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ISSN 1144–0546 CODEN NJCHES 34(12) 2685–3016 (2010)

Cover
See Kaisa Helttunen and Patrick Shahgaldian, pp. 2704–2714.
Amphiphiles based on calixarenes and resorcinarenes have been demonstrated to self-assemble in water to yield a variety of nanometer-sized systems, including the puzzling "spaghetti-like" structures shown on the background scanning electron micrograph.
Image reproduced by permission of Kaisa Helttunen and Patrick Shahgaldian from *New J. Chem.*, 2010, **34**, 2704.

Inside cover
See Janet Blümel *et al.*, pp. 2729–2731.
Rh catalysts immobilized by a rigid linker scaffold, characterized by ^{119}Sn MAS and X-ray analysis, cannot dimerize or touch the silica surface. The batches are recycled 30 times!
Image reproduced by permission of Björn Beele, Johannes Guenther, Melanie Perera, Michaela Stach, Thomas Oeser and Janet Blümel from *New J. Chem.*, 2010, **34**, 2729.

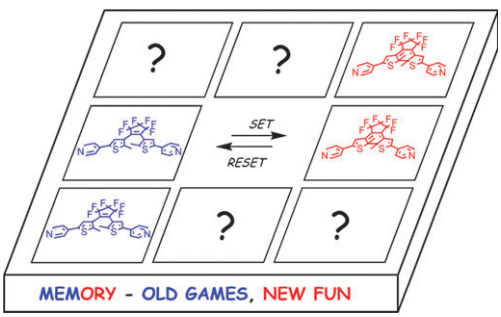
OPINION

2701

A simplicity-guided approach toward molecular set–reset memories

Uwe Pischel* and Joakim Andréasson*

The beauty of the simple: Seemingly complex molecular set–reset latches can be implemented by the application of a few general design conditions.



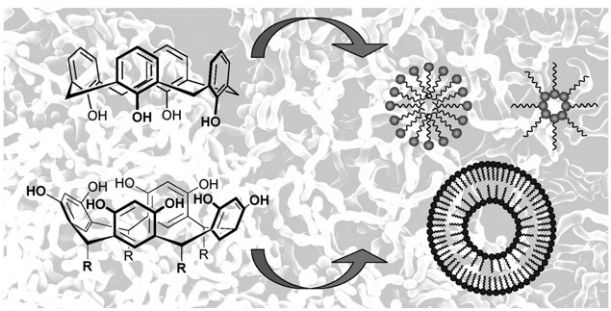
PERSPECTIVES

2704

Self-assembly of amphiphilic calixarenes and resorcinarenes in water

Kaisa Helttunen and Patrick Shahgaldian*

The present perspective article describes the developments of the chemistry of amphiphilic calixarenes and resorcinarenes with a clear focus on the synthetic paths used for their production and their self-assembly properties in water.



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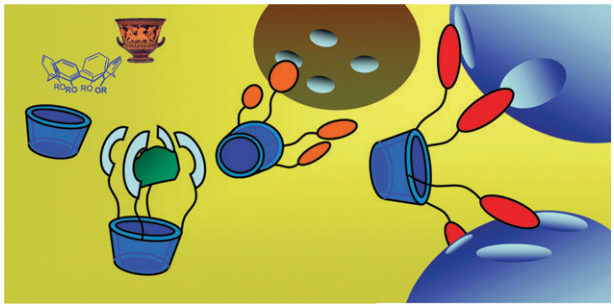
PERSPECTIVES

2715

Calixarenes: from biomimetic receptors to multivalent ligands for biomolecular recognition

Francesco Sansone,* Laura Baldini, Alessandro Casnati and Rocco Ungaro

The evolution of calixarenes, from the design and synthesis of receptors for small molecules of biological interest to the achievement of multivalent ligands for proteins and nucleic acids, is herein presented, and perspectives of these macrocycles in bioorganic chemistry are indicated.



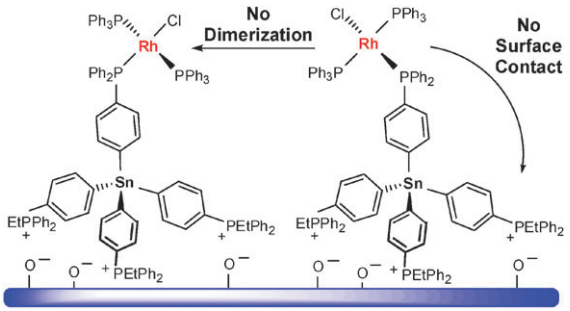
LETTERS

2729

New linker systems for superior immobilized catalysts

Björn Beele, Johannes Guenther, Melanie Perera, Michaela Stach, Thomas Oeser and Janet Blümel*

A new linker scaffold prevents the immobilized Rh catalyst from getting deactivated by dimerization or contact with the support surface, and therefore the catalyst can be recycled for a record 30 times.

