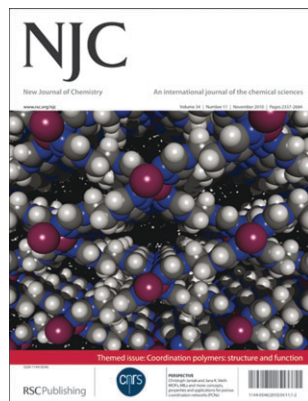
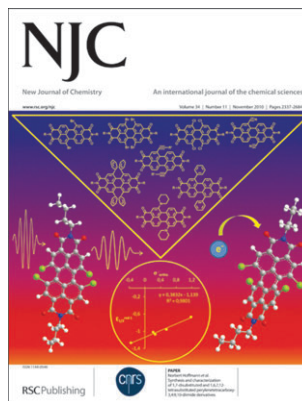


## IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 34(11) 2337-2684 (2010)

**Cover**

See Christoph Janiak and Jana K. Vieth, pp. 2366–2388. Aim for the stars—with MOFs (picturing the 3D-framework in  $[\text{Cu}(\mu_4\text{-btre})]\text{ClO}_4 \cdot 0.25\text{H}_2\text{O}$  from Habib *et al.*, *Inorg. Chem.* 2008, **48**, 2166). Image reproduced by permission of Christoph Janiak and Jana K. Vieth from *New J. Chem.*, 2010, **34**, 2366.

**Inside cover**

See Norbert Hoffmann *et al.*, pp. 2537–2545. The frontier orbital energies of perylene derivatives were determined by optical spectroscopy and cyclic voltammetry. They systematically depend on structural elements such as degree of substitution, electronegativity (Hammett type relationships) and steric hindrance of the substituents. Image reproduced by permission of Mathieu Queste, Cyril Cadiou, Bernard Pagoaga, Louis Giraudet and Norbert Hoffmann from *New J. Chem.*, 2010, **34**, 2537.

## COORDINATION POLYMERS: STRUCTURE AND FUNCTION

## EDITORIALS

2353

**Introduction to the themed issue “Coordination polymers: structure and function”**

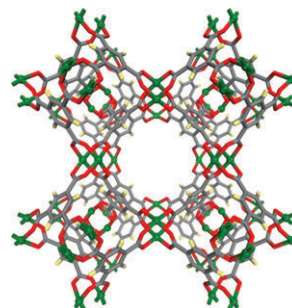
Presenting a collection articles on the theme of Coordination polymers.



2355

**There is plenty of room in the middle: crystal clear opportunities abound for coordination polymers**

The past decade has witnessed an explosion in research activity in the field of coordination polymers, which represent a new paradigm in the context of porous crystalline materials, as exemplified by the prototypal extra-large surface area coordination polymer known as HKUST-1.



## EDITORIAL STAFF

**Editor (RSC)**

Sarah Ruthven

**Deputy editor (RSC)**

Kathleen Too

**Editor (CNRS)**

Denise Parent

**Assistant editor (CNRS)**

Marie Cote

**Senior publishing editor**

Elinor Richards

**Publishing editors**

Mary Badcock, David Barden, Emma Eley, David Parker, Charles Quigg, Michael Townsend

**Publishing assistants**

Anna Anderson, Jackie Cockrill

**Publisher**

Emma Wilson

**Founding editor**

Lionel Salem

For queries about submitted articles please contact Elinor Richards, Senior publishing editor, in the first instance. E-mail [njc@rsc.org](mailto:njc@rsc.org)

For pre-submission queries please contact Sarah Ruthven (RSC), Editor. E-mail [njc-rsc@rsc.org](mailto:njc-rsc@rsc.org)

New Journal of Chemistry (Print: ISSN 1144-0546; electronic: ISSN 1369-9261) is published 12 times a year by the Centre National de la Recherche Scientifique (CNRS), 3 rue Michel-Ange, 75794 Paris cedex 16, France, and the Royal Society of Chemistry (RSC), Thomas Graham House, Science Park, Milton Road, Cambridge, UK CB4 0WF.

All orders, with cheques made payable to the Royal Society of Chemistry, should be sent to RSC Distribution Services, c/o Portland Customer Services, Commerce Way, Colchester, Essex, UK CO2 8HP. Tel +44 (0)1206 226050; E-mail [sales@rscdistribution.org](mailto:sales@rscdistribution.org)

2010 Annual (print + electronic) subscription price: £894; US\$1668. 2010 Annual (electronic) subscription price: £804; US\$1501. Customers in Canada will be subject to a surcharge to cover GST. Customers in the EU subscribing to the electronic version only will be charged VAT.

If you take an institutional subscription to any RSC journal you are entitled to free, site-wide web access to that journal. You can arrange access via Internet Protocol (IP) address at [www.rsc.org/ip](http://www.rsc.org/ip). Customers should make payments by cheque in sterling payable on a UK clearing bank or in US dollars payable on a US clearing bank. Periodicals postage paid at Rahway, NJ, USA and at additional mailing offices. Airfreight and mailing in the USA by Mercury Airfreight International Ltd., 365 Blair Road, Avenel, NJ 07001, USA.

US Postmaster: send address changes to New Journal of Chemistry, c/o Mercury Airfreight International Ltd., 365 Blair Road, Avenel, NJ 07001. All despatches outside the UK by Consolidated Airfreight.

Advertisement sales: Tel +44 (0) 1223 432246; Fax +44 (0) 1223 426017; E-mail [advertising@rsc.org](mailto:advertising@rsc.org)

For marketing opportunities relating to this journal, contact [marketing@rsc.org](mailto:marketing@rsc.org)

NJC

## New Journal of Chemistry

An international journal for the chemical sciences

[www.rsc.org/njc](http://www.rsc.org/njc)

The New Journal of Chemistry is a broad-based primary journal encompassing all branches of the chemical sciences. Published monthly, it contains full research articles, letters, opinions and perspectives.

## EDITORIAL BOARD

**Co-editor-in-chief**

Jerry Atwood, Columbia, MO, USA

**Co-editor-in-chief**

Mir Wais Hosseini, Strasbourg, France

**Consulting editor**

Odile Eisenstein, Montpellier, France

**Board members**

Kumar Biradha, Khargapur, India

Fabrizia Grepioni, Bologna, Italy

Helen Hailles, London, UK

Peter Junk, Monash, Australia

Barbara Nawrot, Lodz, Poland

Alan Rowan, Nijmegen, The Netherlands

Michael Scott, Gainesville, FL, USA

**Associate editors**

Manuscripts should be directed to one of the Editors detailed below.

