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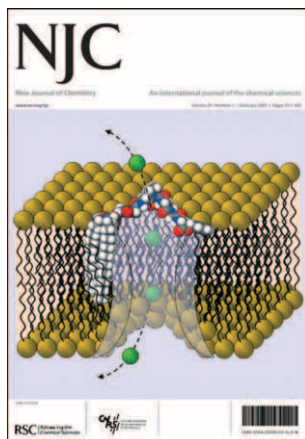
ISSN 1144-0546 CODEN NJCHES 29(2) 253-400 (2005)

In this issue...

Letters from James M. Takacs,
Minghua Qiao, Florence Geneste, Yi Tang,
Joulia Larionova, Angel E. Kaifer,
Julio Belmar and Gwénaél Rapenne



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in this journal also appear in the
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Cover

See George Gokel *et al.*, page 291.
The front cover illustrates the ability of
membrane-active heptapeptides to form
ion channels in phospholipid bilayers
of synthetic liposomes. A range of
heptapeptides form ion channels that
perform many of the functions of complex
proteins even though their molecular
weight of about 1000 is less than 1% of
the natural structures. Both the C- and
N-terminal residues serve as membrane
anchors and small differences in their
structures strongly influence ion transport.

CHEMICAL SCIENCE

C9

Drawing together the research highlights and news from all
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Chemical Science

February 2005/Volume 2/Issue 2

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LETTERS

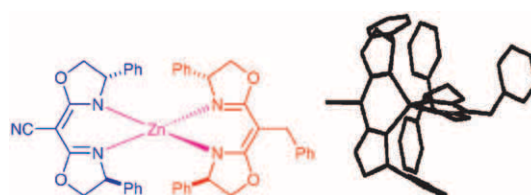
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The selective formation of neutral, heteroleptic zinc(II) complexes *via* self-discrimination of chiral bisoxazoline racemates and pseudoracemates

James M. Takacs,* Paul M. Hrvatin, Jeffery M. Atkins,
D. Sahadeva Reddy and Joanna L. Clark

The reversible metal-directed multi-component self-assembly
of chiral bisoxazolines proceeds with a high level of chiral
self-discrimination and thus defines a simple strategy for the
preparation of neutral, heteroleptic zinc(II) complexes.

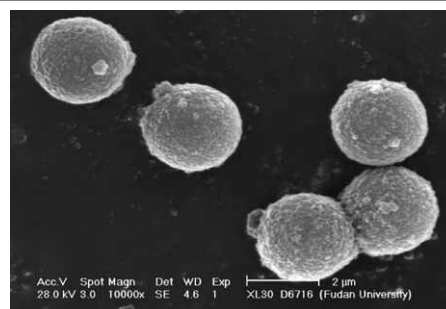


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Amorphous Ni-B hollow spheres synthesized by controlled organization of Ni-B nanoparticles over PS beads *via* surface seeding/electroless plating

Xueying Chen, Wuli Yang, Shuai Wang, Minghua Qiao,*
Shirun Yan, Kangnian Fan and Heyong He*

Hollow spheres made of amorphous Ni-B alloys were prepared
for the first time by a combined surface seeding and electroless
plating method.



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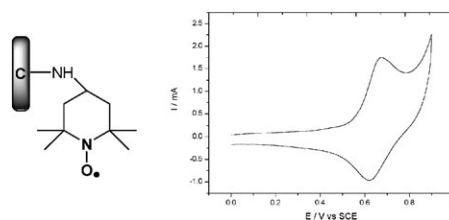
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Electrochemically linking TEMPO to carbon *via* amine bridges

Florence Geneste* and Claude Moinet

The immobilization of TEMPO onto a graphite felt electrode was achieved by anodic oxidation of its corresponding amino derivative at low potentials in aqueous solutions.

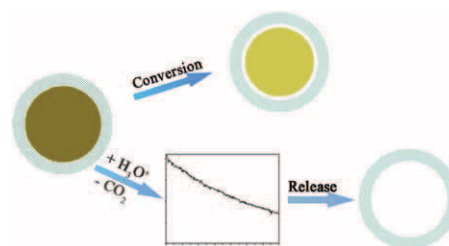


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Controlled release and conversion of guest species in zeolite microcapsules

Deju Wang, Guibo Zhu, Yahong Zhang,* Wuli Yang, Biyun Wu, Yi Tang* and Zaiku Xie

The high microporosity and thermal/chemical stability of zeolite microcapsules allows for the controlled release and conversion of guest species in zeolite microcapsules.

