ISSN 1144-0546 CODEN NJCHES 29(6) 749-856 (2005)

In this issue...

Letters from Janine Cossy, Pierre. H. Dixneuf, Hongbin Zhang, Baowen Zhang and Chun-Ying Duan



The front cover illustrates the formation and disassembly of a host-quest complex. A hydrocarbon, whose shape resembles a tweezer, acts as a host for tetracyanobenzene. There is a charge transfer interaction between the host and guest and luminescence of charge transfer origin is observed from the host-guest complex. The association constant and the association/dissociation barriers for complex formation have been determined by using spectroscopic and electrochemical

Image reproduced by permission of Filippo Marchioni, Alberto Juris, Matthias Lobert, Uta P. Seelbach, Björn Kahlert and Frank-Gerrit Klärner, New J. Chem., 2005, 29, 780.

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, as well as the most significant scientific advances.

Chemical Science

June 2005/Volume 2/Issue 6

www.rsc.org/chemicalscience

OPINION

759



A common misconception about the Eyring equation

Gábor Lente,* István Fábián and Anthony J. Poë

Linearization and direct fitting to the Eyring equation both give the entropy of activation with the same reliability as that of the enthalpy of activation.

$$k = \frac{k_B T}{h} \exp\left(-\frac{\Delta G^{\ddagger}}{RT}\right) = \frac{k_B T}{h} \exp\left(-\frac{\Delta H^{\ddagger}}{RT} + \frac{\Delta S^{\ddagger}}{R}\right)$$
$$\sigma(\Delta S^{\ddagger}) = \frac{1}{T_{av}} \sigma(\Delta H^{\ddagger})$$

EDITORIAL STAFF

Managing editor (RSC)

Mike Corkill

Managing editor (CNRS)

Assistant managing editor

Gérard Calleia (CNRS)

Publishing assistant

Team leader, serials production

Helen Saxton (RSC)

Technical editors

Caroline Moore (RSC) Celia Clarke (RSC) Ken Wilkinson (RSC)

Editorial secretaries

Florence Lepage (CNRS) Sonya Spring Julie Thompson Rebecca Gotobed

Publisher, journals and reviews

Adrian Kybett (RSC)

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 Portland Customer Services, Commerce Way, Colchester, Essex, CO2 8HP, UK. Tel +44 (0) 1206 226050; E-mail sales@rscdistribution.org

2005 Annual (print + electronic) subscription price: £650; US\$1075. 2005 Annual (electronic) subscription price: £585; US\$965. 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. 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 432243; Fax +44 (0) 1223 426017; E-mail advertising@rsc.org

New Journal of Chemistry

An international journal for the chemical sciences

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

Editor-in-chief

Jean-Pierre Majoral, Toulouse, France

Consulting editor

Odile Eisenstein, Montpellier, France

Board members

Laurent Bonneviot, Lyon, France John A Gladysz, Erlangen, Germany George Gokel, St Louis, MO, USA Luca Prodi, Bologna, Italy Paul Raithby, Bath, UK David Reinhoudt, Enschede, The Netherlands

Alan Rowan, Nijmegen, The Netherlands Michael Scott, Gainesville, FL, USA Jonathan W Steed, Durham, UK Michael Veith, Saarbrücken, Germany Vivian Yam, Hong Kong, PR China

Associate editors

Manuscripts should be directed to the appropriate Editor detailed

Supramolecular chemistry and crystal engineering

Dr Jonathan W Steed Department of Chemistry University Science Laboratories University of Durham South Road Durham UK DH1 3LF Fax (+44) (0) 191 384 4737 Tel (+44) (0) 191 384 2085 E-mail jon.steed@dur.ac.uk

Organic & bioorganic

Professor George Gokel Departments of Chemistry and Molecular Biology & Pharmacology Washington University Medical Campus Box 8103 660 S. Euclid Ave. St Louis, MO 63110, USA Fax (+1) 314 362 9298 Tel (+1) 314 362 9297 E-mail ggokel@molecool.wustl.edu Alternatively, any author may submit direct to the

Montpellier Editorial Office

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

International advisory board

Markus Antonietti, MPI, Potsdam, Germany Didier Astruc, Talence, France Jerry Atwood, Columbia, MO, Pierre Braunstein, Strasbourg, France