Professor Peter Junk  
School of Chemistry,  
Monash University, Box 23,  
Victoria 3800,  
Australia  
Fax (+61) 3 9905 4597  
Tel (+61) 3 9905 4570  
E-mail [njc@sci.monash.edu.au](mailto:njc@sci.monash.edu.au)

Professor Michael J. Scott  
Department of Chemistry,  
University of Florida,  
PO Box 117200,  
Gainesville,  
FL 32611, USA  
Fax (+1) 352 392 3255  
Tel (+1) 352 846 1165  
E-mail [njc@chem.ufl.edu](mailto:njc@chem.ufl.edu)

Dr Denise Parent  
New Journal of Chemistry,  
Université Montpellier II,  
Place Eugène Bataillon C.C. 014,  
34095 Montpellier cedex 5,  
France  
Fax (+33) (0) 4 67 14 48 79  
Tel (+33) (0) 4 67 14 48 78  
E-mail [njc@univ-montp2.fr](mailto:njc@univ-montp2.fr)

## ADVISORY BOARD

Markus Antonietti, MPI, Potsdam,  
Germany  
Yasuhiro Aoyama, Kyoto, Japan  
Matthias Bremer, Darmstadt,  
Germany  
Robert Crabtree, New Haven, CT, USA  
François Fajula, Montpellier, France  
John A. Gladysz, College Station,  
TX, USA

George Gokel, St Louis, MO, USA  
Andrew B. Holmes, Melbourne,  
Australia  
Miguel Julve, Valencia, Spain  
Henryk Koslowski, Wroclaw, Poland  
Jean-Pierre Majoral, Toulouse, France  
Luca Prodi, Bologna, Italy  
Jan Reedijk, Leiden, The Netherlands

David Reinhoudt, Enschede,  
The Netherlands  
Kari Rissanen, Jyväskylä, Finland  
Clément Sanchez, Paris, France  
Jeremy K. M. Sanders, Cambridge, UK  
Jean-Pierre Sauvage, Strasbourg,  
France  
Jonathan W. Steed, Durham, UK  
Vivian Yam, Hong Kong, PR China

## INFORMATION FOR AUTHORS

Full details on how to submit material for publication in New Journal of Chemistry are given in the Instructions for Authors (available from <http://www.rsc.org/authors>). Submissions should be made via the journal's homepage: <http://www.rsc.org/njc>.

Authors may reproduce/republish portions of their published contribution without seeking permission from the CNRS and the RSC, provided that any such republication is accompanied by an acknowledgement in the form: (Original Citation) – Reproduced by permission of the CNRS and the RSC

©The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2010. Apart from fair dealing for the purposes of research or private study for non-commercial purposes, or criticism or review, as permitted

under the Copyright, Designs and Patents Act 1988 and the Copyright and Related Rights Regulation 2003, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission in writing of the Publishers or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK. US copyright law is applicable to users in the USA.

The Royal Society of Chemistry takes reasonable care in the preparation of this publication but does not accept liability for the consequences of any errors or omissions.

☞ The paper used in this publication meets the requirements of ANSI/NISO Z39.48–1992 (Permanence of Paper).

Royal Society of Chemistry: Registered Charity No. 207890.

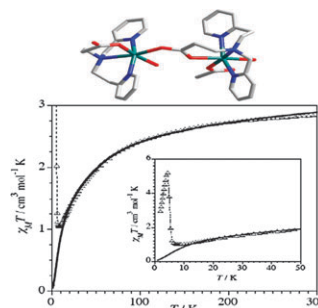
## PERSPECTIVES

2357

**Coordination polymers using (2-pyridyl)alkylamine-appended carboxylates: magnetic properties**

Himanshu Arora and Rabindranath Mukherjee\*

(2-Pyridyl)alkylamine-appended carboxylate ligands can be used to construct coordination polymers of varying dimensionality that exhibit magnetic interactions.

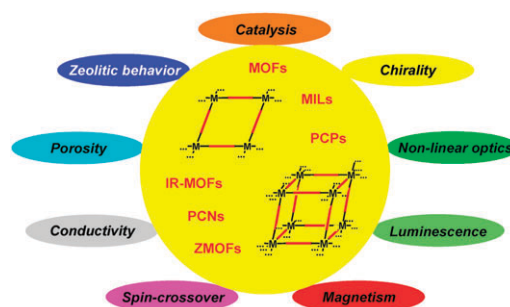


2366

**MOFs, MILs and more: concepts, properties and applications for porous coordination networks (PCNs)**

Christoph Janiak\* and Jana K. Vieth

This review (over 380 references) summarizes metal–organic frameworks (MOFs), Materials Institute Lavoisier (MILs), iso-reticular metal–organic frameworks (IR-MOFs), porous coordination networks (PCNs), zeolitic metal–organic frameworks (ZMOFs) and porous coordination polymers (PCPs) with selected examples of their structure and function.



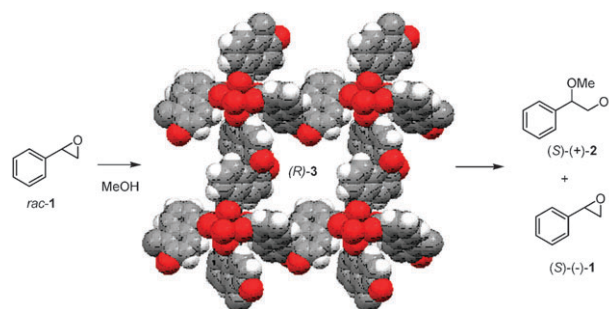
## LETTERS

2389

**Asymmetric alcoholytic kinetic resolution of styrene oxide catalysed by chiral metal–organic framework crystals**

Koichi Tanaka\* and Ken-ichi Otani

The methanolytic kinetic resolution of styrene oxide *rac*-**1** catalyzed by chiral metal–organic framework crystals (*R*)-**3** afforded both 2-methoxy-2-phenylethanol (*S*)-(+)-**2** and unreacted styrene oxide (*S*)-(–)-**1** in good enantiomeric excesses.