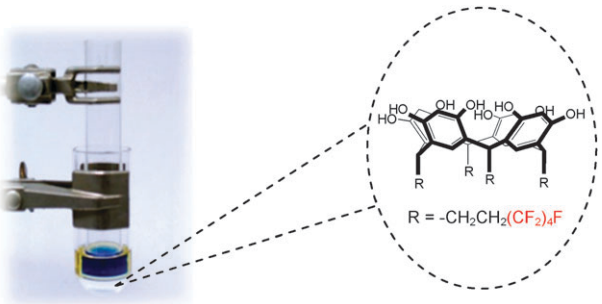


2732

Synthesis, characterization, and applications of fluorous resorcin[4]arenes

Qianli Chu,* Kristi O'Neal, Maksim Osipov, Julius N. Ngwendson, Steven J. Geib, Stephen G. Weber and Dennis P. Curran

The fluorous resorcin[4]arene immobilized in a fluorous bulk membrane is capable of transporting tetramethylammonium cation from an aqueous source phase into an aqueous receiving phase.

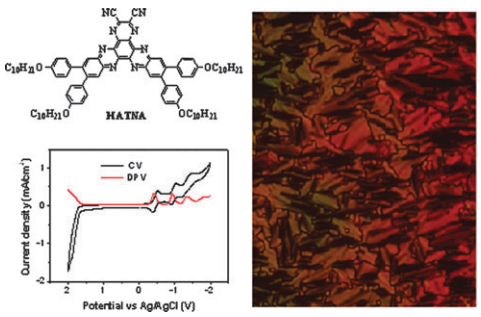


2735

Smectic liquid crystals based on hexaazatriphenylene: potential organic n-type semiconductor

Baoxiang Gao,* Licui Zhang, Qianqian Bai, Ying Li, Junwei Yang and Lixiang Wang*

We report the synthesis of dibenzohexaazatriphenylene derivative **DBHAT**. **DBHAT** shows a high electron-accepting capability and smectic liquid crystalline assembly over a wide temperature range.



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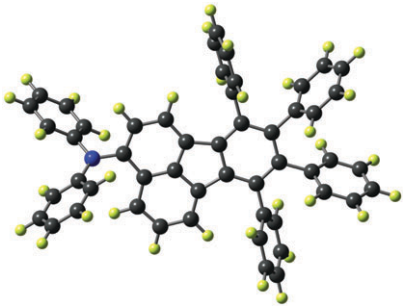
2739

Fluoranthene-based triarylamines as hole-transporting and emitting materials for efficient electroluminescent devices

Neha Kapoor and K. R. Justin Thomas*

Fluoranthene based triarylamines containing Müllen dendron-like structures have been successfully synthesized and demonstrated as hole-transporting and emitting materials in multi-layered organic light-emitting diodes.

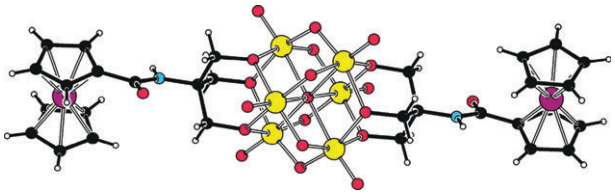


2749

Synthesis, structural characterisation and bonding in an anionic hexavanadate bearing redox-active ferrocenyl groups at the periphery

Jiří Schulz, Róbert Gyepes, Ivana Císařová and Petr Štěpnička*

The salt $(Bu_4N)_2[\{FcC(O)NHC(CH_2O)_3\}_2V_6O_{13}]$ (Fc = ferrocenyl) comprising the first ferrocenyl-modified polyoxovanadate anion (see structure) has been prepared and characterised by a combination of spectroscopic methods, cyclic voltammetry and DFT calculations.

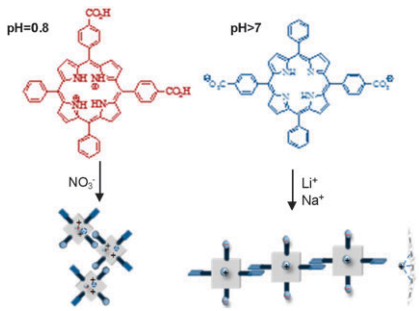


2757

J-aggregate formation in bis-(4-carboxyphenyl)porphyrins in water : pH and counterion dependence

Vanda Vaz Serra, Suzana M. Andrade, Maria G. P. M. S. Neves,* José A. S. Cavaleiro and Sílvia M. B. Costa*

Self-assembly strategy: pH-induced self-aggregation of substituted carboxyphenyl porphyrins depend on the number, charge, relative position of the substituent units in the macrocycle core and on the acid or basic counterion agent.

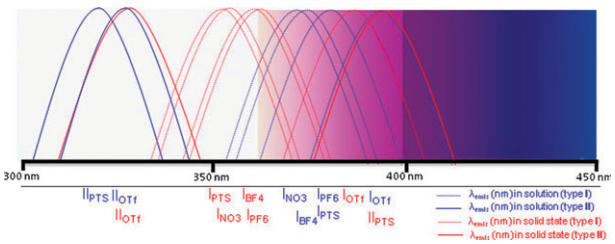


2766

Silver pyrazole complexes with tunable liquid crystals and luminescent properties

María José Mayoral, Paloma Ovejero, José Antonio Campo, José Vicente Heras, María Rosario Torres, Carlos Lodeiro* and Mercedes Cano*

The luminescent and liquid crystal behaviour of ionic silver pyrazole-based complexes can be tuned by controlling the substitution on the pyrazole ring and the nature of the counteranion. Photophysical studies of mesomorphic compounds as a function of the temperature indicate that the emission is maintained in the liquid crystal state.



