

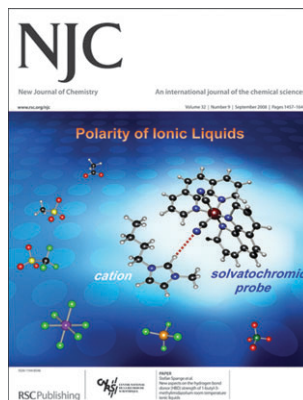
IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 32(9) 1457-1644 (2008)



Cover

See S. T. Hyde *et al.*, pp. 1484–1492. Knotted and linked structures are challenging targets for chemical syntheses due to the inherent connections between tangling, chirality and molecular properties. The image shows a simple example of a "ravelled" structure that is tangled, but contains neither knots nor links. This example is a ravelled tetrahedron. Background image used by permission of Beth Skwarecki. Image reproduced by permission from Toen Castle, Myfanwy E. Evans and S. T. Hyde from *New J. Chem.*, 2008, **32**, 1484.



Inside Cover

See Stefan Spange *et al.*, pp. 1493–1499. Hydrogen bond donor (HBD) strength parameters of 1-butyl-3-methylimidazolium-based ionic liquids with various anions were determined by means of $\text{Fe}(\text{phen})_2(\text{CN})_2$ as the solvatochromic UV/Vis probe. Image reproduced with permission from Ralf Lungwitz, Manfred Friedrich, Wolfgang Linert and Stefan Spange from *New J. Chem.*, 2008, **32**, 1493.

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C65

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Chemical Science

September 2008/Volume 5/Issue 9

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LETTER

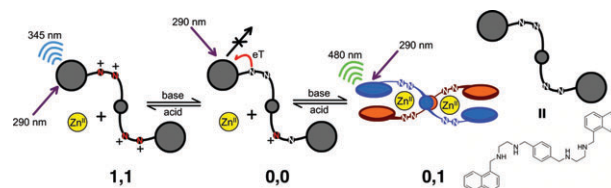


1473

A metallo-supramolecular approach to a half-subtractor

Miguel Vázquez López,* M. Eugenio Vázquez, Clara Gómez-Reino, Rosa Pedrido and Manuel R. Bermejo

The tetraamine dinucleating ligand **L**, which bears naphthalene moieties at both ends, behaves as a combinatorial logic circuit for a molecular half-subtractor in the presence of Zn^{II} ions. The mechanism for this device is based on the assembly of 1 : 1 Zn^{II} –**L** metallo-supramolecular adducts with fluorescent excimer emission properties.



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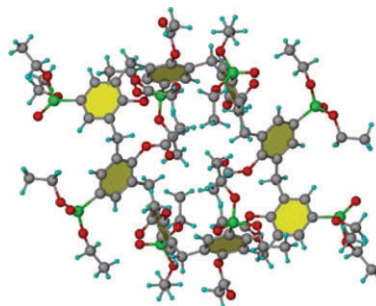
PAPERS

1478

Self-organised nano-arrays of *p*-phosphonic acid functionalised higher order calixarenes

Thomas E. Clark, Mohamed Makha,*
 Alexandre N. Sobolev, Dian Su, Henry Rohrs,
 Michael L. Gross, Jerry L. Atwood and Colin L. Raston*

A general synthetic protocol to the synthesis of water-soluble *p*-phosphonic acid calix[*n*]arenes (*n* = 5, 6 or 8), and solution and gas-phase studies of the formation of nano-arrays of around 20 calixarene units were observed using MALDI-TOF-MS and ESI-MS.

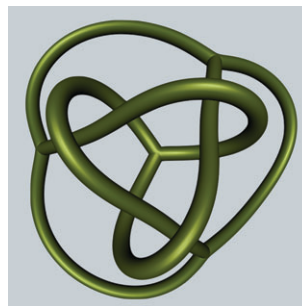


1484

Ravels: knot-free but not free. Novel entanglements of graphs in 3-space

Toen Castle, Myfanwy E. Evans and S. T. Hyde*

Nets can be tangled in a way that avoids any knotting or linking of loops in the net. If the entanglements are localised to a vertex, they are ravelled rather than knotted.

