

IN THIS ISSUE

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Cover

See Odile Eisenstein *et al.*, p. 842.
A well-defined silica supported Re-alkylidene complex shows an unprecedented activity in olefin metathesis compared to homogeneous analogues. DFT periodic calculations show that its structure and electronic properties derive solely from the siloxy group to which Re is attached to silica, hence silica is a large siloxy (solid) ligand. Image reproduced by permission of Xavier Solans-Monfort, Jean-Sébastien Filhol, Christophe Copéret and Odile Eisenstein, *New J. Chem.*, 2006, **30**, 842.

CHEMICAL SCIENCE

C41

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Chemical Science

June 2006/Volume 3/Issue 6

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PERSPECTIVE

823

Looking forward: a glance into the future of organic chemistry

Philippe Compain* *et al.*

What will organic chemistry do in the next forty years? This *Perspective* lists six challenges that have emerged during the first edition of ESYOP, a symposium devoted to the future of organic chemistry.



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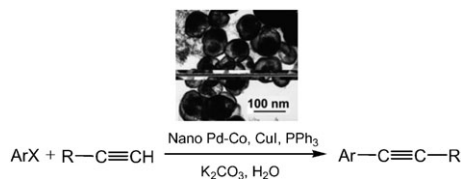
LETTERS

832

A facile synthesis of PdCo bimetallic hollow nanospheres and their application to Sonogashira reaction in aqueous media

Yingguang Li, Ping Zhou, Zhihui Dai, Zhixin Hu, Peipei Sun* and Jianchun Bao*

PdCo bimetallic hollow nanospheres were for the first time synthesized. The Sonogashira reaction catalyzed by these nanoparticles was carried out in aqueous media under mild conditions and with the recycling of the catalyst.

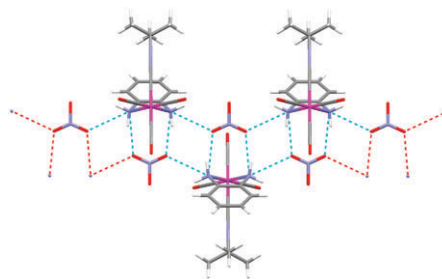


838

Non-covalent interactions between anions and a cationic rhenium diamine complex: structural characterization of the supramolecular adducts

Sonia Nieto, Julio Pérez,* Lucía Riera, Víctor Riera and Daniel Miguel

The formation of supramolecular adducts between the new complex $[\text{Re}(\text{CN}^t\text{Bu})(\text{CO})_3(1,2-(\text{NH}_2)\text{C}_6\text{H}_4)]^+$ and several anions has been detected in solution, and the solid state structures of the nitrate and perchlorate adducts reveal H-bonding between the anions and the N–H groups.



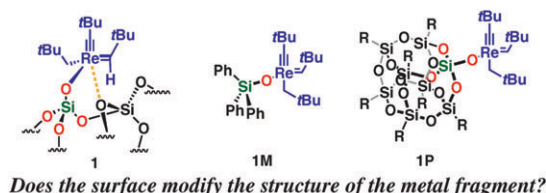
PAPERS

842

Structure, spectroscopic and electronic properties of a well defined silica supported olefin metathesis catalyst, $[(\equiv\text{SiO})\text{Re}(\equiv\text{CR})(=\text{CHR})(\text{CH}_2\text{R})]$, through DFT periodic calculations: silica is just a large siloxy ligand

Xavier Solans-Monfort, Jean-Sébastien Filhol, Christophe Copéret* and Odile Eisenstein*

The structures and properties of alkylidene–alkylidyne Re silica supported olefin metathesis catalysts are due only to the electronic properties of the siloxy group, as there is no influence of the substitution at Si (from H to a piece of silica).

