 g (81%). IR spectrum (in nujol): 1490, 1570, 2580 ($NH_3^+$), 1600 $cm^{-1}$ (benzene ring). $^1H$ NMR spectrum ($DMSO-D_6$): 1.27 and 1.44 (6H, s, $CH_3$), 3.00 (1H, m, $J = -9.8$; 10.0 and 6.1 Hz, $H_{4e}$), 3.07 (1H, m, $J = -9.8$; 5.2 and 1.3 Hz, $H_{4a}$), 3.75 (1H, m, $J = -9.0$; 10.0 and 5.2 Hz, $H_{5e}$), 4.61 (1H, m, $J = -9.0$; 6.1 and 1.3 Hz, $H_{5a}$), 7.3-7.5 (5H, m, $C_6H_5$), 8.2 ppm (3H, s, $NH_3^+$). $^{13}C$ NMR spectrum (in $D_2O$): 22.1 and 22.6 ($CH_3$), 34.5 ($C_{(4)}$), 61.4 (C quaternary), 72.6 (C quaternary), 103.2 ($C_{(2)}$), 128.8 ($C_m$), 129.0 ($C_o$), 129.7 ($C_p$), 140.4 ppm ($C_a$). Elementary analysis of compound II corresponds to the calculated values.

## LITERATURE CITED

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