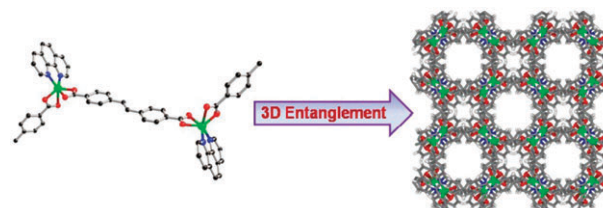


2392

**Solvent-free porous framework resulted from 3D entanglement of 1D zigzag coordination polymer**

Goutam Kumar Kole, Amy J. Cairns, Mohamed Eddaoudi\* and Jagadees J. Vittal\*

The role of solvents and reaction conditions in the formation of an unusual solvent-free porous metal organic framework, built from the entanglement of 1D zigzag coordination polymers is presented.



New  
Journal

# Food & Function

Linking the chemistry and physics of food with health and nutrition

www.rsc.org/foodfunction

Volume 1 | Number 1 | 2010 | Pages 1-100

ISSN 2042-4496

RSC Publishing

## Food & Function

Linking the chemistry and physics of food with health and nutrition

Food science and nutrition is a highly multidisciplinary area. We know it can be difficult to keep abreast of each other's work, especially when there is not enough time in the day and the pile of work keeps growing.

Wouldn't it be great if there was a journal which pulled together high impact chemical and physical research linking to human health and nutrition? Just one platform to find what you need in the field, and reach exactly the right audience when you publish your work.

*Food & Function* provides a dedicated venue for physicists, chemists, biochemists, nutritionists and other health scientists focusing on work related to the interaction of food components with the human body.

**Go to the website now to submit your research  
and register for free access!**

RSC Publishing

[www.rsc.org/foodfunction](http://www.rsc.org/foodfunction)

Registered Charity Number 207890

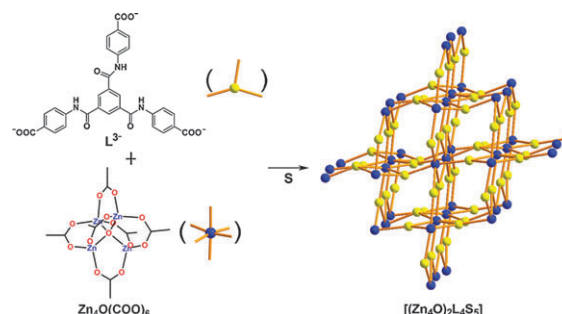
## LETTERS

2396

**A two-fold interpenetrated (3,6)-connected metal–organic framework with rutile topology showing a large solvent cavity**

Xiaokai Song, Yang Zou, Xinfang Liu, Minhak Oh and Myoung Soo Lah\*

A combination of a nanometre-sized tritopic trisbenzoic acid and an octahedral hexatopic  $\text{Zn}_4\text{O}(\text{COO})_6$  secondary building unit led to a two-fold interpenetrated binodal (3,6)-connected network with an **rtl** topology and a large solvent cavity.

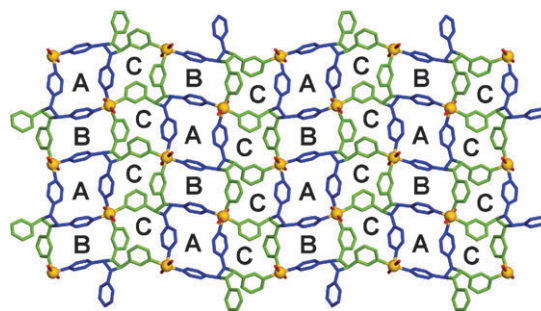


2400

**A metal–organic framework with three cavities based on three-coloured square tiling derived from a cyclobutane constructed in the solid state**

Tamara D. Hamilton, Dejan-Krešimir Bučar and Leonard R. MacGillivray\*

A 2D MOF with a topology that conforms to 3-uniform colour tiling has been achieved using a ligand synthesized by a templated solid-state reaction.



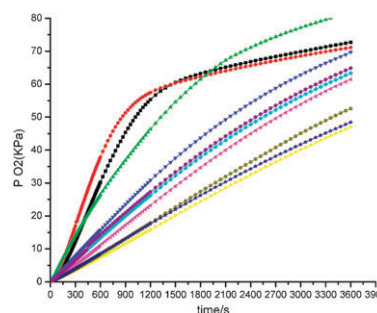
## PAPERS

2403

**Supramolecular assembly under the control of the chelating ligand for the  $\text{Mn}^{\text{II}}$ /bridging ligands/3-sulfobenzoate system and catalytic properties for the disproportionation of hydrogen peroxide**

Xiao-He Miao and Long-Guan Zhu\*

Six  $\text{Mn}^{\text{II}}$  3-sulfobenzoate complexes with neutral ligands show diverse structures and topology and catalytic experiments strongly suggest that these six complexes are catalytically active for the disproportionation of  $\text{H}_2\text{O}_2$  in the presence of imidazole. Complex **3** has the best catalytic activity.

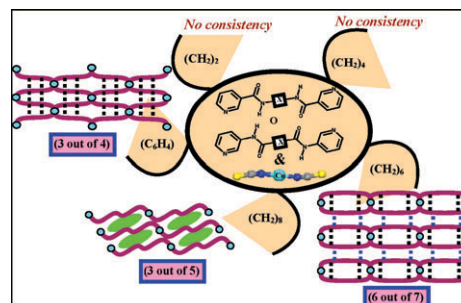


2415

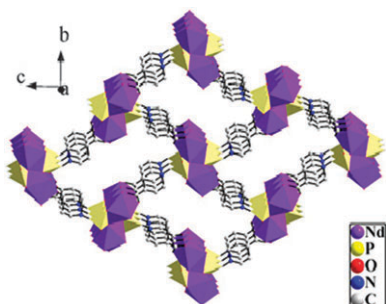
**Assembling coordination networks of bis-amido pyridines *via* hydrogen bonds: isostructurality and large hydrophobic cavities for guest inclusion**

Lalit Rajput and Kumar Biradha\*

Amides and reverse amides were shown to form coordination networks with  $\text{Cu}(\text{II})$  with the ability to include various guest molecules. The ligands with longer spacers such as  $-(\text{CH}_2)_6-$ ,  $-(\text{CH}_2)_8-$  or phenyl have exhibited consistency in network geometries and also iso-structurality between the coordination network geometries of amides and reverse amides.



