

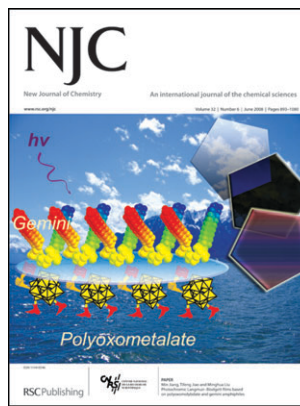
IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 32(6) 893–1080 (2008)



Cover

See Lindsey *et al.*, pp. 947–958. Synthetic bacteriochlorins substituted with auxochromes exhibit sharp absorption and emission bands in the NIR (713–777 nm), enabling diverse applications (polychromatic flow cytometry, photodynamic therapy, solar energy conversion). Cover artwork by Masahiko Taniguchi. Reproduced with permission from Jonathan Lindsey from *New J. Chem.*, 2008, **32**, 947.



Inside Cover

See Liu *et al.*, pp. 959–965. Photochromic hybrid Langmuir–Blodgett films composed of polyoxometalate and gemini amphiphiles were fabricated. A slight dependence of the coloration of the hybrid films on the spacer length was observed. Image reproduced with permission from Minghua Liu from *New J. Chem.*, 2008, **32**, 959.

CHEMICAL SCIENCE

C41

Drawing together the research highlights and news from all RSC publications, *Chemical Science* provides a ‘snapshot’ of the latest developments across the chemical sciences, showcasing newsworthy articles and significant scientific advances.

Chemical Science

June 2008/Volume 5/Issue 6

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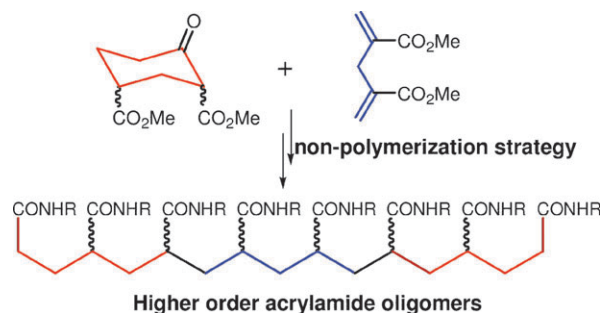
LETTER

909

A tandem non-polymerizing strategy to higher order acrylamide oligomers; potential intermediates for conformational correlations of poly-*N*-acrylamides

Amol M. Kendhale, Pattuparampil R. Rajamohanan and Gangadhar J. Sanjayan*

This letter describes a one-pot procedure to deliver higher order *N*-acrylamide oligomers which are potential intermediates for the correlation of stereochemistry (tacticity) with conformation and hydrogen-bonding propensities in poly (oligo) *N*-acrylamides.



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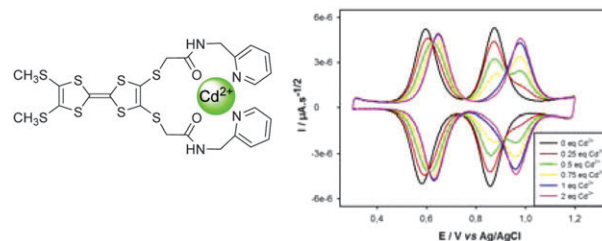
LETTERS

913

Electrochemical M^{2+} recognition by an amidopyridyl-tetrathiafulvalene derivative

Chahrazed Benhaoua, Miloud Mazari, Nicolas Mercier, Franck Le Derf* and Marc Sallé*

A tetrathiafulvalene-based redox-responsive receptor incorporating amide and pyridyl coordinating units exhibits an original multi-wave electrochemical recognition behaviour towards $Cd(II)$.

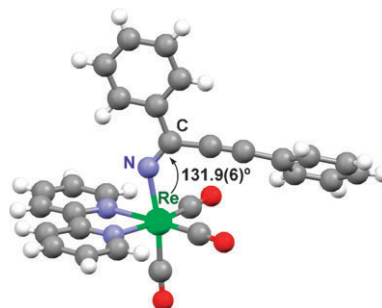


917

A new route for the synthesis of an alkylideneamido complex

Luciano Cuesta, Dolores Morales, Julio Pérez* and Daniel Miguel

The synthesis of the new alkylideneamido complex $[Re\{N=C(Ph)C\equiv CPh\}(CO)_3(bpy)]$ is described. Analysis of its spectroscopic and structural data reveals the absence of π -donation from the nitrogen to the metal.

