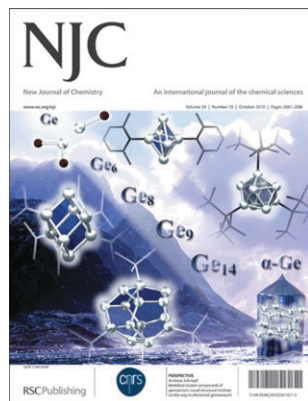
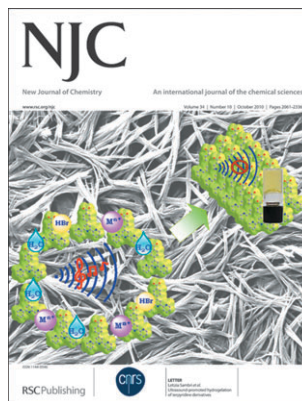


IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 34(10) 2061–2336 (2010)

**Cover**

See Andreas Schnepf, pp. 2079–2092. Metalloid cluster compounds of germanium – metastable intermediates on the way to elemental germanium give a first insight onto the borderland between molecules and the solid state. Dr Christian Schenk is thanked for supporting the construction of the cover image. Image reproduced by permission of Andreas Schnepf from *New J. Chem.*, 2010, **34**, 2079.

**Inside cover**

See Letizia Sambri *et al.*, pp. 2093–2096. Under ultrasound irradiation, terpyridine derivatives “dance” in solution with water, acids and metal cations. When the “music” stops, molecules self-assemble and stable hydrogels are formed. Image reproduced by permission of Letizia Sambri from *New J. Chem.*, 2010, **34**, 2093.

EDITORIAL

2077

NJC. . . a journal for new directions in chemistry

In this Editorial, we wish to inform our authors, reviewers and readers of our new requirements for the content and significance of submitted manuscripts.



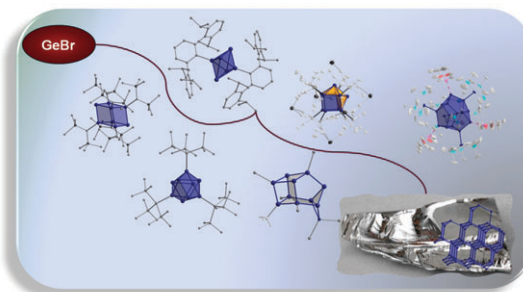
PERSPECTIVE

2079

Metalloid cluster compounds of germanium: novel structural motives on the way to elemental germanium!

Andreas Schnepf*

Metalloid cluster compounds of germanium may be seen as intermediates on the way to elemental germanium, a borderland that is of particular interest, as drastic changes of physical properties take place during reduction from salt like oxidized species to the bulk elemental phase. In this review an account is given of the first steps in this novel field of group 14 chemistry, where special attention is focused on structural features and bonding properties.



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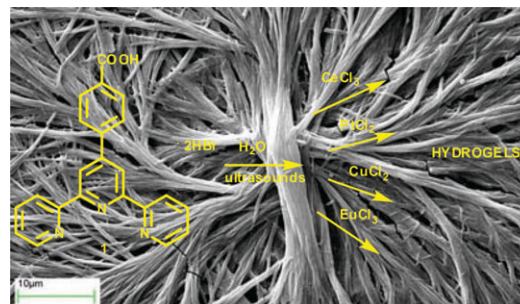
LETTERS

2093

Ultrasound-promoted hydrogelation of terpyridine derivatives

Letizia Sambri,* Fabio Cucinotta, Gabriele De Paoli, Stefano Stagni and Luisa De Cola

Terpyridine derivatives gel water and capture some metal cations giving stable gels with different emissive properties.

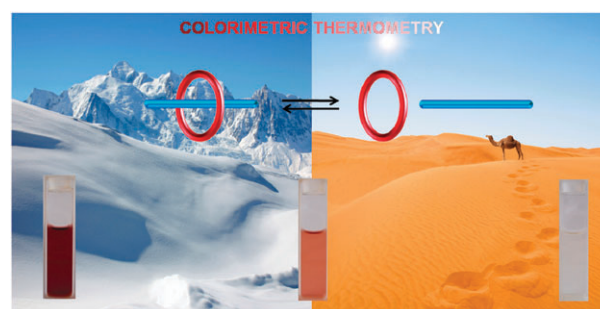


2097

Single-color pseudorotaxane-based temperature sensing

Isurika R. Fernando, Semere G. Bairu, Guda Ramakrishna* and Gellert Mezei*

The continuous and reversible change in optical absorption of charge-transfer based colored pseudorotaxane solutions over large temperature windows suggests that these systems could be exploited in novel temperature sensors.