Kenneth Caulton, Bloomington, IN, USA Robert Crabtree, New Haven,

CT. USA

Pierre Dixneuf, Rennes, France

François Fajula, Montpellier, France Andrew B Holmes, Melbourne, Australia Reinhard W Hoffmann, Marburg, Germany Miguel Julve, Valencia, Spain Peter Junk, Monash, Australia Henryk Koslowski, Wroclaw, Poland

Bernard Meunier, Toulouse,

France

Jan Reedijk, Leiden, The Netherlands Kari Rissanen, Jyväskylä, Finland Clément Sanchez, Paris, France Jeremy K M Sanders, Cambridge, UK Philippe Sautet, Lyon, France Jean-Pierre Sauvage, Strasbourg, France Ulrich Schubert, Vienna, Austria Hideki Sugihara, Tsukuba, Japan

INFORMATION FOR AUTHORS

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 2005. 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 Regulations 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 Royal Society of Chemistry (the Publisher) 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 (the Publisher) 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.

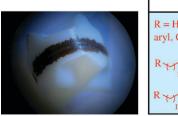
LETTERS

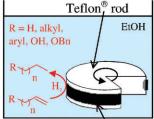
761

Hydrogenation versus hydrogenolysis with a safe, selective and reusable catalyst: palladium black on Teflon

Damien Belotti, Guillaume Cantagrel, Catherine Combellas, Janine Cossy,* Frédéric Kanoufi and Sandra Nunige

Palladium black deposit on the Teflon polymer surface of magnetic stirring bars, deposited by an electrochemical process, can be used to perform hydrogenation of olefins and acetylenic compounds whilst hydrogenolysis is not observed.





Pd/TMSB

Hydrogenation with Pd/TMSB

Pd deposit

765



Direct propargylation of furan and arene by propargylic alcohols promoted by bisoxazoline-ruthenium catalysts

Cédric Fischmeister, Loïc Toupet and Pierre. H. Dixneuf* Synthesis and characterisation of a dicationic rutheniumbisoxazoline complex which shows catalytic activity for the nucleophilic substitution of propargylic alcohols.



769



Efficient synthesis of β -amino- α , β -unsaturated carbonyl compounds

Yuanhong Zhao, Jingfeng Zhao, Yongyun Zhou, Ze Lei, Liang Li and Hongbin Zhang*

An environmentally friendly and high-yielding procedure for the synthesis of β -enamino esters and β -enaminones is presented.

R1 = Alkyl, Aryl; R2 = Alkyl, EtO; R3 = H, Alkyl; R4 = H, Alkyl, Aryl

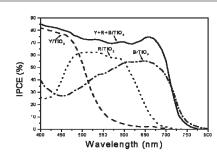
773



Highly efficient co-sensitization of nanocrystalline TiO₂ electrodes with plural organic dyes

Yousheng Chen, Zhanghua Zeng, Chao Li, Weibo Wang, Xuesong Wang* and Baowen Zhang*

A nanocrystalline TiO₂ solar cell co-sensitized by three organic dyes exhibited an overall power conversion efficiency (η) of 6.5% (AM1.5, 80 mW cm⁻²), the highest η to date for dye-sensitized solar cells based on the co-sensitization of plural organic dyes.

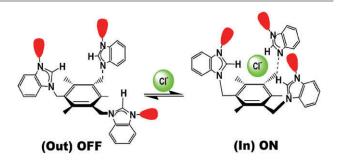


777

Conformational switching fluorescent chemosensor for chloride anion

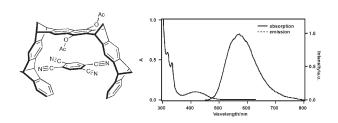
Yan Bai, Bing-Guang Zhang, Jian Xu, Chun-Ying Duan,* Dong-Bin Dang, De-Jun Liu and Qing-Jin Meng*

A new sensor using a guest-induced conformational switching process was achieved by using a positively charged tripodal receptor with naphthyl groups attached to the benzoimidazolium arms.



