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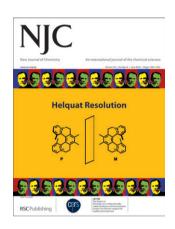
IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 34(6) 1029-1224 (2010)



Cover

See Beatriu Escuder et al., pp. 1044-1054. Supramolecular gels offer great possibilities as media for chemical reactions and catalysis by combining inherent reversibility and recyclability together with the appearance of unexpected valuable supramolecular effects. Beatriu Escuder, Francisco Rodríguez-Llansola and Juan F. Miravet, New J. Chem., 2010, 34, 1044.



Inside cover

See Filip Teplý et al., pp. 1063-1067. A racemic helicene-viologen hybrid can be resolved via diastereomeric dibenzoyltartrate salts. Louis Pasteur, the pioneer of enantioseparations, oversees this resolution scene. Artwork by Filip Teplý and Susan B. Glattstein Design. Image reproduced by permission of Filip Teplý and Susan B. Glattstein Design. Lukáš Severa, Dušan Koval, Pavlína Novotná, Milan Ončák, Petra Sázelová, David Šaman, Petr Slavíček, Marie Urbanová, Václav Kašička and Filip Teplý, New J. Chem., 2010, 34, 1063.

EDITORIAL

1043

A new co-Editor-in-Chief for NJC

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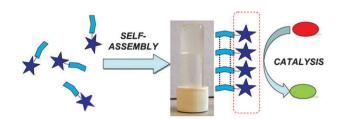
PERSPECTIVE

1044

Supramolecular gels as active media for organic reactions and catalysis

Beatriu Escuder,* Francisco Rodríguez-Llansola and Juan F. Miravet*

Supramolecular gels formed by self-assembled low molecular weight compounds present great potential as media for organic reactions and catalysis.



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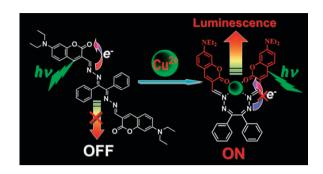
LETTERS

1055

A turn-on PET fluorescence sensor for imaging Cu²⁺ in living cells

Guangjie He, Xiuwen Zhao, Xiaolin Zhang, Hongjun Fan,* Shuo Wu, Huaqiang Li, Cheng He and Chunying Duan*

By the incorporation of coumarin fluorophores within the benzyldihydrazone moiety, a bright Cu²⁺-binding sensor in aqueous media is achieved for the detection of Cu²⁺ in living cells. It features excellent sensitivity, high selectivity, good water solubility and favourable spectroscopic properties.

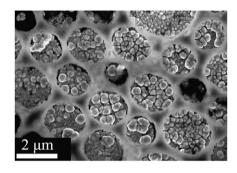


1059

Directionally electrodeposited gold nanoparticles into honeycomb macropores and their surface-enhanced Raman scattering

Peigin Tang and Jingcheng Hao*

The porous honeycomb film of (DODMA)₁₀{Mn₂Bi₂W₂₀} is taken as a good template to directionally electrodeposit gold nanoparticles into their macropores; the prepared hierarchical Au-filled film presents a strong surface-enhanced Raman scattering of rhodamine 6G molecules.



1063

Resolution of a configurationally stable [5]helquat: enantiocomposition analysis of a helicene congener by capillary electrophoresis

Lukáš Severa, Dušan Koval, Pavlína Novotná, Milan Ončák, Petra Sázelová, David Šaman, Petr Slavíček, Marie Urbanová, Václav Kašička and Filip Teplý*

A helicene-viologen hybrid can be resolved via dibenzoyltartrate salts. Capillary electrophoresis with a chiral selector is introduced as a direct way to analyze the enantiocomposition of charged helicene-like species.

racemic
$$(+)-(P)-[5]$$
helquat $>98\%$ ee

1068

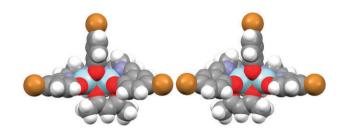
Bridged polysilsesquioxane films via photoinduced sol-gel chemistry

Abraham Chemtob, Cindy Belon, Céline Croutxé-Barghorn,* Jocelyne Brendlé, Michel Soulard, Séverinne Rigolet, Vincent Le Houérou and Christian Gauthier

Two routes towards bridged polysilsesquioxanes were investigated in parallel: a novel photoacid-catalyzed sol-gel process and a traditional HCl-catalyzed sol-gel process.

LETTERS

1073

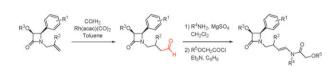


Design of chiral homodinuclear complexes based on the coordinating behaviour of some symmetric ligands

Ana M. García-Deibe,* Matilde Fondo, Noelia Ocampo, Jesús Sanmartín and Esther Gómez-Fórneas

Chiral homodinuclear $Zn(\pi)$ complexes have been designed on the basis of the coordinating behaviours of two symmetric ligands when combined: a compartmental Schiff base and an acetylacetonate anion.

