

MS34-P8 4,2':6',4'' and 3,2':6',3''-terpyridine
Ligands – Coordination polymers with
discrete, up to 3-dimensional assemblies

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Oligopyridines are well known building blocks in coordination chemistry. The popular 2,2':6',2''-terpyridine (tpy) building block adopts a bis(chelating) coordination in octahedral complexes, leading to mainly discrete compounds. By using the less common isomers 4,2':6',4''- and 3,2':6',3''-tpy in combination with a wide range of transition metals, it is observed that the N-atom of the inner pyridine ring does not participate in coordination.¹ Unlike tpy, 4,2':6',4''- and 3,2':6',3''-tpy ligands can no longer form chelates, but favour a variety of multinuclear and multidimensional structures. The ease of introducing substituents in the 4''-position of these tpy's enables facile modification, making the ligands bulkier, as well as introducing additional coordination sites. Taking this one step further, it is possible to synthesise tetra-dentate ditopic bis(tpy) tectons. In the reaction of 1,4-bis(*n*-octoxy)-2,5-bis(3,2':6',3''-terpyridin-4''-yl) benzene (figure) with Co(NCS)₂ a 3-dimensional [4, 8₂] lvt net is obtained.² The assembly of 3-D nets or 2-D sheets as well as discrete assemblies will be presented.

References

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- 2 Y. M. Klein, E. C. Constable, C. E. Housecroft and A. Prescimone, *CrystEngComm*, 2015, **17**, 2070–2073.

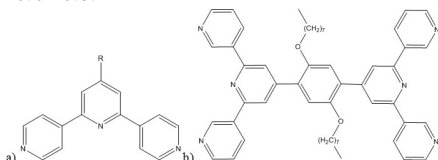


Figure 1. a) 4,2':6',4''-terpyridine with substituent R in 4'' position
b) The ditopic ligand
1,4-bis(*n*-octoxy)-2,5-bis(3,2':6',3''-terpyridin-4''-yl) benzene.

Keywords: Terpyridine, Multidimensional, Self Assembly

MS34-P9 Self-organization of
para-sulfonatocalix[*n*]arenes and selected
aromatic amines in heteromolecular
crystals: structural studies

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Supramolecular chemistry is an interdisciplinary field of science that deals with the design, formation and exploration of complex chemical systems of smaller building blocks joined by non-covalent intermolecular interactions. One of its tasks is to look for new molecular receptors, and acquiring knowledge about molecular recognition which involves the formation of selective bond between a receptor and the substrate molecules, resulting in the host-guest complex formation. The inclusion complexes of *p*-sulfonatocalix[*n*]arenes (*n* = 4, 6, 8) with aromatic amines (1,2-bis(4-pyridyl)-ethane, 1,3-bis(4-pyridyl)-propane, 1,10-phenanthroline) were obtained. *p*-Sulfonatocalix[*n*]arenes show a great ability to interact with the aromatic amines. The obtained supramolecular systems are organic salts formed from deprotonated calixarene and protonated guest molecules. Anion receptors form inclusion complexes with substrates mainly by π - π , C-H... π and N-H... π interactions. New, not described before, conformations of the *p*-sulfonatocalix[8]arene anion was observed and it has been shown that this particular anion may substantially change its conformation depending on the type and the amount of complexed cations. In the obtained complexes, the mechanism of induced fitting is observed in cases where the substrate forces the conformational change of the receptor and the mechanism of mutual induced fitting is observed, when there is a mutual adjusting host and guest molecules. Ions and molecules in described supramolecular compounds contribute to the formation of various structural motifs, such as dimers, trimers, tetramers, infinite stacks, capsules, columns, polymeric chains (Fig.1), channels. The obtained inclusion complexes are characterized by diverse molecular packing in the crystal lattice and diverse topologies from simple, stepped and a "zig-zag" bilayers through the column packing to the three-dimensional network of intersecting channels. The obtained results show structural diversity of these compounds, a great richness of supramolecular chemistry, and demonstrate that these compounds are promising building blocks to construct further supramolecular architectures of high complexity. The information gained about the crystal and molecular structures of *p*-sulfonatocalix[*n*]arenes complexes with aromatic amines can contribute to the development of supramolecular chemistry, crystal engineering and also for materials chemistry, aimed at obtaining new functional materials.

Keywords: calixarene, host-guest complex

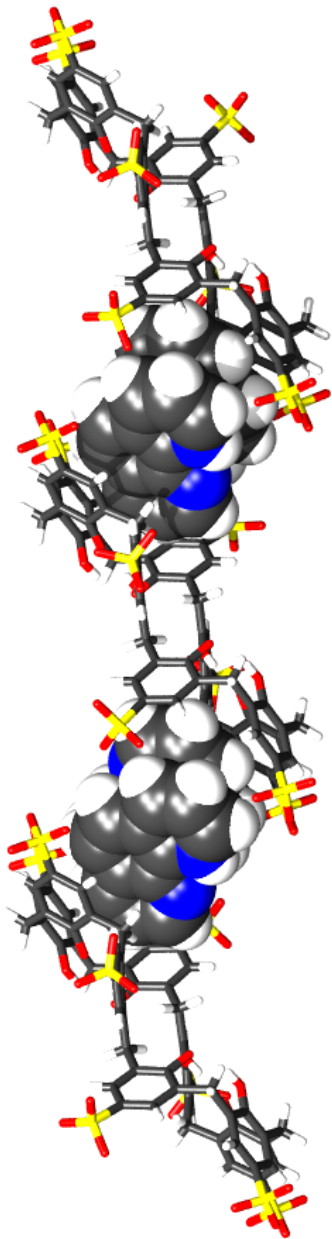


Figure 1. Inclusion polymer formed by *p*-sulfonatocalix[8]arene and 1,10-phenanthroline dimers.