

3D “mot” (4, 4)-c two nodal nets. The interpenetration vector is [0,1,0], Class Ia.

The metal organic nets are constructed from a tetrameric unit and single octahedra linked through the Bpa ligand. The tetrameric unit consists of an edge shared octahedra forming a dimeric unit linked to single octahedra through two Bpa ligand in “Gauche” conformation. Each tetrameric unit is linked to four octahedra via trans-Bpa ligands. This connectivity generates a three dimensional 2 nodal (4,4) connected net with  $\{6^4.8^2\}_2\{6^6\}$  point symbol.

The vanadium oxide subunit consists of twelve corner linked  $\text{VO}_4$  tetrahedra, giving rise to isolated  $\text{V}_{12}\text{O}_{36}$  centrosymmetric cycles. The dimmers of the tetrameric units lie inside the  $\text{V}_{12}\text{O}_{36}$  cycle and the octahedra acts as a linker between adjacent  $\text{V}_{12}\text{O}_{36}$  cycles, generating inorganic-organic chains along the [100] direction. As far as we are concerned, this is the first vanadate in which the  $\text{V}_{12}\text{O}_{36}$  cycle has been isolated in solid state.

The interpenetrating metal organic nets are connected through the vanadium oxide subunit. This way, the  $\text{V}_{12}\text{O}_{36}$  cycle of one of the nets, is corner linked to four octahedra, two of each adjacent nets. The crystal structure possess channels along the [100] direction, in which are located the disordered crystallization water molecules.

The thermal removal of crystallization water molecules (25-85°C) gives rise to a 3% contraction of the crystal structure. Surprisingly, at higher temperatures (85°C – 155°C) the crystal structure presents a continuous structural contraction of 6% without weight loss. The process is totally reversible up to 155°C. However at higher temperatures (200°C) the loss of coordinated water molecules generates an irreversible structural transformation with loss of crystallinity. Finally the structure collapses due to the calcination of the organic ligands.

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**Keywords:** Vanadates, third generation materials, self-catenation

#### FA4-MS29-P04

##### Synthesis and characterization of $\text{B}(\text{OH})_4\text{-H}_2\text{O}$ enclathred gallogermanate sodalite

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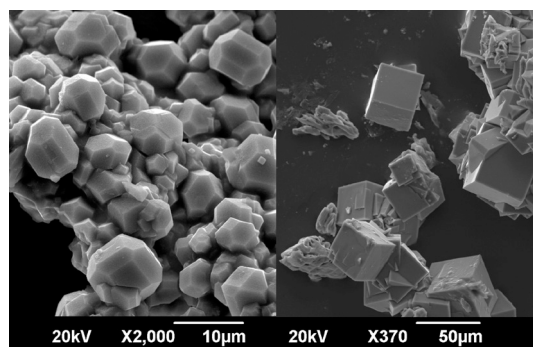
Tetrahydroxoborate and water enclathred sodalite with a gallogermanate host framework was prepared by means of hydrothermal synthesis and characterized by X-ray powder diffraction, IR-spectroscopy, temperature-dependent-IR-(TDIR) spectroscopy as well as scanning electron microscopy

(SEM) and energy dispersive X-ray (EDX)-analysis. The hydrothermal synthesis was performed under mild conditions (i.e. at 393 K) with the beryllonite analogous phase  $\text{NaGaGeO}_4$  as the source of Ga and Ge. Synthesis and crystal structure of the beryllonite type  $\text{NaGaGeO}_4$  are described in detail in [1].

The mild hydrothermal synthesis was carried out in a Teflon coated steel autoclave filled with layers of 1 g of  $\text{NaBH}_4$ -granulate and 1 g of pulverized  $\text{NaGaGeO}_4$ , before 5 ml 1 M sodium hydroxide solution was added. After a reaction time of 24 h the sample was washed with deionized water and dried at 353 K for 12 h.

X-ray powder diffraction shows a mixture of two phases: One is the  $\text{NaGaGeO}_4$  starting material, the other is a typical sodalite phase, which can be indexed in space group P-43n with lattice parameter  $a = 8.995 \text{ \AA}$ . The IR-absorption spectra show typical bands of  $\text{H}_2\text{O}$  at  $1665 \text{ cm}^{-1}$  as well as typical bands of  $\text{OH}^-$  from the  $\text{B}(\text{OH})_4^-$  group at  $3568 \text{ cm}^{-1}$  in good agreement with Pietsch et al. [2]. Furthermore, the presence of the enclathred  $\text{B}(\text{OH})_4^-$  species is confirmed by arising bands in the TDIR- spectra, since  $\text{B}(\text{OH})_4^-$  reacts to  $\text{BO}(\text{OH})_2^-$  at approx. 473 K and subsequently to  $\text{BO}_2^-$  at approx. 873 K by dehydration with increasing temperatures as described by Pietsch et al. [2]. The SEM- investigations show the presence of two different morphologies within the reaction product. As shown in the SEM-images, there are crystallites with rhombic dodecahedral as well as cubic morphology. EDX-analysis shows that the crystallites with cubic morphology tend to have higher Ga/Ge- ratios (average: 1.02) than the crystallites with rhombic dodecahedral morphology (average: 0.86).

Further investigations will aim at controlling the morphology by variation of synthesis parameters and subsequent structural specifications of the two different morphologies as well as studying the behavior of the cage-filling anions.



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**Keywords:** sodalites, synthesis, germinates

#### FA4-MS29-P05

**Robust Alkaline-earth arenedisulfonate Metal-Organic Frameworks materials.** Ana E. Platero-Prats, Natalia Snejko, Angeles Monge, Enrique Gutiérrez-Puebla, *Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC)*.

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Metal-organic Frameworks (MOFs) have been recognized for their great potential to act as crystalline functional solid state materials with interesting structural properties and promising applications, such as carbon dioxide sequestration and drug delivery [1]. In this area, thanks to the use of arenesulfonate ligands, which can provide multiple coordination sites, stable frameworks can be obtained with various dimensionalities [2]. We have been engaged for long time in the new MOFs using arenesulfonate ligands like anthraquinone-2,6-disulfonate (2,6-AQDS, from now on). Our previous studies have shown the ability of this disulfonate ligand to coordinate with rare-earth elements, giving rise to the construction of catalytically active materials [3].

This work deals with the design of a new family of alkaline-earth MOFs based on 2,6-AQDS ligand, synthesized by hydrothermal route as pure phases. Thus, herein we report new four alkaline-earth materials showing different dimensionalities and networks, which have been characterized by means of single-crystal X-ray diffraction. Moreover, topological analysis of these materials has been also carried out.

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