1079

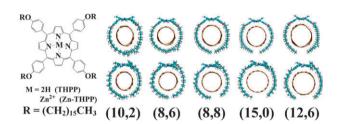


Rhodium-catalysed hydroformylation of N-(2-propenyl)- β -lactams as a key step in the synthesis of functionalised N-[4-(2-oxoazetidin-1-yl)but-1-enyl]acetamides

Stijn Dekeukeleire, Matthias D'hooghe, Christian Müller, Dieter Vogt* and Norbert De Kimpe*

N-[4-(2-Oxoazetidin-1-yl)but-1-enyl]acetamides were prepared starting from N-(2-propenyl)- β -lactams via catalytic hydroformylation of the olefinic moiety and subsequent treatment of the obtained aldehydes with alkoxyacetyl chlorides under Staudinger reaction conditions.

1084



Charge transfer in the non-covalent functionalization of carbon nanotubes

Olayinka O. Ogunro and Xiao-Qian Wang*

A first principles simulation study of type (semiconducting *vs.* metallic) selectability in non-covalent-functionalized carbon nanotubes.

1089

EIO-R-OH HO-R-OEI (Z.Z)-BABCH (E.Z)-BABCH (E.Z)-

The first use of supramolecular recognition to extract and stabilize an enzymatic inhibitor of a coagulation process

Arnaud Grandeury, Claudette Martin, Samuel Petit, Constantin T. Craescu and Géraldine Gouhier*

A supramolecular complex based on salt bridges between an artificial receptor and (Z,Z)-2,7-bis-(4-amidinobenzylidene)-cycloheptan-1-one (BABCH), a synthetic antagonist of tissue-plasminogen activator (t-PA), leads to a notable increase of its stability in solution and a new route of purification for this bioactive isomer.

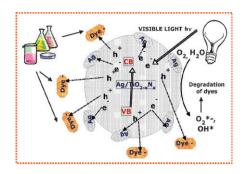
LETTERS

1094

Fabrication and visible light photocatalytic activity of a novel Ag/TiO_{2-x}N_x nanocatalyst

Jurate Virkutyte* and Rajender S. Varma*

A conceptually novel nanocatalyst has been identified that is remarkably efficient, stable and recyclable.

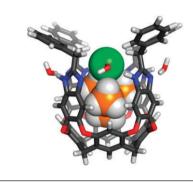


1097

Specific tetramethylammonium recognition drives general anion positioning in tandem sites of a deep cavitand

Miroslav Kvasnica and Byron W. Purse*

Reported here is a new approach to designing heteroditopic receptors for contact ion pairs, using geometric constraints instead of classical recognition motifs to control the position of a diverse set of anions.

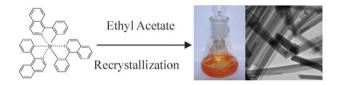


1100

Preparation of phosphorescent crystalline tris(1-phenylisoquinoline) iridium nanobelts via a recrystallization method

Debao Xiao,* Haiyan Xiao, Lili Liu and Xueling Li

Phosphorescent crystalline tris(1-phenylisoquinoline) iridium(III) nanobelts were prepared via a simple recrystallization procedure in ethyl acetate.



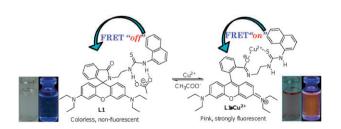
PAPERS

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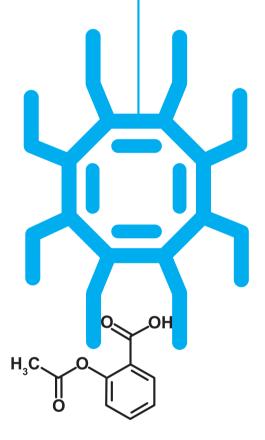
A reversible $E_{\rm m}$ -FRET rhodamine-based chemosensor for carboxylate anions using a ditopic receptor strategy

Chatthai Kaewtong,* Jakkapong Noiseephum, Yuwapon Uppa, Nongnit Morakot, Neramit Morakot, Banchob Wanno, Thawatchai Tuntulani and Buncha Pulpoka

A reversible rhodamine-based sensor (L1) was designed and synthesized using a ditopic receptor. Addition of Cu²⁺ ions to a solution of L1 induced a ring-open conformation of spirolactam ($E_{\rm m}$ -FRET ON), whilst ring closure was induced upon addition of CH_3COO^- (E_m -FRET *OFF*).