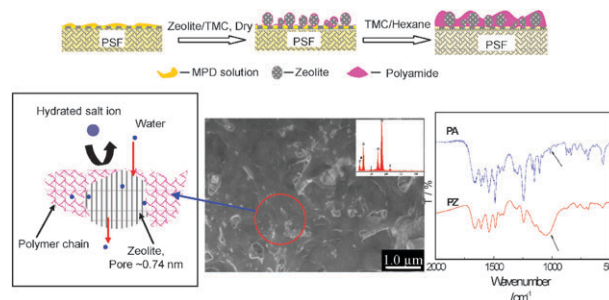


2101

“Pre-seeding”-assisted synthesis of a high performance polyamide-zeolite nanocomposite membrane for water purification

Chunlong Kong, Takuji Shintani and Toshinori Tsuru*

A new type of polyamide-zeolite nanocomposite membrane has been fabricated for use in water purification by a “pre-seeding” method. The incorporated zeolite provides a preferential flow path for water permeability.

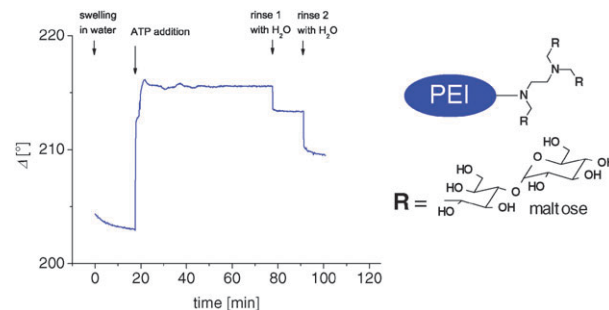


2105

pH-stable hyperbranched poly(ethyleneimine)-maltose films for the interaction with phosphate containing drugs

Anne Richter, Andreas Janke, Stefan Zschoche, Ralf Zimmermann, Frank Simon, Klaus-Jochen Eichhorn, Brigitte Voit and Dietmar Appelhans*

The uptake and release of ATP by hyperbranched poly(ethyleneimine)-maltose (PEI-Mal) hydrogel films is observable by *in-situ* ellipsometric measurements which can be intrigued with other potential bio-applications for establishing multifunctional thin PEI-Mal hydrogel films.



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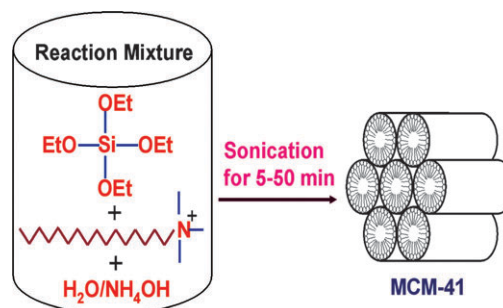
LETTERS

2109

The ultrafast sonochemical synthesis of mesoporous silica MCM-41

Shanmugam Vetrivel, Ching-Ting Chen and Hsien-Ming Kao*

Well-ordered mesoporous silica MCM-41 has been synthesized using cetyltrimethylammonium bromide (CTMABr) as a template under basic media with the aid of ultrasonic irradiation in a very short time period of 5–50 min.

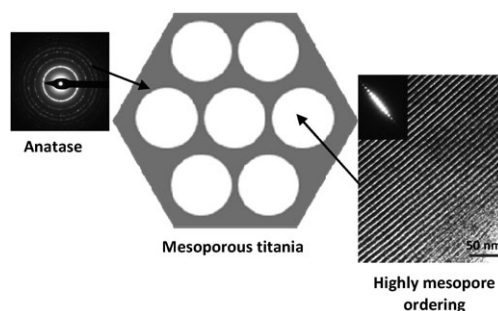


2113

Highly ordered mesoporous titania with semi crystalline framework templated by large or small nonionic surfactants

Kevin Zimny, Jaafar Ghanbaja, Cédric Carteret, Marie-José Stébé and Jean-Luc Blin*

Highly ordered mesoporous titania.

