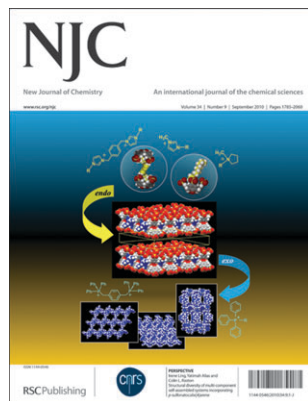


IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 34(9) 1785-2060 (2010)



Cover

See Irene Ling, Yatimah Alias and Colin L. Raston, pp. 1802-1811. Incorporating small organic cations in the cavity of *p*-sulfonatocalix[4]arene through their polar head groups leads to self-assembly in an up-down bilayer arrangement with phosphonium cations interlocked around the *exo* surface of the calixarene. Image reproduced by permission of Irene Ling, Yatimah Alias and Colin L. Raston from *New J. Chem.*, 2010, **34**, 1802.

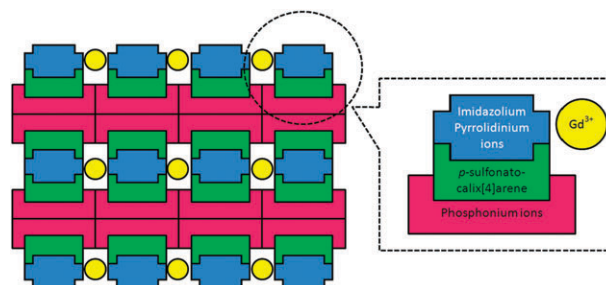
PERSPECTIVE

1802

Structural diversity of multi-component self-assembled systems incorporating *p*-sulfonatocalix[4]arene

Irene Ling, Yatimah Alias and Colin L. Raston*

Bowl shaped *p*-sulfonatocalix[4]arene is a versatile anion in building multi-component self-assembled materials incorporating imidazolium or pyrrolidinium cations within the cavity of the calixarene, which is also established in solution for the two components. The materials also incorporate embracing large phosphonium cations around the outer surface of the calixarene as part of bilayer arrangements.



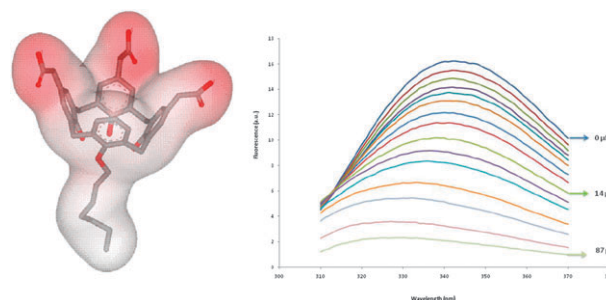
LETTERS

1812

Magnesium dependent complexation of tri-anionic calix[4]arene detergents by the nucleotide binding domain 1 (NBD1) of multidrug resistance protein MRP1

Laurent F. A. Nault, Celine Girardot, Antoine Leydier, Anthony W. Coleman,* Thomas Perrotton, Sandrine Magnard and Helene Baubichon-Cortay*

Amphiphilic tri-carboxylato calix[4]arenes bind to the Nucleotide Binding Domain of MRP1 in a magnesium selective manner, the observed association constant is of the same order as that of the natural substrate ATP.



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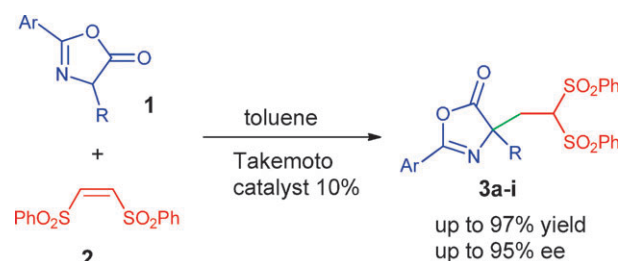
LETTERS

1816

Asymmetric organocatalytic Michael addition of azlactones to *cis*-1,2-bis(phenylsulfonyl)ethene. A simple entry to quaternary α -amino acids

Natalia Bravo, Andrea-Nekane R. Alba, Guillem Valero, Xavier Companyó, Albert Moyano* and Ramon Rios*

In a regio- and enantioselective fashion, azlactones react with 1,2-bis(phenylsulfonyl)ethene under catalysis by simple bifunctional chiral thioureas, affording α,α -disubstituted α -amino acid derivatives in good yields and in moderate to good enantioselectivities.

