LETTERS TO THE EDITOR

REDUCTION OF 1,3,5-TRIMETHYL-5-NITROHEXAHYDROPYRIMIDINE IN THE PRESENCE OF SODIUM METHOXIDE

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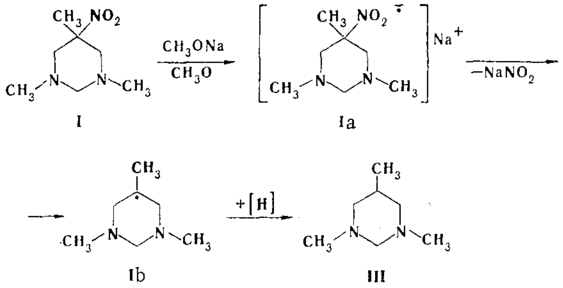
UDC 547.853.4.5:542.958.7

We have established for the first time that 1,3,5-trimethyl-5-nitrohexahydropyrimidine (I) is converted to 1,3-5-trimethylhexahydropyrimidine (III) in 68% yield in the presence of sodium methoxide (II) in methanol at a molar reagent ratio of 1 : 4 at 130°C after 10 min (100% conversion).



The formation of anion radicals from 2,5-dialkyl-5-nitro-1,3-dioxanes under the influence of potassium hydroxide in ethylene glycol was noted in [1]. An anion radical salt, which monomolecularly splits out a nitrite anion to give $NaNO_2$ and hexahydropyrimidinyl radical Ib, is evidently formed from 1,3.5-trimethyl-5-nitrohexahydropyrimidine as a result of electron transfer from the methoxide anion to the nitro group. Radical Ib detaches a hydrogen atom from the solvent to give hexahydropyrimidine III. Sodium nitrite is formed in 100% yield, and this constitutes evidence for the quantitative formation of intermediates Ia, b. Since 5-alkyl-5-nitrohexahydropyrimidines are readily obtained in one step from accessible nitroalkanes, alkylamines, and formaldehyde [2], the reaction under consideration can be regarded as a convenient method for the preparation of polyalkylhexahydropyrimidines.

1,3,5-Trimethylhexahydropyrimidine (III) was isolated by means of column chromatography [ether–hexane (2 : 3)] and had bp 143°C and n_D^{20} 1.4739. ^1H NMR spectrum (CCl_4): 0.68 (3H, d, 5-CH_3), 2.17 (6H, s, 1- and 3-CH_3), 2.05 (4H, m, 4- and 6-H), and 2.98 ppm (2H, m, 2-H). ^{13}C NMR spectrum (CCl_4): 17.7 (q, 5-CH_3), 27.4 (d, C_5), 43.3 (q, 1- and 3-CH_3), 62.3 (t, C_4 and C_6), and 79.1 ppm (t, C_2).

LITERATURE CITED

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2. Houben-Weyl, Methoden der Organischen Chemie, Vol. 4, Georg Thieme Verlag, Stuttgart (1960).

Ufim Petroleum Institute, Ufa 450062. Translated from Khimiya Geterotsiklicheskikh Soedinenii, No. 6, p. 846, June, 1982. Original article submitted August 25, 1981.

0009-3122/82/1806-0644$07.50