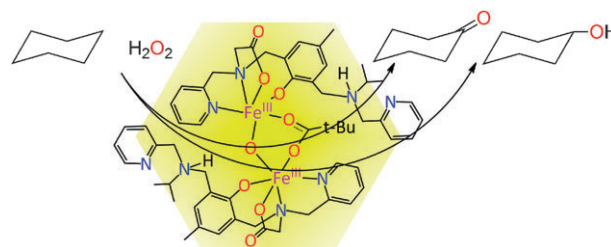


2118

A monocarboxylate-bridged diiron(III) μ -oxido complex that catalyzes alkane oxidation by hydrogen peroxide

Martin Jarenmark, Elena A. Turitsyna, Matti Haukka, Albert A. Shteinman and Ebbe Nordlander*

A new pivalate-bridged μ -oxido diiron complex catalyzes the oxidation of cyclohexane or 1,2-*cis*-dimethylcyclohexane by hydrogen peroxide, forming the corresponding ketones and alcohols.

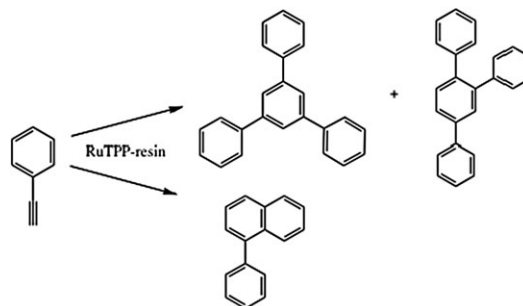


2122

Ruthenium porphyrin bound to a Merrifield resin as heterogeneous catalyst for the cyclooligomerization of arylethynes

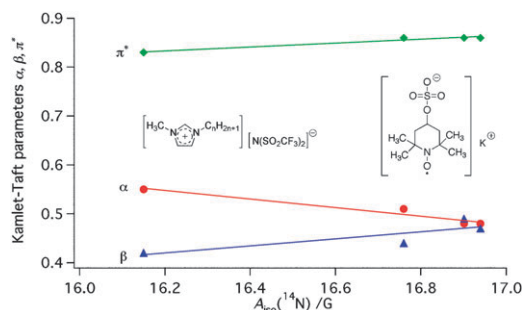
Alina Ciammaichella, Alessandro Leoni and Pietro Tagliatesta*

Ruthenium *meso*-tetraphenylporphyrin bound to the Merrifield resin has been used in the cyclooligomerization of arylethynes, giving heterobiaryl and triphenylbenzenes as final products with a complete recycling of the catalyst.



PAPERS

2125

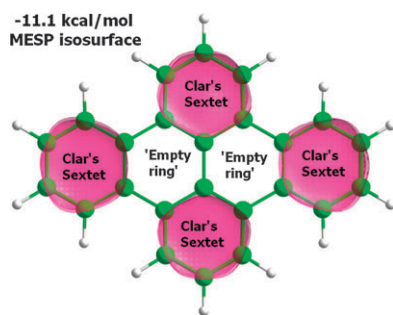


Relationship between hyperfine coupling constants of spin probes and empirical polarity parameters of some ionic liquids

Veronika Strehmel,* Ralf Lungwitz, Hans Rexhausen and Stefan Spange

Polarity of ionic liquids: study with solvatochromic and spin probes.

2132

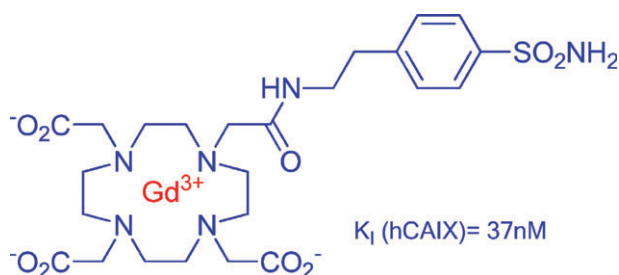


Pictorial representation and validation of Clar's aromatic sextet theory using molecular electrostatic potentials

Kunduchi Periya Vijayalakshmi and Cherumuttathu H. Suresh*

An intimate relationship between molecular electrostatic potential (MESP) and Clar's aromatic sextet theory is reported.