PAPERS

780

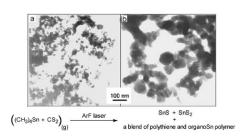


Luminescent host-guest complexes involving molecular clips and tweezers and tetracyanobenzene

Filippo Marchioni, Alberto Juris,* Matthias Lobert, Uta P. Seelbach, Björn Kahlert and Frank-Gerrit Klärner

Luminescence is observed for the first time from charge-transfer excited states in host–guest complexes. Photophysical and electrochemical investigations are used to measure the association constants and to investigate the association/dissociation dynamics.

785

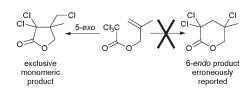


ArF laser photolysis of gaseous CS_2 – $(CH_3)_4Sn$ mixtures: gas-phase reaction between tin and sulfur and deposition of nanosized tin sulfides incorporated in a polymer network

Radmila Tomovska, Vladimír Vorlíček, Jaroslav Boháček, Jan Šubrt and Josef Pola*

Nanosized SnS and SnS₂ tin sulfides are produced by ArF laser photolysis of gaseous mixtures of carbon disulfide and tetramethyltin and are deposited in a blend of polythiene and organotin polymer.

789

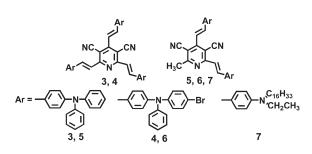


6-endo or not 6-endo, that is the question: correcting an erroneous structural assignment and mechanistic presumption

John Tamine* and Chenbo Wang

CuCl promoted radical cyclization of methallyl trichloroacetate yields the 5-exo product, along with the twelve-membered cyclic dimer, which had previously been mis-identified as the 6-endo cyclization product.

792

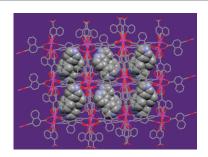


Synthesis and properties of new two-photon absorption chromophores containing 3,5-dicyano-2,4,6-tristyrylpyridine as the core

Hongli Wang, Zhen Li, Pin Shao, Yanke Liang, Hui Wang, Jingui Qin* and Qihuang Gong

New two- and three-branched chromophores based on 3,5-dicyano-2,4,6-tristyrylpyridine show efficient two-photon-induced orange-red fluorescence emission.

798



Second ligand-directed self-assembly of lanthanide(III) coordination polymers with 1,4-naphthalenedicarboxylate

Xiang-Jun Zheng, Lin-Pei Jin,* Song Gao and Shao-Zhe Lu

The addition of a second ligand, 4,4'-bipyridine, directs the self-assembly of two lanthanide coordination polymers with 1,4-naphthalenedicarboxylate, leading to an unprecedented 3D structure having large pores in which 4,4'-bipyridine is enclathrated.

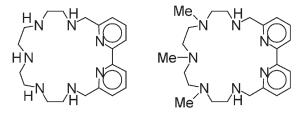
PAPERS

805

Co(II) and Cd(II) complexation with two dipyridinecontaining macrocyclic polyamines in water and dimethyl sulfoxide

Carla Bazzicalupi, Andrea Bencini, Antonio Bianchi,* Silvia Del Piero, Patrizia Fornasari, Claudia Giorgi, Andrea Melchior, Roberto Portanova, Marilena Tolazzi* and Barbara Valtancoli

The different solvation properties of macrocyclic polyamines brought about by N-methylation lead to quite different ligand coordination properties in solution.

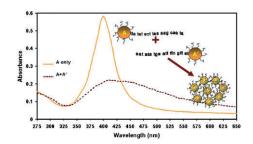


812

Stability and hybridization-driven aggregation of silver nanoparticle-oligonucleotide conjugates

Bernardo C. Vidal Jr.,* Theivanayagam C. Deivaraj, Jun Yang, Heng-Phon Too, Gan-Moog Chow, Leong M. Gan and Jim Y. Lee

Reversible hybridization of complementary DNA strands conjugated to Ag nanoparticles produces a plasmon band signature characteristic of Ag nanoparticle aggregation.

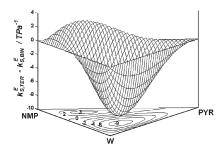


817

Solute-solvent interactions in lactams-water ternary solvents

Rafael Alcalde, Santiago Aparicio, Begoña García, María J. Dávila and José M. Leal*

The strong non-ideal behaviour of lactams-water ternary mixtures, revealed by the excess and mixing properties, is attributed to H-bonding heteroassociations and is analyzed at the microscopic level.