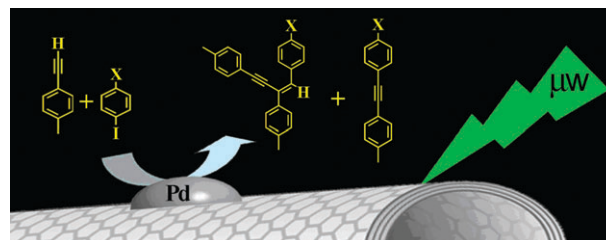


920

Microwave-promoted hydrogenation and alkynylation reactions with palladium-loaded multi-walled carbon nanotubes

Jean-Hubert Olivier, Franck Camerel, Raymond Ziessel,* Pascal Retailleau, Julien Amadou and Cuong Pham-Huu*

Palladium loaded multi-walled carbon nanotubes were used as hydrogenation and alkynylation catalysts under microwave irradiation under eco-friendly conditions.

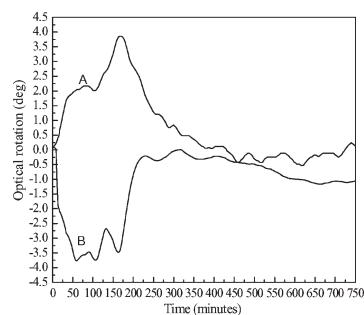


925

Enantioselective crystallization in miniemulsions based on chiral surfactants

Tali Menahem and Yitzhak Mastai*

In this letter we describe new application of a chiral micellar system for the optical resolution of racemic compounds by crystallization.





Surface enhanced Raman scattering

SERS theme issue

Since its discovery over 30 years ago SERS has enjoyed a high level of interest, which has increased significantly in the last few years. *Chem Soc Rev* issue 5, 2008 is a compilation of 2 critical and 15 tutorial reviews on the application of surface enhanced Raman scattering that brings together leading exponents in researching the technique and its applications. The result is a balanced portfolio that covers the main areas of current development and makes this a truly diverse yet up-to-date body of papers on the state of the SERS field.

Papers include:

Elena Bailo and Volker Deckert
Tip-enhanced Raman scattering

De-Yin Wu, Jian-Feng Li, Bin Ren and Zhong-Qun Tian
Electrochemical surface-enhanced Raman spectroscopy of nanostructures

Surbhi Lal, Nathaniel K. Grady, Janardan Kundu, Carly S. Levin, J. Britt Lassiter and Naomi J. Halas
Tailoring plasmonic substrates for surface enhanced spectroscopies

X.-M. Qian and S. M. Nie
Single-molecule and single-nanoparticle SERS: from fundamental mechanisms to biomedical applications

Matthew J. Banholzer, Jill E. Millstone, Lidong Qin and Chad A. Mirkin
Rationally designed nanostructures for surface-enhanced Raman spectroscopy

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"ERS has emerged from the debates over the theory behind the phenomenon to come of age as a powerhouse of the modern spectroscopic world and this theme issue highlights the significant areas where SERS can be applied with unparalleled performance."

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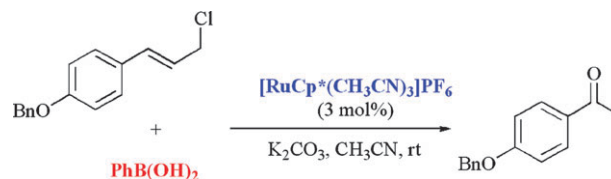
LETTERS

929

Ruthenium-catalyzed tandem allylic substitution/isomerization: a direct route to propiophenones from cinnamyl chloride derivatives

Marion Helou, Jean-Luc Renaud,* Bernard Demerseman, François Carreaux and Christian Bruneau*

A catalytic regioselective allylic substitution/redox isomerization sequence catalyzed by $[\text{RuCp}^*(\text{CH}_3\text{CN})_3]\text{PF}_6$ and involving $\text{PhB}(\text{OH})_2$ as a hydroxy group source.

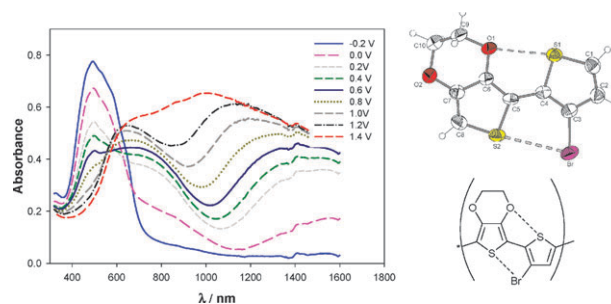


932

Evidence for the contribution of sulfur–bromine intramolecular interactions to the self-rigidification of thiophene-based π -conjugated systems

Noémie Hergué, Philippe Leriche, Philippe Blanchard, Magali Allain, Nuria Gallego-Planas, Pierre Frère* and Jean Roncali

Bithiophene associating 3,4-ethylenedioxythiophene and 3-bromothiophene, and the corresponding polymer exhibit self-rigidified structures resulting from the association of S–Br and S–O non-bonded intramolecular interactions.

