Why is the resolution of certain racemic modifications inefficient? Formation of diastereometric double salts of brucinium.

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Streszczenie

Fractional crystallization of diastereomeric salts remains the most frequently used method for a separation of racemic compounds, and yet it has been performed by trial and error. For a better understanding of the chiral discrimination mechanism that is useful for the rationalization of optical resolution and help in choosing the crucial experimental parameters, structural investigations of products of both successful and unsuccessful racemic resolution are important. The former and the latter typically involve diastereomeric salts precipitating fractionally and the formation of solid solutions of diastereomeric salts or diastereomeric double salts, respectively. In this contribution, a mechanism of recognition leading to formation of the diastereomeric double salts is proposed based on crystal structures of three brucinium double salts (bis(brucinium) *N*-(3,5-dinitrobenzoyl)-dl-alaninate methanol 3-solvate, bis(brucinium) *N*-(3,5-dinitrobenzoyl)-dl-alaninate 5.75-hydrate, and bis(brucinium) *N*-(3,5-dinitrobenzoyl)-dl-serinate 0.10-hydrate) as well as of some relevant diastereomeric salts (containing the d- or l-enantiomer of the alanine or the serine derivative).

Adres publiczny

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