

NJC

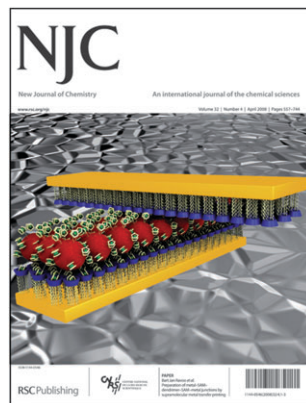
New Journal of Chemistry. An international journal for the chemical sciences

www.rsc.org/njc

RSC Publishing is a not-for-profit publisher and a division of the Royal Society of Chemistry. Any surplus made is used to support charitable activities aimed at advancing the chemical sciences. Full details are available from www.rsc.org

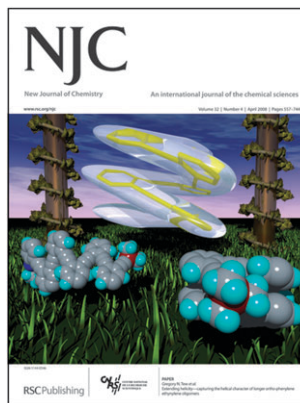
IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 32(4) 557-744 (2008)



Cover

See Ravoo *et al.*, pp. 652–661. The cover shows a supramolecular electronic junction of redox-active ferrocene dendrimers inserted between metal electrodes in a crossed-bar configuration. The dendrimers are held in place by host-guest interaction with cyclodextrins adsorbed on the electrodes. Image designed by Dr. C. A. Nijhuis with the help of Dr. H. Dam, and reproduced with the permission of Bart Jan Ravoo *et al.* from *New J. Chem.*, 2008, **32**, 652.



Inside Cover

See Tew *et al.*, pp. 676–679. Helical structures persist in Nature from macroscopic vines to the well-known alpha-helix. Inspired by folded macromolecules, we have studied synthetic abiotic foldamers based on phenylene ethynylene. Image reproduced with the permission of Ticora V. Jones, Morris M. Slutsky and Gregory N. Tew from *New J. Chem.*, 2008, **32**, 676.

CHEMICAL SCIENCE

C25

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

April 2008/Volume 5/Issue 4

www.rsc.org/chemicalscience

OPINION

571

Music of the elements

Santiago Alvarez

Music may have influenced the development of the periodic system and, in return, the elements have been a source of inspiration for musicians. The dialogue about the elements held for centuries between the worlds of chemistry and music is summarized in this article.



EDITORIAL STAFF

Editor (RSC)

Sarah Ruthven

Editor (CNRS)

Denise Parent

Assistant editors

G rard Calleja (CNRS)

Sarah Dixon (RSC)

Publishing assistants

Jackie Cockrill (RSC)

Florence Lepage (CNRS)

Team leader, serials production

Helen Saxton (RSC)

Technical editors

Celia Clarke (RSC), Nicola Convine (RSC),

Alan Holder (RSC), David Parker (RSC),

Ken Wilkinson (RSC)

Administration coordinator

Sonya Spring (RSC)

Administration assistants

Clare Davies (RSC), Donna Fordham (RSC),

Kirsty Lunnon (RSC), Julie Thompson (RSC)

Publisher

Emma Wilson (RSC)

Founding Editor

Lionel Salem

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

2008 Annual (print + electronic) subscription price: £784; US\$1560. 2008 Annual (electronic) subscription price: £706; US\$1405. 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 432246; 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

Co-editor-in-chief

Jean-Pierre Majoral, Toulouse, France

Co-editor-in-chief

Jerry Atwood, Columbia, MO, USA

Consulting editor

Odile Eisenstein, Montpellier, France

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

Board members

Mats Almgren, Uppsala, Sweden
Yasuhiro Aoyama, Kyoto, Japan
Kumar Biradha, Khargapur, India
Laurent Bonnevot, Lyon, France
Fabrizia Grepioni, Bologna, Italy
Helen Hailes, London, UK
Pascal Le Floch, Palaiseau, France
Barbara Nawrot, Lodz, Poland