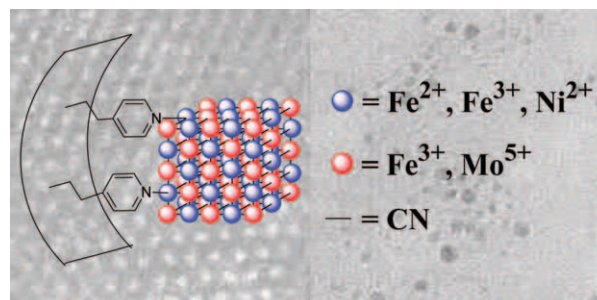


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Formation of cyano-bridged molecule-based magnetic nanoparticles within hybrid mesoporous silica

Guylhaine Clavel, Yannick Guari,* Joulia Larionova* and Christian Guérin

Uniformly sized molecule-based magnetic nanoparticles can be grown into the pores of a functionalized mesostructured hybrid silica matrix.

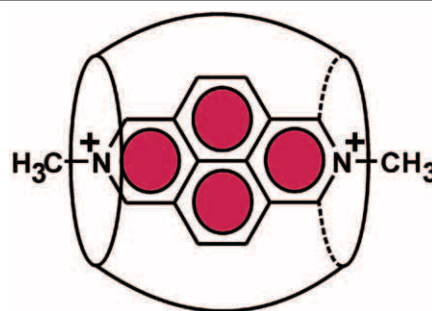


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Tight inclusion complexation of 2,7-dimethyldiazapyrenium in cucurbit[7]uril

Vladimir Sindelar, Mabel A. Cejas, Francisco M. Raymo and Angel E. Kaifer*

Inclusion of the dicationic guest 2,7-dimethyldiazapyrenium in the host cucurbit[7]uril, forming a very stable complex in which the host is distorted by the shape of the guest.

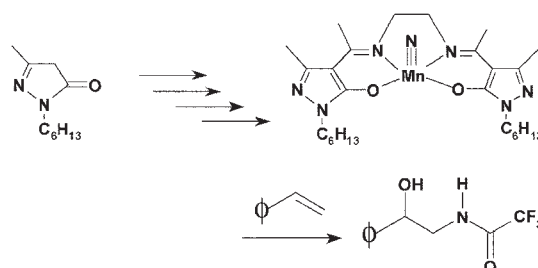


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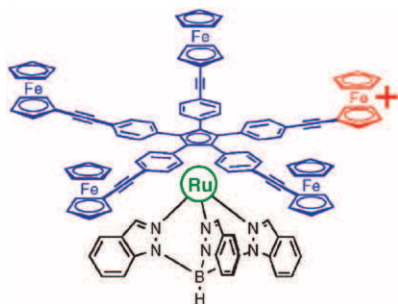
Pyrazolone-based nitrido complexes: synthesis and nitrogen transfer to alkenes

Fredy R. Pérez, Julio Belmar,* Yanko Moreno, Ricardo Baggio and Octavio Peña

The first reported examples of alkylpyrazolone based nitridomanganese(v) complexes are shown to transfer nitrogen in stoichiometric reactions, using styrene with trifluoroacetic anhydride as the test substrates.



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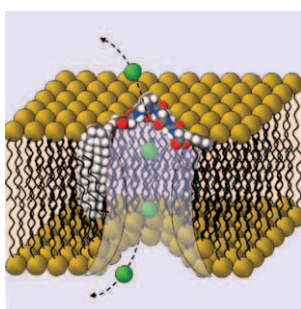


Design and synthesis of the active part of a potential molecular motor

Alexandre Carella, Gwénaél Rapenne* and Jean-Pierre Launay*

A heteroleptic ruthenium(II) complex fulfils all criteria to behave as an electron-driven rotary motor.

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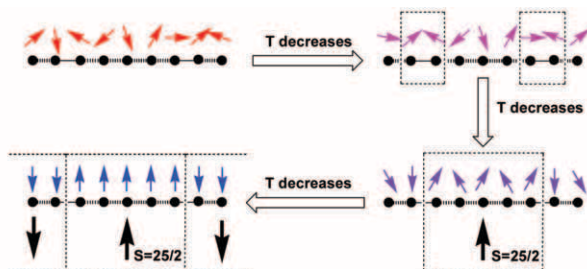


The C- and N-terminal residues of synthetic heptapeptide ion channels influence transport efficacy through phospholipid bilayers

Natasha Djedović, Riccardo Ferdani, Egan Harder, Jolanta Pajewska, Robert Pajewski, Michelle E. Weber, Paul H. Schlesinger and George W. Gokel*

Both the C- and N-terminal chains of the amphiphilic heptapeptide ionophores influence the efficacy of ion transport.

