

FA4-MS02-O1

Bernauer's Bands. Bart Kahr^a, Erica Gunn^a, John Freudenthal^a. ^a*Department of Chemistry, University of Washington, Box 351700, Seattle WA 98195-1700.* E-mail: kahr@chem.washington.edu

Bernauer proposed in 1929 ("Gedrillte" Krystalle) that more than 100 simple crystalline organic compounds (eg. urea, phenol, benzoic acid) that grow as optically banded spherulites do so by twisting helically as they grow radially. While helical growth of high-polymer lamellae has been established, the mechanisms that may apply to polymers are not readily extended to small molecular crystal lattices. The idea that helical twisting with mesoscale periodicity is a common crystal growth mechanism for many simple substances is at variance with contemporary notions of crystal structure of growth and warrants a contemporary reinvestigation. Herein, the evidence of Bernauer is analyzed, and his substances are reexamined with a Mueller matrix imaging polarimeter (MMIP). A Mueller matrix imaging polarimeter can in principle capture all of the linear optical properties of anisotropic substances simultaneously, including linear birefringence, linear dichroism, circular birefringence, and circular dichroism.

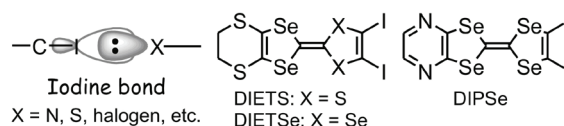
Keywords: spherulites; mueller matrix; polarimetry

FA4-MS02-O2

Supramolecular Organic Conductors Tailored by Strong and Directional Iodine Bonds. Tatsuro Imakubo. *Department of Materials Science and Technology, Nagaoka University of Technology, Niigata, Japan.* E-mail: imakubo@nagaokaut.ac.jp

A large number of organic conductors based on tetrathiafulvalene (TTF) derivatives have been synthesized and it is well recognized today that the design of crystal structure, especially control of the arrangement of the nearest-neighbour molecules, is essential for exploring interesting electronic properties of bulk crystals, such as superconductivity. From a viewpoint of crystal design of organic conductors, we have focused our attention to the iodine-based intermolecular interaction, *i.e.* 'iodine bond' [1,2]. The iodine bond is a special case of the halogen bond [3] and its strength and directionality are outstanding among halogen bonds. It is also noted that the iodine bond is suitable for applications to TTF-based organic conductors because of the lower electronegativity of the iodine atom than that of the carbon atom, which does not reduce donor ability of the TTF skeleton. In this paper, we will present two recent topics of supramolecular organic conductors tailored by the iodine bond together with a brief introduction of the interesting characters of the iodine bond in crystals of organic conductors. The first topic is a search for ambient pressure organic superconductors based on iodine-bonded TTFs. In 2002, we reported superconductivity of θ -(DIETS)₂[Au(CN)₄] [4], however, the superconducting phase appears only under a uniaxial strain and it makes difficult to examine details of the

electronic state of the superconducting phase. Recently, we have synthesized a series of chalcogen derivatives of DIETS and their Au(CN)₄ salts were prepared [5]. Four of them belong to the so-called β -type and the strong donor \cdots anion iodine bonds play a role of 'anchor' to fix the relative arrangement of the donor molecules. Conducting properties of these salts depend on the number and positions of the selenium atoms on the donor molecule and β -(DIETSe)₂[Au(CN)₄] shows superconductivity at around 2 K (onset). The second topic is the discovery of recyclability of supramolecular organic conductors [6]. We have prepared hexagonal cation radical salts based on DIPSe including characteristic supramolecular channels tailored by the strong and directional donor \cdots donor iodine bond. In addition to the metallic conductivity, quantitative recovery of the neutral DIPSe from their conducting salts has been accomplished by a simple chemical reaction. *i.e.* a redox reaction between water and the DIPSe cation radical. This is the first example of the recyclable organic conductor and it will provide a new aspect of organic conductors as a multi-functionalized material.