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

Authors from the Americas

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 mjscott@chem.ufl.edu

Other Fields:
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

ADVISORY BOARD

Markus Antonietti, MPI, Potsdam, Germany
Matthias Bremer, Darmstadt, Germany
Robert Crabtree, New Haven, CT, USA
Fran ois 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
Peter Junk, Monash, Australia
Henryk Koslowski, Wroclaw, Poland
Luca Prodi, Bologna, Italy
Jan Reedijk, Leiden, The Netherlands

David Reinhoudt, Enschede, The Netherlands
Kari Rissanen, Jyv skyl , Finland
Cl ment Sanchez, Paris, France
Jeremy K M Sanders, Cambridge, UK
Jean-Pierre Sauvage, Strasbourg, France

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 2008. 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

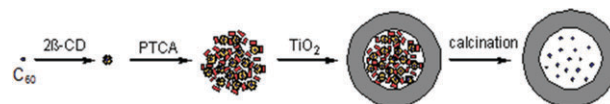
LETTERS

581

Layer-by-layer self-assembled hollow titania composite nanospheres containing [60]fullerene

Wenfeng Jiang, Ying Yu, Dianqing Li, Yingjie Zhao, Maoyou Xu and Zhiqiang Shi*

Core-shell nanospheres, titania composite nanospheres containing [60]fullerene, were fabricated with sizes of about 100 nm by a layer-by-layer self-assembly procedure, and were characterized by TGA, FT-IR and XPS spectroscopy.

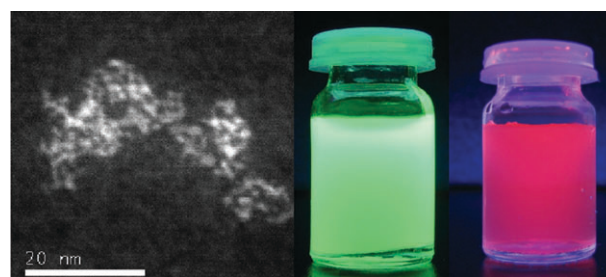


584

Luminescent coordination nanoparticles

Nicolas Kerbellec, Laure Catala, Carole Daiguebonne, Alexandre Gloter, Odile Stephan, Jean-Claude Bünzli, Olivier Guillou and Talal Mallah*

Water-soluble Eu- and Tb-based luminescent nanoparticles are stabilized by the growth confinement of a porous lanthanide-terephthalate three-dimensional network.

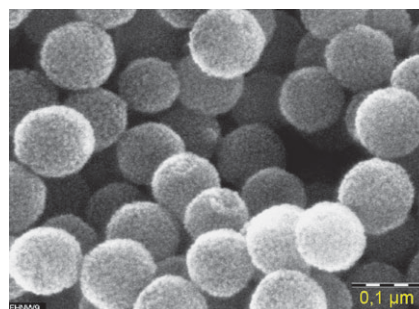


588

Controlling silica nanoparticle properties for biomedical applications through surface modification

Sébastien Legrand, Amélie Catheline, Lucy Kind, Edwin C. Constable, Catherine E. Housecroft, Lukas Landmann, Petra Banse, Uwe Piele and Amina Wirth-Heller*

Can chemistry lock/unlock the fate of nanoparticles?



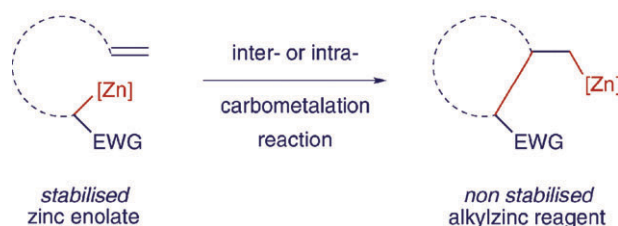
PERSPECTIVE

594

Carbometalation of unactivated alkenes by zinc enolate derivatives

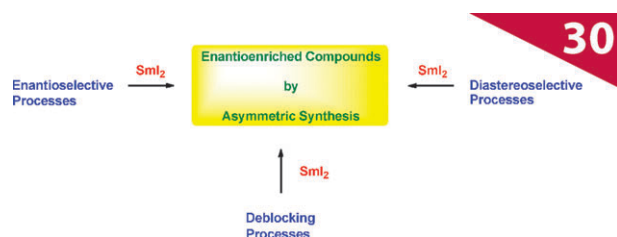
Alejandro Pérez-Luna,* Candice Botuha, Franck Ferreira and Fabrice Chemla*

The carbometalation of unactivated double bonds by zinc enolate derivatives has emerged over the past decade as a mechanistically interesting and synthetically useful reaction. This Perspective is devoted to these challenging and apparently contra-thermodynamic transformations, with a special focus on recent mechanistic considerations.