2429

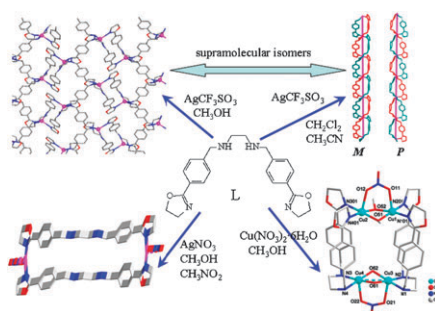


### Synthesis, crystal structure and luminescence properties of eight new lanthanide carboxyphosphonates with a 3D framework structure

Na Zhang, Zhengang Sun,\* Yanyu Zhu, Jing Zhang, Lei Liu, Cuiying Huang, Xin Lu, Weinan Wang and Fei Tong

By using the carboxyphosphonic acid as the ligand, eight new lanthanide carboxyphosphonates,  $\text{Ln}[\text{L}(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$ , have been hydrothermally synthesized and structurally characterized.

2436

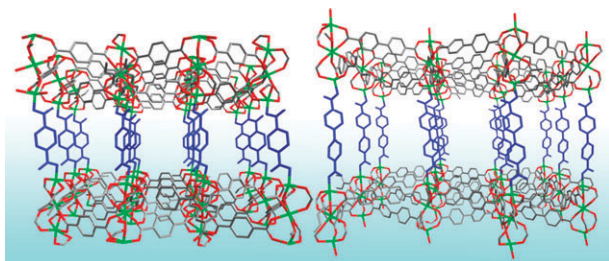


### Syntheses, crystal structures and properties of silver(I) and copper(II) complexes with an oxazoline-containing tetradentate ligand

Yong-Qing Huang, Guang-Xiang Liu, Xia-Ying Zhou, Taka-aki Okamura, Zhi Su, Jian Fan, Wei-Yin Sun,\* Jin-Quan Yu\* and Norikazu Ueyama

Supramolecular isomers with a wavelike cationic two-dimensional network and double-stranded helical chain structures and related frameworks with the same flexible oxazoline-containing tetradentate ligand are reported.

2445

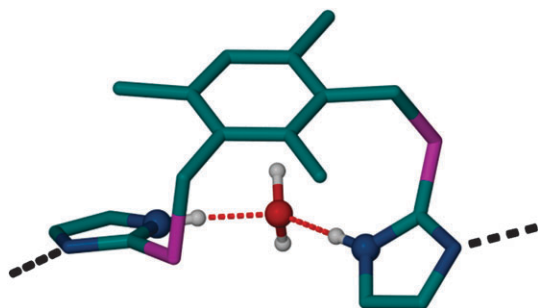


### Synthesis, crystal structures, luminescent and thermal properties of two new metal-organic coordination polymers based on zinc(II) carboxylates

Sergey A. Sapchenko, Danil N. Dybtsev, Denis G. Samsonenko and Vladimir P. Fedin\*

Two novel 3D coordination polymers with anionic framework are synthesized and characterized. Also, it is shown that addition of soluble ionic salts to the reaction media promotes the formation of charged compounds and can be generalized for the synthesis of other porous coordination polymers with ionic nature.

2451



### Solvent-mediated conformational similarities within a series of 1D coordination polymers constructed from a new flexible ditopic bis-imidazole ligand

Storm V. Potts and Leonard J. Barbour\*

Solvated complexes of a new conformationally flexible ditopic ligand 1,3-bis(1-imidazolyl-2-thione)-2,4,6-trimethylbenzene were characterized by means of single-crystal X-ray diffraction and compared with one another by means of Hirshfeld surface analysis.

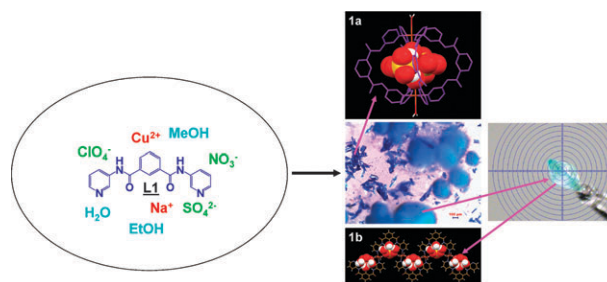
## PAPERS

2458

**Metalla-macro-tricyclic cryptands: anion encapsulation and selective separation of sulfate *via in situ* crystallization**

N. N. Adarsh, Derek A. Tocher, Joan Ribas and Parthasarathi Dastidar\*

An *in situ* crystallization technique under competitive conditions proved to be viable for separating important anions such as  $\text{SO}_4^{2-}$  as concomitantly formed neat crystals of metallacryptand **1a** and 1D zig-zag coordination polymer **1b** from a complex mixture of anions containing  $\text{SO}_4^{2-}$ ,  $\text{NO}_3^-$  and  $\text{ClO}_4^-$ .

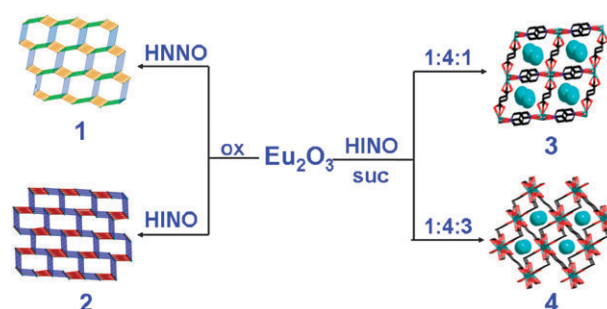


2470

**Design of 3-D europium(III)-organic frameworks based on pyridine carboxylate *N*-oxide and acyclic binary carboxylate: syntheses, structures, and luminescence properties**

Lijuan Zhang, Donghua Xu, Yunshan Zhou\* and Fei Jiang

The ligand coordination mode, the length of the acyclic binary carboxylate, the ligand conformation and the molar ratio of reactants decides the formation of four 3-D europium(III) frameworks of different structures.

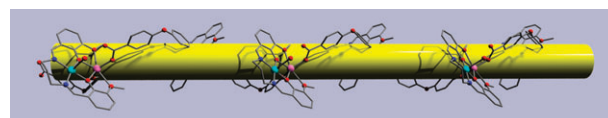


2479

**New heterometallic coordination polymers constructed from 3d–3d' binuclear nodes**

Diana G. Branzea, Augustin M. Madalan, Samuele Ciattini, Narcis Avarvari, Andrea Caneschi and Marius Andruh\*

New heterometallic coordination polymers have been constructed by connecting binuclear nodes  $[\text{Cu}^{\text{II}}\text{Mn}^{\text{II}}]$  and  $[\text{Cu}^{\text{II}}\text{Co}^{\text{II}}]$ , with polycarboxylate anions as spacers.