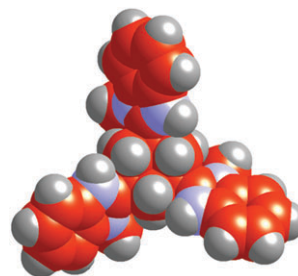


851

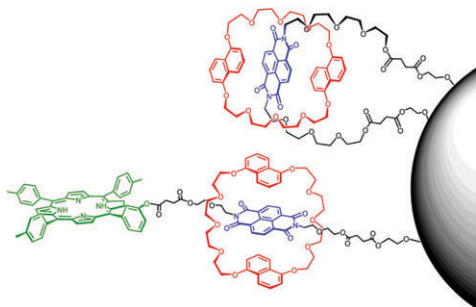
Conformational effects in molecular tectons containing protonated benzimidazole cations

Anita Kübel-Pollak, Craig J. Matthews, Simon Verdan, Bernard Bocquet, Xavier Melich, Alan F. Williams,* Francine Lavergnat, Pierre-Yves Morgantini and Gérald Bernardinelli

N-Methylation of benzimidazole influences the conformation adopted by the cations formed on protonation and thereby the structures formed by cation stacking.



861

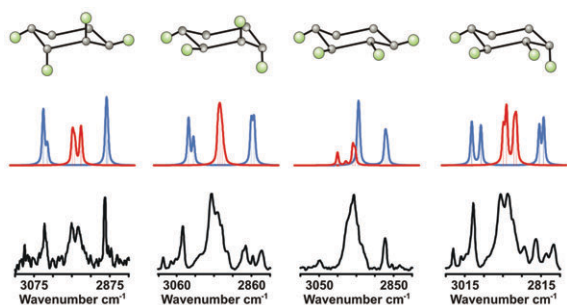


Gel-phase HR-MAS ^1H NMR spectroscopy as a probe for solid-tethered diimide rotaxanes and catenanes

Ken D. Johnstone, Nick Bampos, Jeremy K. M. Sanders and Maxwell J. Gunter*

HR-MAS proton NMR spectroscopy is used to probe the structures of naphthalene diimide-based catenanes and porphyrinic rotaxanes attached to ArgoGel polystyrene beads.

868

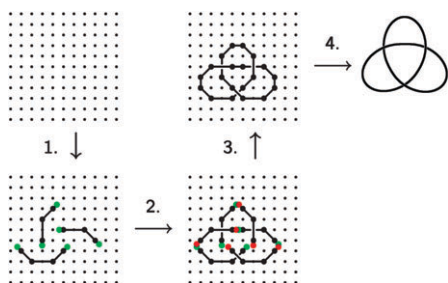


Characterization of 1,2,3,4-tetrabromocyclohexane isomers by GC-matrix isolation FTIR-MS

Daniel L. Vaughn and Ken B. Anderson*

Epimeric 1,2,3,4-tetrabromocyclohexanes have been characterized by GC-matrix isolation FTIR-MS. Results demonstrate that this technique is useful for precise identification of individual BFR derived products, even at trace levels.

873

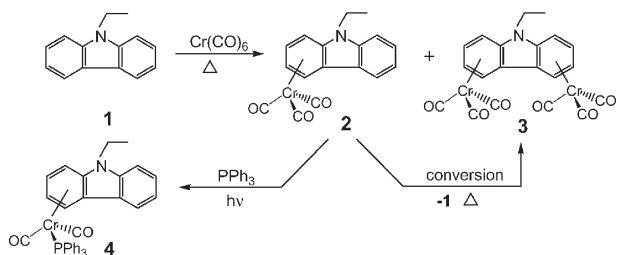


Molecular knots, links, and fabrics: prediction of existence and suggestion of a synthetic route

Dirk Andrae*

Stepwise directed and controlled synthesis of molecular knots and links by the surface template technique (shown schematically for the trefoil knot).

883



Syntheses and third-order NLO properties of η^6 complexes of *N*-ethylcarbazole with $\text{Cr}(\text{CO})_3$ and $\text{Cr}(\text{CO})_2\text{PPh}_3$ moieties

Yanchao Che, Xiaohui Tian,* Hui Chen, Zhenyu Tang and Jiaping Lin

The mono- and bimetallic chromium carbazole derivatives shown here are promising candidates as multi-functional chromophores for the development of third-order NLO materials.

