postulated that these differences are due to the nature of the halogens, or to the increase of the cycloalkane ring, which modify their electronic and steric characteristics.

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Keywords: tellurium complexes, cathepsin, inhibitors

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Structural Variety in Tris(5-acetyl-3-thienyl)methane (TATM) Inclusion Compounds

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Tripodal host molecules form a versatile class of supramolecular materials which include triphenylmethane and analogues such as TATM. TATM host-guest inclusion compounds display a wide variety of stoichiometry and structural motifs and they have demonstrated a propensity for polymorphism. Indeed we have obtained five different forms of the 2:1 host guest compound of TATM / 1,3 dichloropropane. Four of the five polymorphs can be described as polytypes that share both a similar layer motif and a similar conformation of the TATM's thienyl rings. Over the past several years we have examined the structure of more than 20 TATM inclusion compounds. In all but one example the host TATM molecules adopt one of two distinct conformations as first discussed by Herbstein [1]. The TATM frameworks that share a similar conformation may be described as polytypes composed of common layer motifs. Differences in the layer stacking leads to a variety of space groups.

In the TATM frameworks the host molecules interact through π-π and C-H••O interactions to form layers. In all the studies the host and guest interact very weakly through van der Waals forces. The disordered guest molecules are dynamic and located in channels or cages within or between the framework layers. The long-chain guests span more than one layer. Some of the frameworks appear stable upon removal of up to 90% of the guest species.

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Keywords: inclusion compounds, polytypes, molecular packing

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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

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Crystal Structure of a Histidine Schiff Base

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Threonine and histidine are essential aminoacids which have big importance in bioorganic and medicinal chemistry. Their Schiff bases are also important in biological systems because of their functional role in reactions, transaminations, racemizations and decarboxylations [1].

At the beginning of our research program on aminoacid Schiff bases, threonine Schiff base [N-(2-hydroxy-1-naphthylidene)threonine] has been isolated and investigated [2]. In this work, we would like to present an x-ray investigation of a new synthesized histidine Schiff base [N-(2-hydroxy-1-naphthylidene)histidine]as the second part of our studies. The crystal belongs to orthorhombic, space group $P2_12_12_1$ with the following crystallographic parameters: a=6.133(5), b=7.168(5), c=33.639(5) Å , V=1478(2) Å^3. The final R factor: R=0.0394 , wR=0.0784.These type Schiff bases usually show photochromic or thermochromic characters depending on their tautomeric forms [3,4]. According to the present crystallographic results, histidine Schiff base prefer keto-amine tautomerism rather than enol-imine tautomerism which was observed in the structure of threonine Schiff base. A strong intra-molecular hydrogen bond [N-H…O: 2.592(9)Å] indicated that proton transfer from hydroxy group of naphthalidene to the nitrogen atom is favoured by the charge distribution of the (keto-amin) resonance form.

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Keywords: schiff base , histidine, X-ray analysis

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Weak Intermolecular Interactions in Cavitands as Receptors for Mass Sensors

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Cavitands, synthetic organic compounds with enforced cavities of molecular dimensions, are extremely interesting and versatile molecular receptors whose complexation properties mainly derive from H-bonding, CH-π and dipole-dipole interactions [1].

The rational design of organic hosts is particularly appealing to chemical sensor technology, which requires selective, sensitive and stable receptors. The use of supramolecular structures coated as thin layers on quartz crystal microbalances (QCM) has proved to be one of the best approaches to generate new materials with molecular specificity for chemical sensing [2].

Following these studies, convenient phosphorus-bridged cavitands were designed and synthesized to investigate their complexation properties towards linear alcohols [3]. X-ray diffraction on single crystals has been widely used to study the multiple binding interactions in these phosphonate cavitands (hydrogen bonds involving the PO groups and CH-π interactions with the π-basic cavity). It has been thus evidenced that the synergistic behaviour of an increasing number of convergent PO groups enhances the complexation of the guests, giving rise to entropically favoured complexes.

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