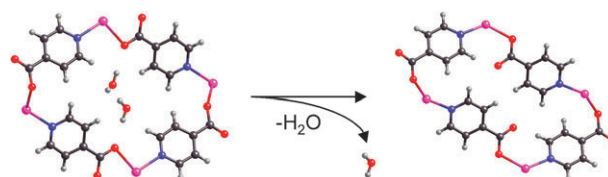


2491

**From crystal to crystal: a new polymorph of (4-carboxylatopyridine)silver(I) by topotactic dehydration of its monohydrate**

Irmgard Kalf, Patrick Mathieu and Ulli Englert\*

A new polymorph of (4-carboxylatopyridine)silver(I) can be obtained by single-crystal-to-single-crystal dehydration. The water molecules leave the reactant crystal, and the coordination framework adapts to a new long-range order.





# International Symposia on Advancing the Chemical Sciences

A new generation of global conferences

## Call for Abstracts

Present your latest research at the International Symposia on Advancing the Chemical Sciences (ISACS) - a significant new global symposia series organised by the RSC. Poster and oral abstracts are invited to supplement the following exceptional plenary speaker line-ups:



### Challenges in Renewable Energy (ISACS4)

5-8 July 2011 • Boston, USA • [www.rsc.org/isacs4](http://www.rsc.org/isacs4)

**Speakers:** Hector Abruña, Fraser Armstrong, James Barber, Allen J Bard, Peter Bruce, Kazunari Domen, Gérard Férey, Leif Hammarström, Cliff Kubiak, Akihiko Kudo, James McCusker, Thomas Moore, Debra Rolison, Michael Strano, Peng Wang, Michael Wasielewski, Andreas Züttel.

Poster deadline **6th May 2011**, oral deadline **21st January 2011**



### Challenges in Chemical Biology (ISACS5)

26-29 July 2011 • Manchester, UK • [www.rsc.org/isacs5](http://www.rsc.org/isacs5)

**Speakers:** Venki Ramakrishnan, Thomas Steitz, Donna Blackmond, Andrew Ellington, Hermann Gaub, Reza Ghadiri, Andrew Griffiths, Bartosz A Grzybowski, Philip Holliger, Clyde Hutchison, Stefan Knapp, Stephen Mann, David Rees, Hugh Rosen, William Shih, Hiroaki Suga, Erik Winfree.

Poster deadline **27th May 2011**, oral deadline **21st January 2011**



### Challenges in Organic Materials & Supramolecular Chemistry (ISACS6)

2-5 September 2011 • Beijing, China • [www.rsc.org/isacs6](http://www.rsc.org/isacs6)

**Speakers:** Takuzo Aida, Harry Anderson, Matthew Francis, Philip Gale, Wenping Hu, Myongsoo Lee, David Leigh, Stefan Matile, Colin Nuckolls, Jian Pei, Julius Rebek Jr, Hanadi Sleiman, Samuel Stupp, Benzong Tang, Xi Zhang.

Poster deadline **8th July 2011**, oral deadline **18th March 2011**

Join in – submit your abstract today!

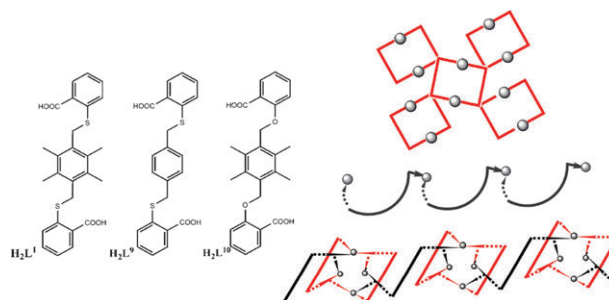
## PAPERS

2496

### The effect of the conformation of flexible carboxylate ligands on the structures of metal–organic supramolecules

Fangna Dai, Shuwen Gong, Peipei Cui, Guoqing Zhang, Xiaoliang Qiu, Fei Ye, Daofeng Sun,\* Zhijian Pang, Lei Zhang, Guilin Dong and Changqiao Zhang\*

Three metal–organic supramolecules constructed from flexible dicarboxylate ligands have been synthesized, and the effect of the conformation of the ligands on the final structures has been discussed.

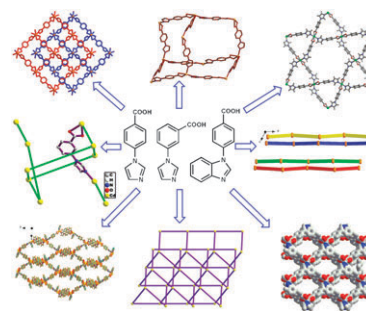


2502

### Coordination polymers of various architectures built with mixed imidazole/benzimidazole and carboxylate donor ligands and different metal ions: syntheses, structural features and magnetic properties

Arshad Aijaz, Prem Lama, E. Carolina Sañudo, Rupali Mishra and Parimal K. Bharadwaj\*

A series of coordination polymers have been synthesized with rigid ditopic ligands having interesting topologies including, square, Kagome, diamondoid, layer, self-penetrating 2D and 3D nets.

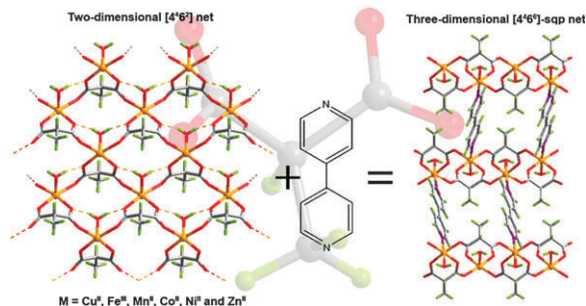


2515

### Metal–organic coordination frameworks based on mixed methylmalonate and 4,4′-bipyridine ligands: synthesis, crystal structure and magnetic properties

Mariadel Déniz, Jorge Pasán, Oscar Fabelo, Laura Cañadillas-Delgado, Francesc Lloret, Miguel Julve and Catalina Ruiz-Pérez\*

We report on three-dimensional networks based on methylmalonate layers of transition metal ions [Cu(II), Fe(III), Mn(II), Co(II), Ni(II) and Zn(II)] pillared by 4,4′-bipyridine ligands.



