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FORMATION OF AN ISOXAZOLE RING FROM PHENYLACETIC ACID AMIDOXIMES

T. R. Vakhitov[1], E. A. Veretennikov[1,2], and O. V. Shtabova[2]

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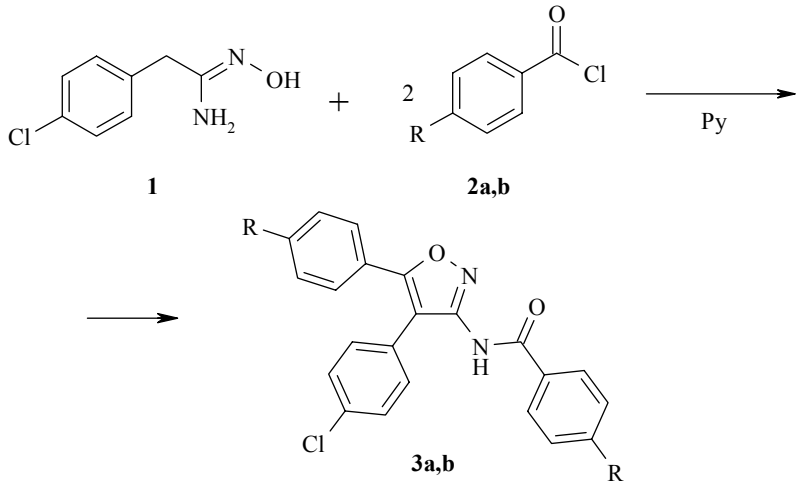
When reacting 4-chlorophenylacetic acid amidoxime **1** with aromatic acid chlorides **2a,b** under reaction conditions in [1], we obtained the isoxazoles **3a,b** in place of the expected 1,2,4-oxadiazoles.

The presence of the isoxazole structure for compounds **3a,b** instead an oxadiazole was confirmed by the absence in the ^{1}H NMR spectra of signals for the methylene group protons and the number of aromatic protons. The course of the reaction towards the formation of the isoxazole is possibly related to the presence of the active methylene group in the amidoxime.

Hence reaction of amidoxime **1** with a two molar excess of the acid chlorides **2a,2b** for 1 h in refluxing pyridine and subsequent dilution with water gives the isoxazoles **3a,3b** respectively.

^{1}H NMR spectra were recorded on a Bruker AM-500 instrument (500 MHz) using DMSO-d_6–CCl_4 (1 : 1) with TMS as internal standard.



2, **3 a** R = H, **b** R = Me

[1]Saint Petersburg State Technical University, Saint Petersburg 190013, Russia. [2"]Contact Service SPb", Saint Petersburg Science Center, Saint Petersburg 193019, Russia; e-mail: toever@yandex.ru. Translated from Khimiya Geterotsiklicheskikh Soedinenii, No. 1, pp. 134-135, January, 2007. Original article submitted June 25, 2006.

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N-[4-(4-Chlorophenyl)-5-phenylisoxazol-3-yl]benzamide (3a). Yield 73%. Mp 226-227°C. ^{1}H NMR spectrum, δ, ppm (*J*, Hz): 7.40 (2H, d, *J* = 8.1, H_{arom}); 7.51 (5H, m, H_{arom}); 7.57 (1H, m, H_{arom}); 7.68 (2H, d, *J* = 8.1, H_{arom}); 8.05 (2H, d, *J* = 7.6, H_{arom}); 8.08 (2H, d, *J* = 7.6, H_{arom}); 10.47 (1H, s, NH). M^+ 375.

N-[4-(4-Chlorophenyl)-5-*p*-tolylisoxazol-3-yl]-4-methylbenzamide (3b). Yield 85%. Mp 233-234°C. ^{1}H NMR spectrum, δ, ppm (*J*, Hz): 2.44 (3H, s, CH_3); 2.45 (3H, s, CH_3); 7.25 (2H, d, *J* = 8.1, H_{arom}); 7.30 (2H, d, *J* = 8.1, H_{arom}); 7.37 (2H, d, J = 8.1, H_{arom}); 7.65 (2H, d, *J* = 8.1, H_{arom}); 7.95 (4H, t, H_{arom}); 10.33 (1H, s, NH). M^+ 403.

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