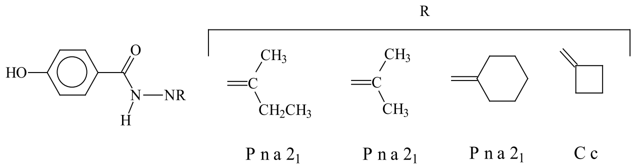
ionic chromophores, or the lowering of the rod-like symmetric shape of the molecule by introducing lateral substituents. Other approaches are based on crystal engineering strategies exploiting directional intermolecular interactions (e.g. H-bonding, halogen bonding), or supramolecular approaches as inclusion compounds and co-crystals [1].

However, all these approaches are highly empirical and fundamentally trial-and-error based. To get a polar crystal is still a challenging task.

Here, we report some preliminary results on the discovery of a class of nonchiral compounds forming polar crystal structures, with favourable orientation of the molecule with respect to the polar axis. Chemical diagrams of the compounds prepared up to now are given in the Scheme below, together with their space groups.

The angle between the polar axis and the long molecular axis joining phenolic oxygen to imino carbon is, respectively, 60°, 41°, 60° and 28° in the four compounds of the Scheme. The functionality resulting from the polar order of the first compound in the scheme has been confirmed by the powder second harmonic generation measurements by the method of Kurtz and Perry, where the efficiency is 120 % that of urea standard at the non-resonant fundamental wavelength of 1907 nm.



[1] M. Jazbinsek, P. Günter, *Introduction to Organic Electronic and Optoelectronic materials and devices*, S.-S. Sun L.R. Dalton Eds., CRC Press, Taylor& Francis Group, Boca Raton **2008**, Ch. 15, 421-466.

Keywords: polar crystals, second harmonic generation, H-bonding synthons.

MS24.P09

Acta Cryst. (2011) A**67,** C359

New coordination polymers with embedded molecular recognition functionality

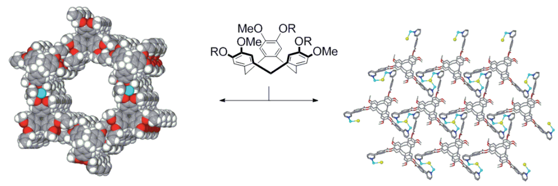
Michaele J. Hardie,[a] Christopher Carruthers,[a] James J. Henkelis,[a] Marc A. Little,[a] Tanya K. Ronson,[a] Christopher J. Sumby,[a,b] [a]*School of Chemistry, University of Leeds, Leeds, LS2 9JT, (UK).* [b]*current address: University of Adelaide, (Australia).* E-mail: m.j.hardie@leeds.ac.uk

The use of molecular hosts as tectons for the self-assembly of coordination polymers promises crystalline materials with embedded molecular recognition sites, as well as the more common lattice-type guest sites [1], [2], [3], [4], [5]. We have developed a range of host molecules based on the cyclotriveratrylene (CTV) framework with additional metal-binding groups at their upper rims.

Tripodal CTV-analogues have a distinctive open pyramidal shape which creates the specific guest-binding site. The rigid “corner-piece” shape also means that coordination polymers resulting from these ligands may have unusual structural and topological aspects to them. For example, 2D networks of linked metallo-cages; [1] rare (3,4)-connected network topologies such as $(4^2.6^2)(4.6^2)_2$; and highly complex and unprecedented 3D topologies [2].

As these tectons are molecular hosts, host-guest interactions may play an important role in both the assembly of the coordination polymers and in their potential applications. Host-guest associations may be structure-directing, and generally, binding large guests in the molecular cavity of the ligand promotes formation of a coordination polymer instead of a discrete species [3], [4]. For example, binding of a large *o*-carborane guests dictates whether a discrete $[Cd_3(OAc)_6L]$ complex or 2D 4.8^2 coordination polymer is formed when L = tris(4-pyridyl)aminocyclotriguaiacylene [3] Self-inclusion motifs also play an important role. Crystalline clathrates of CTV-analogues are known to form a hand-shake dimer where an upper-rim R group of one host is the guest for another host and vice versa, and the same motif is found within coordination chains [5]. Host-guest interactions may also result in associations between networks, including within polycatenation motifs.

Here, different coordination polymers from ligands with N-donor, carboxylate, N-oxide or allyl metal-binding groups will be presented, and the importance of host-guest interactions of these ligands in terms of coordination polymer construction and functionality highlighted.



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Keywords: supramolecular, crystal engineering, coordination polymers

MS24.P10

Acta Cryst. (2011) A**67,** C359-C360

Kinetic assembly of porous coordination networks and ab initio powder structure determination

Masaki Kawano *Division of Advanced Materials Science, Pohang University of Science and Technology (POSTECH), Pohang (South Korea).* E-mail: mkawano@postech.ac.kr

The chemistry of porous coordination networks has undergone explosive growth in the last decade because of fascinating features. Porous coordination networks can be used for gas sorption/separation/storage, molecular recognition, drug delivery, catalysis, and so on. Especially porous materials have been paid much attention as potential hydrogen storage materials for fuel cells. Thanks to the high flexibility in design, a number of porous coordination networks were prepared and were analyzed by single crystal X-ray crystallography. Here we would like to report new aspects in porous coordination network chemistry. A pore of porous materials can be used as crystalline molecular flask in order to not only make a reaction but also directly observe the reaction by X-rays [1-5]. In this talk, especially we will focus on selective kinetic assembly of porous coordination networks, the usage, and the *ab initio* powder structure determination [6-10]. The kinetic study of porous coordination networks compared with zeolite is a totally unexplored field, because of difficulties in powder structure determination. We succeeded in solving powder crystal structures having unit cells larger than 15000 Å^3.

