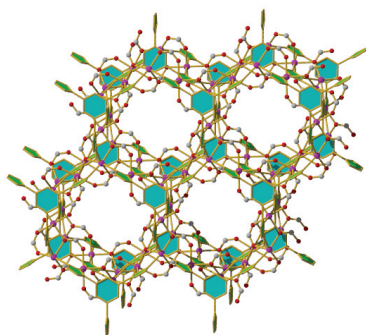


FA4-MS08-P03

Synthesis, Structure Characterization and Hydrogen Adsorption of a Novel Porous Metal-Organic Framework, $Mn_9(btt)_2(HCOO)_{12}$, Where $btt = 1,3,5$ -benzenetristetrazolate. Ju-Hsiou Liao^a, Wan-Ting Chen^a, Cherng-Shiaw Tsai^a. ^aDepartment of Chemistry and Biochemistry, National Chung Cheng University, Min-Hsiung, Chia-Yi 621, Taiwan.
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A novel porous metal-organic framework (MOF), $Mn_9(btt)_2(HCOO)_{12}$, was synthesized solvothermally in mixed H_2O/DMF . Single-crystal X-ray diffraction reveals it crystallizes in a hexagonal space group $P6_3/m$, with $a = b = 11.7410(6)$ Å, $c = 13.3199(13)$ Å, $V = 1590.16(19)$ Å³, $R1/wR2 = 0.0475/0.1030$. Its structure is constructed by cross-linking Mn^{II} ions with 1,3,5-benzenetristetrazolates and formates, which formed *in-situ* from the hydrolysis of dimethylformamide, to form a 3D framework with parallel hexagonal tunnels. Although the Mn^{II} ions at 4f Wyckoff sites are 75% occupied, the framework remains robust and porous, with 264 m^2g^{-1} BET surface area and hydrogen adsorption capacity of ~0.9 wt% at 77K and 1 atm.



Keywords: 1,3,5-benzenetristetrazolate; metal-organic framework; hydrogen adsorption

FA4-MS08-P04

Synthesis and Structural Characterization of Zn(II) Metal Organics Frameworks. Jimmy Restrepo-Guisao^a, Marta E. G. Mosquera^a, Pilar Gomez-Sal^a. ^aUniversidad de Alcalá. Campus Universitario, 28871-Alcalá de Henares, Madrid, Spain.
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The controllable preparation of porous metal-organic frameworks (MOFs) is a desirable objective for many groups [1] since MOFs have applications as materials for exchange, gas storage, catalysis, drug delivery, etc [2]. Although many Zn(II) metal-organic framework have already been described, this metal continues to be in the centre of interest because of its ability to show different coordination modes and its magnetic and biological applications [3].

In this work we report the synthesis and the structural studies of new Zn(II) metal organic frameworks. Thus, using p-aminobenzoic acid (4-abaH) as organic linker and different coligands we have prepared the species $[Zn(4-aba)_2(H_2O)(L)]$, $\{[Zn(4-aba)_2]\}_n$ and $\{[Zn(4-aba)_2(H_2O)]\}_n$. These compounds show a variation of their dimensionality ranging from 0 to 3, and present porous sizes between 4.116 Å and 6.93 Å. An additional interesting feature of these complexes is the multiple binding modes shown by the 4-aba connector, which acts as monodentate, bidentate or quelate ligand, even within the same complex. Different experiments have been made intended to control different aspects of the coordination network. In this communication we analyze the effect of the monodentate coligands, the M:L ratio, the counterions and the pH in the coordination ways and topology of the species obtained.

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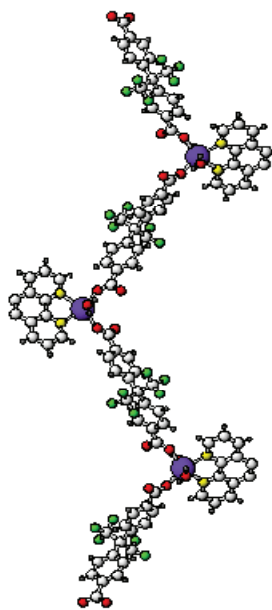
Keywords: framework structures; metal-organic complexes; zinc compounds

FA4-MS08-P05

Elucidation of Crystallization Steps in a New MOF Based on Magnesium. Ana E. Platero-Prats^a, Víctor A. de la Peña-O'Shea^b, Natalia Snejko^a, Ángeles Monge^a, Enrique Gutiérrez-Puebla^a. ^aInstituto de Ciencia de Materiales de Madrid (ICMM-CSIC). ^bInstituto Madrileño de Estudios Avanzados en Energía (IMDEA Energía).
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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].

