# ALKYLATION OF THE 2H-5-NITRO-2-ACETONYL-4,6-DIMETHOXYPYRIMIDINE ANION

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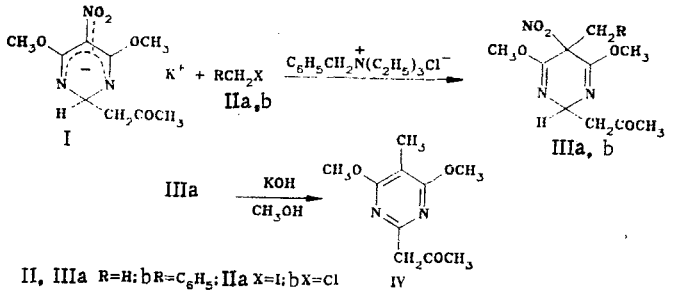
We have shown that alkylation of the acetonyl anionic σ-complex I by methyl iodide or benzyl chloride in benzene with an equimolar amount of benzyltriethylammonium chloride occurs at position 5 of the pyrimidine ring to form a mixture of the cis- and trans-isomers of 2-acetonyl-5-nitro-5-methyl(benzyl)-4,6-dimethoxy-2,5-dihydropyrimidine (IIIa, b).




The location of the alkyl substitutent in the products was established using PMR spectroscopic data. The presence of two sets of PMR spectral signals for IIIa, b points to the formation of a mixture of cis- and trans-isomers but their close similarity in chemical shifts does not permit assignment of the signals individually.

Isomer mixture IIIa was obtained in 40% yield. PMR Spectrum (200 MHz, $CDCl_3$): 5.64 (t, J = 6.4 Hz, CH), 5.58 (t, J = 7.1 Hz, CH), 3.67 (s, $OCH_3$), 3.66 (s, $OCH_3$), 2.77 (d, J = 7.1 Zh, $CH_2$), 2.73 (d, J = 6.4, $CH_2$), 2.19 (s, $CH_3$), 2.14 (s, $CH_3$), 1.87 (s, $CH_3$), 1.79 ppm (s, $CH_3$).

Isomer mixture IIIb was separated using column chromatography with chloroform as eluent. The first eluted component (17%) had mp 84-86°C (from hexane). PMR Spectrum (200 MHz, $CDCl_3$): 7.20 (5H, m, $C_6H_5$), 5.49 (1H, t, J - 7.2 Hz, CH), 3.72 (5H, s, 2 $OCH_3$), 3.66 (2H, s, $CH_2$), 1.87 (3H, s, $CH_3$), 1.27 ppm (wH, d, J = 7.2 Hz, $CH_2$).

Further elution gave an oily product in 11% yield. PMR Spectrum (200 MHz, $CDCl_3$): 7.20 (5H, m, $C_6H_5$), 4.60 (1H, t, J = 7.0 Hz, CH), 3.69 (6H, s, $OCH_3$), 3.63 (2H, s, $CH_2$), 2.58 (2H, d, J = 7.0 Hz, $CH_2$), 2.08 ppm (3H, s, $CH_3$).

2,5-Dihydropyrimidines have been little studied [1] and their alkylation of anionic σ-complexes can be used as one method for their preparation.

Refluxing the isomer mixture IIIa in methanol with potassium hydroxide gave 5-methyl-4,6-dimethoxy-2-acetonylpyrimidine (IV, 72%, mp 110-102°C from methanol), PMR Spectrum (200 MHz, $CDCl_3$): 3.83 (6H, s, 2 $OCH_3$), 3.73 (2H, s, $CH_2$), 2.16 (3H, s, $CH_3$), 1.87 ppm (3H, s, $CH_3$).

Elemental analysis data for the compounds synthesized was in agreement with that calculated.

## LITERATURE CITED

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