

Molecular Recognition of Racemic Salts by Inclusion Complexation with the Chiral BINOL

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Optically active 2,2'-dihydroxy-1,1'-binaphthyl (BINOL) have found many applications, ranging from chiral ligands in catalysts for asymmetric reactions, to hosts for molecular recognition and enantiomeric separation, and as intermediates for the synthesis of chiral materials.

We report here a chiral resolutions of racemic ammonium salts by the inclusion crystallization with (S)-BINOL (**1**) as the optically pure host. Resolution was very efficient for 3-hydroxyquinuclidinium chloride (**2**), but similar resolution of N-methyl-2-hydroxymethyl-piperidinium chloride (**3**) was failed, although (**3**) formed an inclusion complex with (**1**). X-ray structures of these complexes were studied in order to characterize the intermolecular interactions and recognition scheme.

The crystal structure of the complex (S,S)-**1**·**2** consists of the hydrogen bonded chains formed by three OH...Cl bonds, two with two different host molecules and one with the guest. There is also an intramolecular N-H...O bond in guest molecule. In the complex (S,S,S)-**1**·**3** the chloride anion participate in H-bonds in the same manner. However, an extended three dimensional hydrogen bond networks are obtained through the additional N-H...O bonds with one OH group of the host molecules.

Keywords: inclusion complexes, molecular recognition, H-bond