2139

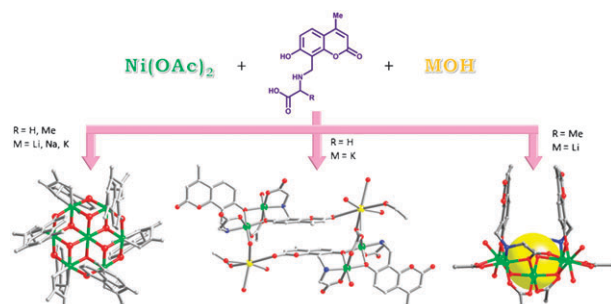


Carbonic anhydrase inhibitors: Gd(III) complexes of DOTA- and TETA-sulfonamide conjugates targeting the tumor associated carbonic anhydrase isozymes IX and XII

Marouan Rami, Jean-Louis Montero, Ludwig Dubois, Philippe Lambin, Andrea Scozzafava, Jean-Yves Winum* and Claudiu T. Supuran*

Gd³⁺ ion-containing sulfonamide complexes have excellent CA IX inhibitory activity and potential for application in both the imaging and treatment of hypoxic tumors.

2145



Alkali metal ion directed self-assembled Ni(II) molecular clusters

Wei Lee Leong and Jagadese J. Vittal*

Self-assembly of Ni²⁺ with coumarin-derived amino acids directed by alkali metal ions furnished interesting oligonuclear structures including heptanickel metallocrowns with highly symmetrical hexagonal shapes, a heterobimetallic molecular cage and a pentanickel cluster with a nanobasket shape.

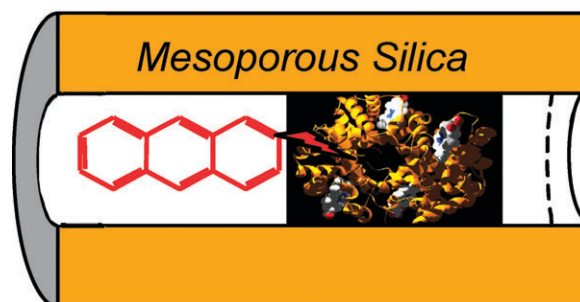
PAPERS

2153

Hemoglobin immobilized on mesoporous silica as effective material for the removal of polycyclic aromatic hydrocarbons pollutants from water

Paco Laveille, Aude Falcimaigne, Françoise Chamouleau, Gilbert Renard, Jullien Drone, Francois Fajula, Sylviane Pulvin, Daniel Thomas, Carole Bailly and Anne Galarneau*

Adsorption of hemoglobin into mesoporous silica leads to a highly efficient biocatalyst able to remove more than 82% of PAH at pH 7 from water using H_2O_2 as oxidant.

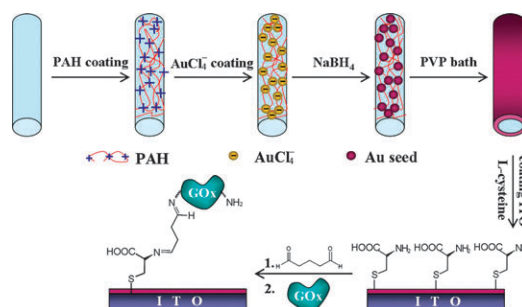


2166

Gold/mesoporous silica-fiber core-shell hybrid nanostructure: a potential electron transfer mediator in a bio-electrochemical system

Haigang Kang, Yihua Zhu,* Xiaoling Yang, Jianhua Shen, Cheng Chen and Chunzhong Li

Mesostructured silica fibers synthesized by electrospinning silica sol were used as templates for the assembly of gold nanoparticles and the formation of continuous gold shells along the fiber axis. The SiO_2/Au fiber hybrid nanostructures are further used as substrates for fabrication of a glucose biosensor, which exhibited excellent bio-electrochemical activity.

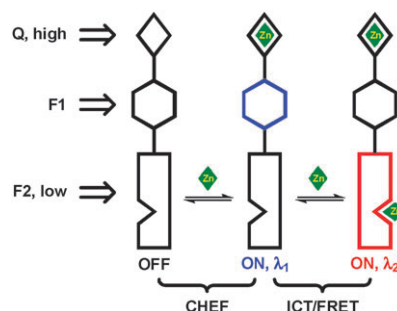


2176

Metal-coordination-mediated sequential chelation-enhanced fluorescence (CHEF) and fluorescence resonance energy transfer (FRET) in a heteroditopic ligand system

Robert J. Wandell, Ali H. Younes and Lei Zhu*

A two-fluorophore heteroditopic ligand system is established for achieving two sequential fluorescence events over a Zn^{2+} gradient.

