DIRECTED CHARACTER OF THE GUANYLATION OF 5-AMINO-1,2,4-TRIAZOLES

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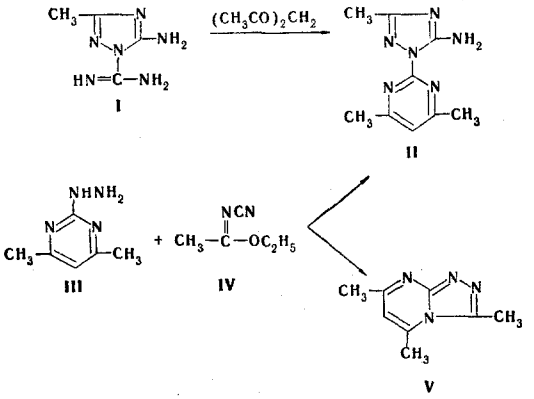
UDC 547.857.7'792

(1,2,4-Triazol-5-yl)guanidine hydrochloride was isolated from the reaction of 5-amino-1,2,4-triazole hydrochloride with cyanamide [1].

In the present study, we have established that guanylation of 5-amino-1,2,4-triazoles with 1-guanylbenzotriazole hydrochloride [2] proceeds at the nitrogen atom in the 1 position.

The structure of 1-guanyl-3-methyl-5-amino-1,2,4-triazole (I) is confirmed by the synthesis of 1-(4,6-dimethyl-2-pyrimidyl)-3-methyl-5-amino-1,2,4-triazole (II) from I and acetylacetone. This same substance (II) was obtained along with 3,5,7-trimethyl-1,2,4-triazolo[4,3-*a*]pyrimidine from 2-hydrazino-4,6-dimethylpyrimidine (III) and N-cyanoacetimino ester IV.



EXPERIMENTAL

1-(4,6-Dimethyl-2-pyrimidyl)-3-methyl-5-amino-1,2,4-triazole (II). A. A 0.35-ml (3.5 mmole) sample of acetylacetone was added to a solution of 0.42 g (3 mmole) of I in 10 ml of absolute ethanol, and the mixture was allowed to stand at room temperature for 24 h. The addition of ether precipitated 0.27 g (45%) of II with mp 227-230° (from benzene). IR spectrum: 1625 and 3295, 3355, 3440 cm^{-1} (deformation and stretching vibrations of the NH_2 group). Found: C 52.8; H 6.0; N 41.7%. $C_9H_{12}N_6$. Calculated: C 52.9; H 5.9; N 41.1%.

B. A 0.61-g (5.5 mmole) sample of IV was added to a solution of 0.7 g (5 mmole) of III in 45 ml of methanol at 50-60°, and the solution was cooled to room temperature and held there for 2 h. The methanol was removed by distillation, and the dry residue was extracted with 30 ml of ethyl acetate to give 0.06 g (7%) of II (the insoluble portion) with mp 227-230° (from benzene). A total of 0.45 g (45%) of V with mp 205-207° (from ethyl acetate) [3] crystallized out from ethyl acetate. Found: N 34.4%. $C_8H_{10}N_4$. Calculated: N 34.5%.

Institute of Organic Synthesis, Academy of Sciences of the Latvian SSR, Riga. Translated from Khimiya Geterotsiklicheskikh Soedinenii, No. 3, p. 423, March, 1973. Original article submitted February 16, 1972.

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3. W. W. Paudler and L. S. Helmick, J. Heterocycl. Chem., 3, 269 (1966).