Crustal Structure of Isosteviol and its Derivatives

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Crystal structure determination of 33 derivatives of plant terpenoid isosteviol and its molecular complexes with small molecules were performed. It was analyzed a molecular geometry and intermolecular interactions in the crystal, and types of crystalline packing. The absolute configuration of chiral centers of the molecule of isosteviol was established.

Shown that for single framework isosteviol derivatives, solvates, or complexes of including are got only at presence of not modified acid group.

For bis-framework derivatives – «tweezers» structures, built on the type «head to head», molecular complexes is not observed, while in crystals of structures, having type of buildings «head to tail» even at short connecting bridge, received solvates with small molecules.

It was established that molecular complexes of isosteviol with small aromatic molecules (benzene, toluene, aniline, dimethilaniline, naphthalene, etc.) are isostructural in the space group $P4_32_12$. The supramolecular structure of these complexes is a double spiral around an axis of fourth order; branches, which formed by hydrogen bonded molecules of isosteviol. Molecules of aromatic «guests» are located in the same areas of crystal, but differently oriented for molecules of isosteviol. Shown that forming of complexes with technical mixtures of nitroanilines and toluene runs regioselective.

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