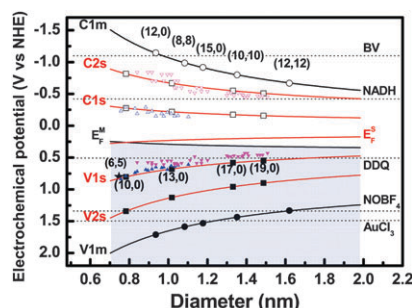


2183

Doping strategy of carbon nanotubes with redox chemistry

Ki Kang Kim, Seon-Mi Yoon, Hyeon Ki Park, Hyeon-Jin Shin, Soo Min Kim, Jung Jun Bae, Yan Cui, Jong Min Kim, Jae-Young Choi* and Young Hee Lee*

The reduction potential of SWCNT as a function of chirality and diameter is obtained based on theoretical calculations. The degree of doping can be controlled by the relative reduction potential between dopant and nanotube. Those phenomena were observed by absorption and Raman spectroscopy.



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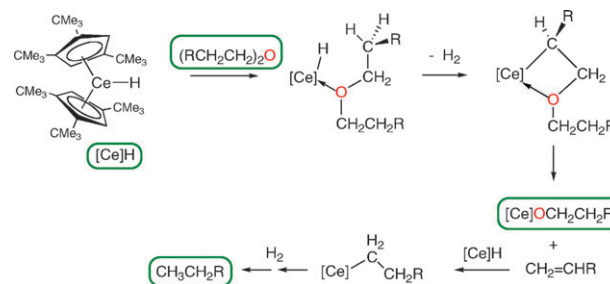
PAPERS

2189

Splitting a C–O bond in dialkylethers with bis(1,2,4-tri-*tert*-butylcyclopentadienyl)cerium hydride does not occur by a σ -bond metathesis pathway: a combined experimental and DFT computational study

Evan L. Werkema, Ahmed Yahia, Laurent Maron,*
Odile Eisenstein* and Richard A. Andersen*

The mechanism of C–O bond cleavage in ethers is shown with reactants and observed products circled in green.

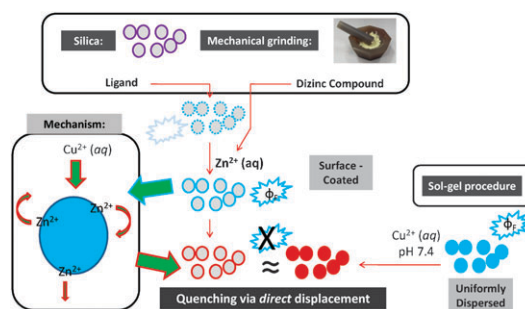


2197

Mechanochemical *versus* sol-gel silica loading of phenolate- and acetate-bridged dizinc complexes: toward instant and inexpensive hybrids for controlled binding and release of Zn^{2+} in pure water

Taehong Jun, Yonghwang Ha, Jina Kang,
Snehadrinarayan Khatua and David G. Churchill*

A chiral ligand and fluorescent dimer were mechanochemically loaded for respective off-on aqueous fluorescence detection of Zn^{2+} and on-off Cu^{2+} detection. Extensive SEM-EDS data enabled the determination of a mechanochemical loading constant.

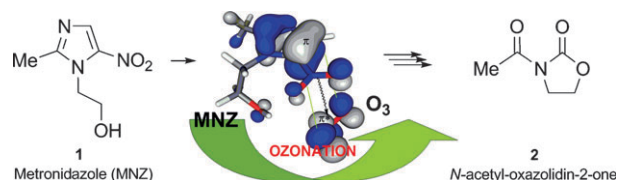


2205

A convenient antibiotic indicator in the ozone treatment of wastewaters. An experimental and theoretical study

Antonio J. Mota,* Gonzalo Prados-Joya,
David Arráez-Román, Manuel Sánchez-Polo,
Rafael Robles, M^a Angeles Ferro-García and
José Rivera-Utrilla*

The ozonation of nitroimidazole-type antibiotics containing wastewaters leads to stable oxazolidinone derivatives.

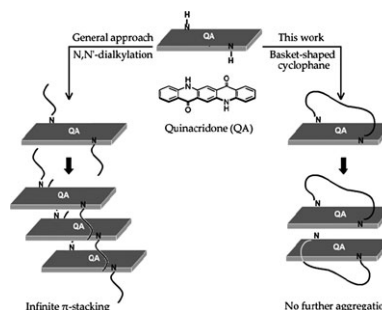


2213

Basket-shaped quinacridone cyclophanes: synthesis, solid-state structures, and properties

