CRYSTAL STRUCTURE OF BROMOALKYL DERIVATIVES OF 6-METHYL-URACIL AND ISOCYANURIC ACID

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Single crystal XRD is used to study the crystal structure of 1-(4-bromobutyl)-3,6-dimethyluracil and 1,3-dimethyl-5-(5-bromopentyl)-isocyanurate in comparison with structurally similar compounds studied previously. It is shown that unlike macrocyclic compound, for which the crystal structure is determined by the presence of the stacking effect, in the crystals of their artificial precursors stacking interactions are not observed. For 1-(4-bromobutyl)-3,6-dimethyluracil, C–H…O interactions and C=O…Br interactions for 1,3-dimethyl-5-(5-bromopentyl)-isocyanurate are found.

Keywords: XRD, pyrimidinophanes, isocyanurate, C=O…Br-interactions, C–H…O-interactions.