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]. [a]*Department of Chemistry and Biochemistry, National Chung Cheng University, Min-Hsiung, Chia-Yi 621, Taiwan.*
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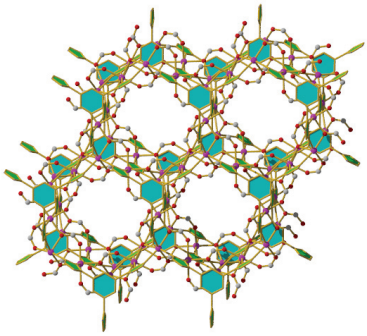
A novel porous metal-organic framework (MOF), $Mn_9(btt)_2(HCOO)_{12}$, was synthesized solvothermally in mixed H_2O/DMF. Single-crystal X-ray diffraction reveals it crystallizes in a hexagonal space group $P6_3/m$, with $a = b = 11.7410(6)$ Å, $c = 13.3199(13)$ Å, $V = 1590.16(19)$ Å^3, *R1/wR2* = 0.0475/0.1030. 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. Jymmy Restrepo-Guisao[a], Marta E. G. Mosquera[a], Pilar Gomez-Sal[a]. [a]*Universidad de Alcalá. Campus Universitario, 28871-Alcalá de Henares, Madrid, Spain.*
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The controllable preparation of porous metal-organic frameworks (MOF's) is a desirable objective for many groups[1] since MOF's 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$_2$O)(L)]*, *{[Zn(4-aba)$_2$]}$_n$* and *{[Zn(4-aba)$_2$(H$_2$O)]}$_n$*. 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

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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]. [a]*Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC).* [b]*Instituto 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'-(hexafluoroisopropyliden)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-lingand (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.