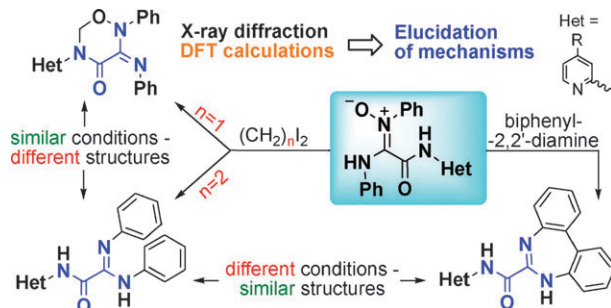
Dingyi Yu, Tai Peng, Hongyu Zhang,* Hai Bi,
Jingying Zhang and Yue Wang*

A comparison of luminescent efficiency in both concentrated solution and EL device with high doping concentration between basket-shaped QA cyclophanes and a non-bridged analogue clearly demonstrates that the basket-shaped bridge has the ability to effectively inhibit molecular aggregation which causes fluorescence quenching in the condensed phases.



PAPERS

2220

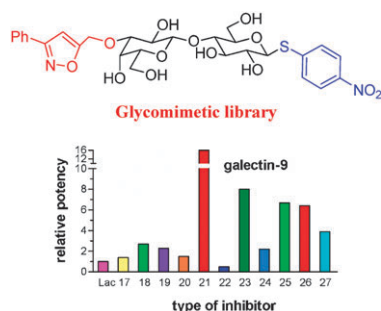


Mechanisms of reactions conducted on α -amido- α -aminonitrones, determined based on the structures of their crystalline products and DFT calculations

Bartosz Trzewik,* Tomasz Seidler, Ewa Broclawik and Katarzyna Stadnicka

The crystal structures of various products, obtained from α -amido- α -aminonitrones, were determined and, along with DFT calculations, allowed us to elucidate the mechanisms of the reactions leading to them.

2229

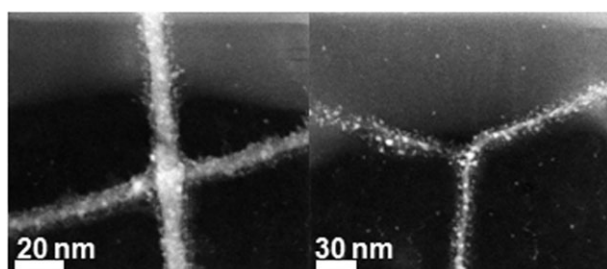


Synthesis and screening of a small glycomimetic library for inhibitory activity on medically relevant galactoside-specific lectins in assays of increasing biorelevance

Sabine André, Denis Giguère, Tarun K. Dam, Fred Brewer, Hans-Joachim Gabius and René Roy*

A panel of galactoside/lactoside derivatives with pharmacophores at the aglycone and O-3/O-3' was evaluated against plant toxin and four human regulatory galectins. Differential sensitivity profiles of lectin binding showing activity increase relative to galactose/lactose were revealed.

2241

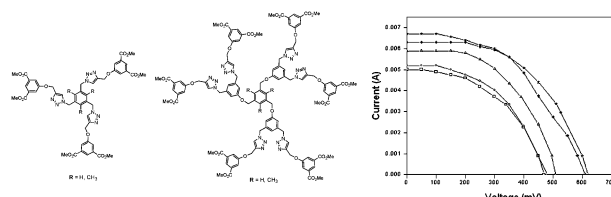


A facile route to self-assembled Hg//MoSI nanowire networks

Valeria Nicolosi,* Zabeada Aslam, Kasim Sader, Gareth M. Hughes, Damjan Vengust, Neil P. Young, Ron Doole, Dragan Mihailovic, Andrew L. Bleloch, Angus I. Kirkland, Nicole Grobert and Peter D. Nellist

The chemical functionalisation of nanowires consisting of molybdenum, sulphur and iodine in conjunction with very low concentrations of molecular mercury leads to self-assembled networks of one-dimensional systems.

2247



Synthesis of triazole dendrimers with a dimethyl isophthalate surface group and their application to dye-sensitized solar cells

Perumal Rajakumar,* Sebastian Raja, Chinnadurai Satheshkumar, Shanmugam Ganesan, Pichai Maruthamuthu and Samuel Austin Suthanthiraraj

A series of novel triazole-carboxylate dendrimers were synthesized *via* 'click' chemistry. Optical and electrochemical properties of the dendrimers and their role in dye-sensitized solar cells are also described.