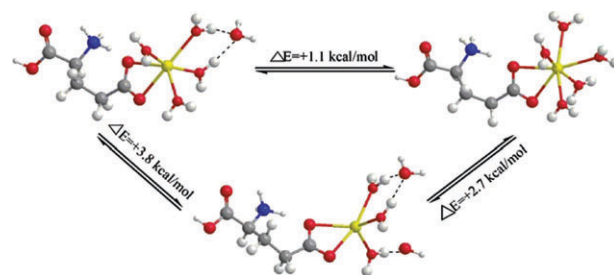
PAPERS

890

Hydration effect on interaction mode between glutamic acid and Ca^{2+} and its biochemical implication: a theoretical exploration

Feng Xiang, Ping Li, Shihai Yan, Lixiang Sun, Robert I. Cukier and Yuxiang Bu*

The hydration effects on the glutamic acid– Ca^{2+} complexes and the correlated biochemical implications have been explored by DFT theoretical calculations.

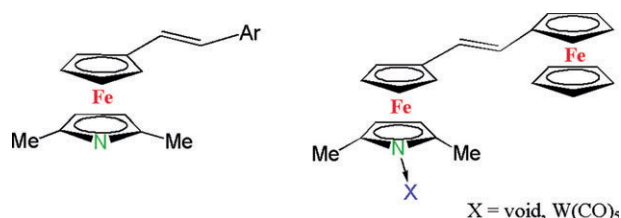


901

Aryl (ferrocenyl)-capped ethenylzaferrocenes: synthesis, structure and electrochemistry

Konrad Kowalski, Janusz Zakrzewski,* Marcin Palusiak and Sławomir Domagała

Cyclic voltammetry showed that electronic properties of aryl (ferrocenyl)-capped ethenylzaferrocenes differ substantially from those of their ferrocenyl counterparts.

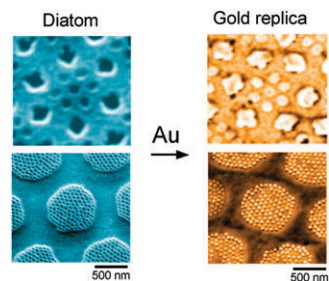


908

Fabrication of gold nanostructures by templating from porous diatom frustules

Dusan Losic,* James G. Mitchell and Nicolas H. Voelcker

Diatom frustules of several different species have been used as templates for the fabrication of gold nanostructures with complex morphologies.

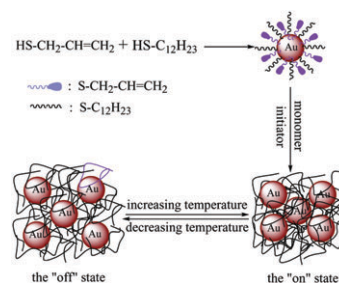


915

A kind of smart gold nanoparticle–hydrogel composite with tunable thermo-switchable electrical properties

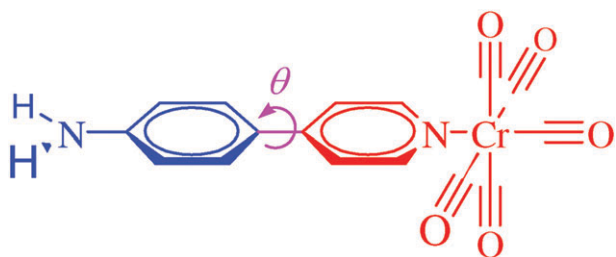
Xiuli Zhao, Xiaobin Ding,* Zhenghua Deng, Zhaohui Zheng, Yuxing Peng,* Chunrong Tian and Xinping Long

A well-dispersed gold nanoparticle–poly-*N*-isopropylacrylamide (PNIPAm) hydrogel composite with thermo-switchable electrical properties was prepared by the co-polymerization of Au nanoparticles with attached vinyl groups with NIPAm.



PAPERS

921

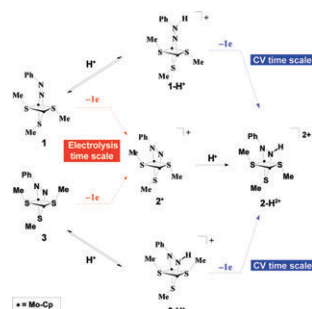


The effect of the conformation on the quadratic nonlinear optical response of metal carbonyl based chromophores with one-dimensional charge transfer capabilities: a computational investigation

Jean-François Lamère, Isabelle Sasaki, Pascal G. Lacroix* and Keitaro Nakatani

The molecular quadratic hyperpolarizability of a phenylpyridine-based chromophore could strictly vanish when the aromatic rings possess a torsion angle (θ) of 63° .

