Mechanism of Mutual Incorporation of Branched Chain Amino Acids and Isomorphic Amino Acids in Batch Crystallization.

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On BCAA (Branched Chain Amino Acids) crystallization process, impurity amino acids (guest amino acids) are easily incorporated to the host amino acid(a purified amino acid). Because host and guest amino acids have similar molecular structures and physical-chemical properties, therefore, in many cases, it is difficult to separate a host amino acid and a guest amino acid each other in the simple crystallization method (such as cooling or concentration crystallization conducted in water solvent). In above cases, HCl or precipitant is added to the mixed solution of a host and guest amino acid in order to separate them by generating the salt of a host amino acid. (A host amino acid crystallizes as a hydrochloride or precipitant process is needed after crystallization to make the products. Therefore, it is thought that development of the simple crystallization method is necessary in order to make a process simpler. In order to develop the simple crystallization method, it is necessary to elucidate the incorporation mechanism of these amino acids at first, and then decide the crystallization condition based on this mechanism.

We explored the mutual incorporation tendency of Branched Chain Amino Acids (Lleucine, L-isoleucine, L-valine) and isomorphic amino acids in cooling crystallization conducted in water solvent. As a result, in most cases, a guest amino acid whose side chain is longer than that of a host amino acid was incorporated easily in a host amino acid. In this case, a solid solution was formed, and the *c*-axis of a host crystal structure was extended. Also the crystal growth was inhibited. Using these results, a mechanism for mutual incorporation of these amino acids was proposed.