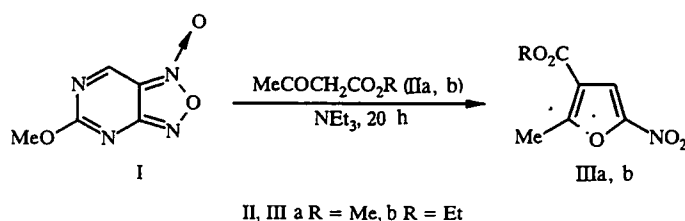


RECYCLIZATION OF 5-METHOXYFUROXANO[4,5-d]- PYRIMIDINE TO DERIVATIVES OF 5-NITROFURAN

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It is known that furoxanopyrimidines are converted by carbanions to pteridine di-N-oxides (the Beirut reaction) [1, 2]. The pyrimidine ring thereby remains unchanged. We established for the first time that the reaction of 5-methoxyfuroxano[3,4-d]pyrimidine (I) with methyl acetoacetate (IIa) or ethyl acetoacetate (IIb) in methylene chloride in the presence of the fivefold excess of triethylamine results in the formation of 2-methyl-5-nitro-3-furancarboxylic esters (IIIa,b) correspondingly.



The mechanism and limits of application of this reaction require further study.

The NMR spectra were taken in CDCl_3 . The IR spectra were taken using tablets of KBr. The UV spectra were taken in ethanol.

Methyl 2-Methyl-5-nitro-3-furancarboxylate (IIIa). The yield is 52%. The mp is 56-57°C (hexane). The IR spectrum (KBr) is as follows: 1730 cm^{-1} (CO ester), 1510 cm^{-1} , and 1360 cm^{-1} (NO_2). The UV spectrum (in ethanol) is characterized by the λ_{max} (log ϵ) 307 nm (4.01). The PMR spectrum (CDCl_3) is as follows: 2.74 ppm (3H, s, OCH_3), 3.90 ppm (3H, s, OCH_3), and 7.54 ppm (1H, s, 4-H). Found, %: C 45.6, H 3.8, and N 7.6. $\text{C}_7\text{H}_7\text{NO}_5$. Calculated, %: C 45.4, H 3.8, and N 7.6.

Ethyl 2-Methyl-5-nitro-3-furancarboxylate (IIIb). The yield is 59%. The mp is 52-54°C (hexane); the literature mp is 52.5°C [3]. The IR spectrum (KBr) is as follows: 1730 cm^{-1} (CO ester), 1535 cm^{-1} , and 1355 cm^{-1} (NO_2). The UV spectrum (in ethanol) is characterized by the λ_{max} (log ϵ) 307 nm (4.01). The PMR spectrum (CDCl_3) is as follows: 1.39 ppm (3H, t, OCH_2CH_3), 2.73 ppm (3H, s, CH_3), 4.35 ppm (2H, q, OCH_2), and 7.55 ppm (1H, s, 4-H). The ^{13}C NMR spectrum is as follows: 14.11 (OCH_2CH_3), 14.19 (CH_3), 61.26 (CH_2), 111.83 ($\text{C}_{(4)}$), 116.96 ($\text{C}_{(3)}$), 150.06 ($\text{C}_{(5)}$), 161.28 (C=O), and 161.61 ($\text{C}_{(2)}$). Found, %: C 48.4, H 4.5, and N 7.0. $\text{C}_8\text{H}_9\text{NO}_5$. Calculated, %: C 48.2, H 4.5, and N 7.0.

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