

FA4-MS04-P01

Multitopic Ligand Approach for the Synthesis of New Mixed Metal Compounds. Fabienne Gschwind^a, Katharina M. Fromm^b. ^a*Department of Chemistry, University of Fribourg, Switzerland.* ^b*Department of Physics, University of Fribourg, Switzerland.*
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Mixed metal materials can be used in different applications, for instance in opto-electronic devices or as metal oxides in high-Tc superconductors (BSSCO, YBCO) [1, 2].

A synthetic strategy to obtain mixed metal oxides is to use decomposition techniques like (metal-organic) chemical vapor deposition (MO-CVD) to combust metal-containing volatile complexes.

We propose the development of new heterometallic complexes with tailored electronic, optical and/or magnetic properties. Combining different metal ions in molecular devices and analyzing their behaviour is interesting for later applications, and also of fundamental interest [3]. For this purpose, we developed a multitopic ligand system based on open polyether molecules and functional N-termini, which allows the coordination to different metal ion types by different ligating atoms.

We will show that this concept works by presenting first results, which could be used for the synthesis of BSSCO or YBCO.

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Keywords: single source precursor; mixed metal complexes; multitopic ligand system

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Dynamic Porous Crystals via Halogen Bonding. Giuseppe Resnati^{a,b}, Pierangelo Metrangolo^a, Tullio Pilati^b, Giancarlo Terraneo^a. ^a*NFMLab, DCMIC, Politecnico di Milano.* ^b*ISTM-CNR, Milano, Italy.*
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Different self-assembled porous architectures with zero-dimensional or infinite one-, two-, and three-dimensional network structures will be described. The systems are constructed from a variety of molecular building blocks which interact under control of the halogen bonding, the attractive interaction involving halogens as electron acceptor sites [1]. In all case iodoperfluoroalkanes and -arenes moieties have been used as halogen bonding donor sites as the strong electron withdrawing effect of fluorine boosts the electron acceptor ability of iodine to the point that the halogen bondings formed with pyridine or anionic donor sites are strong enough to sustain remarkably high porosity in the formed heteromeric architectures. In some architectures halogen bonding and hydrogen bonding or halogen bonding and electrostatic interactions cooperate in locking the modules at their positions in the co-crystals. Coordination-polymer crystals with gated channels [2] or

layered structure will be described. The halogen bonding driven formation of dynamic porous networks from non-porous crystals will be described [3]. On the basis that binding of modules with more than one binding site is largely dependent on structural complementarity with the interacting moieties, we reasoned that matching the size of the halogen-bonded supramolecular dianion with the size of a telechelic hydrocarbon dication should increase the strength of electrostatic binding, thus determining a selective molecular recognition. We thus challenged the densely packed crystalline alfa-omega-bis(trimethylammonium) diiodides with alfa-omega-diiodoperfluoroalkanes of different size and observed a rapid and selective take-up of only the conveniently sized alfa-omega-diiodoperfluoroalkane. Starting from non-porous materials, dynamically porous materials are formed and their structure is controlled by the size matching between the dication and the supramolecular dianion. The selective take-up of the matching diiodoperfluoroalkane occurs in solution and also in solid-gas reactions when powdered telechelic dication diiodides are challenged by vapors of diiodoperfluoroalkane.

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Keywords: crystal engineering; porous solids; supramolecular assemblies

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Silver Coordination Complexes with Fluorescent Ligands. Jing Chen^a, Katharina M. Fromm^a. ^a*Department of Chemistry, University of Fribourg.*
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Recently, metal-organic complexes have attracted extensive attention due to their potential application in electronics, magnetism, optical, and catalytic materials as well as their fantastic structures.^[1-4] Molecular, self-assembled multilayers on selected surfaces based on metal-organic coordination networks may form more complicated structures which can exhibit abundant properties, and even show functionalities not provided by a single subunit building block.^[5,6] So far, a lot of effort has been done to build these kinds of functional surfaces. Our idea is to design and synthesize some new ligands having fluorescent properties and coordinating with silver ions, the latter of which is regarded as a powerful antibacterial material used for many years, to obtain the corresponding fluorescent silver complexes. Furthermore, we want to coat them on a gold surface by molecular self-assembly, to study the structures and the morphologies of the surfaces, and investigate the optical and antibacterial properties. Herein, the structures and fluorescence spectra of some compounds will be presented.