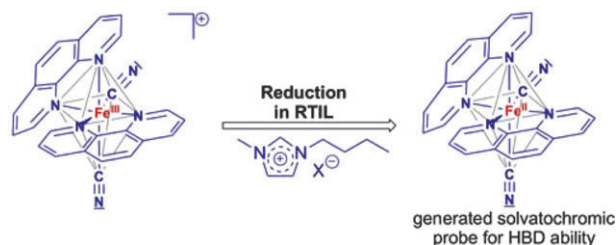


1493

New aspects on the hydrogen bond donor (HBD) strength of 1-butyl-3-methylimidazolium room temperature ionic liquids

Ralf Lungwitz, Manfred Friedrich, Wolfgang Linert and Stefan Spange*

Improved hydrogen bond donor (HBD) strength parameters of room temperature ionic liquids (RTILs) have been determined using Fe(phen)₂(CN)₂ as a solvatochromic UV/Vis probe, which results from dissolution of [Fe(phen)₂(CN)₂]ClO₄.

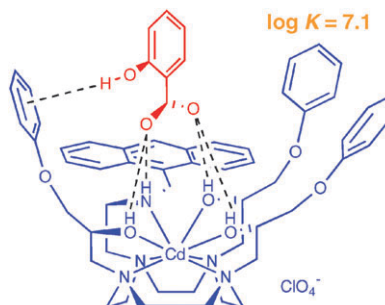


1500

Fluorescent signaling provides deeper insight into aromatic anion uptake by metal-ion activated molecular receptors

Adam J. Bradbury, Stephen F. Lincoln and Kevin P. Wainwright*

Fluorescent signaling of aromatic anion uptake by the metal-ion activated molecular receptor (blue) indicates greatly enhanced binding strength when classical hydrogen bonding is augmented by non-classical hydrogen bonding. Thus, salicylate (log *K* = 7.1), for example, is much more strongly included than benzoate (log *K* = 2.3).



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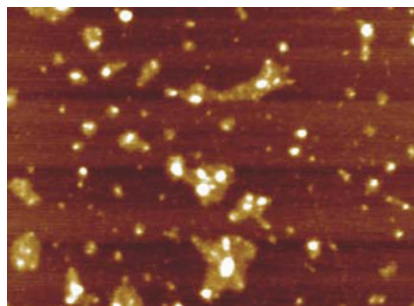
PAPERS

1509

AFM and TEM image of phenylacetylene polymerization on Rh/PVP colloidal nanoparticles

Marta Kopaczyńska, Jurgen H. Fuhrhop,
Anna M. Trzeciak,* Józef J. Ziolkowski and
Robert Choukroun

Rh/PVP nanoparticles were used as a new kind of catalyst in polymerization of phenylacetylene (PA).

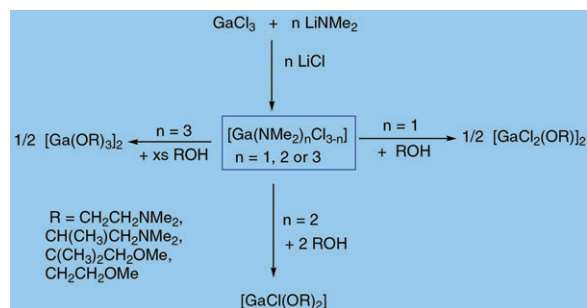


1513

Synthesis and structures of gallium alkoxides

Siama Basharat, Caroline E. Knapp, Claire J. Carmalt,*
Sarah A. Barnett and Derek A. Tocher

The synthesis and characterisation of gallium alkoxides, of the type $[\text{Ga}(\text{OR})_n\text{Cl}_{3-n}]$, incorporating donor functionalised ligands is described.