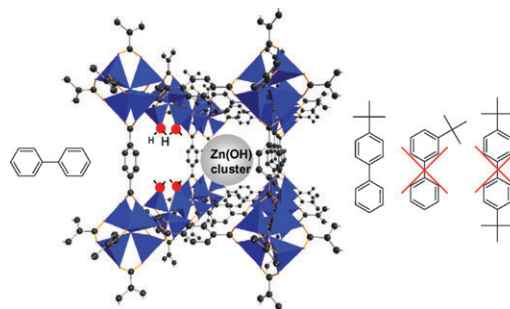


937

MOFs as acid catalysts with shape selectivity properties

Ugo Ravon, Marcelo E. Domine, Cyril Gaudillère, Arnold Desmartin-Chomel and David Farrusseng*

IRMOFs permit the paraalkylation of large polyaromatic compounds with nearly 100% of regioselectivity, offering new alternatives to standard zeolite catalysts.



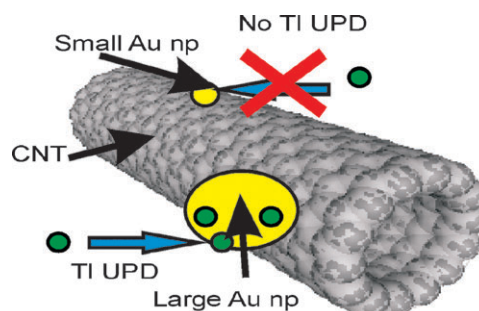
PAPER

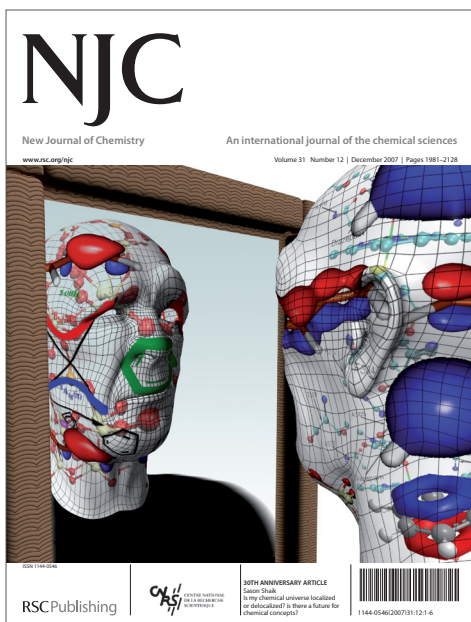
941

The contrasting behaviour of polycrystalline bulk gold and gold nanoparticle modified electrodes towards the underpotential deposition of thallium

Christopher Batchelor-McAuley, Gregory G. Wildgoose and Richard G. Compton

The different size dependent properties of gold nanoparticles supported on MWCNTs are illustrated with respect to the underpotential deposition of thallium(I).





Drawing disciplines together



Introducing Professor Michael Scott

Associate Editor for the Americas

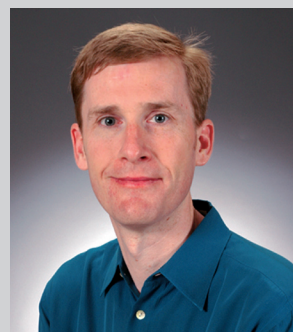
Michael is an associate professor in the Department of Chemistry and the director for the Center for Catalysis at the University of Florida in Gainesville, Florida. He is a fellow of both the Alfred P. Sloan Foundation and the Royal Society of Chemistry. His research interests focus on the design of ligands and metal complexes for the selective recognition and sequestration of cations and anions and for biomimetic catalysis.