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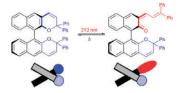


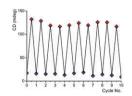
1109

A chiroptical binaphthopyran switch: amplified CD response in a polystyrene film

Anna Kicková, Jana Donovalová, Peter Kasák and Martin Putala*

Confinement of a photochromic binaphthopyran switch in a thin polystyrene film ensured a high fatigue resistance and an amplified CD response upon switching.



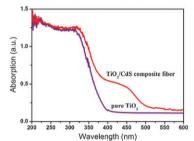


1116

Fabrication of TiO₂/CdS composite fiber via an electrospinning method

Huimin Cao, Yihua Zhu,* Xi Tan, Haigang Kang, Xiaoling Yang and Chunzhong Li

The electrospinning method coupled with a chemical reaction is employed to fabricate a TiO₂/CdS composite fiber. The DRUV-Vis spectra show that the TiO2/CdS composite fiber absorbs both in the UV and visible regions.



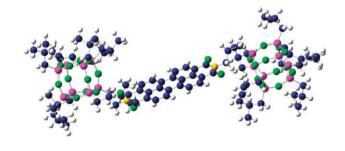


1120

A highly soluble polyhedral oligomeric silsesquioxane end-capped perylenediimide dye

Xiao-Dong Zhuang, Yu Chen,* Bin Zhang, Yongxi Li, Bo Yu and Wenhan Qiao

A highly soluble perylenediimide dye with unusual polyhedral oligomeric silsesquioxanes was synthesized.

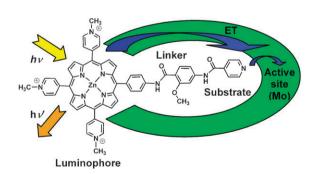




Design and synthesis of water soluble (metallo)porphyrins with pendant arms: studies of binding to xanthine oxidase

Elizabeth A. Gibson, Anne-K. Duhme-Klair* and Robin N. Perutz*

Probes for xanthine oxidase based on a water-soluble porphyrin luminophore covalently attached to a substrate analogue have been synthesised and tested. The probes are designed to report enzyme activity spectrofluorometrically.

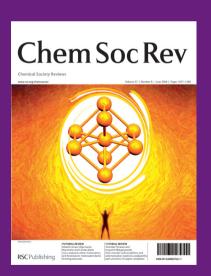


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PAPERS



The dipolarity/polarisability of 1-alkyl-3-methylimidazolium ionic liquids as function of anion structure and the alkyl chain length

Ralf Lungwitz, Veronika Strehmel and Stefan Spange*

The dipolarity/polarisability (π^*) of 1-alkyl-3-methylimidazolium ionic liquids has been determined as function of the alkyl chain length (n) and the anion (X -) by means of the solvatochromic UV/Vis probe 4-tert-butyl-2-(dicyanomethylene)-5-[4-(diethylamino)benzylidene]- Δ^3 -thiazoline.

Dipolarity/Polarisability =
$$\pi^*$$
 $\pi^* = f(\tilde{v}_{max})$
 $\pi^* = f(\tilde{v}_{max})$
 $\pi^* = f(\tilde{v}_{max})$
 $\pi^* = f(\tilde{v}_{max})$

Solvatochromic probe

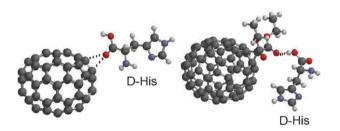
 $\pi = 1, 3, 5, \text{ and } 7$

1141

Enantioanalysis of D-histidine based on its interaction with [5,6]fullerene-C₇₀ and diethyl (1,2-methanofullerene-C₇₀)-71,71-dicarboxylate

Raluca-Ioana Stefan-van Staden*

A molecular interaction between D-histidine and two fullerenes: [5,6]fullerene- C_{70} and diethyl (1,2-methanofullerene- C_{70})-71,71-dicarboxylate, explained the response of two enantioselective, potentiometric membrane electrodes.



1148

A facile synthesis of Ag nanoparticles for mercury ion detection with high sensitivity and selectivity

Wenbing Li, Yanyan Guo, Kaci McGill and Peng Zhang*

Ag nanoparticles (<5 nm), synthesized by a one-step and green method, can be used to detect Hg(II) ions in aqueous media with high sensitivity and selectivity.

