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LETTERS TO THE EDITOR

Synthesis of New Derivatives of 5-Amino-1,3-oxazole Basing on 3-Benzoylamino-3,3-dichloroacrylonitrile

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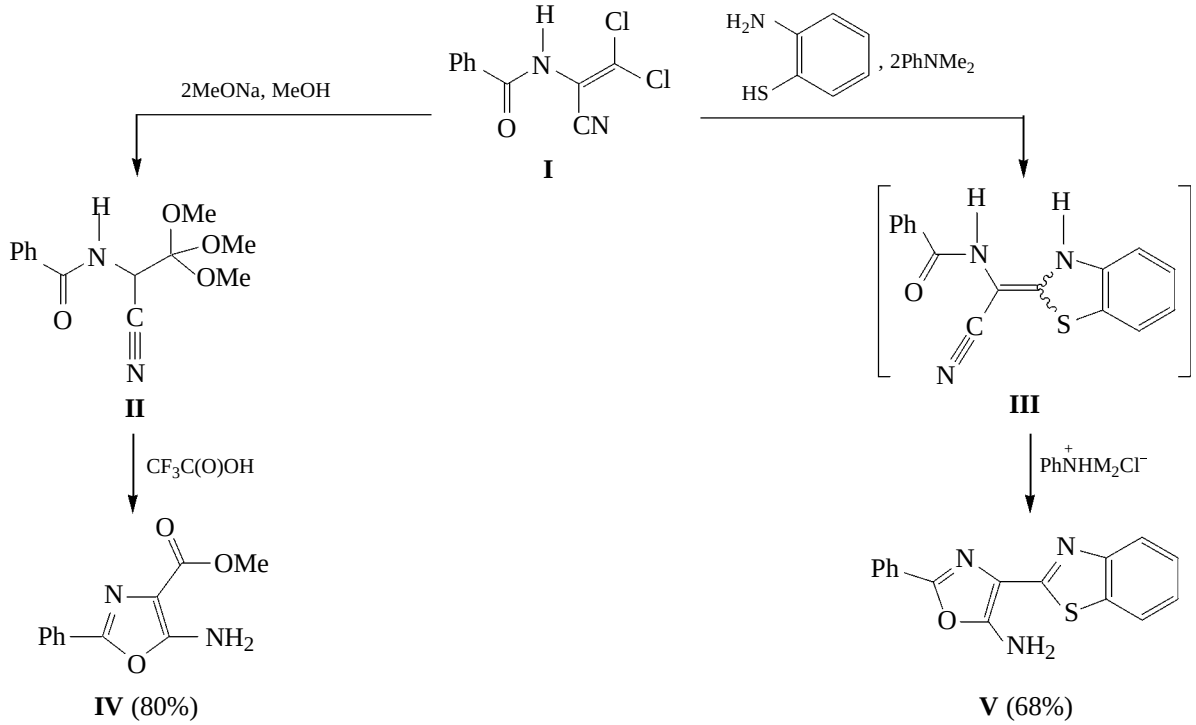
It was shown previously that 2-benzoylamino-3,3-dichloroacrylonitrile (**I**) and its analogs are valuable reagents for heterocyclizations leading to derivatives of mononuclear and condensed heterocycles [1–7]. In our systematic research on such cyclizations we have found two simple transformation sequences **I** → **II** → **IV** and **III** → **III** → **V** leading to new derivatives of 5-amino-1,3-oxazole (see scheme).



The reaction of compound **II** with sodium methylate was studied previously [8], and the cyclization of compound **II** to product **V** in the presence of trifluoroacetic acid was found for the first time. At the same time, the cyclization of compound **III** to product **V** proceeds under the action of another electrophilic catalyst, dimethylaniline hydrochloride. The significance of these two convenient synthetic approaches to 5-amino-1,3-oxazole derivatives will be considered in detail elsewhere. Here we would only

like to mention that the participation of the C≡N bond and amide fragment in the formation of the oxazole ring and primary amino group was confirmed by means of IR and ^{1}H NMR spectroscopy.

Methyl 5-amino-2-phenyl-1,3-oxazole-4-carboxylate (IV). A solution of 0.01 mol of compound **II** [8] in 10 ml of trifluoroacetic acid was stirred for 1 h at 20–25°C, the solvent was removed in a vacuum, and compound **IV** was purified by crystallization from acetonitrile, yield 80%, mp 201–202°C. IR spectrum, ν, cm^{-1}: 1645 (δ_{NH_2}), 1690 (C=O), 3180, 3250 (NH_2). ^{1}H NMR spectrum, δ, ppm: 3.75 s (3H, CH_3), 7.34 br.s (2H, NH_2), 7.44 m ($3H_{arom}$), 7.80 ($2H_{arom}$). Found, %: C 60.37, H 4.48, N 12.61. $C_{11}H_{10}N_2O_3$. Calculated, %: C 60.56, H 4.62, N 12.84.

5-Amino-4-(benzothiazol-2-yl)-2-phenyl-1,3-oxazole (V). To a solution of 0.01 mol of compound **I** in 20 ml of acetonitrile, 0.02 mol of 2-aminothiophenol and 0.025 mol of *N*,*N*-dimethylaniline were added. The resulting mixture was stirred for 2 weeks at 20–30°C. The precipitate was filtered off, washed with water and cold ethanol, and crystallized from acetonitrile to obtain compound **V**, yield 68%, mp 243–244°C. IR spectrum, ν, cm^{-1}: 1650 (δ_{NH_2}), 3170, 3250 (NH_2). ^{1}H NMR spectrum, δ, ppm: 7.31 m ($1H_{arom}$), 7.40–7.90 m ($7H_{arom}$), 7.64 br.s (2H, NH_2), 8.02 d ($1H_{arom}$). Found, %: C 65.37, H 3.53, N 14.02, S 10.57. $C_{16}H_{11}N_3O_2S$. Calculated, %: C 65.51, H 3.78, N 14.32, S 10.93.

The IR spectra were registered on a UR-20 spectrometer in KBr pellets. The ^{1}H NMR spectra were taken on a Varian VXR-300 spectrometer for DMSO-d_6 solutions agains internal TMS.

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