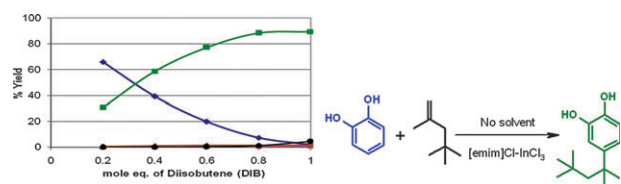


1821

Chloroindate(III) ionic liquids as catalysts for alkylation of phenols and catechol with alkenes

H. Q. Nimal Gunaratne,* Tobias J. Lotz and Kenneth R. Seddon

Chloroindate(III) ionic liquids are shown to be versatile catalysts for the alkylation of phenols and catechol with alkenes, giving high conversions to alkylated phenols with high selectivities.

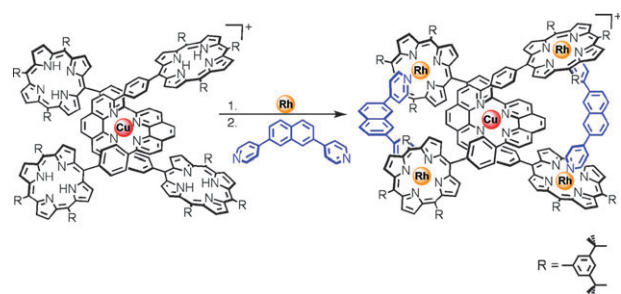


1825

The dual role of Cu(I) as a protective group and a template in the synthesis of a tetra-rhodium(III)porphyrin[2]catenane

Maryline Beyler, Valérie Heitz* and Jean-Pierre Sauvage*

A tetra-rhodium(III)porphyrin[2]catenane is synthesised *via* the formation of four non-covalent but irreversible Rh(III)–pyridine interactions.

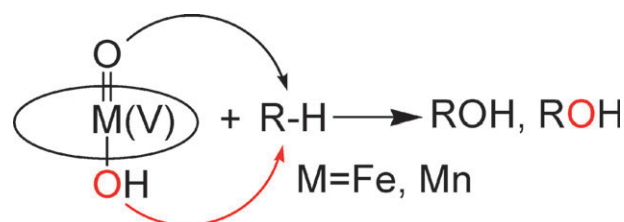


1830

High-valent metalloporphyrins in hydrocarbon activation: metal(v)-oxo or metal(v)-hydroxo?

Radu Silaghi-Dumitrescu*

DFT results show that in Fe(v) and Mn(v) porphyrins with oxo and hydroxo ligands, both oxygen atoms provide routes to hydroxylated hydrocarbons.



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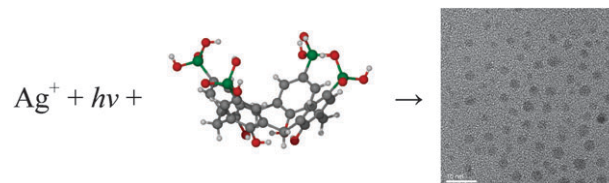
LETTERS

1834

Photochemical generation of small silver nanoparticles involving multi-functional phosphonated calixarenes

Karel J. Hartlieb, Adam D. Martin, Martin Saunders and Colin L. Raston*

Silver nanoparticles less than 5 nm in diameter are accessible by a simple photochemical reduction in water, templated by *p*-phosphonated calix[4]arene and its O-alkyl derivatives, in a way depending on the pH of the reagent solution.

