NEW DATA ON THE DIRECTION OF ALKYLATION OF 5-OXO-7,12-DIHYDRO-5H-ISOQUINO[2,3-*a*]QUINAZOLINE

V. M. Kisil', L. M. Potikha, and V. A. Kovtunenko

It was reported previously [1] that alkylation of 5-oxo-7,12-dihydro-5H-isoquino[2,3-*a*]quinazoline (I) with methyl tosylate occurred at atom $N_{(6)}$ to give a quaternary salt. However this is not the only possible direction of alkylation of compound I. The position of alkylation is determined basically by the nature of the alkylating agent. We have observed that melting the isoquinoquinazoline I with various benzyl halides IIIa-d at 100-120°C gave the products of $C_{(7)}$ alkylation in 50-85% yield — the corresponding 7-benzyl-5-oxo-7,12-dihydro-5H-isoquino[2,3-*a*]quinazolinium halides IV with m.p. 138-140 (IVa), 160-161 (IVb), 191.5-193 (IVc), and 233-235°C (IVd). Alkylation of the isoquinoquinazoline I with the α -bromoacetophenones III e and f by heating in acetonitrile occurred at the same position to give the hydrobromides IV e (m.p. 205-207°C) and IV f (m.p. 176-178°C). The free bases were obtained from the salts IV by treatment with triethylamine: Va (m.p. 181.5-183°C), Vb (m.p. 172-173°C), Vc (m.p. 201-202°C), Vd (196.5-199°C), Ve (187.5-188°C) and Vf (220-221°C).



 $\begin{aligned} \text{III} & - \text{Va } \text{R} = \text{C}_6\text{H}_5, \text{X} = \text{Cl}, \text{ b } \text{R} = \text{C}_6\text{H}_4\text{Cl}\text{-4}, \text{X} = \text{Cl}, \text{ c } \text{R} = \text{C}_6\text{H}_4\text{NO}_2\text{-3}, \text{X} = \text{Cl}, \text{ d } \text{R} = \text{C}_6\text{H}_4\text{CH}_3\text{-2}, \\ \text{X} = \text{Br}, \text{ e } \text{R} = \text{COC}_6\text{H}_5, \text{X} = \text{Br}, \text{ f } \text{R} = \text{COC}_6\text{H}_4\text{Br}\text{-4}, \text{X} = \text{Br} \end{aligned}$

The ¹H NMR spectra (CF₃CO₂D) of salts IV, which are identical with the spectra of the bases V in the same solvent, contain a single proton signal in the 4.86-4.97 ppm region and a two proton signal in the 3.59-3.62 ppm region with a vicinal coupling constant of 7 Hz, corresponding to the $C_{(7)}H-CH_2-R$ fragment. For compounds Vb and Vd, the signals appear as an A₂X system, for the other compounds as an ABX system, with a geminal coupling constant of 14 Hz. Like the hydrogen atoms of the methylene group $C_{(7)}H_2$ in compound I [1], the methyne hydrogens C_7H in compounds IV and V exchange with deuterium: the multiplet for these protons is absent in spectra recorded a day after the solutions were prepared, and there is a corresponding change in the multiplicity for the signals of the protons of the 7-CH₂R group. The molecular asymmetry of these compounds leads to diastereotopy of the protons at $C_{(12)}$, which appear in the spectra as a doublet of doublets with a geminal spin-spin coupling constant of 16 Hz.

Taras Shevchenko Kiev University, Kiev 252017. Translated from Khimiya Geterotsiklicheskikh Soedinenii, No. 3, pp. 423-424, March, 1995. Original article submitted February 14, 1995.

REFERENCES

1. V. M. Kisel', V. A. Kovtunenko, A. V. Turov, A. K. Tyltin, and F. S. Babichev, Khim. Geterotsikl. Soedin., No. 3, 389 (1991).

e