SUPRAMOLECULAR STRUCTURE OF 6-PHENYL-2-CHLOROPYRIMIDINE-4-CARBOXAMIDE AND ITS COMPLEXES WITH DIOXANE AND ETHANOL

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A stable 2:1 complex of 6-phenyl-2-chloropyrimidine-4-carboxamide with dioxane has been synthesized. The structure of the complex was investigated by molecular spectroscopy (chloroform solution), thermoderivatography, and XRD (crystalline phase). A supramolecular structure is formed in the crystal of the complex, which involves centrosymmetric dimer associates of amide molecules, linked by dioxane molecules and intermolecular hydrogen bonds into infinite stepwise ribbons. These ribbons are stacked via π-stacking pair interactions "amidopyrimidine–amidopyrimidine." The complex of the same 2:1 carboxamido derivative of pyrimidine with ethanol is unstable and has a different structure. The ethanol molecules lie in the vacant voids of the stacks formed by the "amidopyrimidine–amidopyrimidine" synthon.

Keywords: 6-phenyl-2-chloropyrimidine-4-carboxamide, complexes with dioxane and ethanol, supramolecular structure, TGA, DTA, XRD.