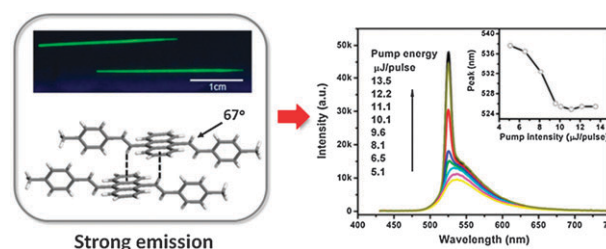


1838

Solid state emission enhancement of 9,10-distyrylanthracene derivatives and amplified spontaneous emission from a large single crystal

Bin Xu, Honghua Fang, Yujie Dong, Feipeng Chen, Qidai Chen, Hongbo Sun and Wenjing Tian*

Tight intermolecular stacking through supramolecular interactions in the crystal is a key point for the solid-state emission enhancement of methyl-substituted 9,10-distyrylanthracene. Amplified spontaneous emission with low threshold was observed from a large single crystal.

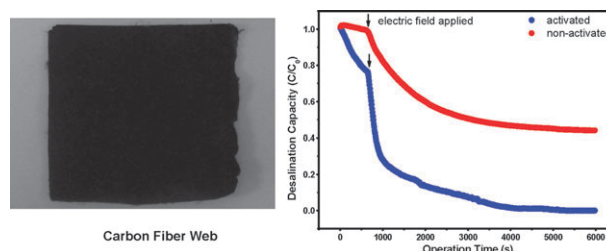


1843

Electrospun ultrafine carbon fiber webs for electrochemical capacitive desalination

Ming Wang, Zheng-Hong Huang,* Lei Wang, Ming-Xi Wang, Feiyu Kang* and Haoqing Hou

The macroscopic, engineered structure of an ultrafine carbon fiber web is produced by electrospinning for a capacitive de-ionization electrode, which exhibits a considerable electrosorption capacity.



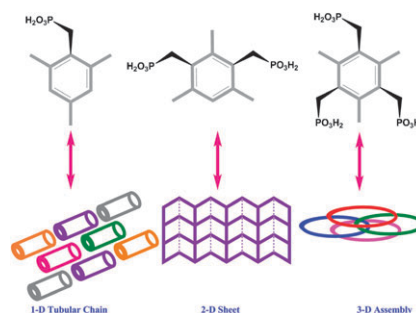
PAPERS

1846

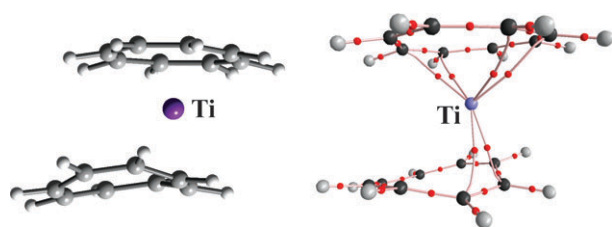
One, two, and three methylene phosphonic acid groups (–CH₂PO₃H₂) on a mesitylene ring: synthesis, characterization and aspects of supramolecular aggregation

Ramaswamy Murugavel* and Mayank Pratap Singh

Up to three phosphonic acid moieties (–PO₃H₂) can be successively added to a central mesitylene ring by a simple synthetic methodology, yielding mesitylene mono-, bis-, and tris-methylene phosphonic acids.



1855

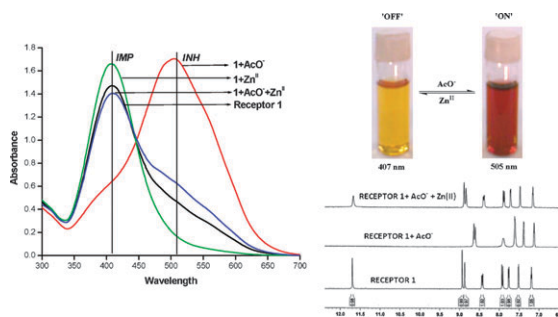


Cyclooctatetraene in metal complexes—planar does not mean aromatic

Justyna Dominikowska and Marcin Palusiak*

The structure of cyclooctatetraene (COT) in metal complexes depends mostly on the efficiency of metal center–ligand interaction, and is not necessarily directly related to its aromatic/nonaromatic character.