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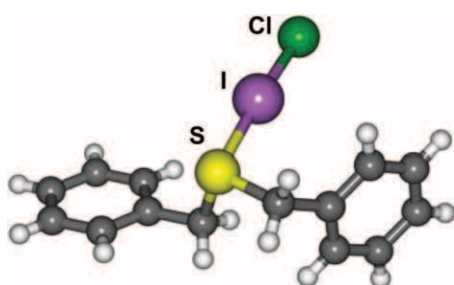


Topological ferrimagnetic behavior of one new chain with the new AF/F/F'/F'/F alternating sequence

Joan Cano,* Yves Journaux, Mohamed A. S. Goher, Morsy A. M. Abu-Youssef, Franz A. Mautner, Guido J. Reiß, Albert Escuer* and Ramon Vicente

A one-dimensional system with an unusual magnetic interaction topology that leads to a new type of ferrimagnetic behavior is analyzed. It has been studied by means of susceptibility, single crystal ESR measurements and Monte Carlo simulations.

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A solid-state structural and theoretical study on the 1 : 1 addition compounds of thioethers with dihalogens and interhalogens I-X (X = I, Br, Cl)

Gabriel A. Asseily, Robert P. Davies,* Henry S. Rzepa* and Andrew J. P. White

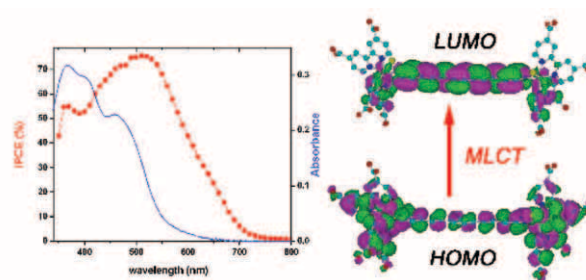
The first solid-state structural characterisation of a thioether I-Cl adduct is presented along with a thorough theoretical study on the accurate modelling of thioether interhalogen and dihalogen adducts.

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A highly efficient redox chromophore for simultaneous application in a photoelectrochemical dye sensitized solar cell and electrochromic devices

Ana F. Nogueira,* Sérgio H. Toma, Marcio Vidotti, André L. B. Formiga, Susana I. Córdoba de Torresi and Henrique E. Toma*

A novel binuclear Ru(II) dicarboxybipyridine complex with a bridging *trans*-1,4-bis[2-(4-pyridyl)ethenyl]benzene ligand exhibits a high IPCE > 70% when applied as a photoanode in a dye sensitized solar cell and high coloration efficiency at 633 nm.

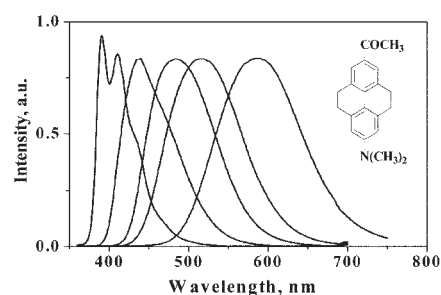


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Synthesis and photophysical studies of donor-acceptor substituted tetrahydropyrenes

S. Sumalekshmy and K. R. Gopidas*

Donor-acceptor substituted tetrahydropyrenes exhibiting very strong photoinduced intramolecular charge transfer undergo deactivation by the twisting of the acceptor group, if it is a strong acceptor, in highly polar solvents.

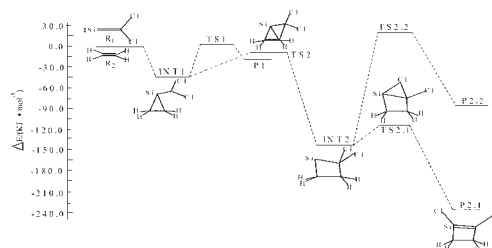


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A theoretical study on the mechanism of the cycloaddition reaction between dichloroalkyldenesilylene and ethylene

Xiuhui Lu,* Haibin Yu and Weirong Wu

The cycloaddition reaction between dichloroalkyldenesilylene and ethylene preferentially forms a 4-membered ring product in which a Cl atom has shifted to the silicon.