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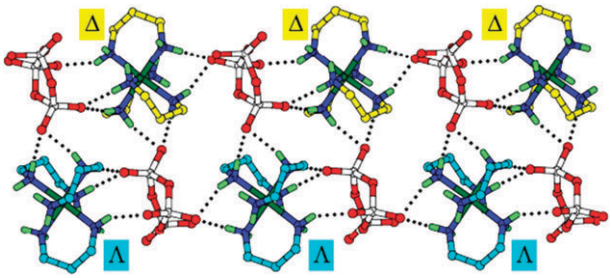
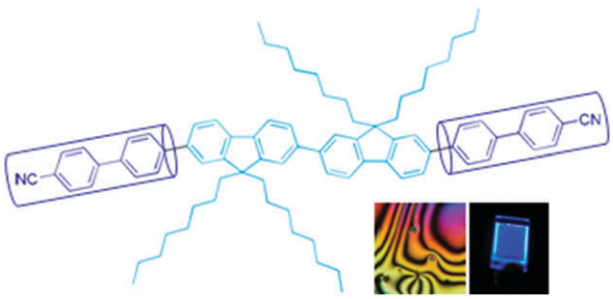


Homochiral column structure of *rac*- and *Λ*-$[M^{III}(tn)_3]P_3O_9$ (M = Co, Cr; tn = 1,3-diaminopropane; P_3O_9 = cyclotriphosphate(3 −)) produced by multiple hydrogen bonds

Yukinari Sunatsuki,* Sho Miyahara, Takayoshi Suzuki, Masaaki Kojima,* Toshio Nakashima, Naohide Matsumoto and Frode Galsbøl

In *rac*-$[Co(tn)_3]P_3O_9 \cdot 7.3H_2O$, the $[Co(tn)_3]^{3+}$ cations with the same absolute configuration and the $P_3O_9^{3-}$ anions are multiply hydrogen bonded to form a homochiral columnar structure.

2785

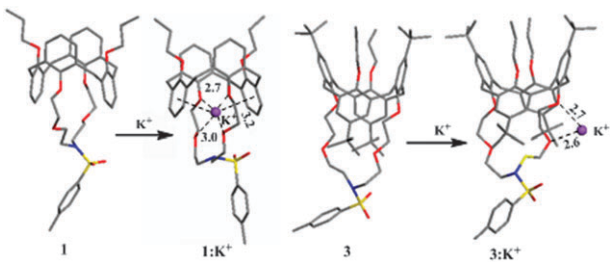


Extended liquid-crystalline oligofluorenes with photo- and electroluminescence

Jesús del Barrio, Luiz Silvino Chinelatto Jr., José Luis Serrano, Luis Oriol,* Milagros Piñol* and Henk J. Bolink

The elongation of an oligofluorene core with pro-mesogenic units provides liquid-crystals with tunable electronic properties and light and electric-stimulated emission. These compounds can be used for polarized photoluminescent films and electroluminescent devices.

2796

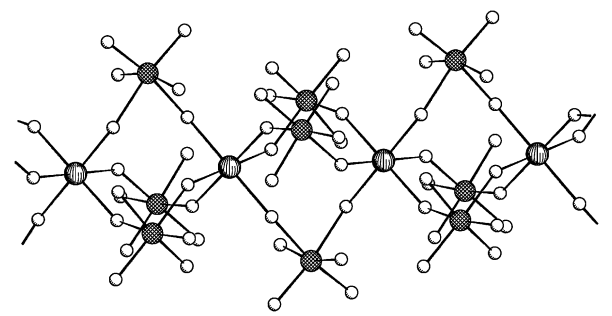


Effect of steric crowding on ion selectivity for calix-crown hybrid ionophores: experimental, molecular modeling and crystallographic studies

Subrata Patra, Debdeep Maity, Anik Sen, E. Suresh, Bishwajit Ganguly* and Parimal Paul*

Experimental and molecular modeling studies on calix[4]arene-azacrown-based ionophores with a large number of cations revealed that steric crowding at both upper and lower rims of the calix and host–guest size matching factors have profound influence on ion-selectivity.

2806



Fluoride ion donor properties of group 13 trifluorides (MF_3, *M* = Al, Ga, In, Tl) and crystal structures of $InF_3 \cdot 3SbF_5$, $TlF_3 \cdot 3SbF_5$ and $TlF_3 \cdot AsF_5 \cdot 2HF$

Zoran Mazej* and Evgeny Goreshnik

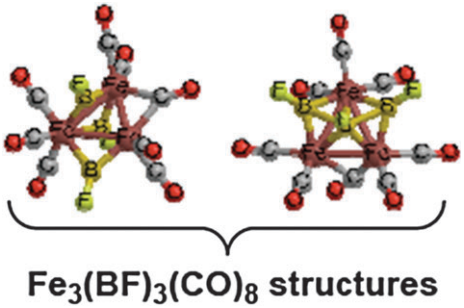
In the crystal structure of $InF_3 \cdot 3SbF_5$ fluorine atoms bridge In and Sb metals (In–F_b–Sb) with very long Sb–F_b bonds, comparable with that in solid SbF_5 (Sb–F_b–Sb).