## GENERAL ARTICLES

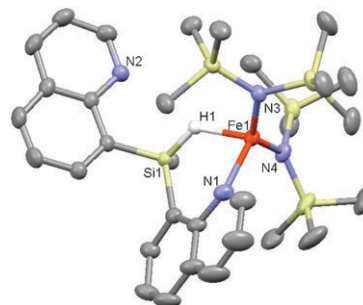
## LETTERS

2528

### (MeQn<sub>2</sub>SiH)Fe[N(SiMe<sub>3</sub>)<sub>2</sub>]<sub>2</sub> (Qn = 8-quinolyl): an unusual δ-agostic iron complex containing an η<sup>1</sup>-SiH interaction

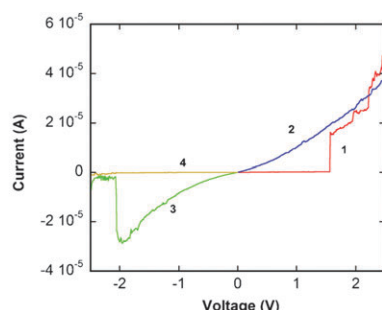
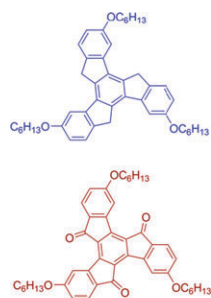
Jian Yang, Meg Fasulo and T. Don Tilley\*

Reaction of MeQn<sub>2</sub>SiH (Qn = 8-quinolyl) (**1**) with Fe[N(SiMe<sub>3</sub>)<sub>2</sub>]<sub>2</sub> at room temperature afforded (MeQn<sub>2</sub>SiH)Fe[N(SiMe<sub>3</sub>)<sub>2</sub>]<sub>2</sub> (**2**), which is an unusual example of a δ-agostic iron complex containing an η<sup>1</sup>-H–Si interaction. Treatment of **2** with excess 3-pentanone at 60 °C produced MeQn<sub>2</sub>SiOCH<sub>2</sub>Et<sub>2</sub> (**3**) in *ca.* 80% yield.



## LETTERS

2530

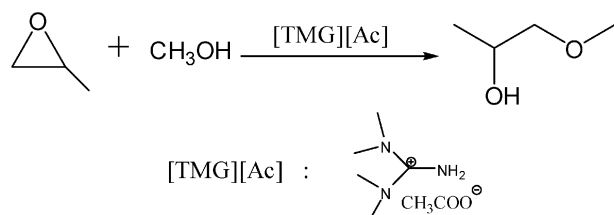


### A co-assembly system of an aromatic donor and acceptor: charge transfer, electric bistability and photoconductivity

Jia Luo, Linfeng Chen, Jie-Yu Wang, Ting Lei, Li-Yi Li, Jian Pei\* and Yanlin Song\*

A co-assembly system organized through the interaction between a donor and an acceptor was developed, in which the charge transfer (CT) process taking place proved to be a key point for achieving both electric bistability and photoconductivity.

2534



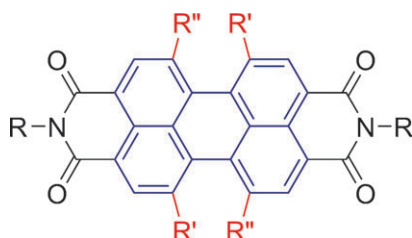
### The tetramethylguanidine-based ionic liquid-catalyzed synthesis of propylene glycol methyl ether

Shuguang Liang, Huizhen Liu, Yinxi Zhou, Tao Jiang\* and Buxing Han\*

1-Methoxy-2-propanol was produced with nearly 90% yield under much milder conditions through the reaction of methanol and propylene oxide using tetramethylguanidine-based ionic liquids as effective and recyclable catalysts.

## PAPERS

2537

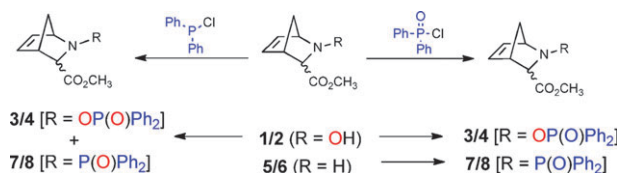


### Synthesis and characterization of 1,7-disubstituted and 1,6,7,12-tetrasubstituted perylenetetracarboxy-3,4:9,10-diimide derivatives

Mathieu Queste, Cyril Cadiou, Bernard Pagoaga, Louis Giraudet and Norbert Hoffmann\*

1-, 6-, 7- or 12- di- and tetrasubstituted perylenetetracarboxydiimide derivatives were synthesized. Using cyclic voltammetry, UV/vis and fluorescence spectroscopy, the energies of the frontier orbitals were determined and the influence of the substituents on these energies is discussed.

2546



### Phosphorylation of 2-azabicyclo[2.2.1]hept-5-ene and 2-hydroxy-2-azabicyclo[2.2.1]hept-5-ene systems: synthesis and mechanistic study

Carlos A. D. Sousa, M. Luísa C. Vale, José E. Rodríguez-Borges\* and Xerardo García-Mera

The *endo/exo* isomers of azabicyclic compounds **1**, **2**, **5** and **6** were treated with OPClPh<sub>2</sub> and ClPPH<sub>2</sub>, respectively, to afford phosphorylated/phosphinoylated bicycles. A mechanistic explanation for the unusual phosphorylation process is proposed.

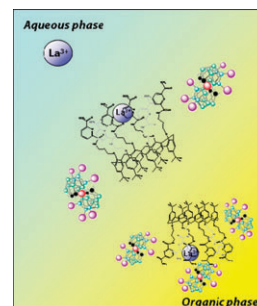
## PAPERS

2552

**Assessing the mechanism of the synergistic action of calixarenes and Co-dicarbollides in lanthanide extractions**

Elena Macerata, Franca Castiglione, Walter Panzeri, Mario Mariani, Francesco Sansone, Alessandro Casnati\* and Andrea Mele\*

The extraction mechanism of lanthanide ions *via* a supramolecular ternary association: *lanthanide/calixarene/Co-dicarbollide* was elucidated by using  $^1\text{H}$  and  $^{11}\text{B}$  NMR, ESI-MS, and FTMS ICR.

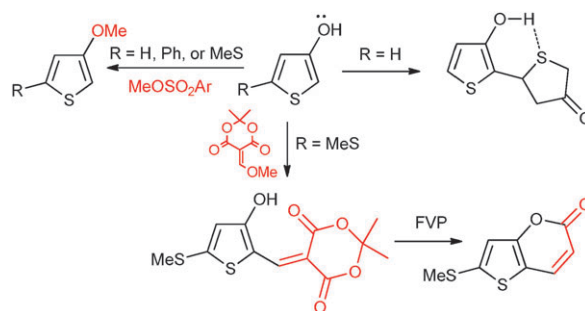


2558

**Chemical and spectroscopic properties of the 3-hydroxythiophene [thiophen-3(2H)-one] system**

Gordon A. Hunter and Hamish McNab\*

The chemistry of 3-hydroxythiophenes is studied, including dimerisation of 3-hydroxythiophene itself, tautomerism, reactivity with electrophiles and nucleophiles and *O*-alkylation and *O*-acylation.