1862

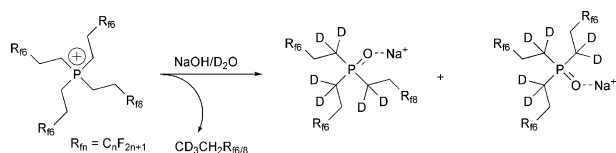


Reversible colorimetric switching of thiophene hydrazone based on complementary IMP/INH logic functions

K. K. Upadhyay,* Ajit Kumar, Rakesh K. Mishra, Thomas M. Fyles, Shalini Upadhyay and Kamlesh Thapliyal

A thiophene hydrazone (receptor **1**) acts as a reversible colorimetric molecular switch showing an ON–OFF function induced by anion and cation recognition. This remarkable color switching is based on two-input complementary IMP/INH logic functions.

1867

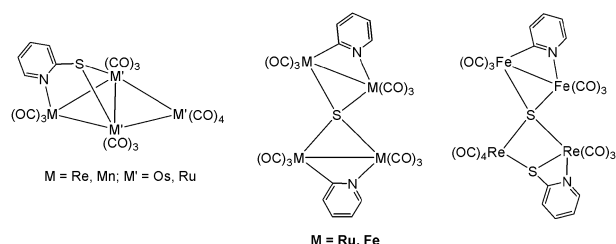


Chemical stability and application of a fluorophilic tetraalkylphosphonium salt in fluorosulfonate anion-selective electrodes

Li D. Chen, Debaprasad Mandal, John A. Gladysz and Philippe Bühlmann*

A fluorophilic tetraalkylphosphonium salt was used to prepare ion-selective electrodes with a high selectivity for perfluorooctanesulfonate and perfluorooctanoate. The sensors were very robust but exposure to 0.1 M OH[−] for 24 h resulted in trialkylphosphine oxide formation.

1875



The rational synthesis of tetranuclear heterometallic butterfly clusters: reactions of [M₂(CO)₆(μ-pyS)₂] (M = Re, Mn) with group VIII metal carbonyls

Shishir Ghosh, Kamrun N. Khanam, G. M. Golzar Hossain, Daniel T. Haworth, Sergey V. Lindeman, Graeme Hogarth* and Shariff E. Kabir*

The reactions of [M₂(CO)₆(μ-pyS)₂] (M = Re, Mn) with [M'₃(CO)₁₀L₂] (M = Os, Ru, Fe; L = MeCN, CO) are described.

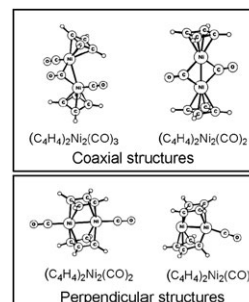
PAPERS

1885

Terminal versus bridging cyclobutadiene rings in binuclear nickel carbonyl derivatives: A cube-antiprism twist of the cyclobutadiene rings in the perpendicular structures

Hongyan Wang,* Zhonghua Sun, Yaoming Xie, R. Bruce King* and Henry F. Schaefer III

The geometries of the binuclear cyclobutadienenickel carbonyls $(C_4H_4)_2Ni_2(CO)_n$ ($n = 3, 2, 1$) are studied by DFT method and compared with the isoelectronic $(C_5H_5)_2Co_2(CO)_n$. The relatively low energy perpendicular structures are predicted for $(C_4H_4)_2Ni_2(CO)_n$ ($n = 1, 2$).

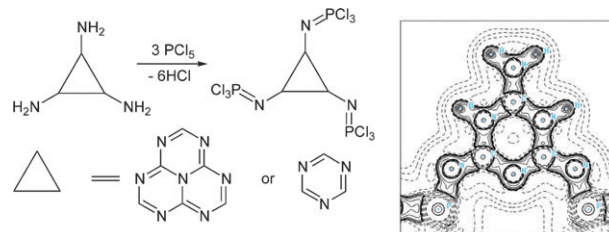


1893

Melem- and melamine-derived iminophosphoranes

Tatyana Saplinova, Christian Lehnert, Uwe Böhme, Jörg Wagler and Edwin Kroke*

The Kirsanov reaction of melamine or melem with phosphorus(v)-compounds allows the syntheses of novel potential flame retarding systems: the s-triazine- and s-heptazine-based iminophosphoranes which were studied by single crystal X-ray diffraction and quantum chemical calculations.

