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Seventeen-membered water cluster resulting from recognition of solvated anions on brucinium corrugated layers.

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Streszczenie

Formation of diastereomeric salts remains the most important method for the separation of racemic acids and bases. Selection of a suitable resolving agent in this method is a key for successful resolution. There are primary, secondary, and tertiary chiral amines among frequently used resolving agents for the separation of racemic acids. Cations of most of them and anions of resolved acids are linked to each other by a characteristic system of hydrogen bonds resulting in common cationic–anionic self-assemblies. In this respect, brucine and strychnine are unique, because incorporation of anionic species into a crystal lattice of their salts usually does not affect common cationic self-assembly. The uniqueness of both resolving agents is also reflected in a high frequency of solvated salt formation. In this paper, we show that the presence of water molecules incorporated into the crystal lattice of the brucinium salt may result from recognition of the resolved compound together with its closest aqueous environment on the common brucinium corrugated layers. Performing racemic resolution of model compounds and studying structural relations between succeeding crystalline fractions, we also point out factors responsible for the successful separation of *N*-(4-nitrobenzoyl)alanine by fractional crystallization of brucinium diastereomeric salts.

Adres publiczny

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