

CRYSTAL STRUCTURE OF SULFINAMIDES OF THE THIAZINE SERIES: FEATURES OF TRANSFERRING THE OPEN-CHAIN SUPRAMOLECULAR SYNTHON FROM THE RACEMIC TO HOMOCHIRAL ENVIRONMENT

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The crystal structures of four representatives of sulfinamides of the thiazine series are comparatively analyzed for the occurrence of different supramolecular associates, inter- and intramolecular interactions. With a similar molecular geometry, different packing motifs occur in the crystals yielding different-type supramolecular associates due to classical N–H···O hydrogen bonds. The features of transferring the sulfinamide open-chain supramolecular synthon from racemic to homochiral environment consisting in the appearance of “secondary cross-linking” are studied.

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INTRODUCTION

Currently, there is a rapid development of crystal engineering – the field of supramolecular chemistry related to the elaboration, design, and study of crystals with desired properties [1-7]. The key concepts of crystal engineering are intermolecular interactions and supramolecular synthons formed through these interactions [8-11]. Studying the stability, reproducibility, interchangeability of the known and new supramolecular synthons and exploring the influence of the crystal environment on their structure is a critical area of modern crystal engineering.

Our previous works on the synthon crystal engineering considered the “synthon structure–crystal environment” relationship in different aspects: strengthening (weakening) of the “synthon-forming” bond due to some secondary intermolecular interaction in the crystal [12], a change in the synthon conformation with a change in the type of the stereochemical environment (homo- or heterochiral) [13], and so on.

We have previously proposed a concept of the “secondary cross-linking” of the hydrogen-bonded supramolecular synthon through non-classical intermolecular interactions, which may differ in crystalline forms. Thus, low- and room-temperature phases of polymorphous cocrystals of diastereomeric pinanyl sulfoxides differ in additional secondary interactions within the same stable hydrogen-bonded synthon [14]. In the crystals of two polymorphs of 1-benzyl-3-bromo-4-

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