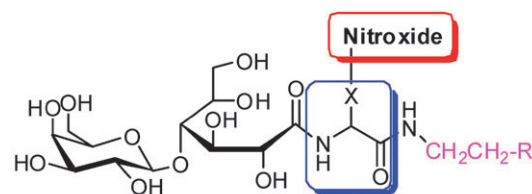


1909

Synthesis, physical-chemical and biological properties of amphiphilic amino acid conjugates of nitroxides

Grégory Durand,* Fanny Choteau, Robert A. Proszak, Antal Rockenbauer, Frederick A. Villamena* and Bernard Pucci

The self-aggregation properties of novel amphiphilic nitroxides as well as their electrochemical properties and relative rates of reduction were determined. Their cytoprotective property against a toxic concentration of hydrogen peroxide using bovine aortic endothelial cells was also investigated.



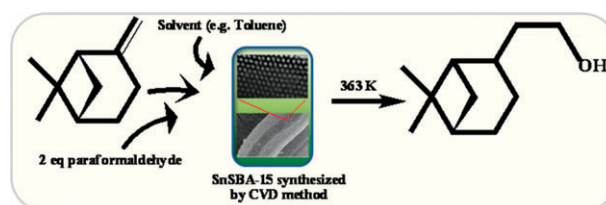
Lysine carrier : X = $-(CH_2)_4-NH-$; Nitroxide = 3-Carboxy Proxyl
Aspartic acid carrier : X = $-CH_2-CO-$; Nitroxide = 4-Amino TEMPO
R = $-C_6H_{13}$ or $-C_6F_{13}$

1921

Highly selective and clean synthesis of nopol over well-ordered mesoporous tin silicate catalysts

M. Selvaraj* and P. K. Sinha

Mesoporous SnSBA-15(CVD) has been successfully used in the production of nopol (N-OH) and it has higher selectivity for N-OH than other mesoporous catalysts, viz. SiSBA-15, Sn/SBA-15(SC) and Sn/SBA-15(SA) and SnMCM-41(40).



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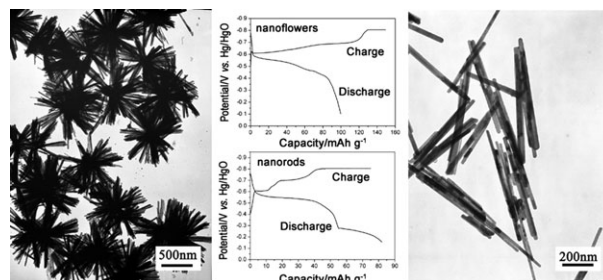
PAPERS

1930

Ionothermal synthesis of bismuth sulfide nanostructures and their electrochemical hydrogen storage behavior

Qingtao Wang, Xiaobo Wang, Wenjing Lou* and Jingcheng Hao*

Bi_2S_3 nanoflowers and nanorods were synthesized by the thermal treatment of a single-source precursor in an ionic liquid ($\text{C}_{16}\text{MIMBF}_4$) solvent. The electrochemical hydrogen storage behavior of these Bi_2S_3 nanostructures is sensitive to the morphology and microstructure.

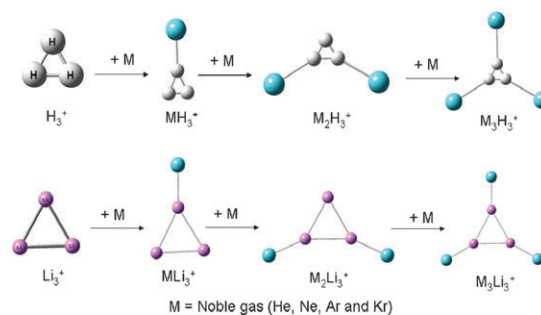


1936

Trapping of noble gases (He–Kr) by the aromatic H_3^+ and Li_3^+ species: a conceptual DFT approach

Arindam Chakraborty, Santanab Giri and Pratim Kumar Chattaraj*

Trigonal aromatic H_3^+ and Li_3^+ systems can trap noble gas atoms to form various small- to medium-sized cationic clusters.

