

frameworks has grown drastically over the past few years. The use of multifunctional ligands, such as organometallic complexes, permits the introduction of other functionalities within the frameworks. We have synthesized and characterized a series of metal-organometallic framework (MOMF) materials, derived from simple [CpFe-(η^6 -arene-carboxylate)] bridging ligands. Depending on the reaction conditions, solid state structures ranging from simple 1D polymer chains to three dimensional square grid structures have been obtained. For example, the reaction of Ni(NO₃)₂·6H₂O with [CpFe]⁺-metalated 1,4-benzenedicarboxylic acid (1) results in [Ni₃(1-H)₄(H₂O)₂(μ -H₂O)₂][NO₃]₂, a 3D framework material constructed of square grid nickel-carboxylate networks that are interconnected in the third dimension through additional nickel ions. The synthesis, structure and characterization of these materials will be presented.

Keywords: coordination polymers, framework structures, ferrocene derivatives

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Cis-trans isomerizations and rearrangements during hydrothermal synthesis of metal carboxylates

Graciela Diaz de Delgado, Jines Contreras, Luis Leon, Marino Gutierrez, Jose Miguel Delgado

Universidad de Los Andes, Facultad de Ciencias, Facultad de Ciencias, Dpto. de Quimica, La Hechicera, Merida, Merida, 5101, Venezuela, E-mail: diaz@ula.ve

Hydrothermal conditions provide clean routes for the synthesis of new hybrid organic-inorganic frameworks. However, at elevated temperature and pressure, it is possible to induce reactions in the organic ligand used. For example, carboxylic acids may undergo isomerization, rearrangements, decompositions, hydrogen abstractions, etc. Unsaturated carboxylic acids may, additionally, suffer dimerization, oligomerization, or polymerization. Even though the hydrothermal reaction may not lead to the desired compound, it may produce an interesting derivative not accessible by other means. For instance, reaction at 160 °C during 48 h of *cis*-4-cyclohexene-1,2-dicarboxylic acid with Ca(OH)₂ afforded *cis*-4-cyclohexene-1,2-dicarboxylato)calcium(II), [CaC₈H₈O₄]. However, when using BaCO₃, under the same conditions, a product which contains the original ligand in the *trans* conformation, diaquabis(*trans*-cyclohex-4-ene-1-carboxylic-2-carboxylato)barium(II), [Ba(C₈H₉O₄)₂(OH₂)₂], is obtained. Other reactions which involve partial decomposition and rearrangement of the organic moiety, leading to mixed ligand compounds will be discussed. We thank R. Benson (Rigaku-USA) and M. Pink (Indiana University), for support with data collection. This work was funded by FONACIT-Venezuela, through grant LAB-97000821.

Keywords: cis-trans isomerization, hydrothermal synthesis, metal carboxylates

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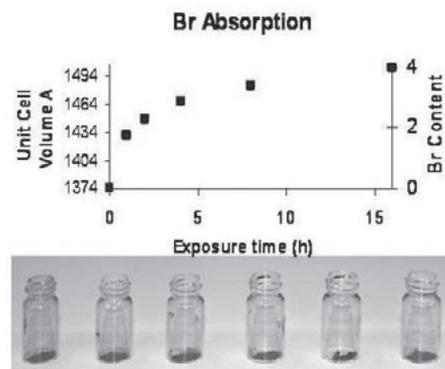
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Real crystal engineering: Solid state reactions in metal-organic compounds

Matteo Lusi, Christopher J. Adams, A. Guy Orpen

University of Bristol, School of Chemistry, Cantock's Close, Bristol, England, BS8 1TS, UK, E-mail: matteo.lusi@bristol.ac.uk

The results of our recent solid state reaction studies applied to the synthesis of hybrid organic-inorganic crystalline solids are presented. Development of methods suitable to prepare solid solutions are reported that allow control of their unit cell dimensions and polymorphism. Mechanochemical reactions are shown to be excellent alternatives to traditional solution methods in preparing coordination polymers and metal-organic hydrogen-bonded networks. Similar products can be prepared by gas-solid methods such as hydrochlorination or dehydrochlorination of crystalline precursors. In some cases reactions proceed under topochemical control to give different products. Precise control over unit cell metrics can be achieved by solid-gas halogen-exchange reactions that enable the modification of the unit cell volume, whilst the formation of a two-metal solid solution allows the coordination geometry of one metal to constrain the other and hence the resulting crystal structure and symmetry. Combined, these methods offer promise helping to control composition, polymorphism and unit cell dimension of the crystal species considered: real crystal engineering.



Keywords: crystal engineering, solid state reactions, polymorphism

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Design of supramolecular complexes: From concept to crystal structures

Cuong Quoc Ton, Ernst Egert

Johann Wolfgang Goethe University, Institute of organic chemistry and chemical biology, cuong.ton@chemie.uni-frankfurt.de, Frankfurt a. M., Hessen, 60438, Germany, E-mail: cuong_ton@hotmail.com

In order to understand the hydrogen bond interaction between an active pharmaceutical ingredient (API) and its receptor, we have investigated small complexes with structurally similar bonding patterns. The co-crystallization of specific supramolecular complexes is not a straightforward procedure. The process, from the pre-selection of potential candidates to the successful co-crystallization of small receptor/ligand models, should not be left to chance. Therefore we have developed a concept for designing these structures. After selection of model compounds with complementary functional groups, we calculate the structures and energies of a multitude of alignments (constellations) by means of our force-field program MOMO [1]. These calculations are time-consuming if the molecules possess a number of torsional degrees of freedom and are thus able to adopt different conformations. Various analytical tools are used to identify the intermolecular hydrogen-bond interactions (especially IR spectroscopy and powder diffraction). The most promising combinations are then selected for further co-crystallization experiments. We have studied many different hydrogen-bond arrangements between at least two acceptor or donor groups at each molecule, advancing our examination to three hydrogen bonds with diverse hydrogen-bonding patterns. We are not only interested in forming the desired hydrogen bonds but also how to prevent undesired ones. The prerequisite for this is a thorough consideration