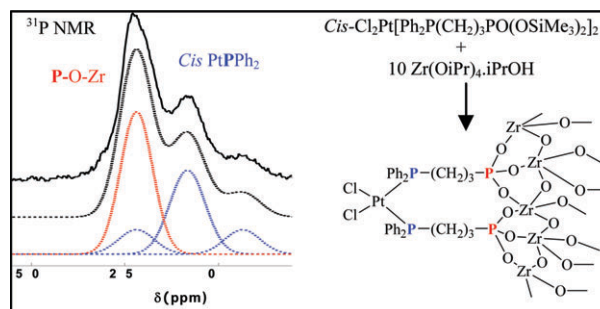


1519

Immobilization of platinum(II) and palladium(II) complexes on metal oxides by sol-gel processing and surface modification using bifunctional phosphine-phosphonate esters

Gilles Guerrero, P. Hubert Mutin,* E. Framery and
André Vioux

Phosphine ligands and Pt(II) and Pd(II) complexes were immobilized on metal oxide supports using phosphonate esters as anchoring groups that provide a valuable alternative to phosphonic acids.

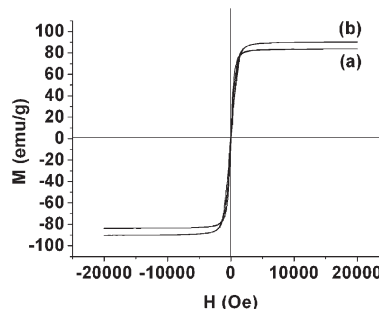


1526

Fe₃O₄ polyhedral nanoparticles with a high magnetization synthesized in mixed solvent ethylene glycol–water system

Shao-Wen Cao, Ying-Jie Zhu* and Jiang Chang

Well-dispersed Fe₃O₄ polyhedral nanoparticles showing superparamagnetism with a high magnetization close to that of bulk Fe₃O₄ were prepared by a solvothermal approach in the ethylene glycol (EG)–H₂O system.



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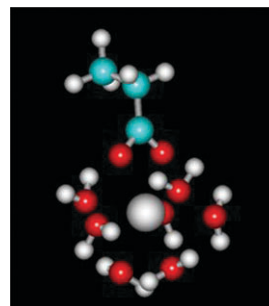
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1531

Luminescence from cerium(III) acetate complexes in aqueous solution: considerations on the nature of carboxylate binding to trivalent lanthanides

M. Emília Azenha, Hugh D. Burrows,* Sofia M. Fonseca,
M. Luísa Ramos, José Rovisco, J. Seixas de Melo,
Abílio J. F. N. Sobral and Ksenija Kogej

A short lived luminescence is seen in aqueous solutions of cerium(III) in the presence of acetate ion and attributed to a 1 : 1 complex involving weak bidentate coordination of the carboxylate ligand.

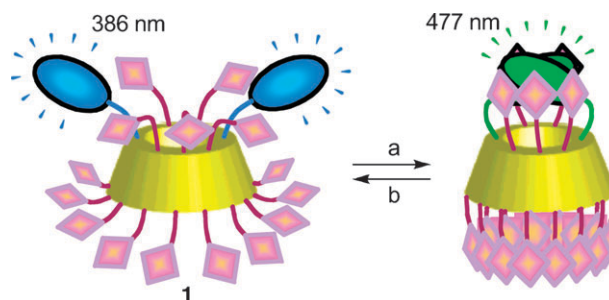


1536

Dual emission of a bis(pyrene)-functionalized, perbenzylated β -cyclodextrin

Cheng Huo, Jean-Claude Chambron* and Michel Meyer

The monomer/excimer fluorescence of **1** is switched by change in solvent composition or presence of the appropriate substrate: (a) H₂O–DMSO (80 : 20 v/v); (b) DMSO or heptanoic acid.

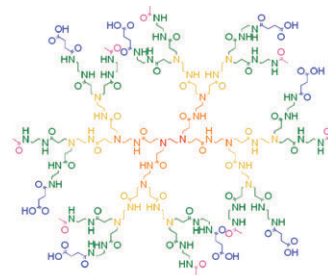


1543

The Dotted Cap Notation: A concise notation for describing variegated dendrimers

Benjamin P. Roberts, Martin J. Scanlon, Guy Y. Krippner
and David K. Chalmers*

A new notation has been developed to concisely describe the surface functionalisation of variegated dendrimers.

