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Supramolecular structures of thymine derivatives

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In the course of our studies of the hierarchy of intermolecular interactions the supramolecular structures of three thymine derivatives have been determined: (1-thyminyl)acetamide (1), 1-(2-cyanoethyl)thymine (2) and 1-(3-cyanopropyl)thymine (3). In all cases the supramolecular structures are primary determined by the strongest interaction, i.e. intermolecular hydrogen bonds N3-H3•••O2 in (1) and N3-H3•••O4 in (2) and (3), respectively, thus forming centrosymmetric dimers. Only consecutive inversion centers of the space group P2₁/c in the case of (1) create then the principal packing motif - molecular tapes which interact between themselves forming the threedimensional structure. The case of (2) is different. The principal packing motif is formed by centrosymmetric dimers which are further connected by weak hydrogen bonds. The dimers are packed in the crystal in a herringbone manner. In the crystals of (3) the same centrosymmetric dimers are formed by using N3-H3•••O4 hydrogen bonds. Moreover, the other two types of centrosymmetric dimers are further created by weak hydrogen bonds and in the end all the intermolecular interactions give rise to two dimensional, folded sheets. In conclusion, the packing motifs are in the given examples determined primary by the strongest intermolecular interactions, although nevertheless a diversity of crystal structures may be reached.

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Conformation angles and hydrogen bond in DL-Phenylglycinium chloride

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D-Phenylglycine is an important starting material in the production of semisynthetic penicillins and cephalosporins and its derivatives are used in the synthesis of antitumor drugs and other pharmacological applications (Satyam et al., [1], Jayasinghe et al. [2]).

In this study we present the angles of conformation and examine the hydrogen bonding in the new crystal structure of DL-Phenylglycinium chloride.

The tilte compound, $C_8H_{10}NO_2+$, Cl- crystallized in Orthorhombic system, with Pbca space group, it has been prepared by slow evaporation of an aqueuos solution of DL-Phenylglycine, tin(II) chloride and hydrochloric acid.

The crystal structure consists of alternating layers of hydrophobic and hydrophilic zones of phenylglycinium along the c axis. The chloride anions are located between hydrophobic zones, forming hydrogen bonds with N and O atoms of the cations, in hydrophilic zones. These ions are linked by cation-cation and cation-anion hydrogen bonds. This three-dimensional complex network of hydrogen bondsreinforces the cohesion of the ionic structure.

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