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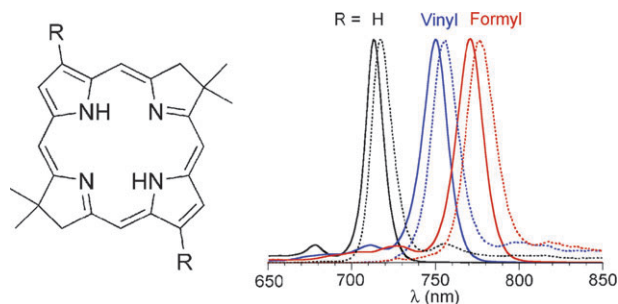
PAPERS

947

Accessing the near-infrared spectral region with stable, synthetic, wavelength-tunable bacteriochlorins

Masahiko Taniguchi, David L. Cramer, Anil D. Bhise, Hooi Ling Kee, David F. Bocian,* Dewey Holten* and Jonathan S. Lindsey*

Synthetic bacteriochlorins substituted with auxochromes exhibit sharp absorption and emission bands in the near-infrared (713–777 nm) spectral region, enabling diverse applications (polychromatic flow cytometry, photodynamic therapy, solar energy conversion).

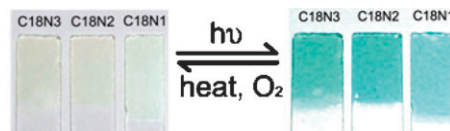


959

Photochromic Langmuir–Blodgett films based on polyoxomolybdate and gemini amphiphiles

Min Jiang, Tifeng Jiao and Minghua Liu*

Hybrid organized molecular films composed of polyoxomolybdate and a series of gemini amphiphile with different hydrophilic spacer length were fabricated by Langmuir–Blodgett (LB) technique and exhibited good photochromic ability.

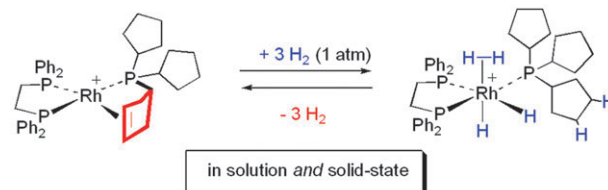


966

Acceptorless, intramolecular, alkyl dehydrogenation in the solid-state in a rhodium phosphine complex; reversible uptake of three equivalents of H₂ per molecule

Thomas M. Douglas and Andrew S. Weller*

A remarkably undemanding reversible acceptorless dehydrogenation of *tris*-cyclopentyl phosphine in the complex [Rh(dppe)(PCyp₃)(H)₂(η^2 -H₂)] [BARF₄⁺] occurs in the solid-state, and results in the storage and release of up to three equivalents of H₂ per molecule. This reactivity mirrors the previously reported solution chemistry.