Carbometalation of Unactivated Alkenes by Zinc Enolates

PERSPECTIVE

607



Use of samarium diiodide in the field of asymmetric synthesis

Kovuru Gopalaiah and Henri B. Kagan*

30th Anniversary article: Samarium diiodide is a versatile reagent for asymmetric synthesis processes, used to release blocking groups under mild conditions, act as an electron donor in C–C bond forming reactions in the presence of a chiral auxiliary, and generate samarium enolates that are undergo asymmetric protonation.

PAPERS

638

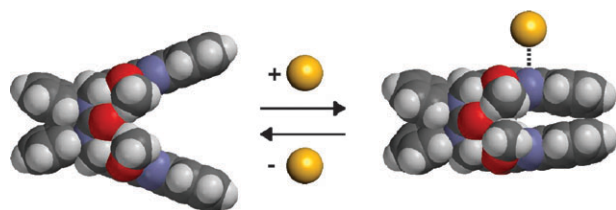


Regularities of the conformations on a single bond; sulfonic esters and sulfonyl derivatives

Otto Exner and Stanislav Böhm*

The so-called *gauche* rule is not a general natural law: the *gauche* conformation is preferred on some sulfonyl derivatives but not with all. Theoretical calculations at a higher level give reliable values of the dihedral angles but not exact values for the population of rotamers; these are obtained more reliably by combination of calculations and experiments.

643

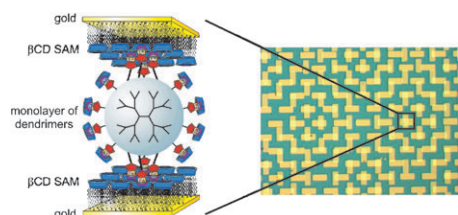


Modulation and binding properties of extended glycoluril molecular clips

Prasad Polavarapu, Helena Melander, Vratislav Langer, Adolf Gogoll* and Helena Grennberg*

The binding properties of a glycoluril type molecular clip are a delicate balance between various molecular interactions.

652



Preparation of metal–SAM–dendrimer–SAM–metal junctions by supramolecular metal transfer printing

Christian A. Nijhuis, Jurjen ter Maat, Satria Z. Bisri, Marcel H. H. Weusthof, Cora Salm, Jurriaan Schmitz, Bart Jan Ravoo,* Jurriaan Huskens and David N. Reinhoudt*

Supramolecular tunnel junctions were fabricated by printing gold electrodes onto self-assembled monolayers. The metal transfer from the stamp onto the substrate was facilitated by multiple specific host–guest interactions.

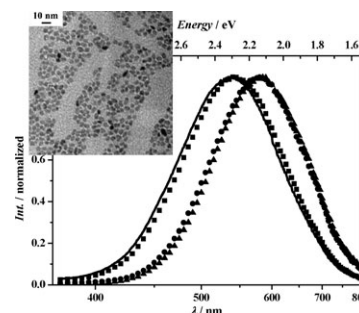
PAPERS

662

Lithium ion as growth-controlling agent of ZnO nanoparticles prepared by organometallic synthesis

Arnaud Glaria, Myrtil L. Kahn,* Thierry Cardinal, François Senocq, Véronique Jubera and Bruno Chaudret*

An organometallic method is developed for the preparation of ZnO nanoparticles of controlled size and shape. The size of the nanoparticles depends directly on the Li amount introduced in the reaction media leading to an effective tuning of the optical properties.

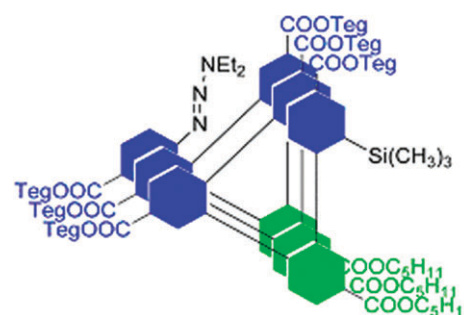


670

Synthesis and characterization of amphiphilic *o*-phenylene ethynylene oligomers

Morris M. Slutsky, Jason S. Phillip and Gregory N. Tew*

New *ortho*-phenylene ethynylene oligomers have been synthesized, incorporating a repeated triad motif of polar–nonpolar–polar sidechains in order to create a hydrophobic stripe in the folded conformation.

