valence chromates, $NH_4Cr(CrO_4)_2$ constitutes a new structure type. The first known compound containing the $CrSO_7^{2-}$ anion is described.
The first rare-earth sulfate containing more than one alkali element structurally characterized is $K_5Na[Ce_2(SO_4)_6]$. Its structure consists of pairs of edge sharing cerium polyhedra, interlinked by edge and corner sharing sulfate groups, forming layers connected by potassium ions. Also the acidic $K_6[Ce(HSO_4)_2(SO_4)_4]\cdot H_2O$ is unique and constitutes a new structure type since it contains rare-earth monomers, $[Ce(HSO_4)(SO_4)_4]^{5-}$.
The existence of alterable oxidation states for the cerium ion may be a base for new attractive applications in the future. In the structure of $K_5Ce_2(SO_4)_6\cdot H_2O$, there are pairs of edge sharing cerium polyhedra with one delocalized f^1 electron. The cerium polyhedra are linked through edge and corner sharing sulfate bridges thereby forming layers joined by potassium ions. The oxidation state of each cerium ion is 3.5. The structure of $CrCe(III)_7Ce(IV)_6(HSO_4)_6(SO_4)_{21}\cdot 75H_2O$ differs significantly from previously known structures of mixed-valence cerium compounds. It extends to form layers through which there are large open channels, c.a 10 Å in diameter.

MS13 P10

Complex Structures of Simple Molybdates.
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Keywords: crystal structure and properties, inorganic synthesis, catalysis

Octamolybdates are the most numerous, important and interesting group of molybdates. They are thoroughly investigated due to their vast applications in catalysis. Octamolybdates are also promising materials for optoelectronic applications. In this report we describe three new octamolybdates. Even though the conditions of their syntheses were very similar and quite simple, different from each other compounds were obtained. All of them are organoammonium octamolybdates, but their structures differ significantly. In **Mo_8O_{26} Ca N_4 C_{10} H_{22} Ca** (**1**), coordination polymeric structure exists, octamolybdate anions are connected by Ca^{2+} cations and create straight chains surrounded by organic cations. **$Mo_8O_{26}.2(C_6H_4(NH_2)_2).4(C_6H_4(NH_2)_2)$ $.4H_2O$** (**2**) belongs to the family of molybdates in which Mo^{+6} cation is directly bonded to N atoms. In **$Mo_8O_{26}.4(C_{10}H_7NH_3).4(C_{10}H_7NH_2).4H_2O$** (**3**) $Mo_8O_{26}^{4-}$ anions are separated by double organic layers consisted of 2-ammoniumnaphthalene cations, 2-aminenaphthalene molecules and molecules of water. The thickness of the layers is about 18Å.
All compounds were synthesised for the first time in our laboratory. In addition to crystal structure studies, they were also characterised by IR spectroscopy and DSC investigations.
Crystallographic data for the investigated compounds:
(**1**) formula: **Mo_8O_{26} Ca N_4 C_{10} H_{22} Ca,** a,b,c,α,β,γ=9.732(2) A, 10.575(2), 11.686(2) A, 65.34(2)°. 65.61(2)°, 86.88(2)°, V=985.2(3) A^3, SG, P-1 (2) Z=2.
(**2**) formula: **$Mo_8O_{26}.2(C_6H_4(NH_2)_2).4(C_6H_4(NH_2)_2)$ $.4H_2O$**, a,b,c,α,β,γ=8.441(4) Å, 12.121(4)Å, 14.646(5)Å, 87.834(4)°, 78.148(4)°, 84.454(4)°,V=1459.3 $Å^3$, SG=P-1 (2), Z=1.
(**3**) formula**: $Mo_8O_{26}.4(C_{10}H_7NH_3).4(C_{10}H_7NH_2).4H_2O.$** a,b,c,α,β,γ= 10.184(5) Å, 10.592(5) Å, 22.737(7) Å, 78.675(5)§, 78.900(5)°, 65.427(5)°, V=2170.1 $Å^3$, SG=P-1 (2), Z=1.

