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SYNTHESIS OF THE FIRST EXAMPLE OF THE IMIDAZO-[5,1-*b*]OXAZOLE HETEROAROMATIC SYSTEM

E. V. Aleksandrova[1] and N. M. Kochergin[2]

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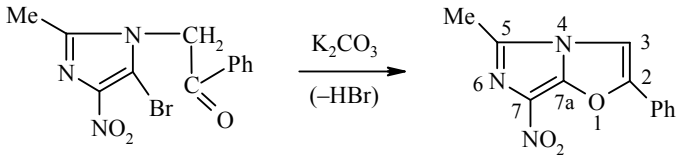
The heteroaromatic system imidazo[5,1-*b*]oxazole and its derivatives have not been described. Only derivatives of 2,3,5,7a-tetrahydro- and 2,3,7,7a-tetrahydroimidazo[5,1-*b*]oxazoles, obtained by multistage syntheses, are known [1,2].

With the objective of discovering new biologically active substances, we have studied the reaction of 1-acylmethyl-5-bromo-4-nitroimidazoles with bases, which readily proceeds with the elimination of hydrogen bromide and closing of the oxazole ring. As a result, a simple synthesis of the previously unknown derivatives of imidazo[5,1-*b*]oxazole has been discovered.

For example, 5-methy-7-nitro-2-phenylimidazo[5,1-*b*]oxazole (**2**) was obtained on heating 5-bromo-2-methyl-4-nitro-1-phenacylimidazole (**1**) [3] with anhydrous potassium carbonate in anhydrous DMF.



1 **2**

The purity, composition, and structure of compound **2** was confirmed by TLC (Silufol UV-254), elemental analysis, mass spectrum, and ^{1}H NMR spectra. The ^{1}H NMR spectrum in DMSO-d_6 solution was recorded on a Varian Unity-400 (400 MHz) instrument and the mass spectrum on a Finnigan SQ-710-MAT (EI, 70 eV ionizing current, direct inlet).

5-Methyl-7-nitro-2-phenylimidazo[5,1-*b*]oxazole (2). A mixture of imidazole **1** (0.324 g, 1 mmol) and anhydrous K_2CO_3 (0.138 g, 1 mmol) in anhydrous DMF (10 ml) was boiled for 5 h. After cooling, methanol (20 ml) was added to the mixture which was heated to boiling, activated charcoal (0.01 g) was added, the mixture boiled again, and filtered. The filtrate was evaporated to dryness and the residue was crystallized from a minimal amount of ethanol to give compound **2** (1.51 g, 62.1%) as yellow crystals with mp 236-237° (dec.), R_f 0.68 (butanol–acetic acid–water, 5:1:4). ^{1}H NMR spectrum, δ, ppm: 8.83 (1H, s, CH); 7.79-7.49 (5H, m, H_{arom}); 3.35 (3H, s, CH_3). Mass spectrum, *m/z*: 243 $[M]^+$. Found, %: C 59.11; H 3.72; N 17.27. $C_{12}H_9N_3O_3$. Calculated, %: C 59.26; H 3.73; N 17.28.

[1]Zaporozhe State Medical University, Zaporozhe 69035, Ukraine. [2]Center for Drugs Chemistry – All-Russian Chemical-Pharmaceutical Research Institute, Moscow 119815, Russia. Translated from Khimiya Geterotsiklicheskikh Soedinenii, No. 5, 792-793, May, 2007. Original article submitted November 27, 2006. Revised article submitted March 14, 2007.

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