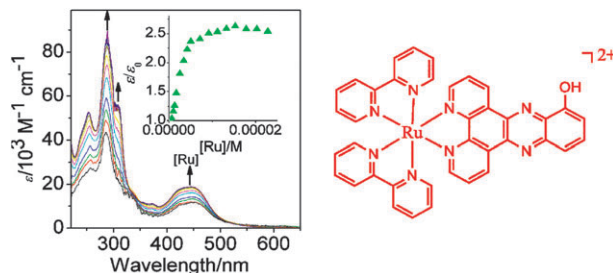


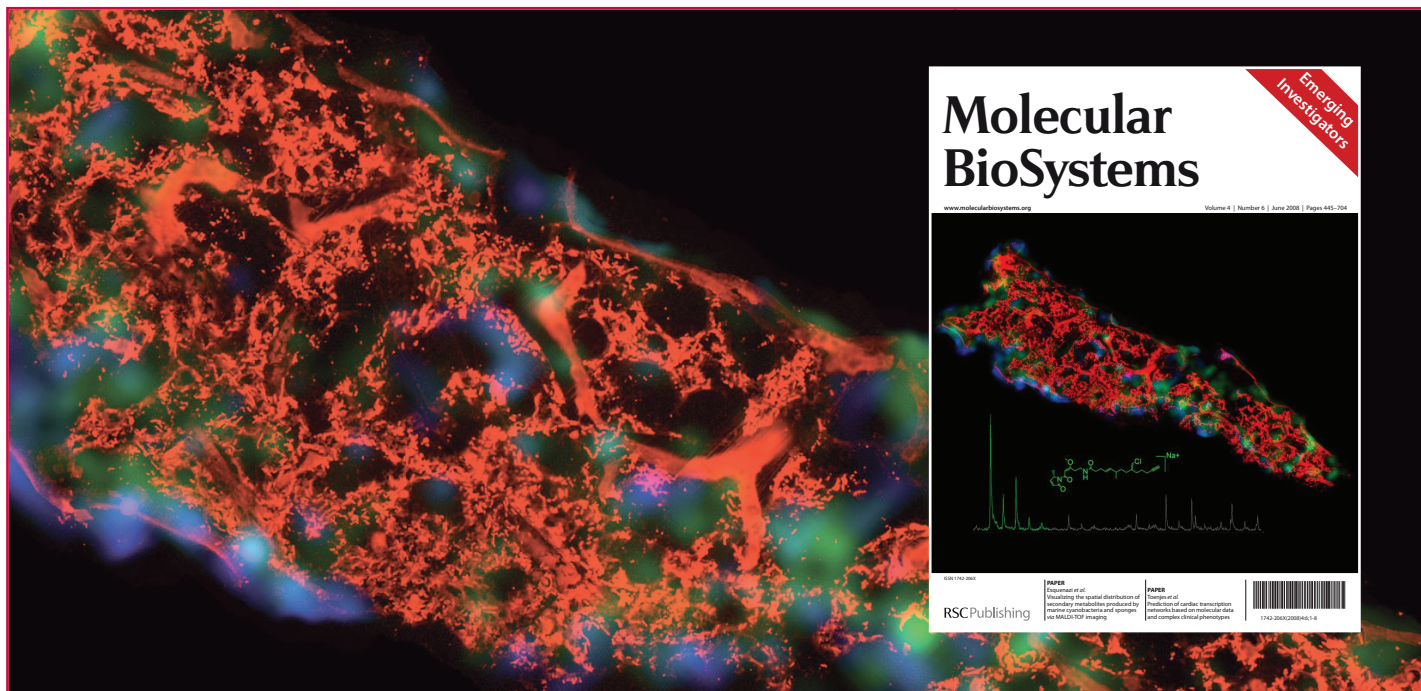
970

Ruthenium(II) complexes of 6-hydroxydipyrido-[3,2-*a*:2',3'-*c*]phenazine: self-association, and concentration-dependent acid–base and DNA-binding properties

Mei-Jiao Han, Yan-Min Chen and Ke-Zhi Wang*

The self-association of the Ru(II) complex profoundly affects its DNA binding properties





Emerging Investigators theme issue

Molecular BioSystems issue 6, 2008, devoted to outstanding young scientists at the chemical- and systems-biology interfaces, features novel methods to visualise and manipulate protein function in living cells, the development of chemical techniques to monitor specific protein post-translational modifications, new insights into metabolomics and much, much more!

Papers include:

Visualization of phosphatase activity in living cells with a FRET-based calcineurin activity sensor

Robert H. Newman and Jin Zhang

Conformation and the sodium ion condensation on DNA and RNA structures in the presence of a neutral cosolute as a mimic of the intracellular media

Shu-ichi Nakano, Lei Wu, Hirohito Oka, Hisae Tateishi Karimata, Toshimasa Kiriha, Yuichi Sato, Satoshi Fujii, Hiroshi Sakai, Masayuki Kuwahara, Hiroaki Sawai and Naoki Sugimoto

A quantitative study of the recruitment potential of all intracellular tyrosine residues on EGFR, FGFR1 and IGF1R

Alexis Kaushansky, Andrew Gordus, Bryan Chang, John Rush and Gavin MacBeath

Direct printing of trichlorosilanes on glass for selective protein adsorption and cell growth

Dawn M. Yanker and Joshua A. Maurer, *Mol. BioSyst.*, 2008

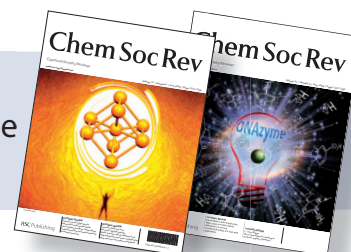
A chemical approach for detecting sulfenic acid-modified proteins in living cells

Khalilah G. Reddie, Young Ho Seo, Wilson B. Muse III, Stephen E. Leonard and Kate S. Carroll

See also:

Chem Soc Rev issue 7, 2008 - Chemistry-Biology Interface theme issue

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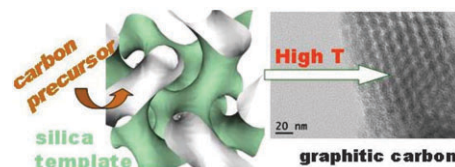
PAPERS

981

High temperature treatment of ordered mesoporous carbons prepared by using various carbon precursors and ordered mesoporous silica templates

Kamil P. Gierszal, Mietek Jaroniec,* Tae-Wan Kim, Jeongnam Kim and Ryong Ryoo*

Adsorption and structural properties of ordered mesoporous carbons prepared by templating *1a3d* silica mesostructures with different precursors are studied upon high temperature treatment in argon ranging from 900 °C to 2400 °C.