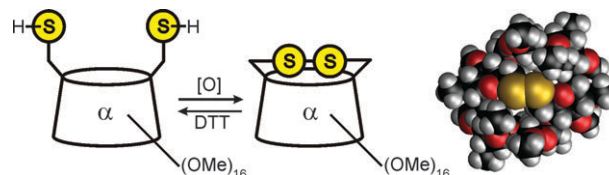
PAPERS

2254

 α -Cyclodextrins reversibly capped with disulfide bonds

Lukáš Kumprecht, Miloš Buděšínský, Petr Bouř and Tomáš Kraus*

Permethyl- α -cyclodextrin capped with a disulfide linkage between the C6^I and C6^{IV} positions can reversibly switch between open-ended and cup-like forms by the application of external stimuli.

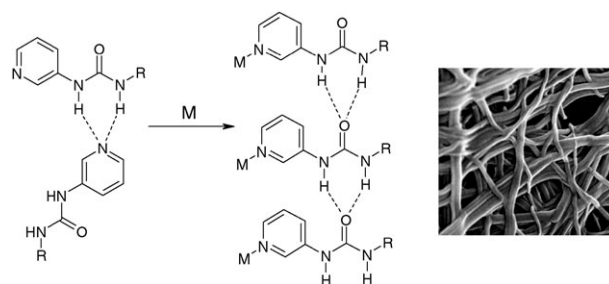


2261

Metal-induced gelation in dipyridyl ureas

Peter Byrne, Gareth O. Lloyd, Lucas Applegarth, Kirsty M. Anderson, Nigel Clarke and Jonathan W. Steed*

Pyridyl bis(urea) ligands form supramolecular gels in the presence of metal ions because of competition between urea-urea and urea-pyridyl hydrogen bonding interactions.

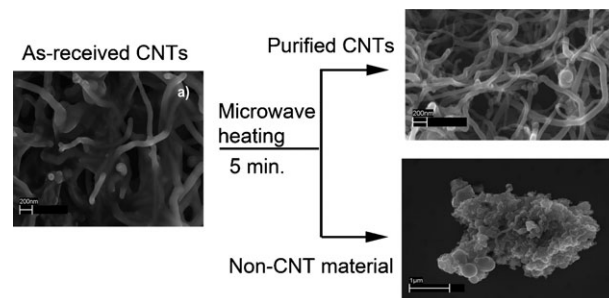


2275

The reagent-free, microwave-assisted purification of carbon nanotubes

Khalil Chajara, Claes-Henrik Andersson, Jun Lu, Erika Widenkvist and Helena Grennberg*

We have developed an extremely fast, microwave-assisted, reagent-free method for the efficient primary purification of MW and SW carbon nanotubes. According to TGA, Raman, IR and SEM, the process rapidly yields pure nanotubes with a low degree of defects.

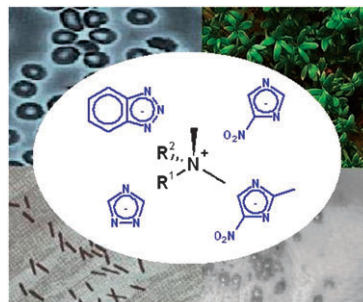


2281

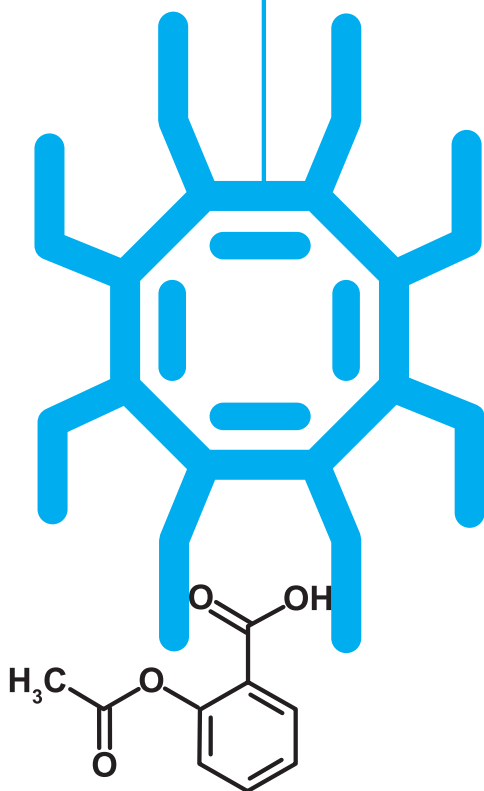
Multifunctional long-alkyl-chain quaternary ammonium azolate based ionic liquids

Filip Walkiewicz, Katarzyna Materna, Aleksandra Kropacz, Alicja Michalczyk, Romuald Gwiazdowski, Tadeusz Praczyk and Juliusz Pernak*

We have synthesized multifunctional quaternary ammonium azolate based ionic liquids of high practical importance.