2813

$Fe_3(BF)_3(CO)_8$ structures with face-semibridging fluoroborylene ligands and a bicapped tetrahedral Fe_3B_3 cluster isoelectronic with $Os_6(CO)_{18}$

Liancai Xu, Qian-shu Li,* Yaoming Xie, R. Bruce King* and Henry F. Schaefer III

Fifteen structures are found for $Fe_3(BF)_3(CO)_8$ within 30 kcal mol^{-1} of the global minimum. None of these structures has any terminal BF groups. One of the singlet $Fe_3(BF)_3(CO)_8$ structures has a B_3F_3 chain as part of an Fe_3B_3 bicapped tetrahedron analogous to $Os_6(CO)_{18}$.

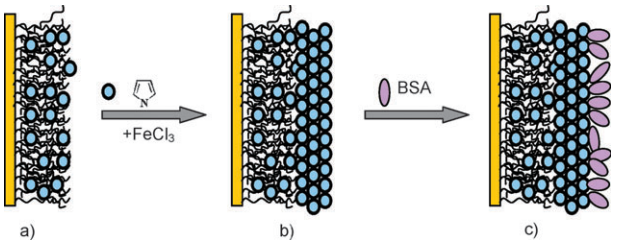


2822

Protein adsorption materials of the soluble conducting polymer poly(acryloyl chloride)-g-polypyrrole

Zhihong Zhang,* Yan Liang, Lijun Yan, Fufeng Yan and Shaoming Fang*

A soluble functionalized conducting graft copolymer of poly(acryoyl pyrrole) (PAP) and polypyrrole, PAP-g-PPy, was synthesized and protein adsorption onto this copolymer surface investigated in detail. The copolymer demonstrates a relative strong electroactivity and high protein fouling properties. The results show that the conducting copolymer PAP-g-PPy can be used as a protein or electrochemical biosensor.

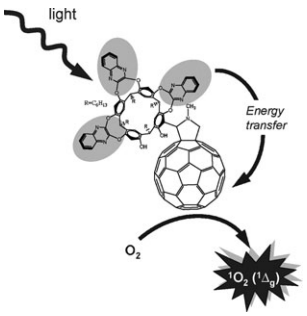


2828

Synthesis and photophysics of a fullerene-triquinoxaline ensemble

Francesco P. Ballistreri, Andrea Pappalardo, Gaetano A. Tomaselli,* Giuseppe Trusso Sfrazzetto, Elisa Vittorino and Salvatore Sortino*

A photophysical investigation on a novel fullerene-triquinoxaline molecular ensemble shows that the light energy absorbed by the quinoxaline antennas is quantitatively transferred to the fullerene centre, which effectively photosensitizes the generation of singlet oxygen.

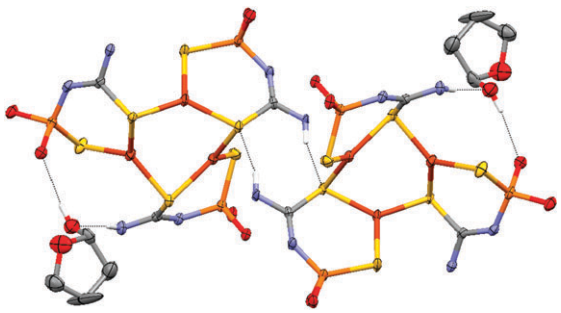


2835

Aerial oxidation of tetrahydrofuran to 2-hydroxotetrahydrofuran in the presence of a trimeric Cu^{I} complex $[Cu_3L_3]$ (HL = *t*BuNHC(S)NHP(S)(O*i*Pr)$_2$) and trapping of the unstable product at recrystallization

Robert C. Luckay, Xia Sheng, Christoph E. Strasser, Helgard G. Raubenheimer, Damir A. Safin,* Maria G. Babashkina and Axel Klein*

The reaction of the potassium salt of *t*BuNHC(S)NHP(S)(O*i*Pr)$_2$ (**HL**) with $Cu(NO_3)_2$ leads to **$[Cu_3L_3]$**. **$[Cu_3L_3]$** provokes the aerobic oxidation of tetrahydrofuran to 2-hydroxotetrahydrofuran.



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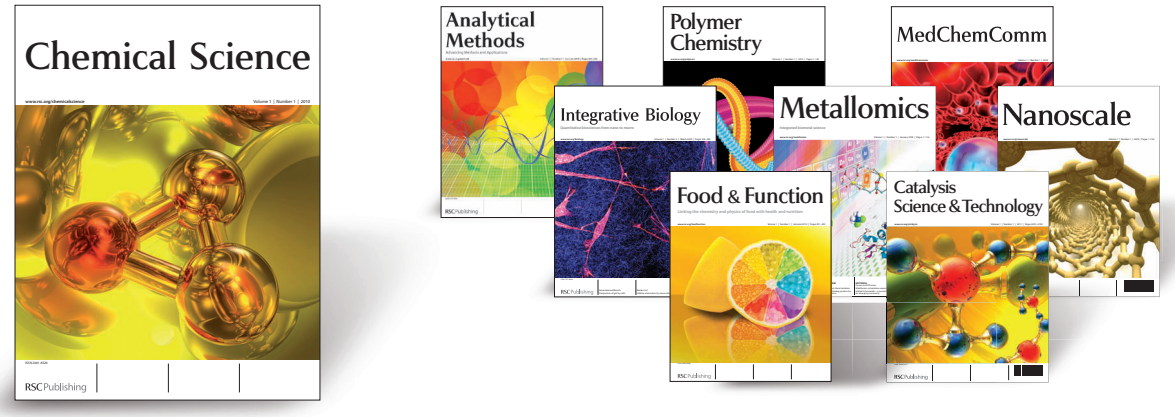