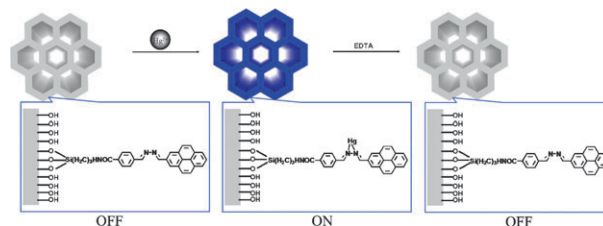


1946

A highly selective regenerable optical sensor for detection of mercury(II) ion in water using organic–inorganic hybrid nanomaterials containing pyrene

Yinghui Wang, Bin Li,* Liming Zhang, Lina Liu, Qinghui Zuo and Peng Li

A novel fluorescent chemosensing hybrid material containing pyrene (Py-SBA-15) for detecting Hg^{2+} ions in water is prepared, and it shows high selectivity, satisfactory detection limit and good regeneration ability.

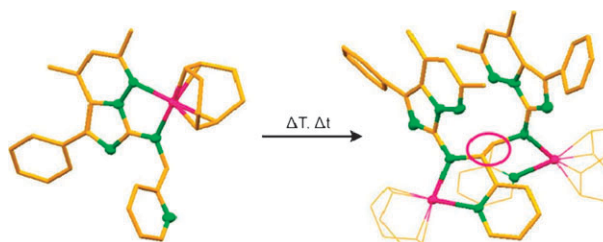


1954

An intermolecular C–C coupling reaction of iridium complexes

Kathrin Kutlescha, Torsten Irrgang and Rhett Kempe*

A novel class of amido-pincer ligands, namely imidazo[1,5-*b*]pyridazine-substituted (pyridyl-methyl)amines, has been synthesized and utilized for the stabilization of iridium complexes, which undergo an intermolecular C–C coupling reaction if enamine tautomerization of the ligand is possible.



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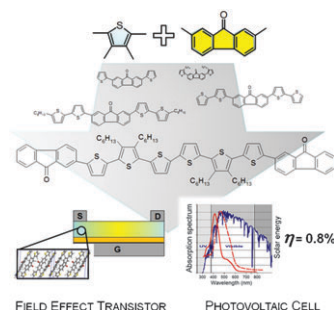
PAPERS

1961

Synthesis and characterisation of fluorenone–thiophene-based donor–acceptor oligomers: role of moiety sequence upon packing and electronic properties

William Porzio,* Silvia Destri,* Mariacecilia Pasini, Umberto Giovanella, Massimo Ragazzi, Guido Scavia, Dariusz Kotowski, Gianni Zotti and Barbara Vercelli

Thiophene and fluorenone oligomers were studied to evaluate the effect on both electronic properties and packing of the moiety sequence. The performance of p-type OFET and BHJ solar cell devices, gave indications of chemical structure requirements.

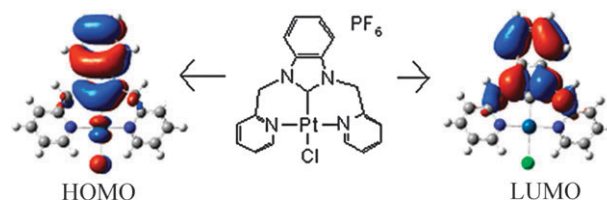


1974

Synthesis, structure and electrochemical behaviour of Ru(II)- and Pt(II)-carbene complexes of the NCN-pincer 1,3-bis(2-pyridylmethyl)-1H-benzimidazolium chloride

S. D. Adhikary, T. Samanta, G. Roymahapatra, F. Loiseau, D. Jouvenot, S. Giri, P. K. Chattaraj and J. Dinda*

The synthesis, structure and electrochemistry of the NCN donor NHC complexes of Ru(II) and Pt(II) have been described, and theoretical calculations undertaken for comparison with the experimental findings.