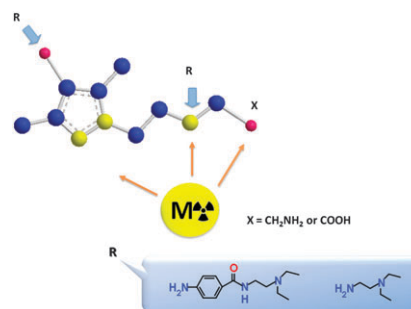


2564

**Synthesis, characterization and biological evaluation of tricarbonyl M(I) (M = Re,  $^{99\text{m}}\text{Tc}$ ) complexes functionalized with melanin-binding pharmacophores**

Carolina Moura, Teresa Esteves, Lurdes Gano, Paula D. Raposo, António Paulo\* and Isabel Santos

The pre-clinical evaluation of  $^{99\text{m}}\text{Tc(I)}$  tricarbonyl complexes anchored by bifunctional pyrazolyl-containing ligands has shown that some of the compounds present a certain degree of selectivity towards melanoma tissue.

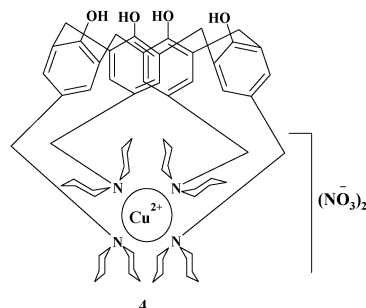


2579

**A highly copper selective chromogenic calix[4]arene derivative**

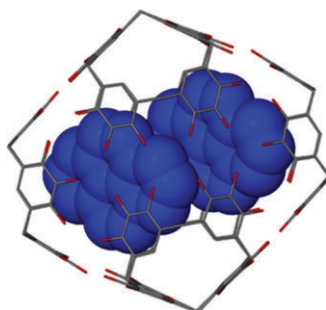
Mansoor Ahmed Qazi, Imdadullah Qureshi and Shahabuddin Memon\*

The synthesized ligand **4** was found to be selective toward  $\text{Cu}^{2+}$  among a series of selected metal ions, which may be due to the compatibility between the metal and ligand. Moreover, ionic radii, nature, number of binding sites, cavity size and geometry of **4** play an important role in selective complexation.



## PAPERS

2587

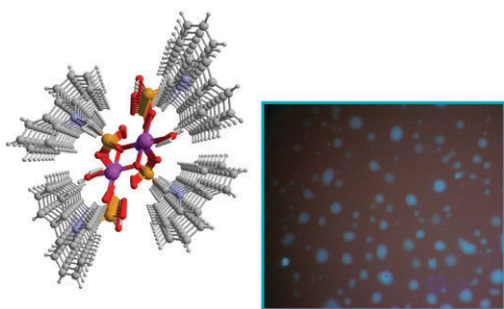


### Spectroscopic investigations of pyrene butanol encapsulated in *C*-hexylpyrogallol[4]arene nanocapsules

Jena L. Whetstone, Katrina K. Kline, Drew A. Fowler, Cheryl M. Ragan, Charles L. Barnes, Jerry L. Atwood\* and Sheryl A. Tucker

A crystallographic perspective of PBOH encapsulated within  $\text{PgC}_6$ .

2592

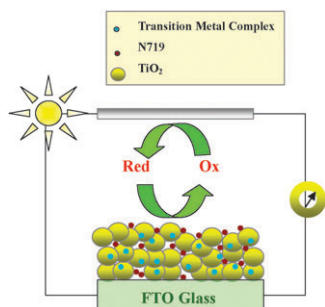


### *N*-Carbazolymethylphosphonic acid—synthesis, metal coordination, emissive aggregate formation and spectroscopic features

Ester Buchaca, Siud Pui Man, Majid Motevalli, John Wilson and Alice Sullivan\*

Diethylcarbazolymethylphosphonic acid **1** forms a 2 : 1 manganese(II) complex with stacked carbazole units bordering a columnar inorganic core. Blue emissive micron size aggregates of **1** form on glass substrates upon spin coating from micromolar solutions of **1**.

2599

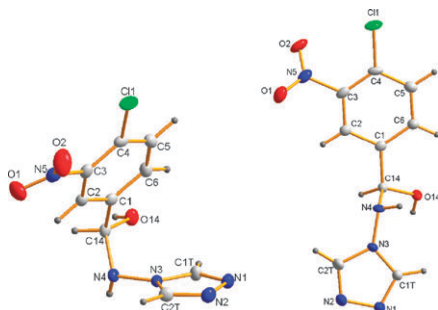


### Co-sensitized dye-sensitized solar cells based on $d^{10}$ coordinate complexes towards their optoelectronic properties

Xin Wang, Yulin Yang,\* Ruiqing Fan\* and Zhaohua Jiang

$d^{10}$  transition metal complexes with a [bis(iminoalkyl)pyridine] ligand connected to N719 as a co-sensitized photoelectrode present an improved optoelectronic performance compared to single dyes in DSSCs.

2605



### Stable hemiaminals containing a triazole ring

Maciej Barys, Zbigniew Ciunik,\* Krzysztof Drabent and Anna Kwiecień

The reaction of nitrobenzaldehyde derivatives with 4-amino-1,2,4-triazole show a new simple route to stable hemiaminals with two chiral centers, in which both conformation and configuration are highly correlated.

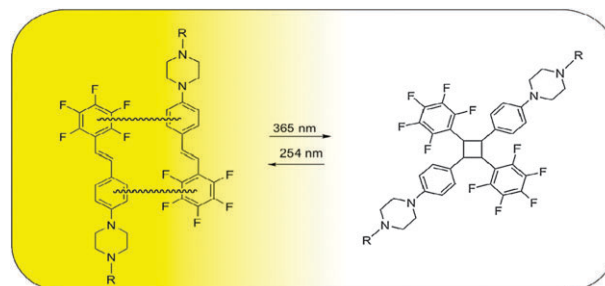
## PAPERS

2612

**Novel fluorinated amino-stilbenes and their solid-state photodimerization**

Antonio Papagni,\* Paola Del Buttero, Chiara Bertarelli, Luciano Miozzo, Massimo Moret, Mary T. Pryce and Silvia Rizzato

Solid state topochemical photodimerizations of polyfluoro-amino-stilbenes are driven by arene-fluoroarene interactions, promoting their reversible photochemical [2 + 2] cyclization in the solid state.

