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A new lanthanide-organic framework (LOF) based on a long (21.2Å) and rigid bid-Gd complex synthon (complex 1) and carbonate anion spacers was discovered. Complex 1 is comprised of two Gd<sup>3+</sup> ions complexed with a pyridine tetracarboxylate ligand and a bridging linear 1,4-diethynylbenzene unit. Two water molecules are coordinated to each Gd ion in order to satisfy its high coordination number. Carbonate anions are coordinated to the Gd<sup>3+</sup> ions linking between two synthons, resulting in the construction of two network types (type A and B). All three oxygen atoms of the carbonate anion are utilized in its function as a spacer between two synthons (complex 1) in the networks. In addition, the carbonate anions also serve as acceptors for hydrogen bonding (O-H...O), with water molecules coordinated to Gd<sup>3+</sup> ions in both the networks. While all the synthons adopt a planar conformation in network A, they are backed alternately in plane and vertical conformation in network B. Auxiliary Na<sup>+</sup> ions and water molecules are positioned around the carbonate ions and connect between the networks. Overall, in this new LOF the synthons are packed in criss-cross fashion and tethered by carbonate spacers, creating a crystal lattice perforated by 10.6 × 15.6Å and 18.6 × 15.6Å wide-open channels.

**Keywords:** supramolecular assembly, gadolinium complexes, crystal design.

## MS24.P39

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**Synthesis and Crystal Structure of a Two-Dimensional Di-Aqua Pyromellitate Strontium(II) Complex:** [Sr<sub>2</sub>{(OOC)<sub>2</sub>-C<sub>6</sub>H<sub>2</sub>(COOH)<sub>2</sub>}(H<sub>2</sub>O)<sub>2</sub>]<sub>n</sub>

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In recent years, metal-organic coordination polymers have attracted considerable attention and been rapidly developed due to their fascinating molecular topologies and crystal-packing motifs along with potential applications as smart optoelectronic, magnetic, and porous materials[1–2]. These specific features are due to the carboxylate group which acts as a linker between inorganic moieties and to the flexible or relatively rigid carbon backbone, which gives a modular nature to the resulting MOFs[3-5]. Most of the bridging ligands used in construction of the porous MOFs are rigid such as benzene-polycarboxylate. Benzene-1,2,4,5-tetracarboxylic acid (H<sub>4</sub>BTC) is an important carboxylate ligand as it has multiple coordinating modes. Moreover, the various coordination geometry of metal ions and the four carboxylic groups of (H<sub>4</sub>BTC) completely or partially deprotonated, have led to the generation of products containing 1D chains, 2D layers and three-dimensional packings[7].

We report here the synthesis and structure of a novel alkaline-earth metal benzene-tetracarboxylate complex [Sr<sub>2</sub>{(OOC)<sub>2</sub>-C<sub>6</sub>H<sub>2</sub>(COOH)<sub>2</sub>}(H<sub>2</sub>O)<sub>2</sub>]<sub>n</sub>. The asymmetric unit consists of two Sr(II) cations, two pyromellitate dianions (H<sub>2</sub>BTC)<sup>2-</sup> and two aqua ligands. The two independent [H<sub>2</sub>BTC]<sup>2-</sup> ligands adopt different coordination mode. They are heptadentate and octadentate and coordinate to five and six metals centers respectively. The coordination polyhedra around

the two Sr atoms can be described as a distorted monocapped square antiprism and a distorted dodecahedron respectively. Among all the nine coordinated oxygen atoms, one come from one coordinated water molecule and the remaining from six [H<sub>2</sub>BTC]<sup>2-</sup> dianions ligands while the eight oxygen atoms around the second metal center belong to one coordinated water molecule and five [H<sub>2</sub>BTC]<sup>2-</sup> dianions ligands.

Each strontium atom is linked to two Sr metals through μ<sub>oxo</sub> bridges leading to the formation of an infinite zigzag chains of one-edge sharing SrO<sub>9</sub>/SrO<sub>8</sub> polyhedra. The chain running parallel to the a axis are further connected through pyromellitate ligands resulting in a two-dimensional network. The crystal structure is further stabilized by hydrogen bonds between chains, involving the four acid groups and the two coordination water molecules as donors.

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**Keywords:** Coordination polymers, pyromellitate, strontium

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**Synthesis and structural study at 100K of a new double metal oxalate Cs<sub>2</sub>Cr(C<sub>2</sub>O<sub>4</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>4</sub>**

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In the course of our studies dealing with oxalate-based bimetallic compounds potentially leading to Metal-organic-frameworks (MOFs) and Coordination polymers (CPs), we have obtained single crystals of [M<sub>x</sub>Cr(C<sub>2</sub>O<sub>4</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>y</sub>]<sub>n</sub>. When M=Rb<sup>+</sup>, a new supramolecular isomer RbCr(C<sub>2</sub>O<sub>4</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]<sub>n</sub> has revealed a 3D extended framework built up from layers containing bi-polyedra surrounding Rb and Cr respectively [1].

This structure is completely different from the previously known<sup>[2]</sup>. When M=Cs<sup>+</sup>, and replacing RbCl by a caesium salt in the same synthesis conditions and mixture, including a Cr<sup>3+</sup> starting salt, few pink prismatic crystals studied by XRD at 100K, brought out a polymeric structure corresponding to a tetraaqua complex, with x=2, owing to the fact that the transition metal has been reduced during synthesis process leading to the unexpected dication Cr<sup>2+</sup>.

This poly[tetraaquad-μ<sub>6</sub>-oxalato]chromium(II)dicaesium(I)] is isotopic with Cs<sub>2</sub>M(C<sub>2</sub>O<sub>4</sub>)<sub>2</sub>.4H<sub>2</sub>O (M=Mg(II); Co(II)) [3], [4]. It belongs to C2/c space group, with a=16.1880(4)Å; b=7.3212(2)Å; c=13.5268(3)Å; β=128.3640(10)°.

The asymmetric unit contains one unique Cs atom, one Cr atom, one oxalate dianion and two water molecules. Only the Cr(II) atom is located on a special position (O y ¼). The nine-coordinated caesium atom is surrounded by six oxalate ligands involving all their donor atoms. One O atom of each functional group chelates to the central alkali in a typical five-membered ring. The coordination sphere is completed by the two independent water molecules. The nearly regular CrO<sub>4</sub>(H<sub>2</sub>O)<sub>2</sub> octahedron consists of four O atoms from two dianions in a η<sup>4</sup>-chelation and two O atoms from two equivalent water molecules in *cis* position. Consequently, the oxalato ligand is bis-bidentate,