

IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 29(8) 981-1096 (2005)

In this issue...

Letters from:

Shaojun Dong *et al.*, CAS, ChangchunMinghua Qiao *et al.*, Fudan UniversityYuan-Gen Yao *et al.*, CAS, Fuzhou

Cover

See Chun-Ying Duan *et al.*, page 1011. The Great Wall of China was built as a defensive fortification. Messages could be relayed along the wall by evenly spaced watch towers to warn against enemy attacks. In Chinese, the pronunciation of "the Great Wall" is close to that of "long distance" so the Great Wall was chosen to symbolise the electron transfer in our dinuclear ruthenium complexes. Image reproduced by permission of Ping Cai, Ming-xue Li, Chun-Ying Duan, Feng Lu, Dong Guo and Qing-Jin Meng, *New J. Chem.*, 2005, **29**, 1011.

CHEMICAL SCIENCE

C57

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

August 2005/Volume 2/Issue 8

www.rsc.org/chemicalscience

EDITORIAL

991

Chemical Science in China

Articles from China are showcased across journals published by the RSC this month, in recognition of the growing importance of Chinese research in the Chemical Sciences.

Chinese
Science

EDITORIAL STAFF

Managing editor (RSC)

Mike Corkill

Managing editor (CNRS)

Denise Parent

Assistant managing editor

G  rard Calleja (CNRS)

Publishing assistant

Jackie Cockrill (RSC)

Team leader, serials production

Helen Saxton (RSC)

Technical editors

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

Administration coordinator

Sonya Spring (RSC)

Editorial secretaries

Lynne Braybrook (RSC), Rebecca Gotobed (RSC), Florence Lepage (CNRS), Julie Thompson (RSC)

Publisher

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 RSC Distribution Services, c/o Portland Customer Services, Commerce Way, Colchester, Essex, UK 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.

PRINTED IN THE UK

Advertisement sales: Tel +44 (0) 1223 432243; Fax +44 (0) 1223 426017; E-mail advertising@rsc.org

NJC

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 Bonnevot, 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, Saarbr  cken, Germany
Vivian Yam, Hong Kong, PR China

Associate editors

Manuscripts should be directed to the appropriate Editor detailed below.

Supramolecular chemistry and crystal engineering

Dr Jonathan W Steed
Department of Chemistry
University Science Laboratories
University of Durham
South Road
Durham
UK DH1 3LE
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
School
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
Universit   Montpellier II
Place Eug  ne 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 EDITORIAL BOARD

Markus Antonietti, MPI, Potsdam, Germany
Didier Astruc, Talence, France
Jerry Atwood, Columbia, MO, USA
Pierre Braunstein, Strasbourg, France
Kenneth Caulton, Bloomington, IN, USA
Robert Crabtree, New Haven, CT, USA
Pierre Dixneuf, Rennes, France

Fran  ois 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, Jyv  skyl  , Finland
Cl  ment 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

Full details of how to submit material for publication in the New Journal of Chemistry are given in the Instructions for Authors (available from <http://www.rsc.org/authors>). Submissions should be sent via ReSource: <http://www.rsc.org/resource>. 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 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

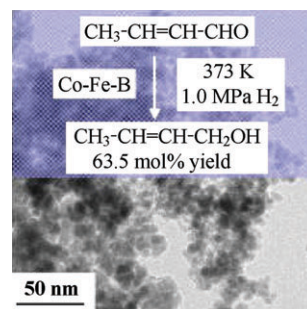
LETTERS

992

A non-noble amorphous Co–Fe–B catalyst highly selective in liquid phase hydrogenation of crotonaldehyde to crotyl alcohol

Yan Pei, Jianqiang Wang, Qiang Fu, Pingjun Guo, Minghua Qiao,* Shirun Yan and Kangnian Fan*

A nanosized amorphous Co–Fe–B catalyst exhibited higher selectivity and yield to crotyl alcohol than noble Pt-based catalysts in the hydrogenation of crotonaldehyde. The catalyst was prepared by a facile chemical reduction method.

