REACTION OF ISOCYTOSINE WITH N-CHLOROCARBONYL ISOCYANATE

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The reaction of isocytosine with chlorocarbonyl isocyanate was found to give a pyrimido[1,2-a][1,3,5]triazine derivative in good yield. The structure of the pyrimidotriazine derivative might be either 1 or 2.

The pyrimidotriazine derivative on treatment with excess benzyl bromide gave two N,N'-dibenzyl derivatives. One was determined to be 3 by X-ray analysis and another to be 4 on the basis of the chemical evidences. The results suggest that the product obtained from the reaction of isocytosine with chlorocarbonyl isocyanate is 1. Namely, chlorocarbonyl isocyanate reacts with both the ring nitrogen at the 1-position and the extranuclear amino group of isocytosine to form a triazine ring.

The reaction of 1 with excess methyl iodide gave the corresponding N,N'-dimethyl derivatives, 5 and 6.

Carbon-13 NMR and Mass spectra of these pyrimidotriazine derivatives showed characteristic patterns depending on the position at which alkyl groups attached. Based on these characteristics, the structure of monobenzyl pyrimidotriazine obtained from the reaction of 1 with one equivalent of benzyl bromide was concluded to be 7.