knowledge, alkaline-earth 2,2'-diphenyldicarboxylate complexes have never been reported.
In this context and following our systematic studies on the alkaline-earth dicarboxylates complexes with 2,2'-diphenyldicarboxylic acid, a new barium(II) compound of formula $[Ba(H_2O)_4(dpdc)]$ 0.25 H_2O has been prepared and structurally characterized by X-ray crystallography.
The Barium (II) ions are nine coordinated by three oxygen atoms from two diphenato groups and six oxygen atoms from six water molecules of which five acting as bridging ligands and one as monodentate. The distances Ba – O range from 2.704(5) to 2.974(4) Å forming a slightly distorted monocapped dodecahedron. The structure of $[Ba(H_2O)_4(dpdc)]_n$ consists of two-dimensional layers, built up from the self-assembly of zigzag chains of face and edge-sharing $\{BaO_9\}$ polyhedra linked by bridging bidendate diphenate anions through different coordination modes of the carboxylate groups. The Ba…Ba distances across these chains are 4.3519(6) and 4.6013(5) Å. The polymer layers form a three-dimensional network *via* O-H···O hydrogen-bond interactions between the coordinated water molecules and the O atoms of the carboxylate groups.

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MS13 P16

Gas sorption and binding in a nonporous single crystal

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Keywords: gas-solid interactions; discrete metallocycles; single crystal diffraction

Recently, coordination chemistry has become an active area of research in the field of crystal engineering of porosity. The coordination-driven motif offers an easier alternative to the synthesis of discrete supramolecular units when considering the classic syntheses involved in producing covalently bonded macromolecules.[1] Despite efforts to predict and define the parameters governing the assembly of discrete coordination compound architectures[2], rational design of these types of molecular structures is still not possible. We are interested in molecules with this topology because, even if efficiently close-packed in the crystalline state, these structural synthons, can yield significant solvated space in the crystal.[3] Here we report an imidazole-derived bridging ligand self-assembling with metal ions to form a series of discrete neutral metallocycles. In these solvent templated systems it is possible to remove guest solvent molecules without concomitant rearrangement of the host lattice. Such structures possess cavities of ca. 110 $Å^3$ and have the notable feature of being structurally flexible during the gas sorption process. Since the desolvation procedure and subsequent gas sorption experiments can all occur as single-crystal to single-crystal transformations, it has been possible to study the gas-solid interactions using X-ray diffraction techniques. These studies are also complemented by gravimetric and volumetric gas sorption experiments.

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MS13 P17

Crystal Structure of 3,4,4-Trichloro-2-nitro-1-propylsulfanyl-1-(4-thiomorpholinly)buta-1,3-diene

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Keywords: organic sulfur compounds, chemical crystallography, biologically important compounds.

Thiomorpholine analogues have found applications in medicine and agriculture [1]. Subsituted thiomorpholino, morpholino and piperidino compounds enhanced the activity against Gram-positive bacteria, but reduced the activity against Gram-negative bacteria [2]. The aim of this study was to determine the conformation of the title compound [3]. In the title compound, $C_{11}H_{15}Cl_3N_2O_2S_2$, the structure contains the expected N,S-substituted butadienyl skeleton, an alkylsulfanyl chain and a thiomorpholine ring. The thiomorpholine ring adopts a chair conformation and the butadiene has a conformation closer to cisoid than to transoid. The C—C bond lengths within the butadiene unit are similar to those in related compounds [4]. The thiomorpholine ring adopts a chair conformation, as shown by the puckering angles of φ = $1(3)^0$and $\theta = 10.2\ (4)^0$ [5].

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Metal-Organic Frameworks using pyridyldiyne ligands

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Keywords: metal-organic frameworks, gas sorption, porosity

The ability to predict and thus control the assembly of networks is an ongoing challenge. It has been proposed that thin, rigid ligands will behave in a more predictable manner, than other, more flexible versions. The assembly of molecular frameworks and network polymers using bidentate ligands such as 4,4'-bipyridyldiynes has been of considerable interest. Their rod-like structures, owing to the alkynyl spacers as well as their conjugated systems that are of a rigid nature, are of specific interest.[0] 4,4'-Bipyridine has previously been used to assemble a variety of crystalline designs such as chains, ladders, squares, diamondoids, etc. as well as a few innovative coordination polymer networks exhibiting a measure of porosity.[0] In