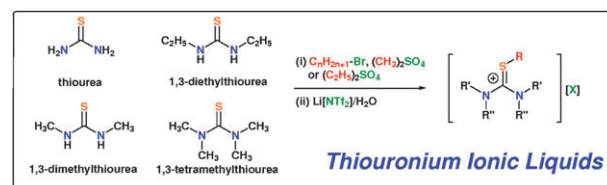


1981

Ionic liquid S-alkylthiuronium salts

Mahpuzah Abai, John D. Holbrey,* Robin D. Rogers and Geetha Srinivasan

Ionic liquids prepared from thiourea, 1,3-dimethylthiourea, 1,3-diethylthiourea and 1,3-tetramethylthiourea are physically and electrochemically characterised. The mutual miscibility limits with octane, dodecane and toluene, and the extraction of dibenzothiophene from dodecane have been investigated.

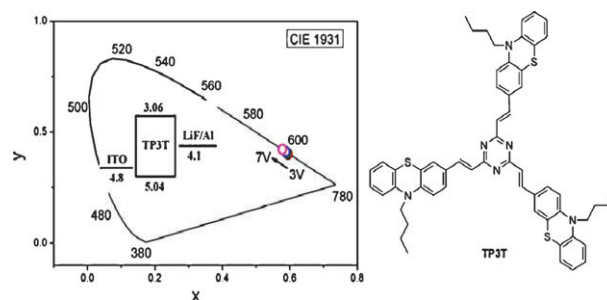


1994

A bright single layer non-doped orange-red light emitting diode using a symmetric starburst material *via* solution process

Sheng Kong, Lixin Xiao,* Yingliang Liu, Zhijian Chen, Bo Qu and Qihuang Gong*

A bright single layer non-doped light-emitting diode with a stable orange-red emission was achieved using a symmetric starburst material as the single combination layer of charge transporting and emitter *via* solution process.



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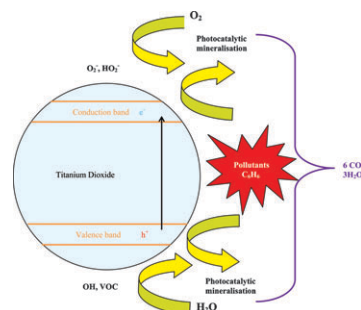
PAPERS

1999

Photocatalytic degradation of acetone and butane on mesoporous titania layers

Václav Štengl,* Vendula Houšková, Snejana Bakardjieva and Nataliya Murafa

From mesoporous titania samples, a 300 μm thin layer on glass desk 10×15 cm was created and the photocatalytic activity of the prepared layers was assessed from the kinetics of the photocatalytic degradation of butane and acetone in gaseous phases.

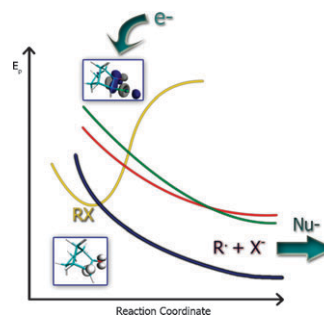


2006

Reactions of halonorbornane and oxo-substituted derivatives with different anions by the electron transfer mechanism; redox catalysis in stabilized radicals

Jorge G. Uranga and Ana N. Santiago*

The reaction coordinates of ET bond breaking were modified depending on the relative orientation of the C=O group and the C-X bond. These breakings were facilitated by the higher orbital interaction between the radical and the carbonyl group. Initial studies on its coupling with nucleophiles are presented.

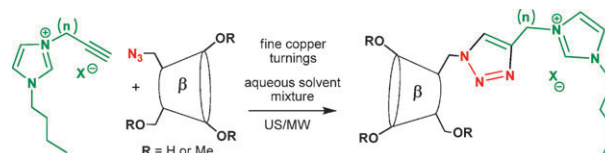


2013

A new class of cationic cyclodextrins: synthesis and chemico-physical properties

Luisa Boffa, Emanuela Calcio Gaudino, Katia Martina, László Jicsinszky and Giancarlo Cravotto*

CuAAC for an easy access to hybrid molecules that combine the properties of ionic liquids and cyclodextrins.