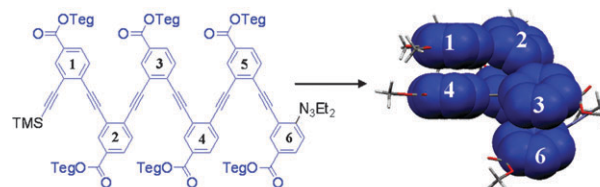


676

Extending helicity—capturing the helical character of longer *ortho*-phenylene ethynylene oligomers

Ticora V. Jones, Morris M. Slutsky and Gregory N. Tew*

New *ortho*-phenylene ethynylene oligomers are shown by 1D and 2D NMR to fold into helices.

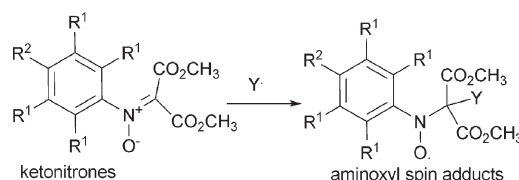


680

Detection and identification of various carbon-centred free radicals using *N*-arylketonitrone: a spin trapping/EPR/MS study

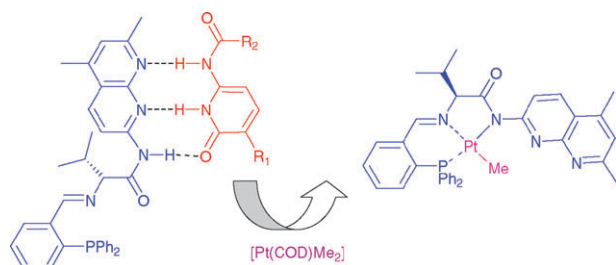
Inas El Hassan, Laurence Charles,* Robert Lauricella and Béatrice Tuccio*

N-Aryl-*C,C*-dimethoxycarbonyl ketonitrone can trap transient free radicals to yield paramagnetic spin adducts. These products are detected by EPR spectroscopy and their structures are elucidated by ESI tandem mass spectrometry.



PAPERS

689

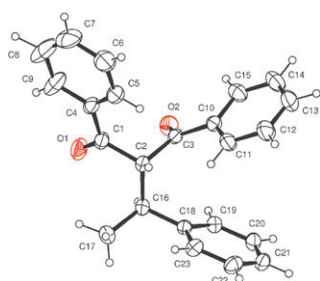


A supramolecular approach to chiral ligand modification: coordination chemistry of a multifunctionalised tridentate amine-phosphine ligand

José A. Fuentes, Matthew L. Clarke* and Alexandra M. Z. Slawin

A novel chiral amine-phosphine tagged with an amido-naphthyridine moiety has been investigated and found to bind complementary pyridinone additives. However, the ligand has a very strong tendency to protonate anionic ligands and form tridentate complexes.

694

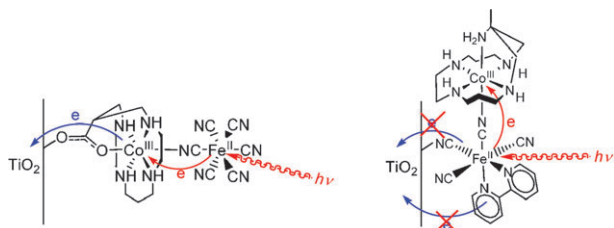


Substituent effects on keto–enol tautomerization of β -diketones from X-ray structural data and DFT calculations

Valerio Bertolasi,* Valeria Ferretti, Paola Gilli, Xiaoquan Yao and Chao-Jun Li

A survey of all the structures of acyclic β -diketones having at least one α -hydrogen, including six new β -diketones, has established that the non-enolized form is stabilized by the steric hindrance of the substituents.