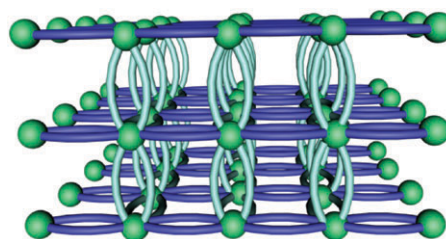


995

A rare metal–organic 3D architecture with a pseudo-primitive cubic topology with double edges constructed from a 12-connected SBU

Yi-Hang Wen, Jian Zhang, Xiao-Qin Wang, Yun-Long Feng, Jian-kai Cheng, Zhao-Ji Li and Yuan-Gen Yao*

A novel metal–organic 3D Cd-MOF coordination polymeric complex, which presents an interesting non-interpenetrated pseudo-pcu topology with double edges constructed from a rare 12-connected SBU, is reported.

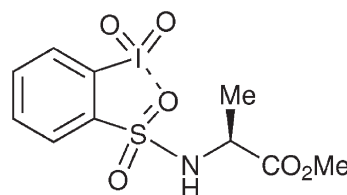


998

Intra- and intermolecular interactions in the solid state structure of 2-iodylbenzenesulfonamides: a heptacoordinated organic iodine(v) compound

Alexey Y. Kuposov, Victor N. Nemykin* and Viktor V. Zhdankin*

Single crystal X-ray structures of two 2-iodylbenzenesulfonamides reveal a combination of intra- and intermolecular I...O interactions leading to a typical hexacoordinated and a unique heptacoordinated iodine(v) center.

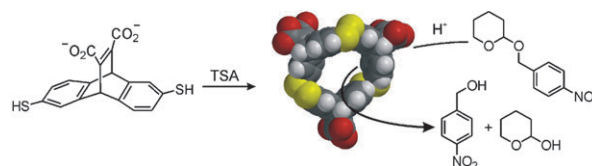


1001

A catalyst for an acetal hydrolysis reaction from a dynamic combinatorial library

Laurent Vial, Jeremy K. M. Sanders and Sijbren Otto*

A transition-state analogue for an acetal hydrolysis reaction was able to select and amplify a catalyst for this reaction from a dynamic combinatorial library of macrocyclic disulfides in water.

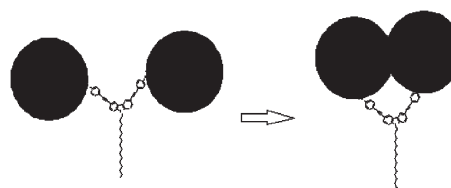


1004

Size-dependent aggregates of gold nanoparticles induced by a “molecular fork”

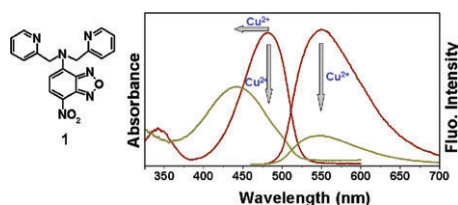
Haifeng Bao, Zhangquan Peng, Yongdong Jin, Shaojun Dong* and Erkang Wang*

A fork-like molecule can induce citrate-capped gold nanoparticles of 2.6 nm diameters to form sintered peanut-like nanoarrays and aggregates. The formation of such aggregates is size-dependent because of steric hindrance between the fork-like molecule and the 5 nm or bigger Au nanoparticles.



LETTERS

1007



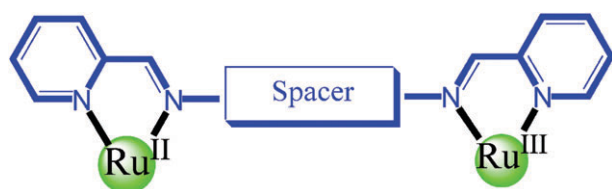
A two-dimensional chromogenic sensor as well as fluorescence inverter: selective detection of copper(II) in aqueous medium

Sandip Banthia and Anunay Samanta*

A new sensor (**1**) has been developed for selective recognition of Cu^{2+} in water. This system shows simultaneous blue shift and intensity loss of the absorption maximum as well as “on-off” fluorescence signalling, selectively, in the presence of Cu^{2+} ions at physiological pH.

