CYCLIZATION OF 1,4,6-TRIAMINO-2(1H)-PYRIMIDINETHIONE

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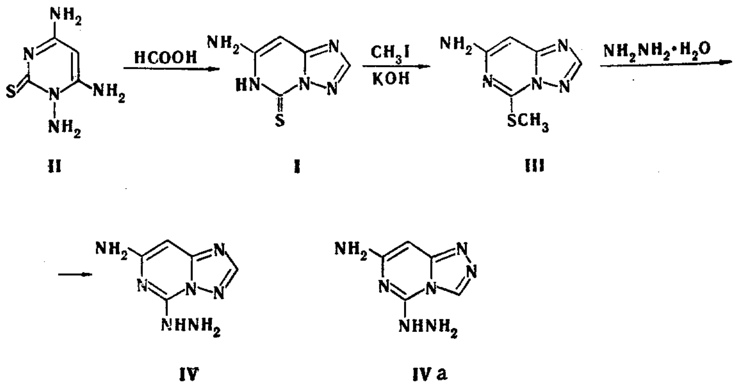
It has been reported [1] that molecular rearrangement to give 2-thiocyanato-4,6-bis(dimethylaminomethyleneamino)pyrimidine occurs during an attempt to obtain an "isopurine" system (I) by heating 1,4,6-triamino-2(1H)-pyrimidinethione (II) with dimethylformamide and $POCl_3$.



We have found conditions for the cyclization of amine II to 5-thioxo-7-amino-S-triazolo[1,5-c]pyrimidine (I). For this, a solution of amine II in 99.7% formic acid was heated in a sealed tube at 170°C for 30 min. Compound I, with mp > 300°C, was obtained in 71% yield after removal of the formic acid in vacuo. The absence in the IR spectrum of this compound of an absorption band at 2500-2600 cm^{-1}, which is characteristic for the mercapto group, constitutes evidence that it exists in the thione form.

The methylation of I gives 5-methylthio-7-amino-S-triazolo[1,5-c]pyrimidine (III) in 69% yield as colorless needles with mp 238°C. When III was refluxed with hydrazine hydrate in ethanol for 1 h, it was converted to 5-hydrazino-7-amino-S-triazolo[1,5-c]pyrimidine (IV), which was obtained in 82% yield as colorless needles with mp 290°C. The Dimroth rearrangement to give isomer IVa is possible for IV. Calculations by the Hückel MO method showed that the IV structure has higher stability.

All of the compounds were purified by crystallization from water (with decolorization by charcoal). The purity of the compounds obtained was monitored by thin-layer chromatography. The results of elementary analysis were in agreement with the calculated values.

LITERATURE CITED

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