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Keywords: organic conductors; supramolecular chemistry; iodine compounds

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Fullerene Fragments-based Molecular Materials: Predicting Properties from Solid State Packing. Marina A. Petrukhina^a, Alexander S. Filatov^a. ^a*Department of Chemistry, University at Albany, SUNY, Albany, NY 12222, USA.* E-mail: marina@albany.edu

A novel class of bowl-shaped polyaromatic hydrocarbons that map onto the surfaces of fullerenes but lack their full closure currently attracts considerable attention. Similar to fullerenes, their convex and concave π -faces exhibit different physical and chemical properties, but the access to their insides is readily available. This makes such open geodesic polyarenes, also referred to as fullerene fragments of buckybowls, very unique objects for studying. However, only a very limited number of such non-planar carbon-rich molecules have been structurally characterized so far. Herein as part of our broad program of studying the structures and reactivity of π -bowls,[1-5] we use a systematic analysis of

their geometry and solid state packing motifs as means to predict functional properties of the resulting solids. These predictions should further stimulate the use of curved carbon-rich molecules in materials chemistry. We also employ several buckybowls as non-planar polyaromatic templates toward coordination of a planar trinuclear mercury complex, $C_{18}F_{12}Hg_3$. The effects of matching/mismatching the planar and non-planar surfaces of interacting partners result in imposing and storing strain energy in the solid state. The photoluminescent properties of such hybrid systems will be discussed.

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Keywords: non-planar polyarenes; molecular geometry; solid state packing

FA4-MS02-O4

Synthesis Procedure vs. Temperature in Cobalt Molecular Magnetic Materials. Catalina Ruiz-Pérez^a, Oscar Fabelo^a, Jorge Pasán^a, Laura Cañadillas-Delgado^a, Mariadel Déniz^a, Ana Belén Lago^a, Pau Díaz-Gallifà^a, Carla Martínez^a, Francesc Lloret^b, Miguel Julve^b. ^aLaboratorio de Rayos X y Materiales Moleculares, Universidad de La Laguna, Spain. ^bICMol, Universitat de València, Spain.

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Recent studies indicate that, in few cases, the thermodynamic considerations outweigh the kinetic ones. The study on the formation of cobalt succinate phases provided the first insight towards this aspect [1], which showed that denser higher dimensional structures are formed on increasing the reaction temperature through entropy driven dehydration pathway. As this respect the existence of eight well-characterized phases of cobalt pyromellitate containing water offers a rare opportunity to examine the role of various reaction variables in determining which structure forms. However, since these cobalt-bta phases have been prepared by different research groups and by different procedures, a retrospective examination of the effect of the reaction conditions on the product formation is difficult, i.e. the synthesis temperature. With this idea in mind we have undertaken a study of the Co(II)-bta system as a function of kinetic (crystal growth/synthesis technique) and thermodynamic parameters (temperature/pressure). In this study, **fifteen phases** have been structural and magnetically characterized, showing a wide variance of structural (from 0D to 3D) and magnetic (from isolated Co(II) ions toward long range order) behaviours and also his structural-magnetic relationship has been done.

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Keywords: crystal engineering; magnetochemistry; magnetic structure

FA4-MS02-O5

Size and Shape Design in Functional Metallorganic Wheel - and - Axle Systems. Alessia Bacchi^a, Mauro Carcelli^a, Paolo Pelagatti^a, Tiziana Chiodo^a. ^aDipartimento di Chimica GIAF, Università di Parma, Italy.

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We are particularly interested in the realization of organic-inorganic systems with flexible dynamic frameworks that can create pores *on demand* to accommodate small guests [1]. Recently we have reported that size and shape of the organic ligands are crucial in determining the inclusion propensity of these materials[2]. In particular, wheel-and-axle *trans*-Pd(II) complexes of carbinol ligands (*waad*) have shown suitable structural requisites to give reversible host-guest properties [3]. Here we investigate the influence on inclusion properties of shape modifications by changing the metal stereochemistry and the wheel hindrance, showing that both axle linearity and wheel bulkiness are needed to realise inclusion. We then present new metal-organic wheel-and-axle (*waamo*) systems based on ruthenium half-sandwich units, designed in order to favour the creation of bistable flexible networks.

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Keywords: meta-organic complexes; inclusion compounds; molecular design