MS13 P11

Synthesis, crystal structures and properties of metal silicates Kwang-Hwa Lii, *Department of Chemistry, National Central University, Chungli, Taiwan.*
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Keywords: silicate, lanthanide, uranium, synthesis, crystal structure

Recently much work has focused on the synthesis of transition metal silicates because of their rich structural chemistry and interesting physical and chemical properties. Most of these compounds were synthesized with alkali metal cations under hydrothermal conditions at 180-240 °C. Our synthetic methods are 2-fold, namely high-temperature, high-pressure hydrothermal reactions at ca. 550-600 °C and 1000-2000 bars with alkali metal counter cations and molten flux reactions at high temperature. We have synthesized a large number of new silicates of transition metals, main group elements, lanthanides, and uranium. For example, we reported the synthesis of $Rb_4(NbO)_2Si_8O_{21}$ and its solid-state NMR spectra. The ^{29}Si MAS NMR spectrum shows multiplet patterns which arise from ^{93}Nb(spin-9/2)-^{29}Si *J*-coupling. This is the first example of two-bond *J*-coupling between a quadrupolar nucleus and a spin-1/2 nucleus in the solid state. The structure $Rb_3In(H_2O)Si_5O_{13}$ consists of 5-membered rings of corner-sharing SiO_4 tetrahedra connected *via* corner sharing to four adjacent 5-membered rings to form a 3D silicate framework which belongs to the $CdSO_4$ topological type. The first pentavalent-uranium silicate, $K(UO)Si_2O_6$, has also been synthesized. In this presentation I will report the syntheses, crystal structures, solid-state NMR spectroscopy, and luminescence properties of a number of new metal silicates.

MS13 P12

2-D and 3-D structures of Luminescent Zinc Metal-Organic Frameworks. Tatiana V. Timofeeva,[a] Christina A. Bauer,[b] Mark D. Allendorf [b]. *[a]Department of Natural Sciences, New Mexico Highlands University, Las Vegas, NM 87701, USA; [b]Sandia National Laboratories, Livermore, CA 94551, USA..*
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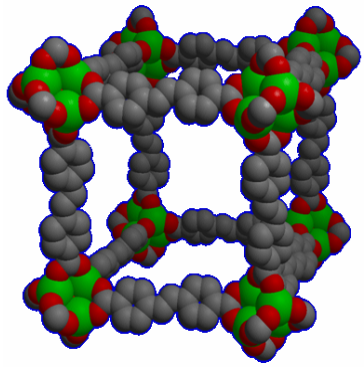
Applications of metal-organic frameworks (MOFs) depend on their structural characteristics such as pores size and availability of absorption. The preparation and characterization of two zinc MOFs based on a flexible and emissive linker molecule, stilbene, is described. Reaction of *trans*-4,4'-stilbene dicarboxylic acid and zinc nitrate in *N,N*-dimethylformamide (DMF) yielded under different conditions in dense 2-D network, **1**, or porous 3-D framework structure, **2**. This framework consists of two interpenetrating cubic lattices, each featuring basic zinc carboxylate vertices joined by *trans*-stilbene. Fragment of one of such lattices is depicted below.



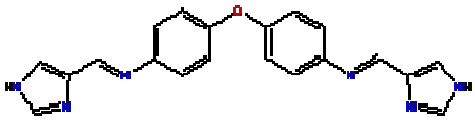
It was shown that optical properties of both **1** and **2** correlate with the local ligand environments observed in the crystal structures. In both cases, the rigidity of the stilbene linker increases upon coordination to the inorganic units through inhibition of torsion about the central ethylene bond, resulting in luminescent crystals with increased emission lifetimes compared to solutions of *trans*-stilbene. The emission spectrum of **2** is found to depend on the nature of the incorporated solvent molecules, suggesting use of this or related materials in sensor applications.