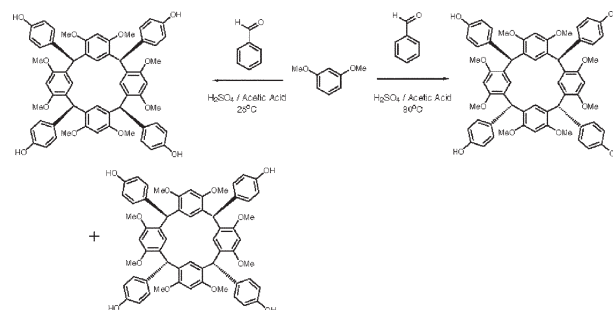


994

Selective formation of the *rc*tt chair stereoisomers of octa-*O*-alkyl resorcin[4]arenes using Brønsted acid catalysis

Deborah Moore, Graeme W. Watson, Thorfinnur Gunnlaugsson* and Susan E. Matthews*

New conditions for the exclusive formation of a single isomer of octa-*O*-alkyl resorcin[4]arenes, from a range of aldehydes, have been developed.

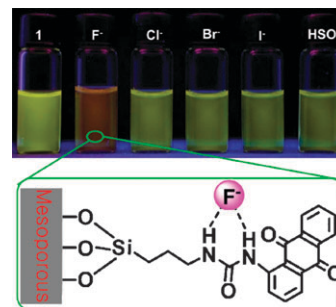


1003

Selective fluoride sensing using organic–inorganic hybrid nanomaterials containing anthraquinone

Eunjeong Kim, Hyun Jung Kim, Doo Ri Bae, Soo Jin Lee, Eun Jin Cho, Moo Ryeong Seo, Jong Seung Kim* and Jong Hwa Jung*

A urea–anthraquinone fluorescent receptor attached to mesoporous silica selectively detects fluoride anions.

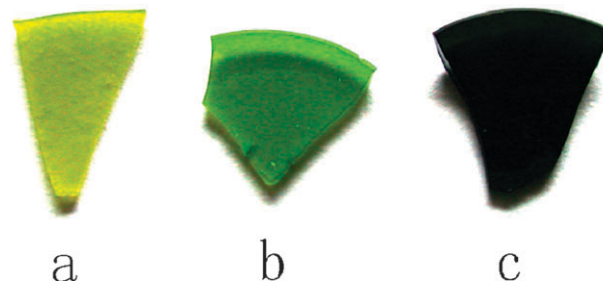


1008

Polyoxometalate-based gasochromic silica

Bingbing Xu, Lin Xu,* Guanggang Gao, Zhikui Li, Yu Liu, Weihua Guo and Liping Jia

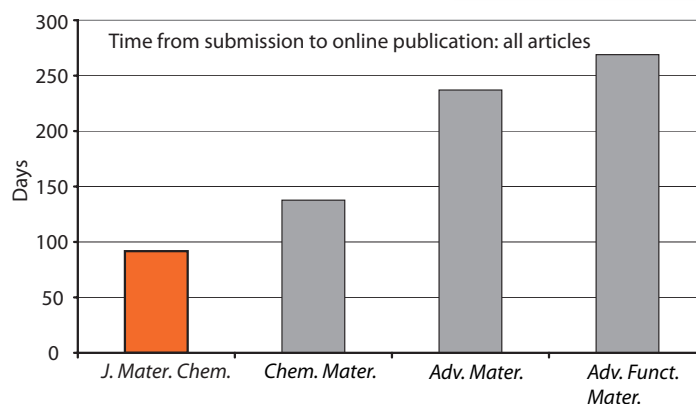
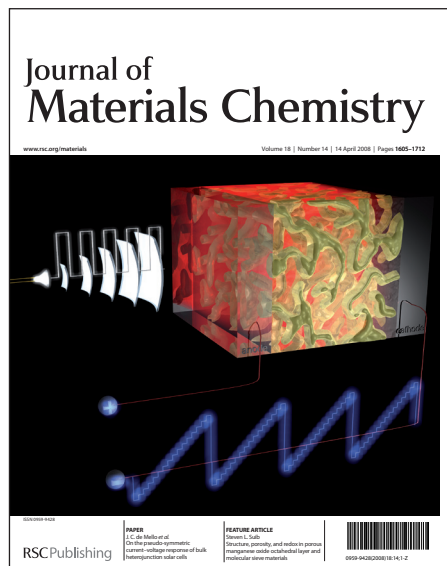
Optical photographs of monolithic pieces after exposure to 7 mg L⁻¹ of H₂S for 0 s (a), 30 s (b) and 300 s (c), respectively. From left to right, the color is yellow, green and dark green.