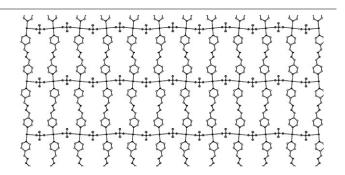


826

Chromophore containing bipyridyl ligands. Part 1: supramolecular solid-state structure of Ag(1) complexes

Alan R. Kennedy,* Karen G. Brown, Duncan Graham, Jennifer B. Kirkhouse, Madeleine Kittner, Claire Major, Callum J. McHugh, Paul Murdoch and W. Ewen Smith

The structures of a series of Ag(I) complexes with azine or azo based bipyridyl ligands have been determined. One-dimensional chains dominate these structures, but the three-dimensional packing of the chains is unpredictable.

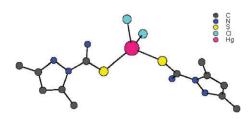


833

Structural, spectroscopic and computational studies of the HgL_2Cl_2 complex (L = 3,5-dimethyl-1-thiocarboxamide pyrazole) and the crystal structure of L

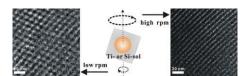
Attila Kovács,* Dénes Nemcsok, György Pokol, Katalin Mészáros Szécsényi,* Vukadin M. Leovac, Željko K. Jaćimović, Ivana Radosavljević Evans, Judith A. K. Howard, Zoran D. Tomić and Gerald Giester

Electronic and steric effects determine the Hg coordination to the ligand through the sulfur atoms instead of the nitrogens in the title HgL₂Cl₂ complex.



PAPERS

841

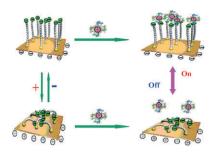


Selective control of cubic and hexagonal mesophases for titania and silica thin films with spin-coating

Jia Hong Pan and Wan In Lee*

Highly ordered cubic and hexagonal mesoporous TiO2 and SiO₂ thin films can be selectively obtained by varying the spin-coating conditions in the evaporation-induced self-assembly process.

847



Selective assembly of specifically charged proteins on an electrochemically switched surface

Li Mu, Ying Liu, Song Zhang, Baohong Liu and Jilie Kong*

A low-density self-assembled monolayer surface can be used for the selective assembly of charged proteins by switching the applied electrical potential.



AUTHOR INDEX

Alcalde, Rafael, 817 Aparicio, Santiago, 817 Bai, Yan, 777 Bazzicalupi, Carla, 805 Belotti, Damien, 761 Bencini, Andrea, 805 Bianchi, Antonio, 805 Boháček, Jaroslav, 785 Brown, Karen G., 826 Cantagrel, Guillaume, 761 Chen, Yousheng, 773 Chow, Gan-Moog, 812 Combellas, Catherine, 761 Cossy, Janine, 761 Dang, Dong-Bin, 777 Dávila, María J., 817 Deivaraj, Theivanayagam C., 812 Del Piero, Silvia, 805 Dixneuf, Pierre. H., 765 Duan. Chun-Ying, 777 Duan, Chun-Ying, 759 Fábián, István, 759 Fischmeister, Cédric, 765 Fornasari, Patrizia, 805 Gan, Leong M., 812 Gao, Song, 798 García, Begoña, 817

833 Giester, Gerald, Giorgi, Claudia, 805 Gong, Qihuang, 792 Graham, Duncan, 826 Howard, Judith A. K., 833 Jaćimović, Željko K., 833 Jin, Lin-Pei, 798 Juris, Alberto, 780 Kahlert, Björn, 780 Kennedy, Alan R., 826 Kanoufi, Frédéric, 761 Kirkhouse, Jennifer B., 826 Kittner, Madeleine, 826 Klärner, Frank-Gerrit, 780 Kong, Jilie, 847 Kovács, Attila, 833 Leal, José M., 817 Lee, Jim Y., 812 Lee, Wan In, 841 Lei, Ze, 769 Lente, Gábor, 759 Leovac, Vukadin M., 833 Li, Chao, 773 Li, Liang, 769 792 Li, Zhen, Liang, Yanke, 792 Liu, Baohong, 847