705

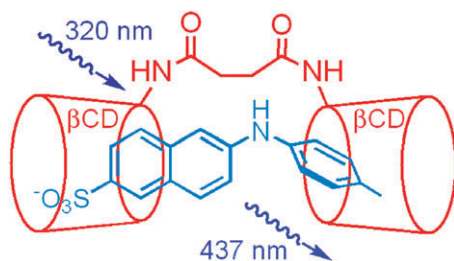


Tailoring mixed-valence $\text{Co}^{\text{III}}/\text{Fe}^{\text{II}}$ complexes for their potential use as sensitizers in dye sensitized solar cells

Paul V. Bernhardt, Gerrit K. Boschloo, Fernando Bozoglian, Anders Hagfeldt, Manuel Martínez and Beatriz Sienra

Tailoring discrete mixed-valence cyanide bridged $\text{Co}^{\text{III}}/\text{Fe}^{\text{II}}$ complexes to obtain characteristics of electron injection processes dominated by the MMCT band is possible; the band is important to disrupt injection from the iron centre and promote electron transfer from the cobalt centre.

712



Complexation of 6-(4'-(toluidinyl)naphthalene-2-sulfonate by β -cyclodextrin and linked β -cyclodextrin dimers

Duc-Truc Pham, Philip Clements, Christopher J. Easton, John Papageorgiou, Bruce L. May and Stephen F. Lincoln*

The 6-(4'-(toluidinyl)naphthalene-2-sulfonate–*N,N*-bis(6 Λ -deoxy-6 Λ - β -cyclodextrin)-succinamide complex exemplifies five linked β -cyclodextrin dimer complexes studied by UV-Vis, fluorescence and ^1H NMR spectroscopy.

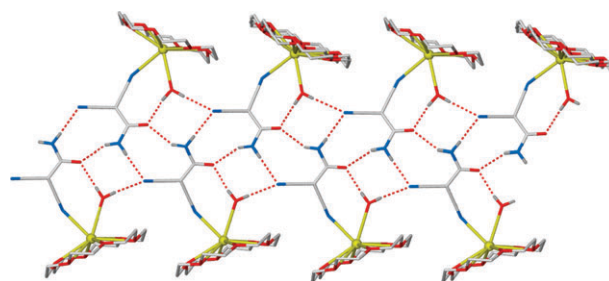
PAPERS

719

Amide-water hydrogen-bond motifs in alkali-metal/crown ether complexes of carbamoyldicyanomethanide, $C(CONH_2)(CN)_2^-$

David R. Turner, Sze Nee Pek and Stuart R. Batten*

A series of complexes have been obtained from the crystallisation of $M(cdm)$ ($M = Na, K$; $cdm =$ carbamoyldicyanomethanide) with crown ethers from aqueous solution. The structures of these complexes display a range of hydrogen-bonding tape and sheet motifs incorporating both coordinated and lattice water molecules.

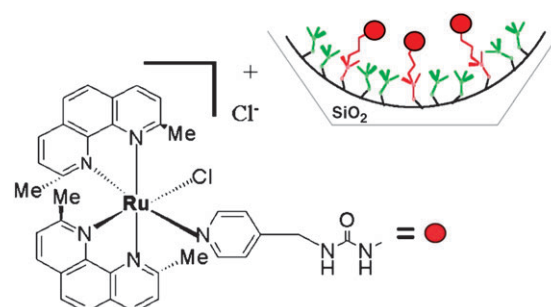


727

Multistep anchoring of a catalytically active ruthenium complex in porous mesostructured silica

St phanie Calmettes, Bel n Albela, Olivier Hamelin, St phane M nage, Fabien Miomandre and Laurent Bonneviot*

$[Ru(dmp)_2Cl_2]$ is reacted with pyridinyl terminated tether $Py@LUS$ to produce a $[Ru(dmp)_2(Py@LUS)Cl]Cl$ species active in selective oxidation of methyl phenylsulfide into sulfoxide.

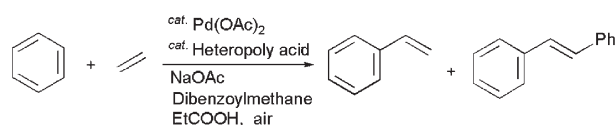


738

Oxidative arylation of ethylene with benzene catalyzed by $Pd(OAc)_2$ /heteropoly acid/ O_2 system

Tomoyuki Yamada, Aki Sakakura, Satoshi Sakaguchi, Yasushi Obora and Yasutaka Ishii*

The reaction of benzene with ethylene in the presence of catalytic amounts of $Pd(OAc)_2$ combined with heteropoly acids, $NaOAc$, and dibenzoylmethane under air produced oxidative coupling products, styrene and stilbene, in fair yields.