PAPERS

1011

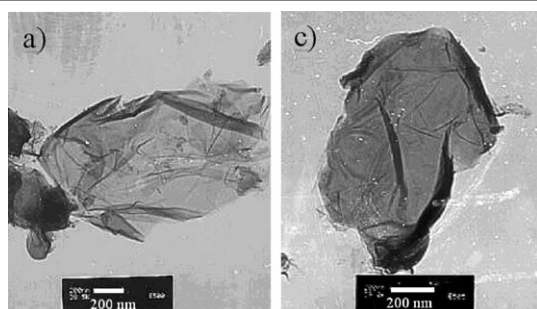


Syntheses, crystal structure and electrochemical properties of dinuclear ruthenium complexes containing saturated and unsaturated spacers

Ping Cai, Ming-xue Li, Chun-Ying Duan,* Feng Lu, Dong Guo and Qing-Jin Meng

The study on the electrochemical and spectral properties of a series of binuclear complexes of ruthenium demonstrated that the Schiff base bridging ligands exhibited high efficiency for mediating the metal-metal coupling and approached molecular wire behavior.

1017

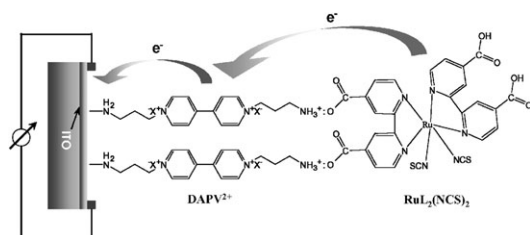


Surface modification of as-synthesized lamellar mesostructured silica obtained by liquid crystal templating

C. Henrist,* C. Vogels, A. Rulmont and R. Cloots

Mesostructured silica silylated directly after synthesis obtained in (a) acidic and (c) basic medium is constituted of very thin silica sheets with poor rigidity and an extremely high aspect ratio.

1022



Molecular photosensors of self-assembled monolayers: electron acceptor-photosensitizer dyad on an ITO surface

Kyung-Hee Hyung, Dong-Young Kim and Sung-Hwan Han*

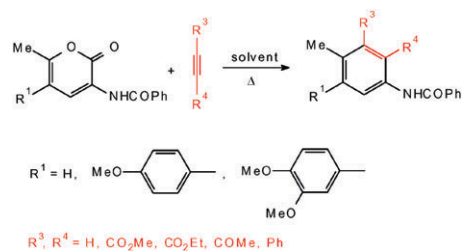
The energy level alignment through the SAMs of di-(3-diaminopropyl)-viologen successfully facilitates electron transfer and alters the ITO conductivity.

1027

Diels–Alder reaction of highly substituted 2*H*-pyran-2-ones with alkynes: reactivity and regioselectivity

Krištof Kranjc and Marijan Kočevár*

Efficient and completely regioselective Diels–Alder reaction of substituted 2*H*-pyran-2-ones with various alkynes under thermal and high-pressure conditions is presented; effects of substituents and reaction conditions on the reactivity were investigated.

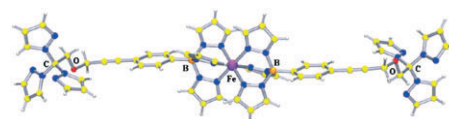


1035

Multitopic third generation tris(pyrazolyl)methane ligands built on alkyne structural scaffolding: first preparation of mixed tris(pyrazolyl)methane/tris(pyrazolyl)borate ligands

Daniel L. Reger,* James R. Gardinier, Selma Bakbak, Radu F. Semeniuc, Uwe H. F. Bunz and Mark D. Smith

Sonogashira and related alkynyl coupling reactions were used to prepare new third-generation scorpionate compounds including the first metal complexes that contain both the tris(pyrazolyl)methane and tris(pyrazolyl)borate ligating units.

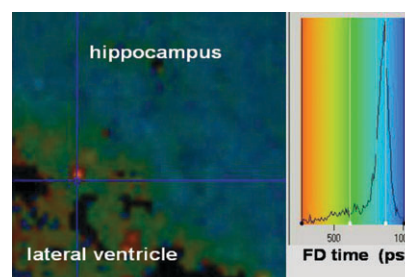


1044

Time-resolved emission upon two-photon excitation of bis-*N*-carbazolyl-distyrylbenzene: mapping of water molecule distribution in the mouse brain

Evgenia Vaganova,* Shlomo Yitzchaik,* Mark Sigalov, Jan W. Borst, Antonie Visser, Haim Ovadia and Vladimir Khodorkovsky*

Water molecule distribution in a brain was visualized by incorporation of water sensitive chromophore-bis-*N*-carbazolyl-distyrylbenzene and the FLIM technique.