Liu, De-Jun, 777 Liu, Ying, 847 Lobert, Matthias, 780 Lu, Shao-Zhe, 798 Major, Claire, 826 Marchioni, Filippo, 780 McHugh, Callum J., 826 Melchior, Andrea, 805 Meng, Qing-Jin, 777 Mészáros Szécsényi, Katalin, 833 Mu, Li, 847 Murdoch, Paul, 826 Nemcsok, Dénes, 833 Nunige, Sandra, Pan, Jia Hong, 841 Poë, Anthony J., 759 Pokol, György, 833 Pola, Josef, 785 Portanova, Roberto, 805 Qin, Jingui, 792 Radosavljević Evans, Ivana, 833 Seelbach, Uta P., Shao, Pin, 792 Smith, W. Ewen, Šubrt, Jan, 785

Tamine, John, 789 Tolazzi, Marilena, 805 Tomić, Zoran D., 833 Tomovska, Radmila, 785 Too, Heng-Phon, 812 Toupet, Loïc, 765 Valtancoli, Barbara, 805 Vidal Jr., Bernardo C., 812 Vorlíček, Vladimír, 785 Wang, Chenbo, 789 Wang, Hongli, 792 Wang, Hongli, 7 Wang, Hui, 792 Wang, Weibo, 773 Wang, Xuesong, 773 Xu, Jian, 777 Yang, Jun, 812 Zeng, Zhanghua, 773 Zhang, Baowen, 773 Zhang, Bing-Guang, 777 Zhang, Hongbin, 769 Zhang, Song, 847 Zhao, Jingfeng, 769 Zhao, Yuanhong, 769 Zheng, Xiang-Jun, Zhou, Yongyun, 769

FREE E-MAIL ALERTS

Contents lists in advance of publication are available on the web via www.rsc.org/njc – or take advantage of our free e-mail alerting service (www.rsc.org/ej_alert) to receive notification each time a new list becomes available.

* Indicates the author for correspondence: see article for details.

Electronic supplementary information (ESI) is available via the online article (see http://www.rsc.org/esi for general information about ESI).

ADVANCE ARTICLES AND ELECTRONIC JOURNAL

Free site-wide access to Advance Articles and the electronic form of this journal is provided with a full-rate institutional subscription. See www.rsc.org/ejs for more information.

Find a SOLUTION

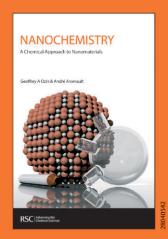
... with books from the RSC

Choose from exciting textbooks, research level books or reference books in a wide range of subject areas, including:

- Biological science
- Food and nutrition
- Materials and nanoscience
- Analytical and environmental sciences
- · Organic, inorganic and physical chemistry

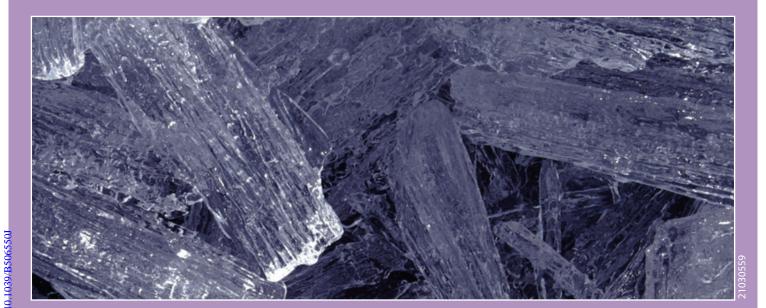
Look out for 3 new series coming soon ...

- RSC Nanoscience & Nanotechnology Series
- Issues in Toxicology
- RSC Biomolecular Sciences Series



www.rsc.org/books

RSC | Advancing the Chemical Sciences



CrystEngComm

The electronic journal for crystal engineering

CrystEngComm provides a forum for the publication of high impact articles in all aspects of crystal engineering. Its high quality is reflected in CrystEngComm's first impact factor – an impressive 2.730!

- Fast times to publication typically 50 days
- Full reference linking
- Fully interactive features
- International authorship and world-wide circulation