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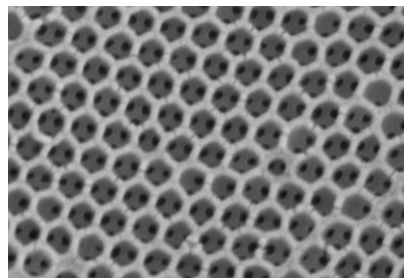
PAPERS

1014

Fabrication of three-dimensionally ordered macroporous gadolinia-doped ceria films

Jiu-Peng Zhao,* Yao Li, Zhong Cao and Wu-Hong Xin

Three-dimensionally ordered macroporous (3-DOM) gadolinia-doped ceria (CGO) thin films were prepared by aqueous organic gel method through the interstitial spaces between polystyrene spheres assembled on glass substrates.

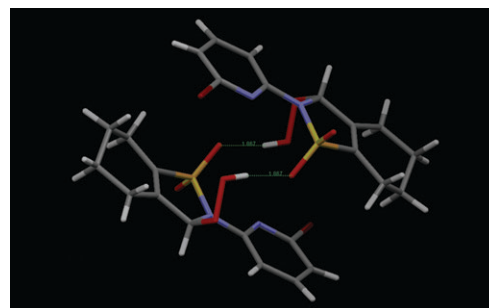


1020

Novel hydroperoxy sultam, 2-(6-bromo-pyrid-2-yl)-2,3,4,5,6,7-hexahydro-1,2-benzisothiazol-3-hydroperoxy 1,1-dioxide: synthesis, crystal structure and kinetics of catalytic interaction with cyclooctene

O. Makota,* A. Eilfeld, Yu. Trach, B. Schulze and J. Sieler

The novel hydroperoxy sultam was synthesized, its solid-state structure was established and kinetics of interaction with cyclooctene in the presence of molybdenum boride was investigated.

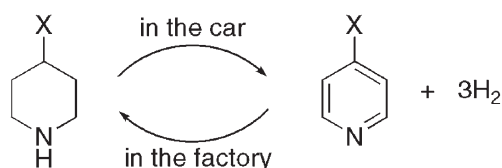


1027

The effect of substitution on the utility of piperidines and octahydroindoles for reversible hydrogen storage

Yi Cui, Samantha Kwok, Andrew Bucholtz, Boyd Davis, Ralph A. Whitney and Philip G. Jessop*

Substituents greatly affect the suitability of piperidines and octahydroindoles to serve as reversible organic hydrogen storage liquids for hydrogen-powered fuel cells. Strategies are described for the design of optimum hydrogen storage liquids.

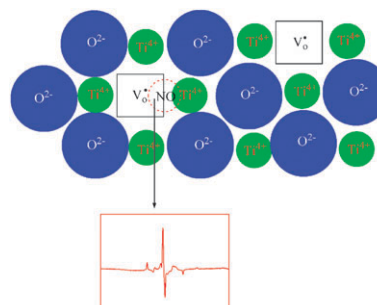


1038

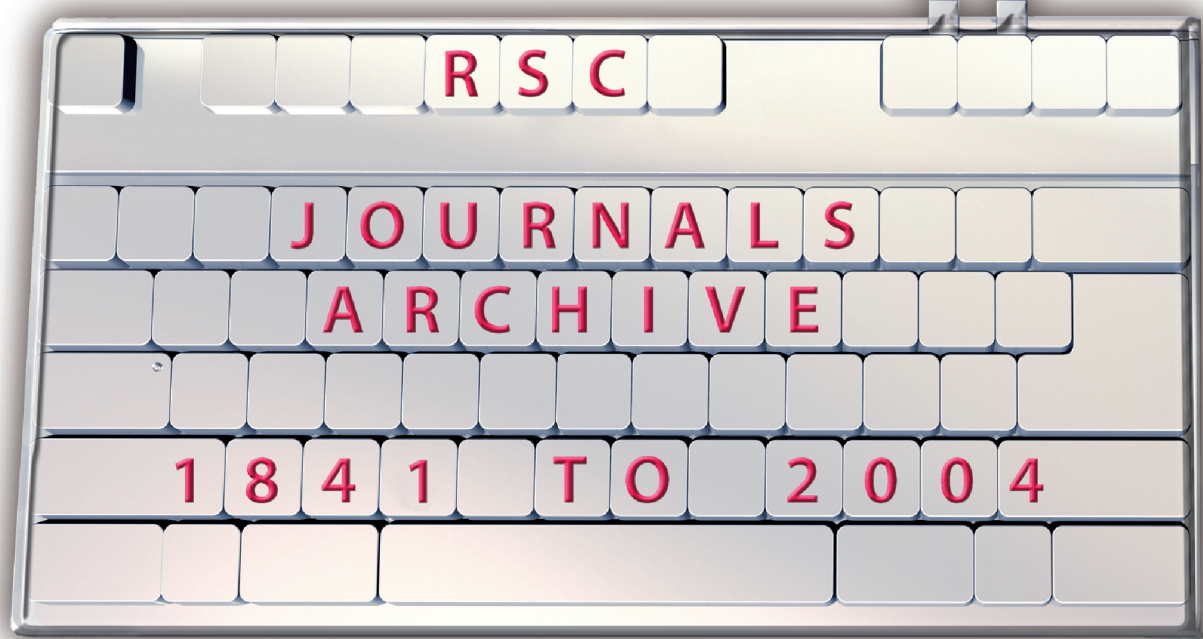
Photoactive centers responsible for visible-light photoactivity of N-doped TiO₂

