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IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 31(12) 1981-2128 (2007)



Cover

See Sason Shaik, p. 2015.
Crossing the mirror between conceptual worlds creates an integrated insight and a higher degree of understanding, as exemplified by the *homo-chemicus* inspecting its chemical ideas in the looking glass.

Artistic drawing by Yifat Shaik.
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CHEMICAL SCIENCE

C89

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Chemical Science

December 2007/Volume 4/Issue 12

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EDITORIAL

1995

Reflections on 30 years in the life of a journal

The *NJC* Editors reflect on 30 years of *NJC* and the anniversary celebrations over the last year.



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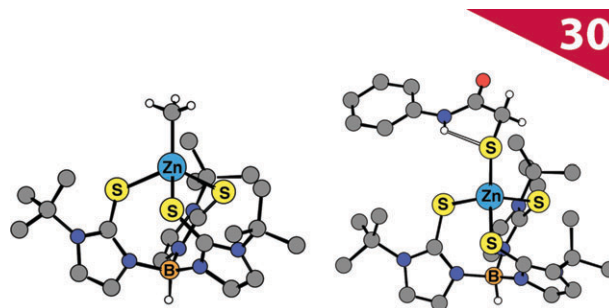
PERSPECTIVE

1996

Applications of tripodal $[S_3]$ and $[Se_3]$ L_2X donor ligands to zinc, cadmium and mercury chemistry: organometallic and bioinorganic perspectives

Gerard Parkin*

30th Anniversary article: The tripodal tris(2-mercapto-1-*R*-imidazolyl)hydroborato ligand system, $[Tm^R]$, and its selenium counterpart, $[Tse^R]$, provide useful platforms for investigating organometallic and bioinorganic aspects of the chemistry of zinc, cadmium and mercury in sulfur-rich and selenium-rich coordination environments.



2015

Is my chemical universe localized or delocalized? is there a future for chemical concepts?

Sason Shaik

30th Anniversary article: Crossing through the looking glass between conceptual worlds intensifies the chemical insight.

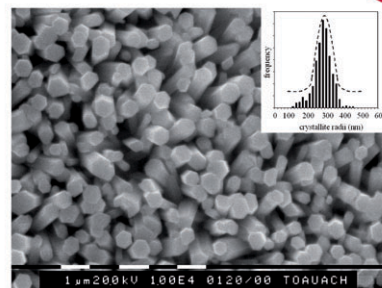


2029

Preparation of zinc containing materials

Mohammad Afzaal, Mohammad A. Malik and Paul O'Brien*

30th Anniversary article: Methods for growing zinc oxide or chalcogenide materials are described and discussed.



LETTER

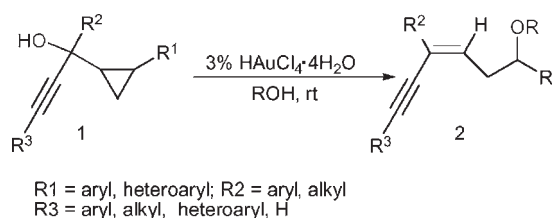


2041

Au(III)-catalyzed ring opening reaction of 1-cyclopropyl-2-yn-1-ols with nucleophiles: highly efficient approach to (*Z*)-conjugated enynes

Hui-quan Xiao, Xing-zhong Shu, Ke-gong Ji, Chen-ze Qi and Yong-min Liang*

A highly efficient approach to (*Z*)-conjugated enynes has been developed by utilizing an Au(III)-catalyzed ring-opening reaction of 1-cyclopropyl-2-yn-1-ols with nucleophiles under mild conditions.



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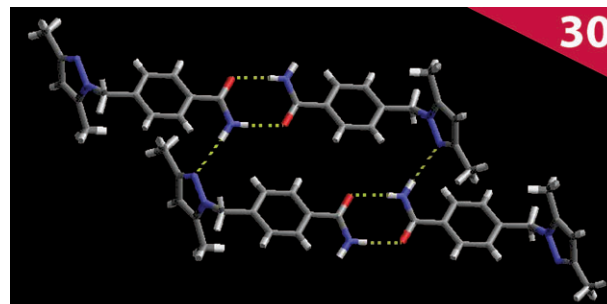
PAPERS

2044

How robust is the hydrogen-bonded amide 'ladder' motif?

