

Role of hydrogen bonding in molecular recognition of L-phenylalanine to D/L-mandelic acid for diastereomeric crystallization

Xuan-Hung Pham, 김인호¹, 김종민², 장상목², 김우식*
경희대학교; ¹충남대학교; ²동아대학교
(wskim@khu.ac.kr*)

In the present study we have examined the difference in the molecular structure of both two diastereomers L-mandelic acid.L-phenylalanine and D-mandelic acid.L-phenylalanine to explain the preferential crystallization of former. The presence of hydrogen bond in two diastereomeric salts has been manifested by the decrease of the stretching vibration frequency of $-\text{COOH}$ and $-\text{NH}_3^+$ peak of IR and Raman. In addition, the broad and shift of proton NMR at NH_2 and $-\text{OH}$ peaks have confirmed the hydrogen bonding existence. However, the number and strength of hydrogen bond was different in two salts. By using SXRD and DSC analysis, it's shown that there are five hydrogen bonds and 162 kJ/ mol enthalpy in L-mandelic acid.L-phenylalanine. Meanwhile, D-mandelic acid.L-phenylalanine has 117 kJ/ mol enthalpy and six hydrogen bonds, one of which is bifurcated hydrogen bond. At the same time, it is attempted at measuring the attractive force between the resolving agent and mandelic acid by using Chemical force microscopy (CFM). Consequently, the interaction of L-mandelic acid with L-phenylalanine preferentially than D-mandelic acid has been presented.