

عنوان مقاله:

Theoretical Investigations on the Separation of Medetomidine Enantiomers

محل انتشار:

نشریه متدهای شیمیایی، دوره 4، شماره 6 (سال: 1399)

تعداد صفحات اصل مقاله: 10

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خلاصه مقاله:

The enantiomeric separation of racemic compounds is of special importance. Conglomerate mixture is of considerable interest, since it corresponds to the possibility of spontaneous resolution of the two enantiomers. The aim of this paper is to find the achiral anions causing conglomerate formation of Medetomidine salts. For this purpose, the effect of 9 anion (X) on the heterochiral structure of Medetomidine enantiomers salts have been studied by Material Studio software. The crystal structures of all systems were determined by quantum calculations of CASTEP module. Investigation of the crystal structures and their respective energy show that Medetomidine salts, formed by Oxalic acid, Maleic acid and Fumaric acid crystalize as conglomerate, favoring preferential crystallization. The AIM results confirmed the more stability of conglomerate crystal in these cases while in the presence of other salting agent as Hydrochloric acid, Acetic acid, Carbonic acid, Formic acid, Malic acid and Lactic acid racemic crystal form is calculated as the more stable crystal. Using Forcite module, the total energy of the crystalline systems (calculated as the sum of the energies of the bonded and non-bonded interactions) are in agreement with those predicted by .CASTEP module and AIM calculations

کلمات کلیدی:

Medetomidine, Racemic Compound, Conglomerate Mixture, Crystal Structure Prediction, Preferential Crystallization

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