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Keywords: MOF, kinetic assembly, powder structure determination

MS24.P11

Acta Cryst. (2011) A**67,** C360

Structure and gas adsorption study on metal organic frameworks

Rahul Banerjee, *Physical/Materials Chemistry Division, National Chemical Laboratory, Pune 411008, (India).* E-mail: r.banerjee@ncl.res.in

Recent work in the field of hydrogen storage and CO_2 sequestration has been overwhelmingly dominated by the use of a narrow range of materials, specifically high surface area carbons (including carbon nanotubes) zeolites and metal hydrides. Activated carbons have the attraction that they are very cheap, their capacities on a weight % basis are very good due to their very low densities, and the adsorption process is readily reversible under mild conditions. Their shortcomings stem from the fact that the fundamental interactions between carbons and hydrogen are non-bonding in nature (i.e. they involve physisorption) and are therefore rather weak. Metal hydrides, adsorb hydrogen by a chemisorption process that is accompanied by dissociation of the dihydrogen molecules. The interaction is much stronger, but facile reversibility is a problem in many cases and such systems are often prone to irreversible poisoning by oxygen. There is clearly an urgent need to develop new classes of materials that have the potential to provide superior performance for hydrogen storage and CO_2 sequestration. Some of the more recent developments in this area include the use of Metal Organic Frameworks (MOFs). Our strategy is aimed at the development of new materials systems where the host-guest interactions are intermediate between those found in the carbons and the metal hydrides.

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Keywords: porous, zeolytic, adsorption

MS24.P12

Acta Cryst. (2011) A**67,** C360

Photo-responsive Pores of Porous Coordination Polymers

Hiroshi Sato,[a,b] Ryotaro Matsuda,[a,b] Susumu Kitagawa,[a,b,c] [a]*Exploratory Research for Advanced Technology (ERATO), (Japan) Science and Technology Agency (JST), Kyoto, (Japan).* [b]*Institute for Integrated Cell-Material Sciences, Kyoto University, Kyoto, (Japan).* [c]*Department of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University, Kyoto, (Japan).* E-mail: hiroshi.sato@kip.jst.go.jp

Porous coordination polymers (PCPs) or metal–organic frameworks (MOFs), which are constructed from metal ions and organic ligands, have been extensively investigated to provide the nanometer-sized space that is potentially applicable in separation, heterogeneous catalysis, and gas separation/storage. Recently, we reported porous crystalline materials that can be activated by photostimulation [1] and demonstrated that photochemical modification is a powerful method for the control of physical properties of PCPs or MOFs.

In this report, synthesis and properties of new PCPs containing *trans*-1,2-bis(4-pyridyl)ethene (bpe) as a photoreactive module will be presented. The photoreactive PCPs adsorb gaseous molecules such as carbon dioxide. The bpe molecules quantitatively take place topochemical [2+2] cycloaddition reactions and the PCPs show single-crystal to single-crystal (SCSC) transformations upon UV irradiation (> 300 nm). We will discuss not only the SCSC transformations but also the impact on the photochemical transformations on the sorption properties.

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Keywords: microporous, photoreaction, adsorption

MS24.P13

Acta Cryst. (2011) A**67,** C360

Pressure-induced magnetic switching in molecular framework materials

Gregory J. Halder,[a] Karena W. Chapman,[a] John A. Schlueter,[b] Jamie L. Manson,[c] Peter J. Chupas,[a] [a]*X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, Illinois, (USA).* [b]*Materials Science Division, Argonne National Laboartory, Illinois, (USA).* [c]*Department of Chemistry & Biochemistry, Eastern Washington University, Cheney, Washington, (USA).* E-mail: halder@aps.anl.gov

The design and characterization of molecular materials with targeted functionalities, such as magnetism and/or nanoporosity, is part of a major international push aimed at developing systems with technologically important applications (e.g., molecular sensing and storage). As such, the accurate elucidation of their often complex structure-function relationships presents a crucial step in their advancement. For molecular magnetism, these approaches are commonly focused on variations of temperature and/or magnetic field, while comparatively little attention has been given to how these materials behave as a function of pressure. Here, we report magneto-structural investigations of magnetic molecular materials using synchrotron-based structural studies (powder diffraction and pair distribution function) and magnetic susceptibility measurements at high pressures. These studies have revealed a range of interesting phenomena such as orbital reorientations, spin crossover, phase transitions, and extreme compressibility [1].

[1] G.J. Halder, K.W. Chapman, J.A. Schlueter, J.L. Manson, *Angew. Chem. Int. Ed.* **2011**, *50*, 419-421.

Keywords: high pressure, magnetism, phase transition

MS24.P14

Acta Cryst. (2011) A**67,** C360-C361

The crystal structure of Ziegler-Natta catalyst supports

Giuseppe Cruciani,[a] Federica Malizia,[b] Anna Fait,[b] [a]*Departament of Earth Sciences, University of Ferrara, Ferrara (Italy).* [b]*Basell*