Poster Sessions

composed of achiral building blocks resulting in most of the polymeric chains being aligned relative to each other in a centrosymmetric manner. There is however, one example in which an interesting high symmetry chiral structure has been formed. As is to be expected, the cobalt structure has been found to have magnetic properties.



Keywords: crystal engineering, coordination polymer, magnetism

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A single-crystal-to-single-crystal apical ligand exchange process in a 2D coordination network

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Crystal engineers are becoming more and more aware of the potential coordination chemistry holds. The successes in the design and synthesis of new functional materials, based on metal-organic complexes, are most noticeable in the continuously growing group of porous coordination compounds, with applications such as guest encapsulation, ion exchange and catalysis. As crystalline materials are the main focus of most preliminary studies, reports dealing with structural transformations in the solid state are presently more often, yet still rarely, encountered in the literature. In continuation of our studies on the development of new functional materials and our interest in solid-to-solid interconversions, we report a singlecrystal-to-single-crystal ligand exchange process. The copper centers have been incorporated in corrugated square-grid coordination layers which provide big channels occupied by water and/or solvent molecules and chloride ions. The copper coordination geometry is square pyramidal with the chloride ion in the apical position and four ditopic imidazole type ligands at the equatorial positions. Upon immersion of crystals in a saturated methanolic solution of NaBr (3 h), a color change was noticed. X-ray analysis revealed that the apical chloride was substituted by a bromide ion. During the exchange process, the crystals didn't lose their crystallinity, as was monitored by atomic force microscopy (AFM). These results and the use of other anions for exchange will be presented, as well as supporting analyses.

Keywords: crystal engineering, single-crystal-to-single-crystal transformations, polymeric coordination compounds

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Boronic acids as hydrogen-bond bridges between metal coordinated carboxylates

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Boronic acids have been the subject of several recent papers describing their H-bonding ability in supramolecular chemistry. There have been papers on the functionalised acids (Pedireddi), calixarene derivatives (Atwood) and those linking metal complexes (Orpen, Braga) among others. Applications are varied for boronic acids and their derivatives and range from fluorescent sensors, to organic reagents to supramolecular assemblies and beyond. Our studies focus on the use of such acids to link metal carboxylate complexes together. Such complexes normally fail to link due to a lack of H-bond donors. Reaction of (PPh₃)₂Cu(BH₄) with a pyridine or pyrazine carboxylate in a sealed reaction vessel results in hydrolysis of BH₃ to B(OH)₃. The B(OH)₃ is then available in situ and co-crystallises with the Cu(I) complex to form motifs as shown in fig.1. We have exploited this reaction and used a range of boronic acids to form a number of 0D, and 1D architectures. Some data sets have been collected with the use of SR. We note that the Etter graph set descriptions fail to distinguish between the central, head-to-tail and boronic acid-carboxylate double donor $R^2_2(8)$ motifs, yet they are different.

Keywords: hydrogen bonding recognition, boronic acids, supramolecular assemblies

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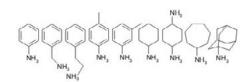
Noncovalent interactions in a family of cyclic ammonium nitrates

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The aim of crystal engineering is the design of crystal structures, and as a result, materials with desired properties. A fundamental requirement of crystal engineering is the understanding of the role of non-covalent interactions present in the solid-state structure. This study focuses on the identification of non-covalent interactions in a family of cyclic ammonium nitrate salts, as indicated below. All the compounds crystallize in layered structures, with the organic layer containing the cyclic ammonium moiety, while the ammonium groups and nitrate anions comprise the inorganic layer. Trans-1,4-diammonium nitrate exhibits polymorphism. Non-covalent interactions present in the structures include pi-pi interactions, nitrate...nitrate interactions and strong, charge assisted N+-H...Ointeractions. The hydrogen bonding networks observed are compared, and trends relating to the interactions are identified. The effect of the bulkiness, saturation, charge, number of hydrogen bonding donors and directionality, ring-size and alkyl chain length of the cation

on the structure obtained, and on the non-covalent interactions present is highlighted.



Keywords: crystal engineering, nitrates, hydrogen-bond patterns