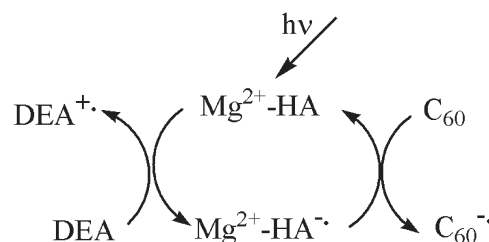

$$A \cdot B \cdot A \cdot B \cdots A \cdot B \cdot A \cdot B \cdots A \cdot B \cdot A \cdot B \cdots A \cdot B \cdot A \cdot B$$

1555

Photodynamic properties of supramolecular assembly constructed by magnesium complex of hypocrellin A and fullerene C₆₀

Yunyan Gao, Zhize Ou,* Jingrong Chen, Guoqiang Yang,*
Xuesong Wang,* Baowen Zhang, Mimi Jin and Lihua Liu

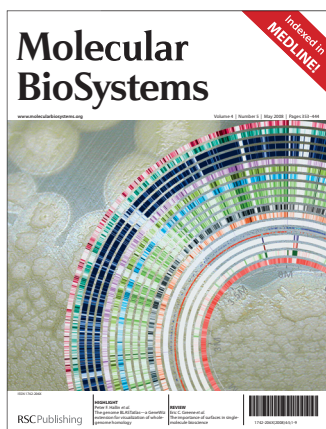
Mg^{2+} –HA acts as a light-harvesting antenna in the supramolecular system Mg^{2+} –HA/ C_{60} and mediates electron transfer from diethylaniline (DEA) to C_{60} .



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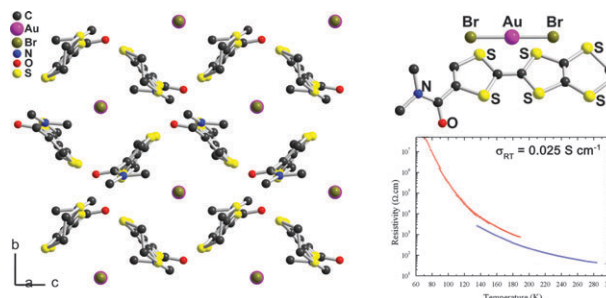
PAPERS

1561

Square-lattice hybrid organic–inorganic conducting layers in the τ phase of a TTF tertiary amide derivative

Pascal Cauliez, Cécile Mézière, Pascale Auban-Senzier, Rodolphe Clérac and Marc Fourmigué*

A rare stoichiometric τ phase is identified in τ -(EDT-TTF-CONMe₂)₂(AuBr₂)₂·TCE, characterised by a square lattice of orthogonal radical cations and a sizeable conductivity for a 1 : 1 salt.

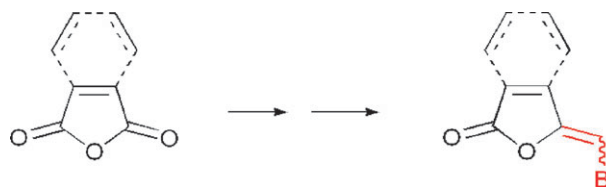


1567

Synthesis of 5-(bromomethylene)furan-2(5*H*)-ones and 3-(bromomethylene)isobenzofuran-1(3*H*)-ones as inhibitors of microbial quorum sensing

Tore Benneche, Zainab Hussain, Anne Aamdal Scheie and Jessica Lönn-Stensrud

5-Bromomethylenefuran-2(5*H*)-ones and 3-(bromomethylene)isobenzofuran-1(3*H*)-ones inhibit bacterial communication and can be readily made from maleic anhydrides and phthalic anhydrides, respectively.

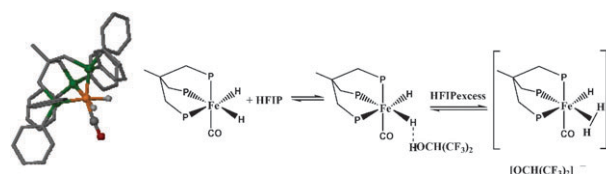


1573

Synthesis and characterisation of [(triphos)Fe(CO)H₂] and its protonation to a dihydrogen complex *via* an unconventional hydrogen-bonded intermediate

Gemma Guilera, G. Sean McGrady,* Jonathan W. Steed,* Richard P. L. Burchell, Peter Sirsch and Anthony J. Deeming

Protonation of an iron(II) dihydride complex proceeds *via* an unconventionally hydrogen bonded intermediate to give a stretched H₂ complex.