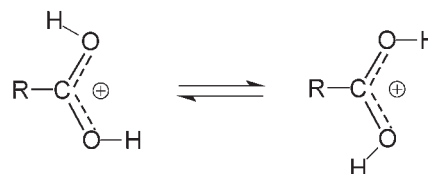


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Basicity of carboxylic acids: resonance in the cation and substituent effects

Stanislav Böhm and Otto Exner*

Carboxylic acids are moderately strong bases in the gas phase. Their protonated forms prefer the unsymmetrical conformation and are stabilized by resonance that is stronger than the resonance in the carboxylate anion. This resonance makes carboxylic acids somewhat stronger bases and compensates partly the stronger inductive effect, which makes them distinctly weaker bases than ketones.

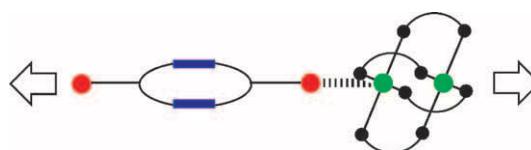


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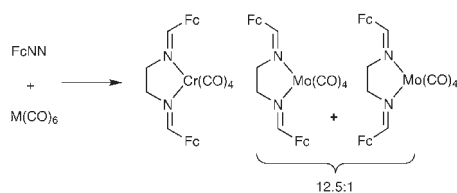
Molecular tectonics: design of coordinating tectons based on diazamacrocycles bearing pyridine units and formation of 1D copper coordination networks

Ernest Graf, Mir Wais Hosseini,* Jean-Marc Planeix and Nathalie Kyritsakas

Bis monodentate tectons based on diazamacrocyclic cores bearing pyridine units generate in the crystalline phase 1D coordination networks in the presence of copper diacetate.



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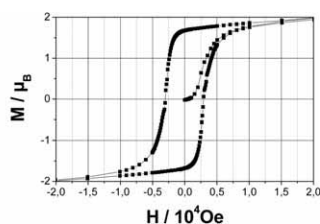
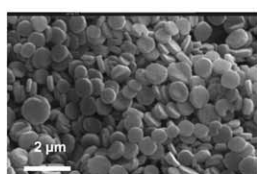


Synthesis of ferrocenyldiimine metal carbonyl complexes and an investigation of the Mo adduct encapsulated in cyclodextrin

Željko Petrovski, Susana S. Braga, Sandra S. Rodrigues, Cláudia C. L. Pereira, Isabel S. Gonçalves,*
Martyn Pillinger, Cristina Freire and Carlos C. Romão*

New heterometallic tetracarbonyl adducts were prepared by the reaction of a ferrocenyldiimine ligand with chromium or molybdenum hexacarbonyl. The change from Cr to Mo is sufficient to induce isomerisation of the ligand.

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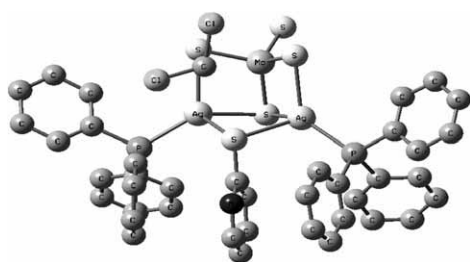


Synthesis, characterization and magnetic properties of disk-shaped particles of a cobalt alkoxide: $\text{Co}^{\text{II}}(\text{C}_2\text{H}_4\text{O}_2)$

Nassira Chakroune, Guillaume Viau,* Souad Ammar, Nouredine Jouini, Patrick Gredin, Marie Josèphe Vaulay and Fernand Fiévet

The cobalt alkoxide $\text{Co}(\text{OCH}_2\text{CH}_2\text{O})$ presents a brucite-like structure that, below 20 K, exhibits a 3D ferromagnetic order with a hysteresis loop showing a very high remanence-to-saturation ratio typical of uniaxial magnetocrystalline anisotropy.