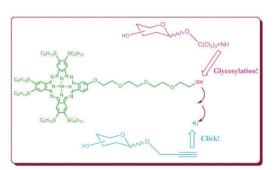
$$\underbrace{\text{PEG}}_{\text{(PEG)}} + \text{Ag}^{+} \Longrightarrow \underbrace{\underbrace{\text{Ag}^{0}}_{\text{Ag particles in PEG}}}_{\text{Ag particles in PEG}}$$

1153

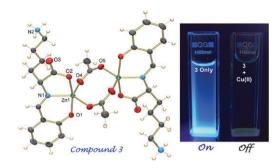
Amphiphilic carbohydrate-phthalocyanine conjugates obtained by glycosylation or by azide-alkyne click reaction

Mahmut Ali Ermeydan, Fabienne Dumoulin, Tamara V. Basova, Denis Bouchu, Ayşe Gül Gürek, Vefa Ahsen* and Dominique Lafont*

Two series of amphiphilic carbohydrate-phthalocyanine conjugates have been prepared, either by glycosylation or by copper-catalyzed click coupling. Functionalized versatile precursors: hydroxylated or azido phthalocyanines have been easily substituted by different carbohydrates.



1163



Direct dizinc displacement approach for efficient detection of ${\rm Cu}^{2^+}$ in aqueous media: acetate *versus* phenolate bridging platforms

Snehadrinarayan Khatua, Jina Kang and David G. Churchill*

Blue-fluorescent dizinc complexes 1–3 have been synthesized. 3 is a new diactate-bridged species, structurally different from closely related compounds 1 and 2, and acts as a highly selective ON–OFF fluorescent probe for Cu²⁺ *via* direct displacement of zinc ion in water at physiological pH.

1170

$$CI$$
+ $-SnMe_3$
 $-CI^ CO_2Me$
 CO_2Me
 CO_2Me
 CO_2Me

Regioselectivity of methyl chlorobenzoate analogues with trimethylstannyl anions by radical nucleophilic substitution: theoretical and experimental study

Juan P. Montañez, Jorge G. Uranga and Ana N. Santiago* Reactions of methyl 2,5-dichlorobenzoate, methyl 4-chlorobenzoate, methyl 2-chlorobenzoate and methyl 3-chlorobenzoate with Me₃Sn⁻ ions gave the corresponding substitution products by the S_{RN}1 mechanism.

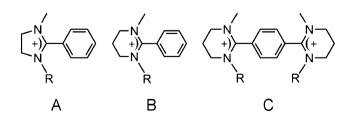
1176



Synthesis and structure of a series of new luminescent Ag-Ln coordination polymers and the influence of the introduction of an Ag(1) ion on NIR luminescence from the Ln(III) centre

Jing Jin, Shuyun Niu,* Qian Han and Yuxian Chi Four unusual Ag-Ln coordination polymers (Ln = Eu (1), Yb (2), Er (3), Ho (4)) with a 2D layer structure have been hydrothermally synthesized and characterized. The Ag-Ln polymers show peculiar emission bands in the NIR region owing to formation of the Ag-Ln coordination polymers.

1184



Amidinium based ionic liquids

Pierre Dechambenoit, Sylvie Ferlay,* Nathalie Kyritsakas and Mir Wais Hosseini*

Three new series of mono- and bis-cyclic amidinium cations bearing alkyl chains of different length were synthesized and several of their salts were found to behave as ionic liquids.

PAPERS

1200

Improving intramolecular hydroamination Rh(I) and Ir(I) catalysts through targeted ligand modification

Sophie R. Beeren, Serin L. Dabb, Gavin Edwards, Matthew K. Smith, Anthony C. Willis and Barbara A. Messerle*

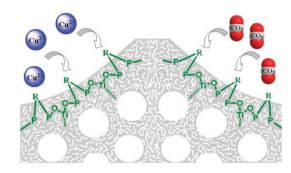
Catalysed intramolecular hydroamination of 4-pentyn-1-amine was achieved with a turnover rate of 1500 h (>98% conversion in 6 minutes). Activation of catalysts in situ through chloride abstraction was also investigated.

1209

High surface area titanium phosphonate materials with hierarchical porosity for multi-phase adsorption

Tian-Yi Ma, Xiu-Zhen Lin, Xue-Jun Zhang and Zhong-Yong Yuan*

Hierarchical meso-/macroporous hydroxyethylidene-bridged titanium phosphonate materials with high surface area (>370 m² g⁻¹) were synthesized by a mild solvent evaporation strategy in the presence of triblock copolymers F127 and P123, and proved to be low-cost and efficient adsorbents for heavy metal ions and CO₂ with good reusability.

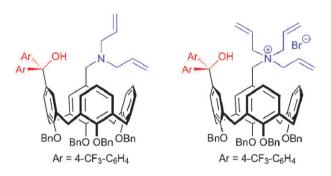


1217

Improved design of inherently chiral calix[4]arenes as organocatalysts

Seiji Shirakawa and Shoichi Shimizu*

An improvement of the design of inherently chiral calix[4]arenes as organocatalysts was accomplished via the introduction of a diarylmethanol structure.



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