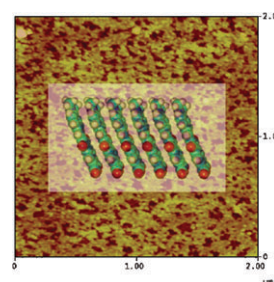


1049

Studies of Langmuir and Langmuir–Blodgett films of NLO-active amphiphilic 1,3-indanedione derivatives

Somobrata Acharya, Pnina Krief, Vladimir Khodorkovsky,* Zvi Kotler, Gerry Berkovic, Jacob T. Klug and (the late) Shlomo Efrima

SHG from alternate LB films of 1,3-indanedione-5,6-dicarboxylic acid derivatives.

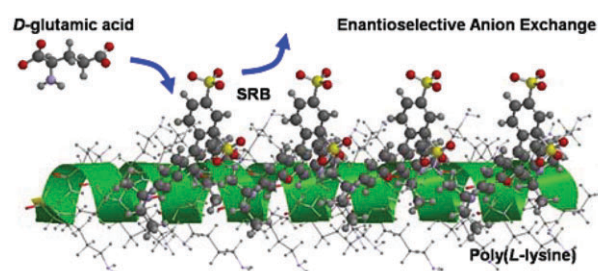


1058

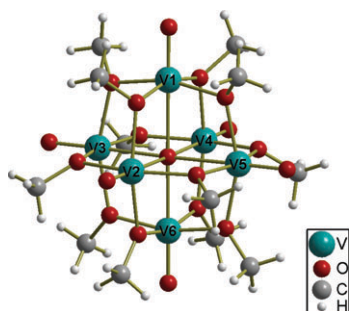
Enantioselective anion exchange on a positively charged poly(L-lysine) layer assembled on thin TiO₂-gel films

Sharmistha Paul, Jianguo Huang and Izumi Ichinose*

Fluorescent dye was electrostatically adsorbed on a molecularly thin poly(L-lysine) layer prepared on thin TiO₂-gel films. The enantioselective release of the dye molecules into the solutions of chiral glutamic acids was observed, as monitored by fluorescence measurements.



1064

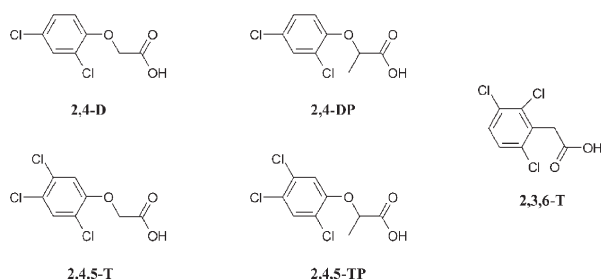


EPR study of the magnetic states of a mixed-valence $V^{IV}_4V^{V}_2$ alkoxypolyoxovanadium cluster

Maria A. Augustyniak-Jablokow, Serguei A. Borshch, Charles Daniel, Hans Hartl and Yurii V. Yablokov*

An EPR study of the $[V^{IV}_4V^{V}_2O_7(OCH_3)_{12}]$ single crystal shows that in the studied cluster an electron transfer between V^{IV} and V^V takes place. A phase transition at about 190 K was also discovered.

1072

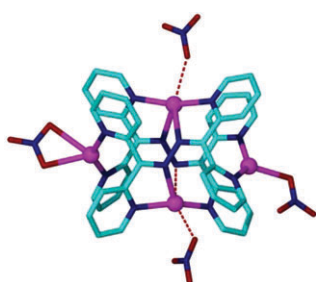


Partition and transfer of chlorophenoxy acids (herbicides) in water–non-aqueous media

Angela F. Danil de Namor,* Jorge A. Zvietcovich-Guerra, Viatcheslav Grachev, Walther B. Aparicio-Aragón, Katherine Zegarra-Fernandez and F. J. Sueros-Velarde

The distribution, K_d , and the dimerisation, K_{dim} , constants of chlorophenoxy acids (herbicides) are reported. K_d values in mutually saturated solvent systems are compared with those derived from solubility data in water and in anhydrous non-aqueous media.

1077

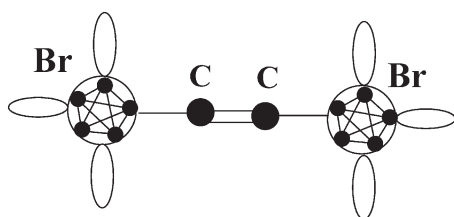


An investigation of the coordination chemistry of the hexadentate ligand di-2-pyridylketone azine; the formation of a discrete tetranuclear complex with silver nitrate

Christopher J. Sumby and Peter J. Steel*

Reaction of the ligand di-2-pyridylketone azine with silver nitrate leads to the formation of a discrete $Ag_4L_2(NO_3)_4$ complex.