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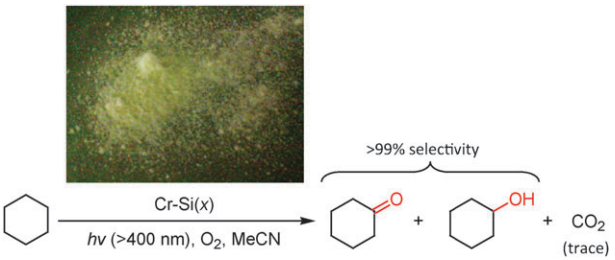
2841

Hydrophobic Cr–Si mixed oxides as a catalyst for visible light-induced partial oxidation of cyclohexane

Yasuhiro Shiraishi,* Hiroshi Ohara and Takayuki Hirai

Hydrophobic Cr–Si mixed oxides prepared with an organosilane promote efficient and selective photocatalytic oxidation of cyclohexane to cyclohexanone and cyclohexanol with molecular oxygen under visible light irradiation.

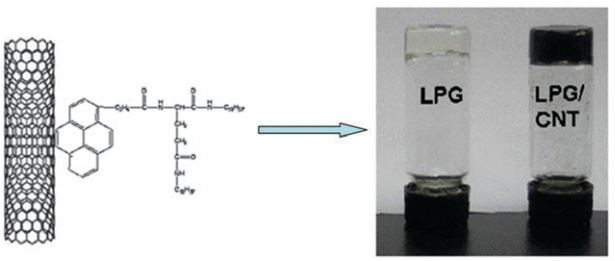


2847

Fabrication of organogels composed from carbon nanotubes through a supramolecular approach

Ye Tian, Li Zhang, Pengfei Duan, Fuyong Liu, Baoqing Zhang, Chenyang Liu and Minghua Liu*

A pyrene based low molecular gelator was synthesized and it was used to fabricate a stable organogel composed of pristine single-walled carbon nanotubes.

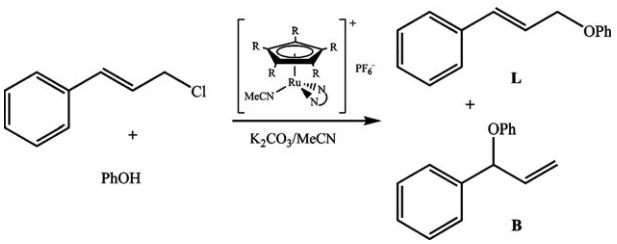


2853

Basicity and bulkiness effects of 1,8-diaminonaphthalene, 8-aminoquinoline and their alkylated derivatives on the different efficiencies of η^5-C_5H_5 and η^5-C_5Me_5 ruthenium precatalysts in allylic etherification reactions

Giovanna Brancatelli,* Dario Drommi, Giusy Feminò, Maria Saporita, Giovanni Bottari and Felice Faraone*

N,*N*-Ligands with different basicity nitrogen donor atoms and bulkiness features were used in allylic etherification reactions of cinnamyl chloride catalyzed by $[(\eta^5\text{-}C_5R_5)Ru(N,N)(NCMe)]PF_6$ (R = H, Me) complexes.

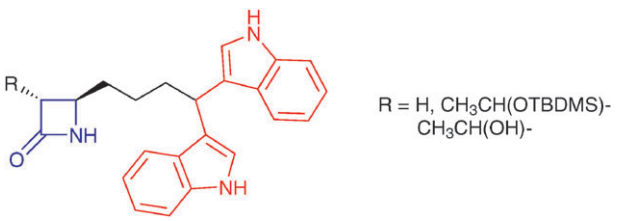


2861

2-Azetidinones: synthesis of new bis(indolyl)butyl-β-lactams

Paola Galletti, Arianna Quintavalla, Caterina Ventrici, Giuseppe Giannini, Walter Cabri and Daria Giacomini*

New β-lactam compounds containing a bis(indolyl)-framework were synthesized.



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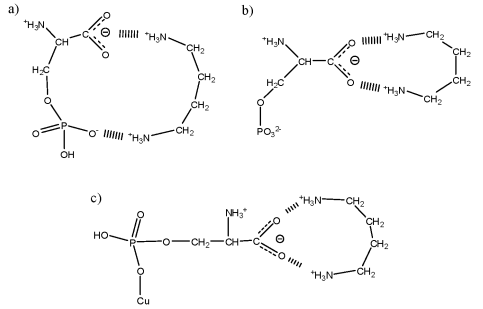
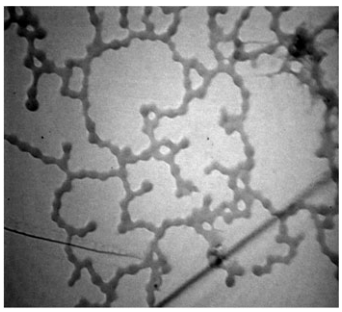


The influence of copper(II) ions on noncovalent interactions in the systems including phosphoserine and biogenic amines

Renata Jastrzab*

Ternary systems of copper(II) complexes with phosphoserine and biogenic amines (putrescine or spermidine or spermine) have been investigated.