Caixia Feng, Yan Wang, Zhensheng Jin,* Jiwei Zhang, Shunli Zhang, Zhishen Wu and Zhijun Zhang*

Single-electron-trapped oxygen vacancy (V_o^{\bullet}) formed in well-crystallized TiO₂ surface layer, which accompanied with chemisorbed NO, should be the key structure for the appearance of visible-light photoactivity.



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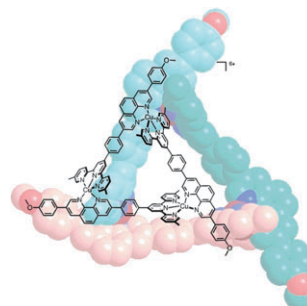
PAPERS

1048

A highly rigid ditopic conjugate with orthogonal coordination axes and its zinc(II) and copper(II) complexes

Benoît Champin, Valérie Sartor and Jean-Pierre Sauvage*

A highly rigid phen–terpy conjugate is synthesised, and forms a surprisingly strained dinuclear complex with zinc(II), whereas a trinuclear complex is also obtained with copper(II).

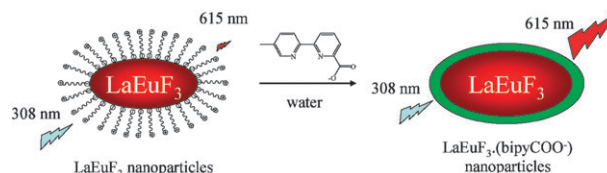


1055

Highly luminescent water-soluble lanthanide nanoparticles through surface coating sensitization

Loïc J. Charbonnière,* Jean-Luc Rehspringer, Raymond Ziessel and Yvan Zimmermann

The luminescence of water-soluble Eu doped LaF_3 nanoparticles can be improved by more than two orders of magnitude upon surface coating with antenna chromophores.

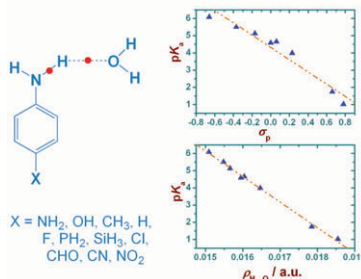


1060

Substituent effects on the hydrogen-bonded complex of aniline– H_2O : a computational study

Menghui Cheng, Xuemei Pu,* Ning-Bew Wong, Menglong Li and Anmin Tian

Substituent effects on the hydrogen-bonded complex of *para*-substituted aniline with one water molecule are studied at the B3LYP/6-311++G(d,p) level. The nature of H-bond interactions and the origin of substituent effects are explored by means of NBO and AIM analysis as well as a series of good correlation equations obtained.

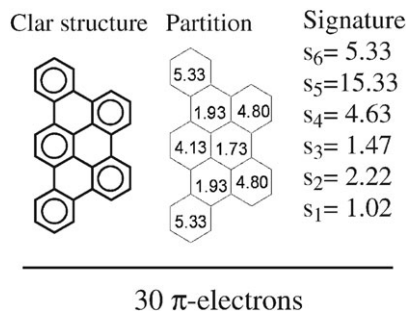


1071

Correlations between various ways of accounting for the distribution of π -electrons in benzenoids

Alexandru T. Balaban and Milan Randić

Our two recently proposed ways of accounting for the π -electrons in polycyclic benzenoids (partition and signature) based on all-Kekule structures or on Pauling bond orders can be reconciled with the help of Fries, anti-Fries, and quasi-Clar structures, proving that they reflect differently the spirit of Clar structures



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