Christer B. Aakeröy,* Benjamin M. T. Scott and John Desper

30th Anniversary article: The well-known hydrogen-bonded ladder displayed by amides in the solid state, is readily disrupted and reduced to an $R_2^2(8)$ motif if a competitive hydrogen-bond acceptor is incorporated in the molecular structure of the amide.

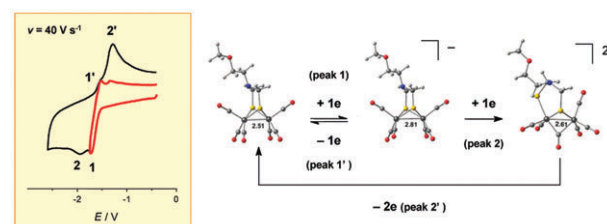


2052

Electrochemical and theoretical investigations of the reduction of $[\text{Fe}_2(\text{CO})_5\text{L}\{\mu\text{-SCH}_2\text{XCH}_2\text{S}\}]$ complexes related to $[\text{FeFe}]$ hydrogenase

Jean-François Capon, Salah Ezzaher, Frédéric Gloaguen, François Y. Pétillon, Philippe Schollhammer, Jean Talarmin,* Thomas J. Davin, John E. McGrady* and Kenneth W. Muir

The overall 2e reduction of three $[\text{Fe}_2(\text{CO})_5\text{L}(\mu\text{-dithiolate})]$ complexes (L = CO or NHC) can be split into two 1e steps.

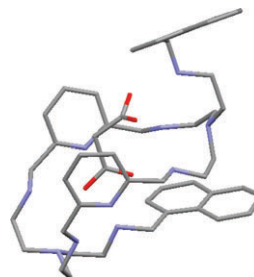


2065

A bibracchial lariat aza-crown ether as an abiotic catalyst of malonic acid enolization

M. Paz Clares, M. Teresa Albelda,* Juan Aguilar,* Luis R. Domingo, Juan C. Frías, Roberto Tejero, Conxa Soriano and Enrique García-España*

A bibracchial lariat aza-crown ether (L) consisting of 2-aminoethylnaphthyl moieties appended to a 2 : 2 azapyridinophane structure displays significant activation of H–D exchange in malonic acid and can be used to obtain clues about the reaction mechanism.

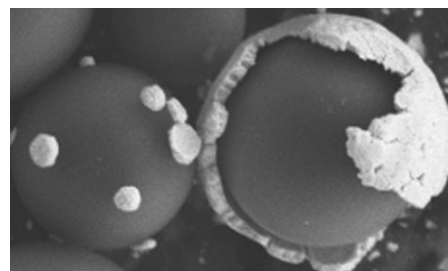


2071

The expansion/contraction of gold microparticles during voltammetrically induced amalgamation leads to mechanical instability

Laura E. Barrosse-Antle, Lei Xiao, Gregory G. Wildgoose, Ronan Baron, Chris J. Salter, Alison Crossley and Richard G. Compton*

Mercury is electrochemically deposited on and then stripped from gold microparticles, which experience morphological and chemical changes, going from ordered polycrystalline formations to irregular cuboid crystals and from gold to a gold–mercury amalgam, respectively.



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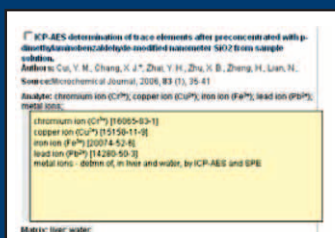


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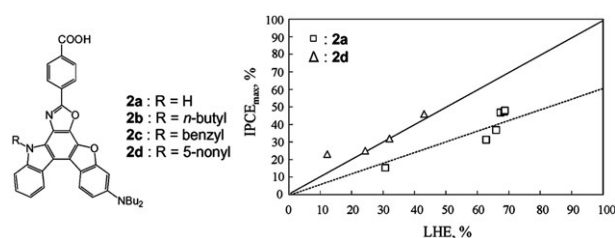
PAPERS

2076

Dye-sensitized solar cells based on novel donor–acceptor π -conjugated benzofuro[2,3-*c*]oxazolo[4,5-*a*]carbazole-type fluorescent dyes exhibiting solid-state fluorescence

Yousuke Ooyama, Akihiro Ishii, Yusuke Kagawa, Ichiro Imae and Yutaka Harima*

Dye-sensitized solar cells (DSSCs) based on novel donor–acceptor π -conjugated benzofuro[2,3-*c*]oxazolo[4,5-*a*]carbazole-type fluorescent dyes exhibiting solid-state fluorescence are fabricated and their photovoltaic performances are investigated.

