

MS30-P01 | FEATURES OF CRYSTAL FORMATION OF CHIRAL DERIVATIVES OF 1,5-DIHYDRO-2H-PYRROLE-2-ONE

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1,5-Dihydro-2H-pyrrol-2-ones represent an important class of five-membered nitrogen-containing heterocycles. Their structural moiety is found in different natural molecules and synthesized compounds having a wide range of biological activities. Among the compounds of this class, substances with antimicrobial, anti-inflammatory, antitumor, analgesic, antiviral, nootropic, antiaggregant and other types of biological activities have been found.

We have studied series of halogen derivatives of 1,5- dihydro-2H-pyrrol-2-ones. The presence of a chiral center in the studied compounds leads to the formation of three types of crystals: racemates, conglomerates and solid solutions with a different composition. All types of crystals were studied by single-crystal, powder X-Ray diffraction and DSC methods. It was found, that crystallization of conglomerates in a high-symmetric crystal systems (as opposed to racemic crystals) is a characteristic feature of the compounds under investigation.

The classical hydrogen bonds between the hydroxyl and carboxyl groups leads either to the formation of a centrosymmetric H-dimers or to H-bounded chains in the crystals. Powder diffraction and DSC studies have shown that during the melting of racemic crystals the processes of racemate melting, followed by the formation of a conglomerate from a supercooled solution and its further melting are observed. The reasons for such phase transitions in the crystals are discussed. The conclusion about the greater thermodynamic stability of highly symmetric conglomerates derived on the basis of the study of the rapid crystallization of compounds from various solvents by powder diffraction.

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