929

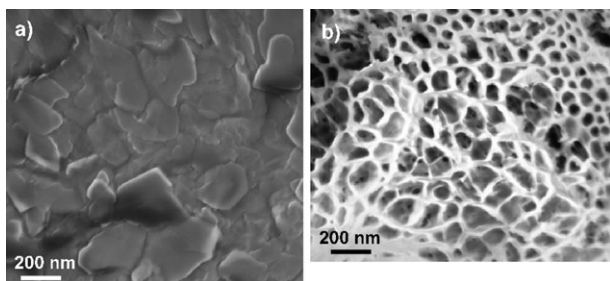


Oxidatively-induced $\mu\text{-}\eta^1 \rightarrow \mu\text{-}\eta^1\text{:}\eta^1$ rearrangement of $\{\text{N}=\text{N}\}$ ligands at a $\{\text{Mo}_2(\mu\text{-SMe})_3\}$ site and protonation of the oxidized diazenido complex

Alan Le Goff, Christine Le Roy, François Y. Pétillon, Philippe Schollhammer and Jean Talarmin*

Oxidatively-induced processes comprising $\mu\text{-}\eta^1 \rightarrow \mu\text{-}\eta^1\text{:}\eta^1$ linkage isomerism of diazenido and hydrazido ligands bound to a dimolybdenum-sulfur core, and inversion at an equatorial SMe, are reported.

939

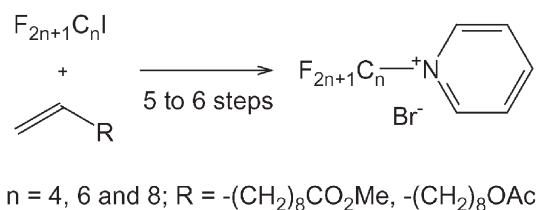


[2.2]Paracyclophanes incorporated within poly(3-butylthiophene): synthesis and photoelectrical properties

Luca Valentini,* Francesco Mengoni, Aldo Taticchi, Assunta Marrocchi, Selvaggia Landi, Lucio Minuti and José M. Kenny

Linearly functionalized [2.2]paracyclophane derivatives interacting with poly(3-butylthiophene) are largely responsible for the generation of photo-charge carriers in semiconducting conjugated polymers.

944



Synthesis and biocompatibility evaluation of partially fluorinated pyridinium bromides

Sandhya M. Vyas, Jaroslav Turánek, Pavlína Knöťigová, Andrea Kašná, Veronika Kvardová, Venkat Koganti, Stephen E. Rankin, Barbara L. Knutson and Hans-Joachim Lehmler*

The synthesis and biocompatibility assessment of partially fluorinated pyridinium surfactants is described.

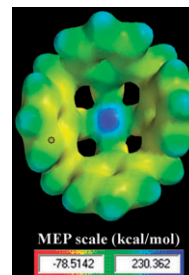
PAPERS

952

Organic guests inclusion by tungsten-calix[4]arene hosts

Arturo Arduini, Chiara Massera, Andrea Pochini,*
Andrea Secchi and Franco Ugozzoli*

The binding mode of a series of lower rim tungsten-calix[4]arenes toward different neutral organic guests has been investigated in the solid state and through *ab initio* computational studies.

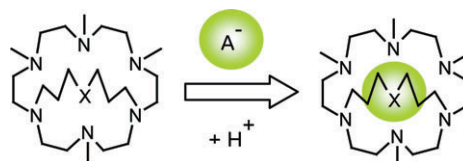


959

Inclusive coordination of F⁻, Cl⁻ and Br⁻ anions into macrobicyclic polyammonium receptors

Carla Bazzicalupi, Andrea Bencini, Antonio Bianchi,*
Andrea Danesi, Claudia Giorgi, Maria Angeles Martinez
Lorente and Barbara Valtancoli

Two macrobicyclic cage-like ligands, based upon [18]aneN₆, display uncommon selectivity trends in the binding of halogenide ions.