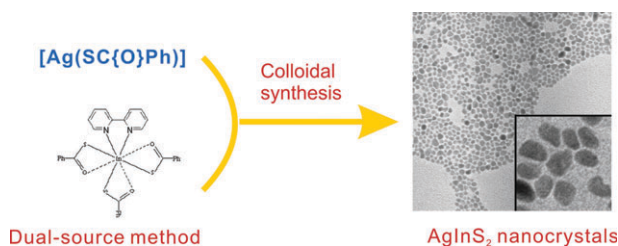


2083

Synthesis and characterization of ternary AgInS₂ nanocrystals by dual- and multiple-source methods

Lu Tian and Jagadees J. Vittal*

The precursors [In(bipy)(SC{O}Ph)₃] and [Ag(SC{O}Ph)] have been used to prepare monodispersed polyhedral shaped AgInS₂ nanocrystals (NCs).

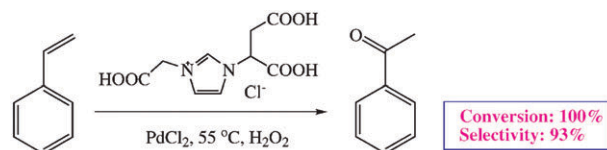


2088

Synthesis of multicarboxylic acid appended imidazolium ionic liquids and their application in palladium-catalyzed selective oxidation of styrene

Xuehui Li,* Weiguo Geng, Jixiang Zhou, Wei Luo, Furong Wang, Lefu Wang and Shik Chi Tsang*

A series of novel multicarboxylic acid appended imidazolium ionic liquids (McaILs) have been synthesized and McaIL/PdCl₂ catalytic systems have been investigated for the selective oxidation of styrene to acetophenone.

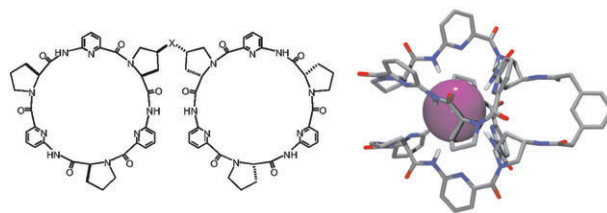


2095

Influence of linker structure on the anion binding affinity of biscyclopeptides

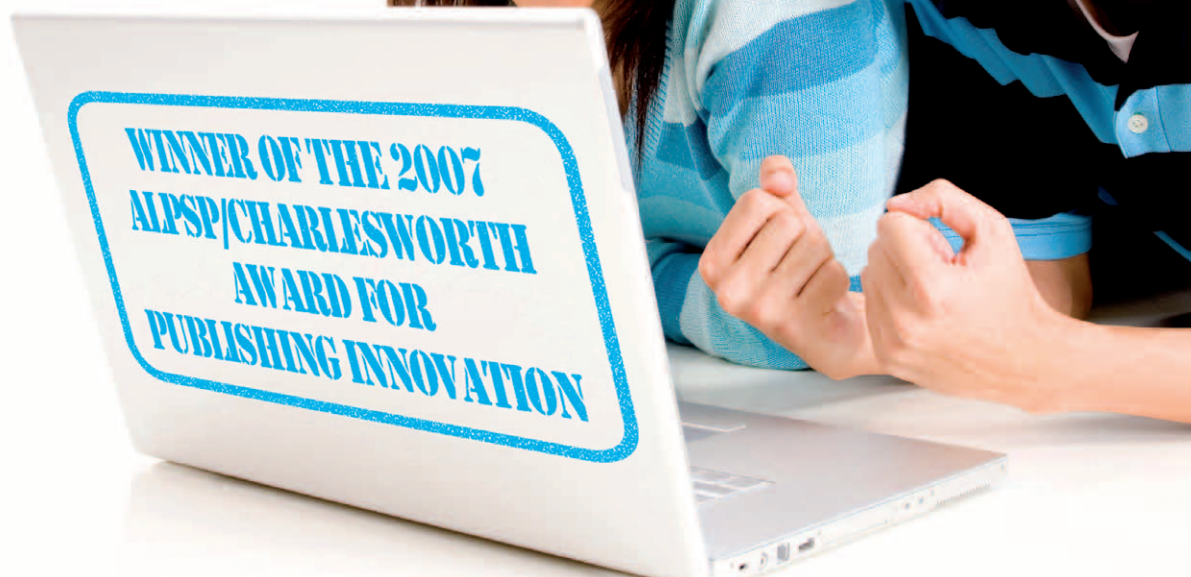
Carsten Reyheller, Benjamin P. Hay and Stefan Kubik*