1082

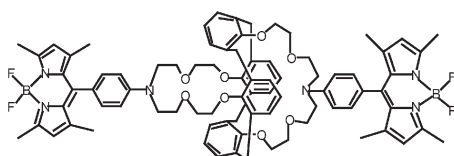


A natural graph-theory model for partition and kinetic coefficients

Lionello Pogliani

The hydrogen-depleted chemical pseudograph (or general graph) plus complete graphs of $Br-CH_2=CH_2-Br$. Odd complete graphs, K_5 and K_1 , are used to encode the core electrons for Br and C, respectively.

1089



A highly selective fluorescent molecular sensor for potassium based on a calix[4]bisazacrown bearing boron-dipyrrromethene fluorophores

Jean-Pierre Malval, Isabelle Leray* and Bernard Valeur

A calix[4]bisazacrown bearing boron dipyrrromethene fluorophores was used as a fluorescent molecular sensor for K^+ with high selectivity.

AUTHOR INDEX

- Acharya, Somabrata, 1049
 Aparicio-Aragón, Walther B., 1072
 Augustyniak-Jablokow, Maria A., 1064
 Bakbak, Selma, 1035
 Bantia, Sandip, 1007
 Bao, Haifeng, 1004
 Berkovic, Gerry, 1049
 Borshch, Serguei A., 1064
 Borst, Jan W., 1044
 Bunz, Uwe H. F., 1035
 Cai, Ping, 1011
 Cheng, Jian-kai, 995
 Cloots, R., 1017
 Daniel, Charles, 1064
 Danil de Namor, Angela F., 1072
 Dong, Shaojun, 1004
 Duan, Chun-Ying, 1011
 Efrima, Shlomo, 1049
 Fan, Kangnian, 992
 Feng, Yun-Long, 995
 Fu, Qiang, 992
 Gardinier, James R., 1035
 Grachev, Viatcheslav, 1072
 Guo, Dong, 1011
 Guo, Pingjun, 992
 Han, Sung-Hwan, 1022
 Hartl, Hans, 1064
 Henrist, C., 1017
 Huang, Jianguo, 1058
 Hyung, Kyung-Hee, 1022
 Ichinose, Izumi, 1058
 Jin, Yongdong, 1004
 Khodorkovsky, Vladimir, 1044, 1049
 Kim, Dong-Young, 1022
 Klug, Jacob T., 1049
 Kočevár, Marijan, 1027
 Kopolov, Alexey Y., 998
 Kotler, Zvi, 1049
 Kranjc, Krištof, 1027
 Krief, Pnina, 1049
 Leray, Isabelle, 1089
 Li, Ming-xue, 1011
 Li, Zhao-Ji, 995
 Lu, Feng, 1011
 Malval, Jean-Pierre, 1089
 Meng, Qing-Jin, 1011
 Nemykin, Victor N., 998
 Otto, Sijbren, 1001
 Ovadia, Haim, 1044
 Paul, Sharmistha, 1058
 Pei, Yan, 992
 Peng, Zhangquan, 1004
 Pogliani, Lionello, 1082
 Qiao, Minghua, 992
 Reger, Daniel L., 1035
 Rulmont, A., 1017
 Samanta, Anunay, 1007
 Sanders, Jeremy K. M., 1001
 Semeniuc, Radu F., 1035
 Sigalov, Mark, 1044
 Smith, Mark D., 1035
 Steel, Peter J., 1077
 Sueros-Velarde, F. J., 1072
 Sumby, Christopher J., 1077
 Vaganova, Evgenia, 1044
 Valeur, Bernard, 1089
 Vial, Laurent, 1001
 Visser, Antonie, 1044
 Vogels, C., 1017
 Wang, Erkang, 1004
 Wang, Jianqiang, 992
 Wang, Xiao-Qin, 995
 Wen, Yi-Hang, 995
 Yablokov, Yurii V., 1064
 Yan, Shirun, 992
 Yao, Yuan-Gen, 995
 Yitzchaik, Shlomo, 1044
 Zegarra-Fernandez, Katherine, 1072
 Zhang, Jian, 995
 Zhdankin, Viktor V., 998
 Zvietcovich-Guerra, Jorge A., 1072

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.