2875

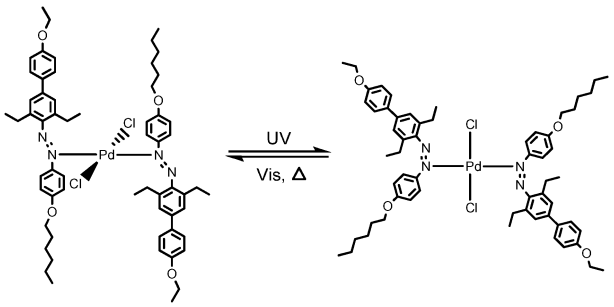


Fabrication and characterization of single walled carbon nanotubes-iron phthalocyanine nano-composite: surface properties and electron transport dynamics of its self assembled monolayer film

Isaac Adebayo Akinbulu and Tebello Nyokong*

Transition electron microscopy image of a nano-composite of single walled carbon nanotubes and iron phthalocyanine, peripherally tetra-substituted with diethylaminoethanethiol, showed the latter was attached in a continuous manner to the walls of the carbon nanotubes.

2887



A reversibly photoswitchable mononuclear palladium(II) complex with *ortho*-diethylated azobenzene ligands

Mina Han,* Tomohiro Hirade and Masahiko Hara

A mononuclear palladium(II) complex ($PdCl_2(2Et\text{-}Azo)_2$) containing two *ortho*-diethylated azobenzene ligands was designed to achieve reversible photoswitching originating from a reversible change in its molecular structure.

2892

Light-driven modulation of fluorescence color from azobenzene derivatives containing electron-donating and electron-withdrawing groups

Mina Han,* Yasuo Norikane, Ken Onda, Yoko Matsuzawa, Masaru Yoshida and Masahiko Hara

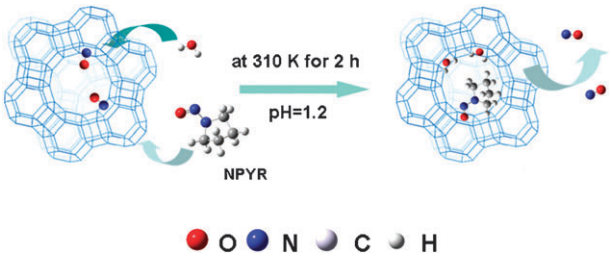
We report that the fluorescence wavelength of the UV-exposed azobenzene solution can be modulated from blue to yellow by simply changing the substituents to ones with different electronic properties.

2897

Moisture-saturated zeolites – A new strategy for releasing nitric oxide

Feng Wei, Jia Yuan Yang, Qian Hou and Jian Hua Zhu*

Zeolite pre-adsorbed with nitric oxide, when added to a gastric juice mimic, releases NO and captures nitrosamines, making it a potential functional material for reducing the risk of ulcers and cancers in the digestive system.

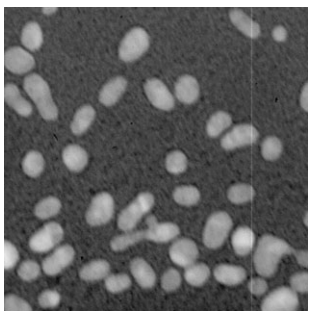


2906

The effect of initiation method on the size, monodispersity and shape of gold nanoparticles formed by the Turkevich method

Madeeha A. Uppal, Andreas Kafizas, Michael B. Ewing and Ivan P. Parkin*

The Turkevich method is adapted to investigate the effect of initiation method on the size, monodispersity and shape of gold colloids formed; with thermal and microwave energy, sonication and UVA light being studied.

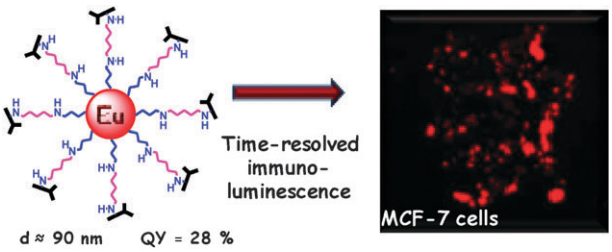


2915

Increasing the efficiency of lanthanide luminescent bioprobes: bioconjugated silica nanoparticles as markers for cancerous cells

Svetlana V. Eliseeva, Bo Song, Caroline D. B. Vandevyver, Anne-Sophie Chauvin, Josias B. Wacker and Jean-Claude G. Bünzli*

Lanthanide binuclear helical luminescent bioprobes are introduced into IgG conjugated silica nanoparticles and used to detect the 5D10 antigen expressed by breast cancer MCF-7 cells *via* a time-resolved immunoluminescent assay.

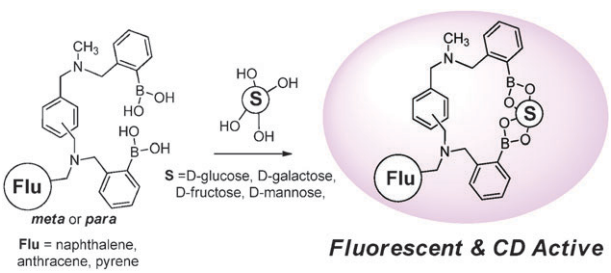


2922

Boronic acid based photoinduced electron transfer (PET) fluorescence sensors for saccharides

Joseph D. Larkin, Karine A. Frimat, Thomas M. Fyles, Stephen E. Flower and Tony D. James*

A modular approach to the synthesis of saccharide selective fluorescence sensors has been developed.