MS13 P13

Spin crossover and supramolecular organization of a new family of iron (II) dinuclear complexes Bernard Tinant[a], Nicolas De Crom[b], Yann Garcia[b] [a]*Unité de chimie structurale et des mécanismes réactionnels.* [b] *Unité de chimie des matériaux inorganiques et organiques, Université Catholique de Louvain, Louvain-la-Neuve, Belgium.* E-mail: tinant@chim.ucl.ac.be

Keywords: Molecular switches; Spin-crossover; Iron (II) dinuclear complexes

Spin crossover materials are important coordination compounds wherein the spin state can be reversibly switched by external stimuli [1]. A novel family of dinuclear iron(II) compounds with a triple-helicate architecture has been recently synthesized [2] and their spin pairs population studied [3]. In the present work, new iron(II) complexes have been obtained with L as bis-bidentate ligand which could offer more H-bonding possibilities.



L

By varying the counter-anions and the conditions for crystallization, we obtained suitable single crystals and solved three structures:

$[Fe_2L_3](PF_6)_2Cl(C_3H_3O_4)\cdot 5CH_3OH\cdot 3H_2O$

$[Fe_2L_3](C_6H_4BrSO_3)_4\cdot 7CH_3OH\cdot H_2O$

$[Fe_2L_3](PF_6)_3Cl\cdot 5CH_3OH\cdot 2H_2O$

The structure was refined at two temperatures for the third compound. Two iron sites are in the high-spin state at 250 K and are found in an intermediate state at 120 K (high-spin/low-spin). Complementary ^{57}Fe Mössbauer studies are in progress to shed more light on the spin crossover behaviour of this dinuclear compound. The structures will be presented in details.

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MS13 P14

Hydrogen bond in Tri (2-hydroxyanilinium) hexachlorostin (IV) chloride trihydrate. Sofiane Bouacida[a,b]*, Hocine Merazig[b] and Patricia Benard-Rocherulle[c] *a)Dpt de Chimie, Université de Béjaia ,Alegria. b) Lacmom, Université Constantine, Algeria . c) UMR 6226 CNRS,Université´ de RennesI, France .*
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Keywords: Hydrogen bond, Single crystal, Hybrid materials.

Organic-inorganic hybrid materials of formula $(R\text{-}NH_3)$, SnXn, where X = F, Cl, Br or I, exhibit interesting magnetic, optical and electronic properties [1], [2]. Within our research of hybrid compounds based on tin a new crystal structure has been investigated.
The title compound, $3(C_6H_8NO^+(SnCl_6)^{2-}Cl\ .3(H_2O)$, crystallized in Monoclinic system, with P $2_1/n$ space group.
The crystal structure can be described as double layers of $[SnCl_6]$ octahedral and 2-hydroxyanilinium cations parallel to (10-1) plane, with the chloride ions and the water molecules sandwiched between the double layers.
In this structure, four types of hydrogen bonds are observed,
viz. cation-cation, cation-anion, cation-water and water-water,
with the N and O atoms of the cation and the water molecules acting as donors and with the Cl^- ions and the O atoms of the water molecules acting as acceptors .
These intermolecular bonds link the molecules within the layers and also link the layers together, delineating a three-dimensional network and reinforcing the cohesion of the structure.

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MS13 P15

Synthesis, Characterization and Crystal Structure of a Three–Dimensional Alkaline-Earth Diphenatete Complex: $[Ba(H_2O)_4(OOC\text{-}(C_6H_4)_2\text{-}COO)]\ 0.25\ H_2O$

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Keywords: diphenate, barium compounds, crystal structure analysis

Intense research activity during the last few years employing benzene carboxylic acids such as 2,2'-diphenyldicarboxylic acid (H_2dpdc) has resulted in many new compounds with fascinating structures. These coordination polymers possess one-, two- and three-dimensionally extended structures and are attractive for their diverse coordination modes, intriguing structures, porosity and many potential uses in the areas of catalysis, sorption and luminescence [1-4]. To the best of our