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Repozytorium

Plik pochodzi z repozytorium Wydziału Chemii Uniwersytetu Wrocławskiego

Dielectrically controlled priority of interactions in molecular recognition.

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Rok wydania

2015

Czasopismo

Crystal Growth and Design

Numer woluminu

15

Strony

358-365

DOI

10.1021/cg501456n

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

It was shown previously that formation of brucinium double salts during attempts of racemic resolution of *N*-(3,5-dinitrobenzoyl)amino acid (alanine or serine) by fractional crystallization of brucinium diastereomeric salts is related to the self-recognition of anions of the amino acid derivatives into dimeric units stabilized by a set of hydrogen bonds (Białońska, A. and Ciunik, A. Why Is the Resolution of Certain Racemic Modifications Inefficient? Formation of Diastereomeric Double Salts of Brucinium. *Cryst. Growth Des.***2013**, *13*, 111−120). Similar dimeric units were observed in brucinium diastereomeric salts precipitated from methanol solutions containing brucine and one enantiomer of the amino acid derivative. To test if the ability of the anions to form dimeric units can be weakened, an increase of dielectric constant of solutions from which the brucinium salts precipitated was applied. In this approach, three new crystalline forms of brucinium salts with enantiomeric *N*-(3,5-dinitrobenzoyl)serine were obtained. Two of them belong to Z' > 1 structure, and occurrence of the Z' > 1 structures is discussed. In the new crystalline forms, a set of hydrogen bonds that stabilizes the dimeric units is replaced by interactions of the anions with solvent molecules, and the anions are linked to each other at most by lone hydrogen bonds. Recognition between cationic and anionic species by ionic $N–H^{+}\cdots O^{-}$ hydrogen bonds, observed in the previously reported crystal structures of brucinium *N*-(3,5-dinitrobenzoyl)-l-serinate 3.88-hydrate and in the new form, brucinium *N*-(3,5-dinitrobenzoyl)-l-serinate brucine 11.5-hydrate, is precluded by formation of π···π stacking interactions between the anions and brucine molecules as well as by separation of the anions and cations by the extended net of hydrogen-bonded water molecules.

Adres publiczny

http://dx.doi.org/10.1020/cg501456n

Strona internetowa wydawcy

https://www.acs.org/content/acs/en.html

Plik został wygenerowany dnia 2026-11-03 19:27:53

Adres w repozytorium https://old.chem.uni.wroc.pl/pl/repozytorium/XRbGkdF.