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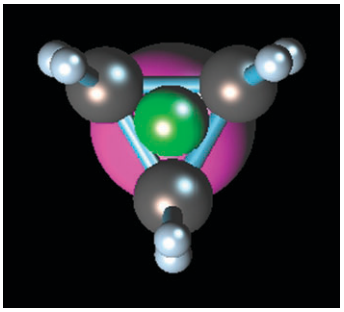
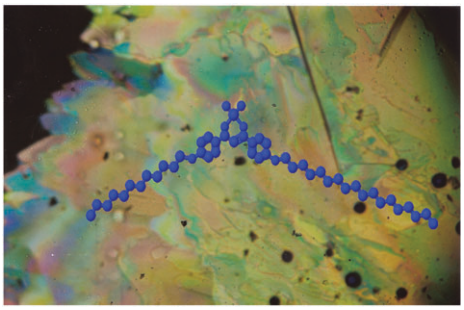


Insertion complexes of an organic molecule trapped in ion-pairs

Gurpaul Kochhar and Fedor Y. Naumkin*

Small cyclic organic molecules can be trapped between two atomic/molecular counter-ions, forming metastable systems with very large dipoles and energy storage capability.

2937

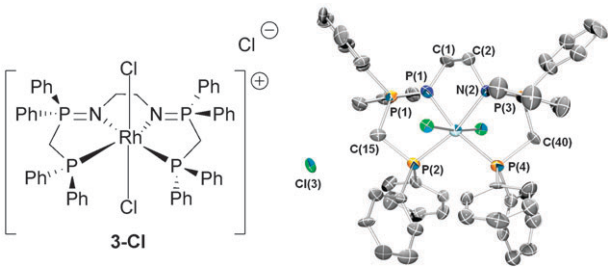


Luminescent liquid crystal materials based on unsymmetrical boron difluoride β-diketonate adducts

Ignacio Sánchez, María José Mayoral, Paloma Ovejero, José Antonio Campo, José Vicente Heras, Mercedes Cano* and Carlos Lodeiro

Bent-core compounds based on boron difluoride adducts with unsymmetrically 1,3-alkyloxyphenyl substituted β-diketonate ligands are luminescent liquid crystals exhibiting high fluorescence quantum yield. These materials open new opportunities for electro-optical devices.

2943

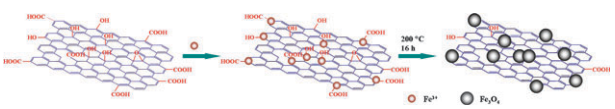


Iminophosphorane-based [P_2N_2] rhodium complexes: synthesis, reactivity, and application in catalysed transfer hydrogenation of polar bonds

Antoine Buchard, Elina Payet, Audrey Auffrant,* Xavier Le Goff and Pascal Le Floch*

Rh(I) and Rh(III) complexes featuring a mixed tetradentate phosphine-iminophosphorane ligand were synthesised. As reduction of the Rh(III) derivative could be performed with silanes or in the presence of sodium isopropoxide, this complex was used for the transfer hydrogenation of polar bonds.

2950



One-pot preparation of graphene/Fe_3O_4 composites by a solvothermal reaction

Kangfu Zhou, Yihua Zhu,* Xiaoling Yang and Chunzhong Li

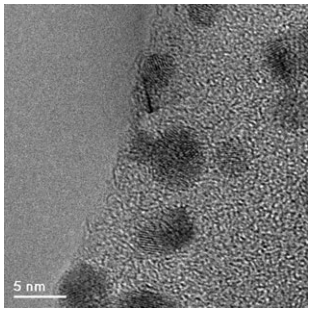
Graphene/Fe_3O_4 composites were prepared through a one-pot solvothermal reaction by using graphite oxide and $FeCl_3 \cdot 6H_2O$ as starting materials. Fe_3O_4 microspheres were distributed on graphene sheets uniformly. The obtained composites show a considerable saturation magnetization and high doxorubicin hydrochloride loading.

2956

Template controlled synthesis of monometallic zerovalent metal nanoclusters inside cross-linked polymer frameworks: the effect of a single matrix on the size of different metal nanoparticles

Paolo Centomo,* Patrizia Canton, Matteo Ferroni and Marco Zecca

The characterization in the swollen state of a cross-linked functional polymer and of nanostructured Ag, Au, Pd, Pt, Ru and Rh metal phases, shows the ability of this class of polymer materials to control the growth of nanoparticles.

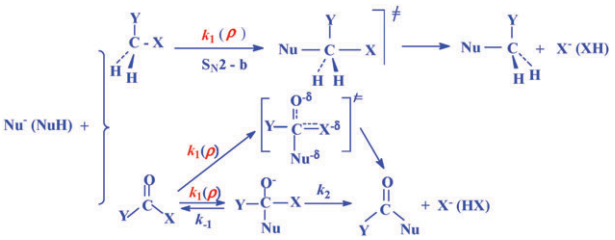


2962

Substituent effects in substrates on activation parameters in the bimolecular nucleophilic reactions in solution

Vladislav M. Vlasov

$\Delta H^{\neq} = \delta\Delta H^{\neq}\sigma + \Delta H_0^{\neq}$; $\delta\Delta H^{\neq} = \delta\Delta H_{ext}^{\neq} + \delta\Delta H_{int}^{\neq}$; $\delta\Delta H_{int}^{\neq} = (-0.1 \pm 0.5) - (6.1 \pm 0.2)\,\rho(r = 0.989, s = 1.9, n = 38)$ where $\rho = \rho(k_1)$. The charge development in the transition state (k_1) in S_N2, S_NAr and acyl-transfer reactions is mainly governed by the internal part of the activation enthalpy change, $\delta\Delta H_{int}^{\neq}$.

