SUBSTITUTION OF BROMINE ATOM IN 8-BROMOTHEOPHYLLINE BY PYRIDINE IN THE PRESENCE OF o-PHENYLENEPHOSPHORIC ACID ISOCYANATE

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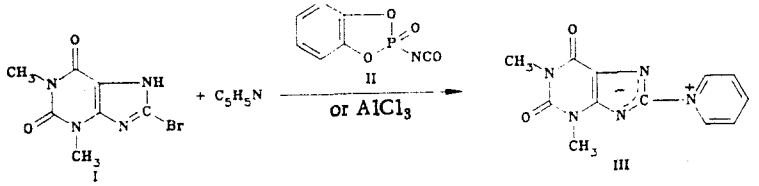
In general, isocyanates of P(V) phosphoric acids readily carbomoylate various derivatives containing at N–H bond [1].

In the reaction of 8-bromotheophylline I with isocyanate II in pyridine, instead of the carbamoyl derivative, we have unexpectedly obtained betaine III in a high yield. It is possible that in this reaction, isocyanate II displays the properties of a Lewis acid, since its replacement by $AlCl_3$ also leads to the formation of betaine III in a high yield. Compound III has already been obtained in a 53% yield by prolonged boiling of 8-chlorotheophylline in pyridine [2].



8-Pyridiniotheophyllinate (III) is obtained by heating (100°C, 2 h) a solution of 5 mmoles of compound I in 40 ml of pyridine with 10 mmoles of isocyanate II or with 11 mmoles of $AlCl_3$; the yield is 77 and 81%, respectively. mp 335...337°C (from water). PMR spectrum (DMSO-D_6): 2.73 (3H, s, 3-CH_3), 2.89 (3H, s, 1-CH_3); 7.70...7.95 ppm (5H, m; C_5H_5N). IR spectrum: 1680, 1640, (C=O), 1525, 1560 cm^{-1} (Ar). The data of elemental analysis of betaine III for C, H, and N correspond to the calculated values.

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