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Keywords: silver coordination complexes; fluorescence; antibacterial properties

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From X-ray Structure to Gel – Can We Predict Gelation Abilities of Small Molecules? Roman Luboradzki^{a,b}, Monika Pyzalska^b, Zbigniew Pakulski^c. ^a*Institute of Physical Chemistry, Polish Academy of Sciences, Poland.* ^b*Cardinal Stefan Wyszyński University, Warsaw, Poland.* ^c*Institute of Organic Chemistry, Polish Academy of Sciences, Poland.*

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In recent years, gels derived from low-molecular-mass compounds have attracted special interest on account of their unique features, potential applications and relative simplicity of the gelator molecules [1], [2]. These gels fall within the physical gels (in contradistinction to chemical gels) since, only non-covalent interactions between the gelator molecules are involved. The formation of the gel based on spontaneous self-assembly of gelator molecules under non-equilibrium conditions such as the cooling of oversaturated solutions which is used as the typical preparation method. Despite gels are, in general, amorphous an x-ray crystallography may be used as a tool for predicting the presence (or absence) of gelation abilities since the basic feature of the gelator molecules is their ability to stack into one-dimensional chains (e.g. by using intermolecular hydrogen bonds). Moreover, crystallographic data can be an inspiration for design more complicated systems, as two component gels [3]. The authors acknowledge the financial support from the Polish Ministry of Science and Higher Education (Grant No. N204 058 32/1514)

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FA4-MS04-P05

β -Cyclodextrin Inclusion Complexes of L- and D-tryptophan. Chiral Discrimination. Irene M. Mavridis^a, Spyros D. Chatziefthymiou^a, Anastasia Paulidou^a. ^a*National Center for Scientific Research “Demokritos”, Athens, Greece.*

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Cyclodextrins (CDs) are well known cyclic oligosaccharides, consisting mainly of six (α CD), seven (β CD) or eight (γ CD) glucopyranose residues, which are water soluble and they are used for micro encapsulation of organic molecules inside their relatively apolar cavity. CDs are chiral hosts forming diastereomeric inclusion complexes with chiral substrates, a feature that makes them potential agents for enantiomeric discrimination, which is the basis of enantiomeric resolution of racemic mixtures by chiral gas and liquid chromatography. Enantiomeric discrimination by CDs is achieved by weak intermolecular interactions that may or may not include H-bonding, established by the embrace of the guest by the CD host, in order to obtain maximum contact. Resolution of racemates by natural α -, β -, and γ -CDs is generally poor, because the secondary hydroxyl groups of adjacent glucose units form strong intramolecular H-bonds that keep the cavity rigid and symmetrical. As a consequence, strict shape complementarity with a particular chiral guest, of the type “lock and key”, is required for complete enantioselective complexation. On the other hand, in per-derivatized CDs the above strong H-bonding network has been destroyed and the macrocycles can be distorted readily, thus they can perform enantiomeric discrimination via “induced fit”, leading even to complete resolution of racemates [1-2]. Presently, we report the crystal and molecular structures of the inclusion complexes of N-acetyl-L-tryptophan and N-acetyl-D-tryptophan with β CD, which are isomorphous, triclinic P1, $a=17.760$, $b=15.158$, $c=15.237$, $\alpha=102.774$, $\beta=99.346$, $\gamma=112.997$. The host forms dimers that include two guest molecules (host:guest ratio 1:1), their aromatic moieties being in parallel arrangement ($\pi\cdots\pi$ interactions). The host-guest interactions involve H-bonding of the carboxylic terminal group and the indole part. Chiral discrimination of β CD is discussed based on similarities and differences of the inclusion complexes of the two enantiomeric guests and the corresponding complexes of the N-acetyl-L- and D-phenylalanine.

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Conformational Adaptations of Podands as a Base for Selective Binding of Stereoisomers. Krunoslav Užarević^a, Ivica Đilović^a, Marina Cindrić^a, Dubravka Matković-Čalogović^a. ^a*Laboratory of General and Inorganic Chemistry, Chemistry Department, Faculty of Science and Mathematics, University of Zagreb, Zagreb, Croatia.*

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Flexible anion receptors draw significant scientific attention in the last few decades.[1] Although they usually display lower binding constants than rigid hosts, many interesting features are connected with this class of compounds. Binding