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Neutral *ansa*-bis(fluorenyl)silane neodymium borohydrides: synthesis, structural study and behaviour as catalysts in butadiene–ethylene copolymerisation

A series of new neutral *ansa*-bis(fluorenyl)silane neodymium borohydrides were found to be active in the butadiene-ethylene copolymerisation reaction; the activity of the catalyst is independent of the substituents at silicon.



The transfer of neutral molecules, ions and ionic species from water to ethylene glycol and to propylene carbonate; descriptors for pyridinium cations

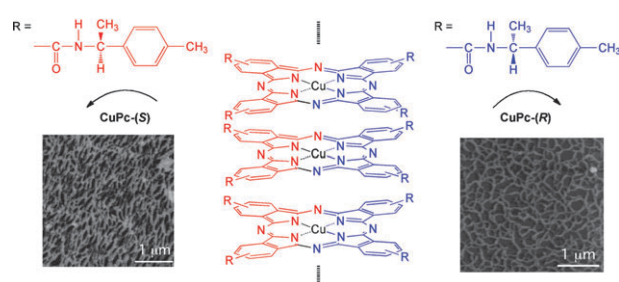
Equations have been constructed for the transfer of neutral molecules and ions from water to ethylene glycol and to propylene carbonate; the ions include pyridinium cations that are strong hydrogen bond acids, but are not hydrogen bond bases at all.



The photoinduced substitution of the 2-naphthoxide anion was carried out using diethylphosphite, benzenethiolate or 2-naphthalenethiolate anions in the presence of an electron acceptor. The corresponding products were afforded in good yield.

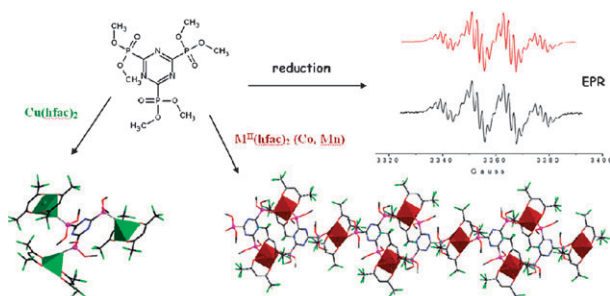


Copper(II) phthalocyanine with four chiral groups, that can form ambidextrous optically active self-assemblies in solutions, generated worm-like polymeric and circle-like structures on mica surface.



PAPERS

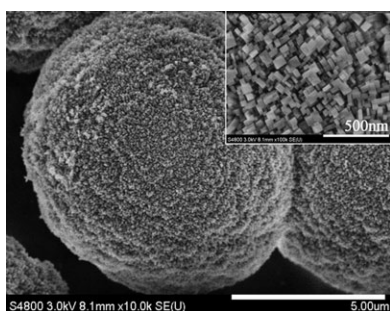
2319

**C₃ symmetric tris(phosphonate)-1,3,5-triazine ligand: homopolymetallic complexes and its radical anion**

Catalin Maxim, Adil Matni, Michel Geoffroy,*
Marius Andruh, Nigel G. R. Hearn, Rodolphe Clérac and
Narcis Avarvari*

The ligand 2,4,6-tris(dimethoxyphosphonate)-1,3,5-triazine **L**, for which EPR investigations and theoretical calculations have been performed on its radical anion, provided paramagnetic homopolymetallic complexes, which were structurally characterized.

2328

**One-step synthesis of hierarchical pentasil zeolite microspheres using diamine with linear carbon chain as single template**

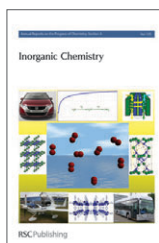
Li Chen, Shu Yan Zhu, Yi Meng Wang* and
Ming-Yuan He

Hierarchical pentasil zeolite microspheres of 5–8 μm in size containing nanocrystals were synthesized *via* a one-step method using a diamine with a linear carbon chain as the single template.

Annual Reports on the Progress of Chemistry

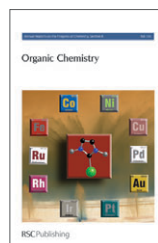
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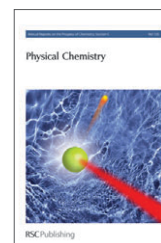
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