CYCLIC TRIMER OF BENZIMIDAZOLE

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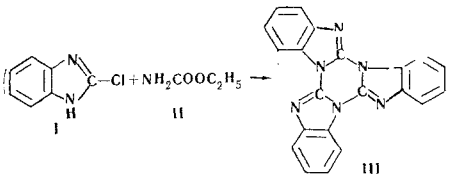
The reaction of 2-chlorobenzimidazole (I) with ethylurethane was studied in order to develop a direct method for the preparation of ethyl 2-benzimidazolyl carbamate. However, a study of the condensation product indicated that a cyclic trimer of benzimidazole (III) is formed instead of the expected compound.



The mass spectrum of this compound contains a molecular ion peak at 348 m/e and a doubly charged ion peak at 174 m/e, which corresponds to the molecular weight of structure III. The spectrum does not contain any other intense peaks; this is probably associated with the stability of the benzimidazole rings. The literature contains data regarding the fact that 2-chlorobenzimidazole forms a linear, chlorine-containing polymer when it is heated at 5 to 10 deg above the melting point [1].

EXPERIMENTAL

Cyclic Trimer of Benzimidazole (III). A tube was charged with 0.25 g (0.002 mole) of I and 0.25 g (0.003 mole) of ethylurethane in 3 ml of toluene and heated in a micro Carius tube for 18 h at 180-200 deg. The tube was opened and the reaction product was filtered, washed with sodium carbonate solution and water, and refluxed in methanol. Compound III was obtained as yellowish crystals with mp 353-356 deg which were slightly soluble in organic solvents. Found %: C 71.91; H 3.91; N 24.61. $C_{21}H_{12}N_6$. Calc. %: C 72.41; H 3.47; N 24.10.

The mass spectrum was obtained with a series MKh-1303 spectrometer equipped with a glass system for input of the sample into the ion source; the ionizing voltage was 40 eV at 130 deg.

LITERATURE CITED

1. D. Harrison, I. T. Rolph, and A. C. B. Smith, J. Chem. Soc., 2930 (1963).

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