Chemistry of Heterocyclic Compounds, Vol.35, No. 3, 1999

DESTRUCTIVE HYDRATION OF 7-BENZYL-1-ISOPROPYL-5-METHYL-1,2,4-TRIAZOLO[4,3-*c*]-PYRIMIDINE DURING DIMROTH REARRANGEMENT

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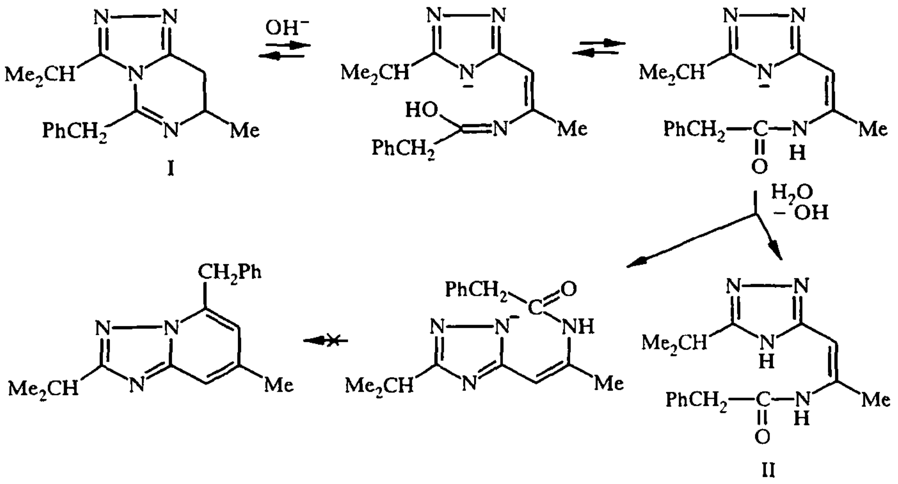
We previously used the Dimroth rearrangement to produce isomeric 1,2,4-triazolo[2,3-*c*]pyrimidines by the action of sodium ethoxide in alcohol on several 7-benzyl-1,2,4-triazolo[4,3-*c*]pyrimidines [1, 2]. The attempted analogous isomerization of 7-benzyl-1-isopropyl-5-methyl-1,2,4-triazolo[4,3-*c*]pyrimidine (I) by KOH in ethanol led only to the isolation of an intermediate, a cleavage product that converted during work up and separation into the hydration product II.



The PMR spectrum of II contains signals characteristic of an olefinic proton at 5.25 ppm, the amide and triazole NH groups. In addition to the absence of a singlet for the pyrimidine proton at weaker field, which is characteristic of triazolo[4,3-*c*]pyrimidines, this is consistent with the formation of an intermediate and not the recyclization product. Apparently the intermediate that formed during opening of the pyrimidine cycle does not cyclize owing to the low electrophilicity of the amide carbonyl group. In the previously published work [1], we noted that the molecule is destroyed on boiling with base. However, the intermediate cleavage product was not isolated.

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Phenylacetic Acid 1-(3-Isopropyl-1,2,4-triazol-5-yl)-1-propen-2-ylamide (II, $C_{16}H_{20}N_4O$). Compound I (0.42 g, 2 mmol) was refluxed in ethanol (15 ml) containing KOH (0.86 g, 15 mmol) for 6 h. After the spot of the initial material disappeared (TLC control), the reaction mixture was neutralized by HCl in ether. The precipitated salt was filtered off. The solvent was evaporated from the filtrate. The solid was crystallized from hexane. Yield 0.26 g (57%) of II; mp 76-78°C. R_f 0.41 (Silufol UV-254, benzene–acetone, 3:1). ^{1}H NMR spectrum ($CDCl_3$): 1.38 (6H, d, J = 6.5 Hz, $(CH_3)_2C$), 2.51 (3H, s, CH_3), 3.18 (1H, q, J = 6.5 Hz, $\underline{CH}(CH_3)_2$), 3.4 (1H, br. s, NH), 4.53 (2H, s, CH_2), 5.25 (1H, s, CH=C), 7.18-7.43 (5H, m, C_6H_5), 8.15 ppm (1H, br. s, NH).

The work was supported by the Grant 96-559 with a subsidy from the State Central Finance of the Republic of Armenia and by a collaborative grant NACH 006 98/AC 1-955 of the National Foundation for Science and Conversion Technologies of Armenia and the U.S. Civilian Research and Development Foundation.

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