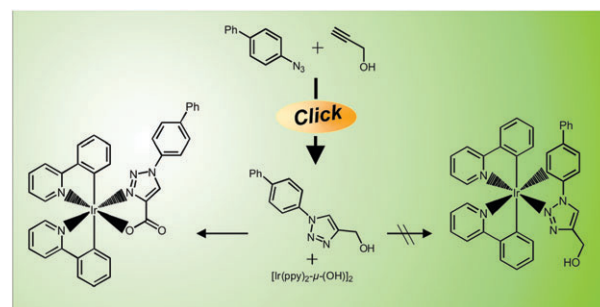


2622

**Unexpected metal-mediated oxidation of hydroxymethyl groups to coordinated carboxylate groups by bis-cyclometalated iridium(III) centers**

Beatrice Beyer, Christoph Ulbricht, Andreas Winter, Martin D. Hager, Richard Hoogenboom, Nicole Herzer, Stefan O. Baumann, Guido Kickelbick, Helmar Görls and Ulrich S. Schubert\*

The “click” reaction approach was used to synthesize a series of functionalized 1-phenyl- and 4-phenyl-1*H*-[1,2,3]-triazoles.

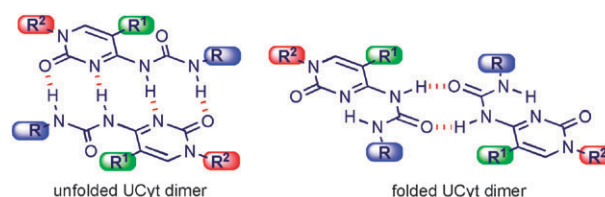


2634

**Cytosine modules in quadruple hydrogen bonded arrays**

Elisabetta Greco, Abil E. Aliev, Valerie G. H. Lafitte, Kason Bala, David Duncan, Laura Pilon, Peter Golding and Helen C. Hailes\*

Cytosine modules have been investigated for applications in supramolecular quadruple hydrogen bonded arrays, including variation at R and R<sup>2</sup> (different alkyl chain lengths) and R<sup>1</sup> (H or F), and the influence on the ratio of the unfolded : folded rotamers determined. A polyadipate telechelic polymer was also used to prepare novel cytosine polymers.

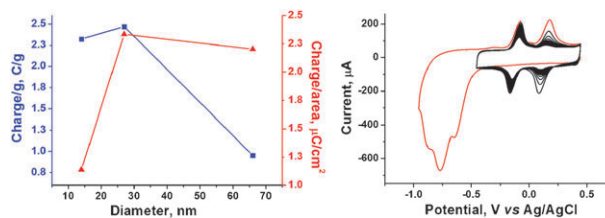


2643

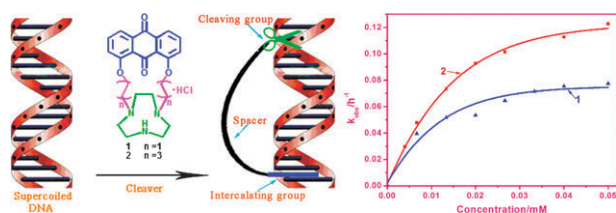
**Size-effects in the chemical modification of carbon black nanoparticles with 4-nitroaniline**

Janjira Panchompoo, Leigh Aldous and Richard G. Compton\*

A range of carbon black primary nanoparticle sizes were investigated; conditions required in order to obtain strongly bound redox compounds are discussed and size effects noted.



2654

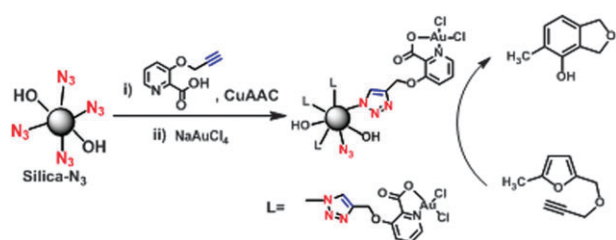


### Synthesis and DNA cleavage activity of triazacrown-anthraquinone conjugates

Weihong Xu, Xiaoli Yang, Lian Yang, Zhao-Li Jia, Li Wei, Fang Liu and Guo-Yuan Lu\*

Two triazacrown-anthraquinone conjugates were synthesized as new metal-free DNA cleaving reagents, and their cleavage efficiency, interactions with DNA were studied by spectroscopic techniques and agarose gel electrophoresis.

2662

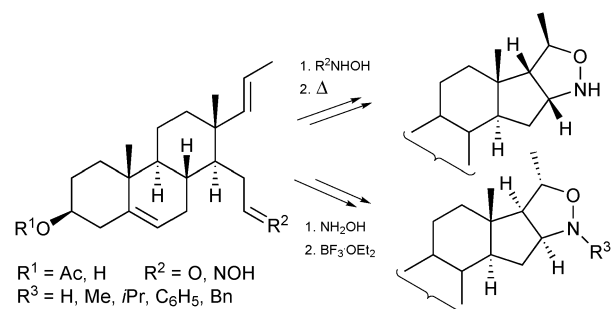


### 'Clicking' molecular hooks on silica nanoparticles to immobilize catalytically important metal complexes: the case of gold catalyst immobilization

Anal Kr. Ganai, Rima Bhardwaj, Srinivas Hotha,\* Sayam Sen Gupta\* and B. L. V. Prasad\*

An Au(III) complex has been "clicked" onto silica nanoparticles by using alkynalated picolinic acid as a "molecular hook", and this nano-conjugate's catalytic activity on furanyl propargyl ethers to give isobenzofurans has been investigated.

2671



### Intramolecular approach to some new D-ring-fused steroidal isoxazolidines by 1,3-dipolar cycloaddition: synthesis, theoretical and *in vitro* pharmacological studies

Éva Frank,\* Zoltán Mucsi, Mihály Szécsi, István Zupkó, János Wölfling and Gyula Schneider

Novel androstene-fused isoxazolidines have been obtained diastereoselectively *via* thermally induced and Lewis acid-catalysed intramolecular [3 + 2] cycloaddition of a D-secopregnene aldehyde and its aldoxime derivative.