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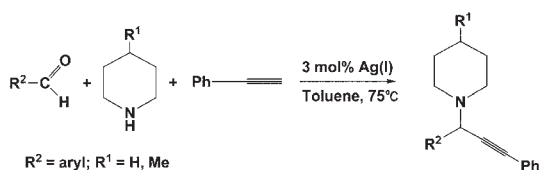


Large hyperpolarizabilities of trinuclear transition metal clusters $[\text{MAg}_2\text{X}_4(\text{C}_5\text{H}_5\text{NS})(\text{PPh}_3)_2] \cdot \text{CH}_2\text{Cl}_2$ ($\text{M} = \text{Mo}, \text{W}$; $\text{X} = \text{S}, \text{Se}$): a DFT study

Kechen Wu,* Rongjian Sa and Chensheng Lin

DFT calculations of static and dynamic first hyperpolarizabilities of a series of trinuclear transition metal molecular clusters have been carried out with evaluation of the different types of charge-transfer contributions to significant nonlinear optical activities.

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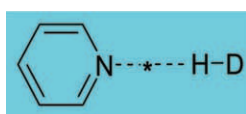


Organonitrile ligated silver complexes with perfluorinated weakly coordinating anions and their catalytic application for coupling reactions

Yanmei Zhang, Ana M. Santos, Eberhardt Herdtweck, Janos Mink and Fritz E. Kühn*

Acetonitrile ligated silver salts with three different non coordinating anions $[\text{B}(\text{C}_6\text{F}_5)_4]^-$, $[\text{B}(\text{C}_6\text{H}_3(\text{CF}_3)_2)_4]^-$ and $[(\text{C}_6\text{F}_5)_3\text{B}-\text{C}_3\text{H}_4\text{N}_2-\text{B}(\text{C}_6\text{F}_5)_3]^-$ were synthesized and characterized. They contain tetrahedrally or linearly coordinated $\text{Ag}(\text{I})$ cations. Their activity towards coupling reactions of terminal alkynes with aldehydes and amines was examined.

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Is there a hydrogen bond radius? Evidence from microwave spectroscopy, neutron scattering and X-ray diffraction results

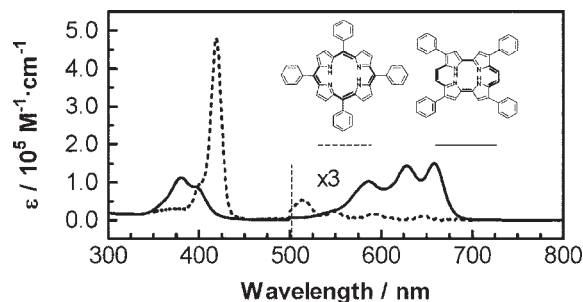
B. Lakshmi, A. G. Samuelson, K. V. Jovan Jose, S. R. Gadre and E. Arunan*

Hydrogen bond radius is the difference between the average $\text{H}\cdots\text{A}$ distance in $\text{D}-\text{H}\cdots\text{A}$ ($\text{D} = \text{O}/\text{N}/\text{C}$) hydrogen bonded contacts and the distance from the minimum (*) in the electrostatic potential of an acceptor (ex. pyridine) to the bonded atom (N).

A comparison between the photophysical and photosensitising properties of tetraphenyl porphycenes and porphyrins

Noemí Rubio, Ferran Prat, Núria Bou, José I. Borrell, Jordi Teixidó, Ángeles Villanueva, Ángeles Juarranz, Magdalena Cañete, Juan C. Stockert and Santi Nonell*

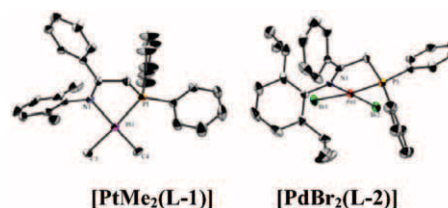
The photophysical properties of 2,7,12,17-tetraphenylporphycene and its Pd(II)- and Cu(II)-complexes are compared to those of tetraphenylporphyrins for assessing their potential advantages in photodynamic therapy.



New group 10 complexes of the bulky iminophosphine ligands [Ph₂PCH₂C(Ph)=N(2,6-R₂C₆H₃)], where R = Me, ^tPr

Sofia I. Pascu,* Karl S. Coleman, A. R. Cowley, Malcolm L. H. Green* and Nicholas H. Rees

Ni(II), Pd(II) and Pt(II) complexes of **L1**: [Ph₂PCH₂C(Ph)=N(2,6-Me₂C₆H₃)] and **L2**: [Ph₂PCH₂C(Ph)=N(2,6-^tPr₂C₆H₃)] have been prepared. The Pd(II) complexes catalyse the Heck coupling of 4-bromoacetophenone with *n*-butyl acrylate.



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