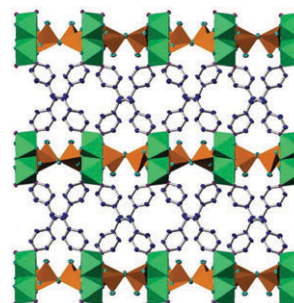


1582

Topological description of a 3D self-catenated nickel hybrid vanadate Ni(bpe)(VO₃)₂. Thermal stability, spectroscopic and magnetic properties

Roberto Fernández de Luis, José L. Mesa,* Miren K. Urtiaga, Luis Lezama, María I. Arriortua and Teófilo Rojo

Crystal structure of 3D self-catenated NiBpe(VO₃)₂.



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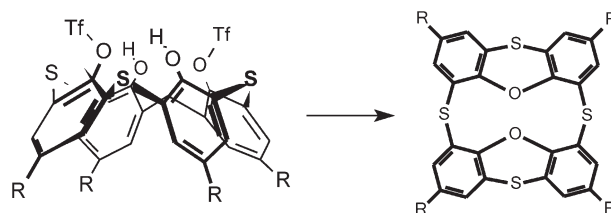
PAPERS

1590

Reactions of thiacalix[4]arene 1,3-bistriflate: formation of thiacalix[2]phenoxathiins—structural and complexation studies

Almeqdad Habashneh, Chester R. Jablonski, Julie Collins and Paris E. Georghiou*

Sonogashira reactions with thiacalix[4]arene bistriflate fail to produce arylethynyl products. Instead, a novel thia[2]phenoxathiin is produced, likely *via* an Ullmann-type mechanism. An unprecedented Pd(0)-mediated hydride-displacement of a lower-rim triflate was also observed. Five new X-ray structures are reported.

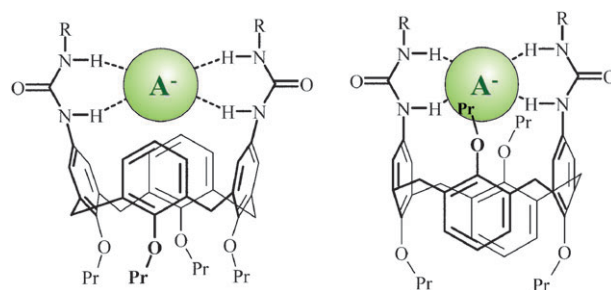


1597

Systematic approach to new ligands for anion recognition based on ureido-calix[4]arenes

Ivan Stibor,* Jan Budka, Veronika Michlová, Marcela Tkadlecová, Michaela Pojarová, Petra Cuřínová and Pavel Lhoták*

Mono-, di-, tri- and tetraureido-calix[4]arenes were synthesised and systematically studied for their complexation ability towards anions. A new type of very efficient ligands based on a 1,3-*alternate* conformation was discovered.

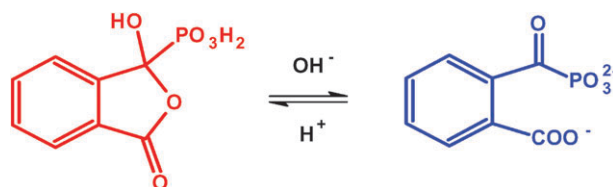


1608

Ring-chain tautomerism and protolytic equilibria of 3-hydroxy-3-phosphonoisobenzofuranone studied by ^1H , ^{13}C and ^{31}P NMR-controlled titrations

Sven Augner, Jan Kehler, Zoltán Szakács, Eli Breuer* and Gerhard Hägele*

Multinuclear NMR and potentiometric titrations revealed concerted ring-chain and protolytic equilibria involving 3-hydroxy-3-phosphonoisobenzofuranone and *ortho*-(phosphonatoformyl)benzoate.



