It is very hard to imagine modern supramolecular chemistry without principles of anion binding.<sup>1</sup> Despite all progress in this field, significant anion binding rate in this type of assembly is hard to achieve due to the properties of anions.<sup>2</sup> Anion binding is interesting because of its potential applications and roles in many biological systems and industrial processes.<sup>3</sup> Herein we describe a solid-state study of several supramolecular complexes based on a podand L, containing three potential binding sites, and anions with various geometries and basicities. L adapts its conformation in order to respond to the anion's requests, thus forming two kinds of supramolecular rings with hydrophilic and hydrophobic interiors. Since the assembly is highly anion specific, the occurrence of the

complexes in systems with high concentrations of competing anions has been explored. The role of the solvent in structural stabilization will be also discussed.

1) S. O. Kang et al, Angew. Chem. Int. Ed. 2006, 45, 7882-7894. 2) P. D. Beer, P. A. Gale, Angew. Chem. Int. Ed. 2001, 40, 486-516. 3) J. L. Sessler et al, Chem. Commun. 2004, 1276-1277.



Keywords: supramolecular chemistry, template synthesis, anion recognition

#### P07.04.27

Acta Cryst. (2008). A64, C407

# Triple-stranded helical metal complex of quaterimidazole and its highly-symmetrical network

Yumi Yakiyama<sup>1</sup>, Tsuyoshi Murata<sup>2</sup>, Yasushi Morita<sup>1</sup>,

Kazuhiro Nakasuji3

<sup>1</sup>Graduate School of Science, Osaka University, Chemistry, Machikaneyama1-1, Toyonaka, Osaka, 560-0043, Japan, <sup>2</sup>Graduate School of Science, Kyoto University, Kyoto, Japan, <sup>3</sup>Fukui University of Technology, Fukui, Japan, E-mail:yakiyaki@chem.sci.osaka-u.ac.jp

In this study, we focused 4,4':2',2'':4'',4'''-quaterimidazole (424-Qim), the tetramer of imidazole, and prepared complexes with various metal ions. As a consequence, we have turned out a high potential of 424-Qim for the versatile and general building block for constructing triple-stranded helical metal complex (triple-helicate) having a multi-dimensional network in the crystal. In this context, we have newly investigated the binding isomer of 424-Qim, 2,2': 4',4'':2'',2'''-quaterimidazole (242-Qim) and found that 242-Qim can also form triple-helicate with two Ni(II) ions (Figure.1). In this presentation, we will report the synthetic method for 242-Qim and its triple-stranded helical dinuclear Ni(II) complex and highly-symmetrical multi-dimensional network structure of the complex. In

the crystal structure, triple-helical structure was constructed by three **242-Qim** molecules that coordinate to two Ni(II) ions with largely twisting structure in the center of their skeletons. Unlike the triple-helicate



composed of **424-Qim**, **242-Qim**-based helicate formed highlysymmetrical two-dimensional sheet structure connected through Hydrogen bonds via counter anions.

Keywords: hydrogen bonding of coordination compounds, supramolecular chemistry, nickel compounds

### P07.04.28

Acta Cryst. (2008). A64, C407

# Design of crystalline space for constructing ferroelectric rotators in [Ni(dmit)<sub>2</sub>]- salts

Tomoyuki Akutagawa, Takayoshi Nakamura

Hokkaido Univesrity, Research Institute for Electronic Science, N12W6 kita-ku, Sapporo, Hokkaido, 060-0812, Japan, E-mail:takuta@es.hokudai. ac.jp

The cation units of aryl ammonium  $(R-NH_3^+)$  - crown ethers in metal dithiolate complex,  $[Ni(dmit)_2]$ , are one of the useful building blocks to construct supramolecular rotors in crystalline solid. Here, we present the crystal structures, magnetic properties, and ferroelectric properties of (meta-substituted anilinium)(dibenzo[18] crown-6) supramolecualr cations associated with the molecular motion in  $[Ni(dmit)_2]$  salts (R = F and NH<sub>2</sub>). Figure 1 shows the unit cell of (m-F-anilinium+)(dibenzo[18]crown-6)[Ni(dmit)<sub>2</sub>]salt viewed along the a-axis. Alternate arrangement of cations and anions was observed along the c-axis. Within the cation layer, the  $\pi$ -plane of m-F-anilinium was interacted with two [Ni(dmit)2]anions. The temperature dependent dielectric constant showed a frequency dependent behavior above 240 K, suggesting that

the dielectric response was associated with molecular rotation of m-F-anilinium+ cations in the crystal. From the electric filed - polarization (P - E) measurement at 300 K, a hysterics behavior was confirmed. The relation between molecular motion and ferroelectric behavior will be mentioned.



Keywords: ferroelectric properties, supramolecular structure, metal coordination complex

## P07.04.29

Acta Cryst. (2008). A64, C407-408

#### The diabolecules: Some unexpected copper clusters

Laura J. McCormick, Brendan F Abrahams, Richard Robson University of Melbourne, Department of Chemistry, Parkville, Victoria, 3010, Australia, E-mail:1.mccormick2@pgrad.unimelb.edu.au

Saccharic acid (sacc, I) is a chiral dicarboxylic acid which, when deprotonated, has the ability to bridge metal centres, which can lead to the formation of chiral coordination networks<sup>1</sup>. In efforts to further explore the coordination chemistry of this ion we combined it with metal ions in the presence of co-ligands such as 1,10-phenanthroline. With two coordination sites on the metal centre blocked by the terminal 1,10-phen we hoped that a macrocyclic species may form with a chiral hydrophilic void at the centre and aromatic groups on the outside of a macrocyclic ring. A mixture of Cu(NO<sub>3</sub>)<sub>2</sub>, KHsaccharate and 1,10-phen afforded blue crystals of