RSC Biomolecular Sciences

A new series from the RSC

Editor-in-Chief:

Professor Stephen Neidle, *University of London, UK*

Series Editors:

Dr Simon F Campbell

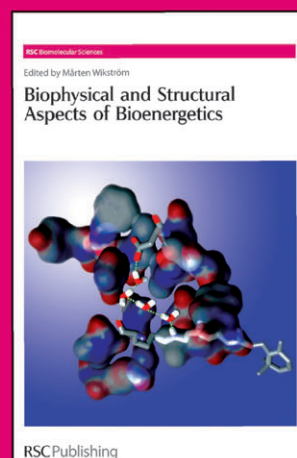
Dr Marius Clore, *National Institutes of Health, USA*

Professor David M J Lilley, *University of Dundee, UK*

This series provides an authoritative insight into research at the interface between chemistry and biology. It comprises a range of research monographs, edited by high profile, international scientists working in the field. Each book will be on an individual topic, published in full colour format and fully referenced to the primary literature.

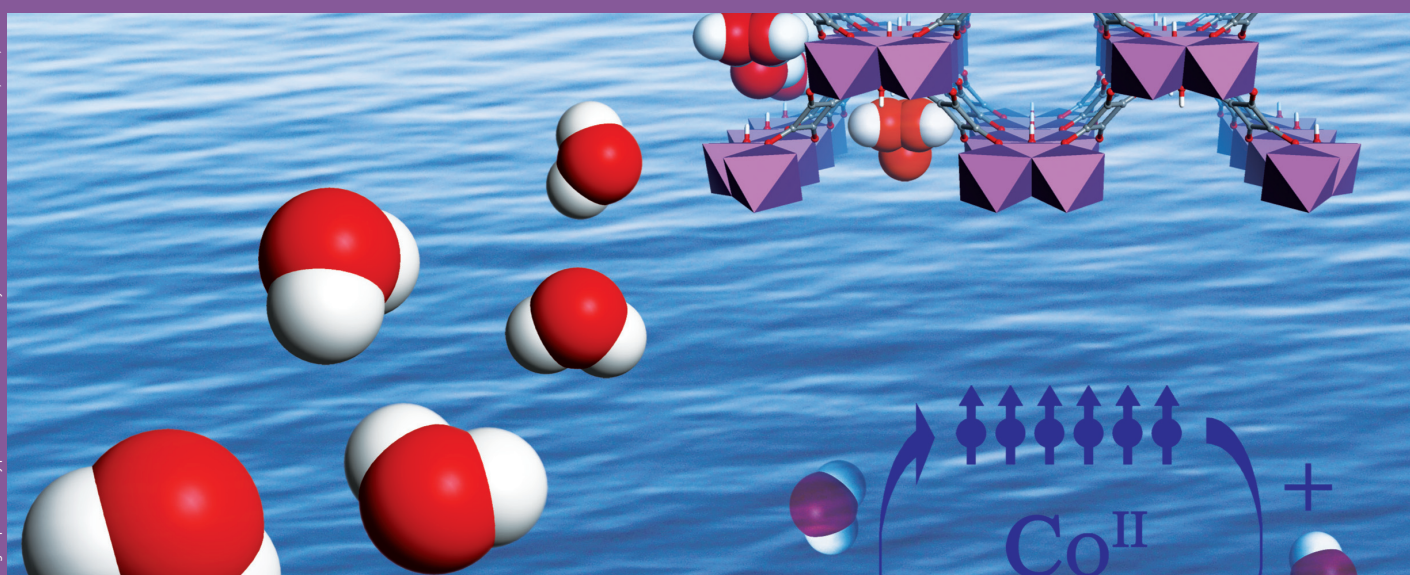
Readership: academic researchers, graduate students, government institutions, industry

Market: structural biology, drug discovery and biophysical chemistry



RSC Publishing

www.rsc.org/biomolecularsciences



ChemComm

The leading international journal for the publication of communications on important new developments in the chemical sciences.

- Weekly publication
- Impact factor: 4.031
- Rapid publication – typically 60 days
- 3 page communications – providing authors with the flexibility to develop their results and discussion
- 40 years publishing excellent research
- High visibility – indexed in MEDLINE
- Host of the RSC's new journal, *Molecular BioSystems*