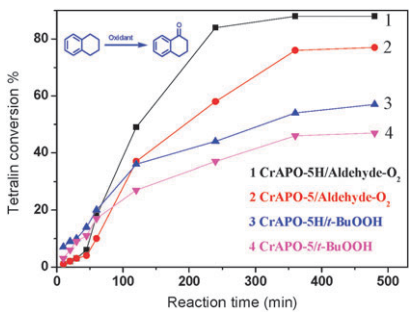


2971

CrAPO-5 catalysts having a hierarchical pore structure for the selective oxidation of tetralin to 1-tetralone

Jun Kim, Samiran Bhattacharjee, Kwang-Eun Jeong, Soon-Yong Jeong, Minkee Choi, Ryong Ryoo and Wha-Seung Ahn*

A novel CrAPO-5 material having a unique microporous–mesoporous hierarchical pore structure (CrAPO-5H) showed high activity and selectivity in the liquid phase oxidation of tetralin to 1-tetralone, and outperformed the conventional microporous CrAPO-5.

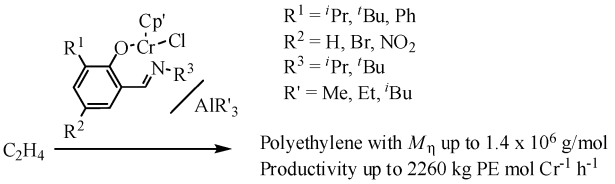


2979

Synthesis, structures and ethylene polymerization behavior of half-metallocene chromium(III) catalysts bearing salicylaldiminato ligands

Mingtai Sun, Ying Mu,* Qiaolin Wu, Wei Gao and Ling Ye

Half-sandwich chromium(III) complexes bearing a salicylaldiminato ligand with an electron-withdrawing group show good catalytic activity for ethylene polymerization upon activation with AlR_3.



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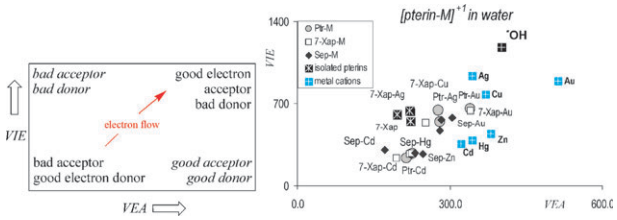
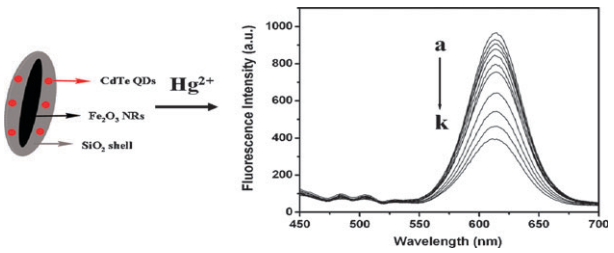


Electron donor–acceptor properties of metal atoms interacting with pterins

Ana Martínez* and Rubicelia Vargas

Metal cations and di-cations form very strong complexes with pterins and consequently, they intensely modify donator–acceptor properties, *i.e.*, the ionization energy (VIE) and the electron affinity (VEA).

2996

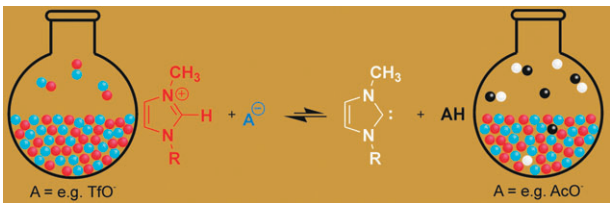


Synthesis and characterization of multifunctional $CdTe/Fe_2O_3@SiO_2$ core/shell nanosensors for Hg^{2+} ions detection

Hengguo Wang, Yapeng Li, Xiaoliang Fei, Lei Sun, Ligong Zhang, Zhenzhong Zhang, Yue Zhang, Yaoxian Li and Qingbiao Yang*

Novel multifunctional magnetic-photoluminescent-Hg^{2+} ion sensing nanocomposites were developed by applying SiO_2 as the encapsulation agent to package Fe_2O_3 NRs and CdTe QDs, resulting in $CdTe/Fe_2O_3@SiO_2$ core/shell nanostructures.

3004



Carbenes in ionic liquids

Oldamur Hollóczki, Dirk Gerhard, Klemens Massone,* László Szarvas, Balázs Németh, Tamás Veszprémi* and László Nyulászi*

Sufficiently basic counteranions such as acetate are able to deprotonate imidazolium based ionic liquids to a certain extent resulting in an observable carbene content.

ADDITIONS & CORRECTIONS

3010

Additions and corrections published in 2010

