chemical modifications of the molecular structures are very reliable and accessible, prediction of the supramolecular behavior is not always easy and in some cases can be very complex.

In this paper, examples of these new hosts will be presented as well as their design and synthesis procedures. Furthermore, the crystal structures of some of these new inclusion compounds will be described in detail.

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Keywords: inclusion compounds, host, crystal structure

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Interactions of Supramolecular Synthons Formed by Secondary Propargylic Alcohols

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Chiral secondary propargylic alcohols are used in the enantioselective synthesis of natural products and as synthetic precursors of several optically active compounds. Secondary propargylic alcohols with aryl substituents possess three important functional groups: the hydroxyl group, the π system of the alkyne moiety, and a variety of aryl rings that can be involved in π˜ π stacking as well as other interactions. The combination of the three functional groups attached to one chiral carbon makes secondary propargylic alcohols well suited for applications in supramolecular chemistry and crystal engineering [1-3].

The competition between O-H…O hydrogen bonds and weaker interactions such as C-H…π and π˜ π stacking leads to the formation of a diverse set of synthons, including non-planar hexamers. The cooperativity between intermolecular forces is essential for the stabilization of these synthons.

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Keywords: supramolecular chemistry, crystal engineering, organic molecule

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Stereochemistry in Crystal Engineering

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Molecular recognition by hydrogen bonding between organic molecules has been explored in supramolecular chemistry to a great extent. [1,2] Most of the recognition motifs are however two-dimensional in nature. By employing organic compounds in the context of supramolecular chemistry and utilizing their chiral attributes the three-dimensional nature of intermolecular hydrogen bonding may be revealed.

This project, to date, has been focused on the design and synthesis of sulfides, sulfoxides and sulfones. Sulfoxides are ideally suited as a recognition motif as they are extremely polar and have the potential to participate in hydrogen bonding. The intrinsic chirality at sulfur introduces the three-dimensional nature of the study. The effect of the oxidation state of sulfur on the hydrogen bonding array is also investigated, along with other substituent effects.

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Keywords: hydrogen bonding, chirality, sulfur

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Ringing the Changes with Tetrazole: Hydrogen Bonding Studies

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Tetrazoles are acidic heterocycles and used in angiotensin II receptor antagonists for the treatment of high blood pressure. The binding mode is still controversial [1], as yet the only published crystal structure of a tetrazole-protein complex shows close contacts between two of the tetrazole nitrogen atoms and two lysine residues within the enzyme binding site. [2]

Tetrazoles are used as bioisosteric replacements for carboxylic acids in modern drug design. Transmembrane receptors are notoriously difficult to study, so model systems can provide further insight into non-covalent binding interactions.

This work describes the hydrogen-bonding patterns seen for readily available ionic model complexes, developing earlier studies of hydrogen-bonding tetrazolate anion [3] and illustrate how the tetrazole, or simple derivatives bind to acetamidine (arginine model), propranolol (an antihypertensive drug) and spermine (a natural hormone). These will be compared with analogous carboxylic acid complexes to provide insight into the hydrogen bonding interactions favoured by tetrazoles as well as difference in binding properties.

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Keywords: drug binding, hydrogen bonding, heterocyclic compounds

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Structure of *N,N*-dimethylaminopyridinium *L*-malate

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The crystal structure of a new *L*-malic acid salt, N,N- dimethyl-aminopyridinium *L*-malate has been determined at room temperature using single crystal X-ray diffraction techniques. The space group is orthorhombic $P2_12_12_1$ with lattice parameters a= 7.461(1), b= 7.945(1) and c= 20.774(4)Å. Similarly to other *L*-malic salts, the malate anions form hydrogen-bonded head-to-tail (carboxylic and carboxylate groups) infinite chains parallel to the [100] crystal direction. On the other hand, the dimethylaminopyridinium cations are arranged with their mean plane approximately perpendicular to the [100] crystal direction. The N-H group of every cation forms two hydrogen bonds with oxygen atoms of different anion chains connecting *L*-malate chains along the [010] crystal direction. The whole crystal packing can be viewed as parallel two-dimensional hydrogen-bonded molecular arrangements perpendicular to the [001] direction. As in other *L*-malic salts, preliminary measurements show optical second-harmonic generation.

Keywords: nonlinear optical materials, molecular crystals, crystal engineering

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Complexes of Non-chiral Surfactant Molecules with Chiral and Racemic Compounds

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