Isothermal titration calorimetry revealed pronounced effects of linker structure on the thermodynamic parameters of complex formation in biscyclopeptide-based anion receptors.



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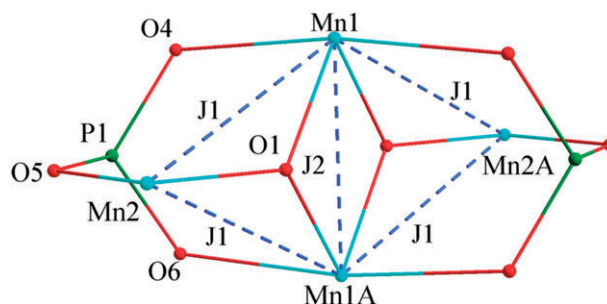
PAPERS

2103

Synthesis and characterization of a family of tetranuclear manganese(III) phosphonate complexes

Mei Wang, Chengbing Ma, Daqiang Yuan, Mingqiang Hu, Changneng Chen* and Qiutian Liu

Butterfly-shaped tetranuclear manganese(III) complexes containing phosphonate ligands with triply bridging oxygen atoms have been synthesized and characterized. The spin topology of two of the complexes leads to antiferromagnetic interactions through the μ_3 -O, O-C-O and O-P-O bridges.

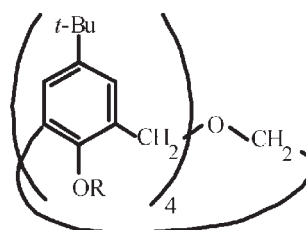


2111

Complexation and transport of transition and heavy metal cations by *p*-*tert*-butyldihomoxacalix[4]arene tetraketones and X-ray crystal structure of the *tert*-butyl ketone derivative

Paula M. Marcos,* Sandra Félix, José R. Ascenso, Manuel A. P. Segurado, Pierre Thuéry, Besma Mellah, Sylvia Michel, Véronique Hubscher-Bruder and Françoise Arnaud-Neu*

The binding properties of **2a–d** have been assessed.

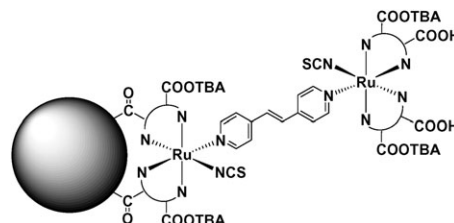
**2a** R = CH₂COMe**2b** R = CH₂COBu^t**2c** R = CH₂COAd**2d** R = CH₂COPh

2120

Dinuclear Ru(II) dyes for improved performance of dye-sensitized TiO₂ solar cells

Youngju Lee, Song-Rim Jang, R. Vittal and Kang-Jin Kim*

An N719 dye linked to another TiO₂-attached N719 dye through the linker *trans*-1,2-bis(4-pyridyl)ethylene (*tbpe*) renders higher conversion efficiency to the pertinent dye-sensitized solar cell, compared with those of the cells sensitized by the other mononuclear or dinuclear Ru(II) dyes.



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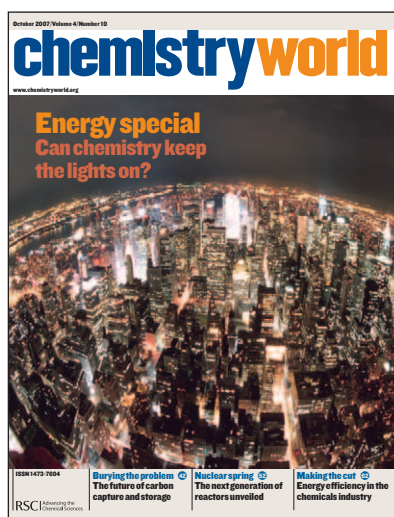


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