1617

Investigation on the flexibility of chiral tricyclic derivatives

Maria Altamura, Paolo Dapporto, Antonio Guidi, Nicholas J. S. Harmat, Loïc Jerry, Elisa Libralesso, Paola Paoli* and Patrizia Rossi

Results of the investigations, by *ab initio* calculations and NMR spectroscopy, on the inversion barrier of enantiomeric conformers of tricyclic compounds bearing different heteroatoms on the central seven-membered ring, are presented.



Dynamic Stereochemistry of Chiral Compounds

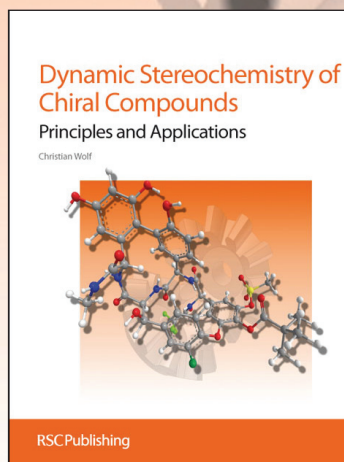
This book provides an overview of fundamental concepts of asymmetric synthesis highlighting the significance of stereochemical and stereodynamic reaction control. Topics include kinetic resolution (KR), dynamic kinetic resolution (DKR), dynamic kinetic asymmetric transformation (DYKAT), and dynamic thermodynamic resolution (DTR). In-depth discussions of asymmetric synthesis with chiral organolithium compounds, atropisomeric biaryl synthesis, self-regeneration of stereogenicity (SRS), chiral amplification with chiral relays and other commonly used strategies are also provided. Particular emphasis is given to selective introduction, interconversion and translocation of central, axial, planar, and helical chirality.

A systematic coverage of stereochemical principles and stereodynamic properties of chiral compounds guides the reader through the book and establishes a conceptual linkage to asymmetric synthesis, interconversion of stereoisomers, molecular devices that resemble the structure and stereomutations of propellers, bevel gears, switches and motors, and topologically chiral assemblies such as catenanes and rotaxanes. Racemization and diastereomerization reactions of numerous chiral compounds are discussed as well as the principles, scope and compatibility of commonly used analytical techniques.

- More than 550 figures, schemes and tables illustrating mechanisms of numerous asymmetric reactions and stereomutations of chiral compounds
- Technical drawings illustrating the conceptual linkage between macroscopic devices such as turnstiles, ratchets, brakes, bevel gears, propellers or knots and molecular analogs
- More than 3000 references to encourage further reading and facilitate additional literature research
- A comprehensive glossary with stereochemical definitions and terms which facilitate understanding and reinforce learning

This book will be of particular interest to advanced undergraduates, graduates and professionals working and researching in the fields of synthetic organic chemistry and stereochemistry.

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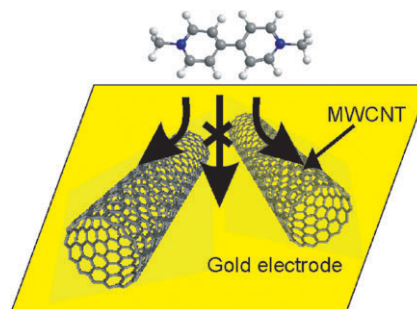
PAPERS

1628

Investigating the voltammetric reduction of methylviologen at gold and carbon based electrode materials. Evidence for a surface bound adsorption mechanism leading to electrode 'protection' using multi-walled carbon nanotubes

Lei Xiao, Gregory G. Wildgoose and Richard G. Compton*

The mechanistic redox behaviour of methylviologen in water is reported for several electrode materials. It was also found that multi-walled carbon nanotubes provides diffusional protection to underlying substrates.

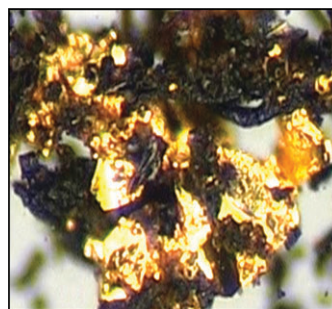


1634

Recovery of precious metals by using chemically modified waste paper

Chaitanya Raj Adhikari, Durga Parajuli, Katsutoshi Inoue,* Keisuke Ohto, Hidetaka Kawakita and Hiroyuki Harada

Chemically modified waste paper reduces Au(III) in acidic solution to elemental form.



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