We have been engaged for long time in the design of sophisticated new MOFs using flexible ligands like 4,4'-(hexafluoroisopropylidene)bis(benzoic acid) (H_2L , from now on). Our previous studies have shown the ability of this ligand to coordinate with different metal ions giving rise to the construction of MOFs with interesting properties (catalytic, magnetic, luminescence, among others) [2]. However, the use of alkaline-earth metals has been much less studied, despite their interesting sorption properties (e. g. H_2 , CH_4 , CO_2 fixation) [3] and catalytic behaviour. This work deals with the design of a new 1D Mg-MOF involving the use of H_2L and a nitrogenated co-ligand (phenantroline). The main objective is the study and understanding the effect of the synthesis conditions in the hydrothermal crystallization procedure since they are crucial in order to form this Mg-MOF as a pure phase. Thus, by means of single-crystal X-ray diffraction, two new non-polymeric precursors of this organo-inorganic hybrid structure have been characterized.



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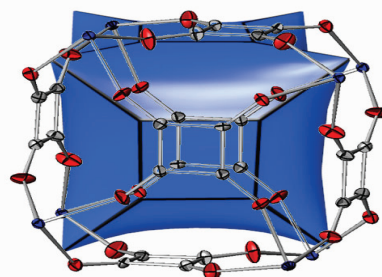
Keywords: organic inorganic hybrid materials; hydrothermal synthesis; materials science

FA4-MS08-P06

A New Sc MOF Built up from Octadecasil Zeolitic Cages as Heterogeneous Catalyst. Felipe Gándara^a, Berta Gómez-Lor^a, Marta Iglesias^a, Natalia Snejko^a, Enrique Gutiérrez-Puebla^a, Angeles Monge^a. ^a*Department of Synthesis and Structure of Oxides, Instituto de Ciencia de Materiales de Madrid-CSIC.*
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Metal-organic Frameworks (MOFs) continue receiving a great attention since they are a very attractive type of materials due to their potential applications in several fields^[1]. Specific organic and inorganic units, with predefined geometric characteristics, are employed to obtain predesigned secondary building blocks, with the aim of obtaining networks with preferred features, and therefore, desired properties. We have selected an organic ligand with a well defined geometry, like is the squarate dianion and scandium, a trivalent cation that is usually found in octahedral environment. The combination of these two well geometrically defined building elements has led to the formation of a new Metal-organic framework with a zeolite related structure, and with interesting properties as heterogeneous catalyst. The new framework is constructed with presence of zeolitic cages of the AST type, formed by six 4MR and twelve 6MR. Each scandium atom belongs to two adjacent cages since they are coordinated to six O atoms from six different squarate anions: The result is a new binodal net, 3 and 6 connected net with point symbol

(4.6²)₆(6⁶.12⁹). The new material is stable above 400 °C and it has been tested as an acid heterogeneous catalyst in cyanosilylation and acetalization of carbonyl compounds. A high degree of conversion is achieved with the new Sc-MOF as catalyst, which can also be easily recovered and reused in several cycles of reaction.



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Keywords: metallorganic compounds; crystal structure topology; heterogeneous catalysis

FA4-MS08-P07

Axial Ligand Removal and Subsequent Pillaring of a Layered Zinc Dicarboxylate MOF. P. Smart^a, C. Mason^a, A. J. Florence^b, L. Brammer^a. ^a*Department of Chemistry, University of Sheffield, UK,* ^b*Department of Pharmaceutical Sciences, University of Strathclyde, Glasgow, UK.*

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Vapour diffusion of pyridine into an ethanolic solution of zinc nitrate and (+)-camphoric acid produces a MOF comprising of Zn₂ paddlewheel units bridged by camphorate to form a 2D layered structure. The axial sites of the paddlewheel are occupied by coordinated pyridine and the remaining inter-layer space is occupied by ethanol. Heating this framework removes the trapped ethanol and the coordinated pyridine in a two step process. The alcohol-free framework remains crystalline and several other alcohols can then be taken up into the framework including the chiral alcohol 1,2-propanediol. Heating the framework removes the coordinated pyridine ligands to produce a semi-crystalline material of the formula [Zn₂(Camphorate)₂]. This semi-crystalline 2D material can then be used as a starting material to produce frameworks with various ligands coordinated in the axial position of the Zn₂ paddlewheel. Reaction with solutions of ditopic diimine pillaring molecules such as pyrazine and 4,4'-bipyridine result in 3D MOFs with large pores. Reaction with substituted pyridines produces frameworks which have proved difficult to make by other methods. X-ray powder diffraction using both lab and synchrotron radiation was used to follow the ligand uptake reactions and to structurally characterise the pillared MOFs.