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AUTHOR INDEX

- Anderson, Ken B., 868
 Andrae, Dirk, 873
 Arduini, Arturo, 952
 Bampos, Nick, 861
 Bao, Jianchun, 832
 Barboiu, Mihail, 823
 Bazzicalupi, Carla, 959
 Belmont, Philippe, 823
 Bencini, Andrea, 959
 Bernardinelli, Gérard, 851
 Bianchi, Antonio, 959
 Blériot, Yves, 823
 Bocquet, Bernard, 851
 Bolze, Frédéric, 823
 Bouquillon, Sandrine, 823
 Bourguet, Erika, 823
 Braid, Benoît, 823
 Bu, Yuxiang, 890
 Che, Yanchao, 883
 Chen, Hui, 883
 Compain, Philippe, 823
 Constantieux, Thierry, 823
 Copéret, Christophe, 842
 Cukier, Robert I., 890
 Dai, Zhihui, 832
 Danesi, Andrea, 959
 Deng, Zhenghua, 915
 Désaubry, Laurent, 823
 Desvergnès, Valérie, 823
 Ding, Xiaobin, 915
 Domagala, Sławomir, 901
 Dupont, Delphine, 823
 Eisenstein, Odile, 842
 Filhol, Jean-Sébastien, 842
 Gastaldi, Stéphane, 823
 Giorgi, Claudia, 959
 Gunter, Maxwell J., 861
 Hu, Zhixin, 832
 Jérôme, François, 823
 Johnstone, Ken D., 861
 Kašná, Andrea, 944
 Kenny, José M., 939
 Knötigová, Pavlína, 944
 Knutson, Barbara L., 944
 Koganti, Venkat, 944
 Kowalski, Konrad, 901
 Kübel-Pollak, Anita, 851
 Kvardová, Veronika, 944
 Lacroix, Pascal G., 921
 Lamère, Jean-François, 921
 Landi, Selvaggia, 939
 Lavernat, Francine, 851
 Le Goff, Alan, 929
 Le Roy, Christine, 929
 Legoupy, Stéphanie, 823
 Lehmler, Hans-Joachim, 944
 Li, Ping, 890
 Li, Yingguang, 832
 Lin, Jiaping, 883
 Long, Xiping, 915
 Losic, Dusan, 908
 Marat, Xavier, 823
 Marrocchi, Assunta, 939
 Martinez Lorente, Maria Angeles, 959
 Massera, Chiara, 952
 Matthews, Craig J., 851
 Melich, Xavier, 851
 Mengoni, Francesco, 939
 Migaud, Marie, 823
 Miguel, Daniel, 838
 Minuti, Lucio, 939
 Mitchell, James G., 908
 Moitessier, Nicolas, 823
 Morgantini, Pierre-Yves, 851
 Nakatani, Keitaro, 921
 Nieto, Sonia, 838
 Ollivier, Cyril, 823
 Palusiak, Marcin, 901
 Papot, Sébastien, 823
 Peng, Yuxing, 915
 Pérez, Julio, 838
 Peri, Francesco, 823
 Pétilon, François Y., 929
 Petit, Marc, 823
 Pochini, Andrea, 952
 Py, Sandrine, 823
 Rankin, Stephen E., 944
 Riera, Lucia, 838
 Riera, Victor, 838
 Robert, Frédéric, 823
 Sanders, Jeremy K. M., 861
 Sasaki, Isabelle, 921
 Schollhammer, Philippe, 929
 Schulz, Emmanuelle, 823
 Secchi, Andrea, 952
 Solans-Monfort, Xavier, 842
 Sun, Lixiang, 890
 Sun, Peipei, 832
 Suzenet, Franck, 823
 Talarmin, Jean, 929
 Tang, Zhenyu, 883
 Taticchi, Aldo, 939
 Tian, Chunrong, 915
 Tian, Xiaohui, 883
 Tranoy-Opalinski, Isabelle, 823
 Turánek, Jaroslav, 944
 Ugozzoli, Franco, 952
 Valentini, Luca, 939
 Valtancoli, Barbara, 959
 Vaughn, Daniel L., 868
 Vauzeilles, Boris, 823
 Vayron, Philippe, 823
 Verdan, Simon, 851
 Vergnes, Laurent, 823
 Vidal, Sébastien, 823
 Voelcker, Nicolas H., 908
 Vyas, Sandhya M., 944
 Williams, Alan F., 851
 Wilmouth, Serge, 823
 Xiang, Feng, 890
 Yan, Shihai, 890
 Zakrzewski, Janusz, 901
 Zhao, Xiuli, 915
 Zheng, Zhaohui, 915
 Zhou, Ping, 832

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