AUTHOR INDEX

- Albela, Belén, 727
 Alvarez, Santiago, 571
 Banse, Petra, 588
 Batten, Stuart R., 719
 Bernhardt, Paul V., 705
 Bertolasi, Valerio, 694
 Bisri, Satria Z., 652
 Böhm, Stanislav, 638
 Bonneviot, Laurent, 727
 Boschloo, Gerrit K., 705
 Botuha, Candice, 594
 Bozoglian, Fernando, 705
 Bünzli, Jean-Claude, 584
 Calmettes, Stéphanie, 727
 Cardinal, Thierry, 662
 Catala, Laure, 584
 Catheline, Amélie, 588
 Charles, Laurence, 680
 Chaudret, Bruno, 662
 Chemla, Fabrice, 594
 Clarke, Matthew L., 689
 Clements, Philip, 712
 Constable, Edwin C., 588
 Daguebonne, Carole, 584
 Easton, Christopher J., 712
 El Hassan, Inas, 680
 Exner, Otto, 638
 Ferreira, Franck, 594
 Ferretti, Valeria, 694
 Fuentes, José A., 689
 Gilli, Paola, 694
 Glaria, Arnaud, 662
 Gloter, Alexandre, 584
 Gogoll, Adolf, 643
 Gopalaiah, Kovuru, 607
 Grennberg, Helena, 643
 Guillou, Olivier, 584
 Hagfeldt, Anders, 705
 Hamelin, Olivier, 727
 Housecroft, Catherine E., 588
 Huskens, Jurriaan, 652
 Ishii, Yasutaka, 738
 Jiang, Wenfeng, 581
 Jones, Ticora V., 676
 Jubera, Véronique, 662
 Kagan, Henri B., 607
 Kahn, Myrtil L., 662
 Kerbellec, Nicolas, 584
 Kind, Lucy, 588
 Landmann, Lukas, 588
 Langer, Vratislav, 643
 Lauricella, Robert, 680
 Legrand, Sébastien, 588
 Li, Chao-Jun, 694
 Li, Dianqing, 581
 Lincoln, Stephen F., 712
 Mallah, Talal, 584
 Martínez, Manuel, 705
 May, Bruce L., 712
 Melander, Helena, 643
 Ménage, Stéphane, 727
 Miomandre, Fabien, 727
 Nijhuis, Christian A., 652
 Obora, Yasushi, 738
 Papageorgiou, John, 712
 Pek, Sze Nee, 719
 Pérez-Luna, Alejandro, 594
 Pham, Duc-Truc, 712
 Phillip, Jason S., 670
 Pieleus, Uwe, 588
 Polavarapu, Prasad, 643
 Ravoo, Bart Jan, 652
 Reinhoudt, David N., 652
 Sakaguchi, Satoshi, 738
 Sakakura, Aki, 738
 Salm, Cora, 652
 Schmitz, Jurriaan, 652
 Senocq, François, 662
 Shi, Zhiqiang, 581
 Sienna, Beatriz, 705
 Slawin, Alexandra M. Z., 689
 Slutsky, Morris M., 670, 676
 Stephan, Odile, 584
 ter Maat, Jurjen, 652
 Tew, Gregory N., 670, 676
 Tuccio, Béatrice, 680
 Turner, David R., 719
 Weusthof, Marcel H. H., 652
 Wirth-Heller, Amina, 588
 Xu, Maoyou, 581
 Yamada, Tomoyuki, 738
 Yao, Xiaoquan, 694
 Yu, Ying, 581
 Zhao, Yingjie, 581

FREE E-MAIL ALERTS AND RSS FEEDS

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.



Try our RSS feeds for up-to-the-minute news of the latest research. By setting up RSS feeds, preferably using feed reader software, you can be alerted to the latest Advance Articles published on the RSC web site. Visit www.rsc.org/publishing/technology/rss.asp for details.

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.

* 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).