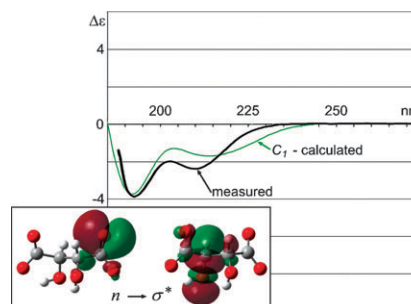


2020

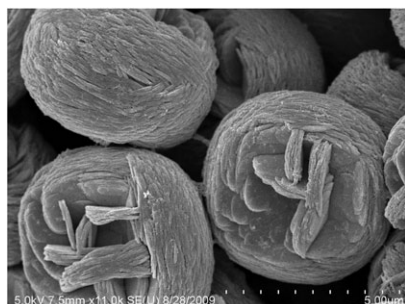
Extending the applications of circular dichroism in structure elucidation: aqueous environment breaks the symmetry of tartrate dianion

Marcin Hoffmann,* Jakub Grajewski and Jacek Gawronski

As seen from the CD spectra and quantum mechanical calculations, the interactions with water solvent favor the C_1 symmetry structure of (*R,R*)-tartrate molecular anion although the anion itself prefers the C_2 symmetry structure.



2027

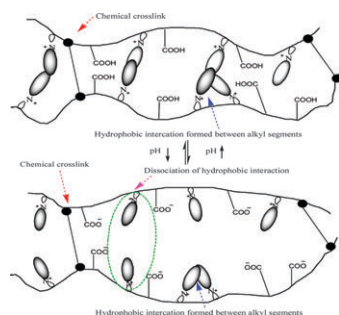


Pancake-like $\text{Fe}_2(\text{MoO}_4)_3$ microstructures: microwave-assisted hydrothermal synthesis, magnetic and photocatalytic properties

Lei Zhang, Xiao-Feng Cao, Ying-Li Ma, Xue-Tai Chen* and Zi-Ling Xue

A fast and economical route based on microwave-assisted hydrothermal process has been developed to synthesize pancake-like $\text{Fe}_2(\text{MoO}_4)_3$ microstructures. This study provides a facile pathway to prepare hierarchical $\text{Fe}_2(\text{MoO}_4)_3$ nanoarchitectures using nanosheets as building blocks.

2034

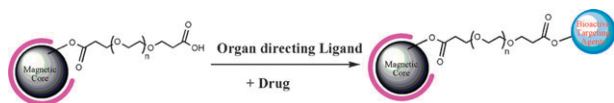


Synthesis of pH-responsive hydrophobically-modified hydrogels of poly(methacrylic acid-co-diallyl ammonium salt) in aqueous solution

Dang-Ge Gao, Jian-Zhong Ma* and Hai-Qing Guo*

The crystallization of hexadecyl groups in the side-chain of P(CC16-MAA) gels occurred at low pH. The ionization of the carboxylic acid groups occurred and their electrostatic repulsions can destroy the physical cross-linking between the hexadecyl groups at high pH, resulting in a high swelling ability for the gels.

2040

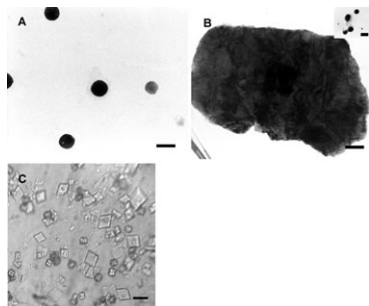


One-pot fabrication of carboxyl-functionalized biocompatible magnetic nanocrystals for conjugation with targeting agents

Chichong Lu,* Zhe-Shan Quan, Jung Chul Sur, Sun-Hee Kim, Choong Hun Lee and Kyu Yun Chai*

Biocompatible, water-soluble, superparamagnetic, manganese-doped and magnetism-engineered iron oxide nanocrystals were prepared *via* a one-pot fabrication. Our results demonstrate that the nanocrystals provide carboxyl functional groups for targeting agent immobilization.

2047



Self-aggregation behaviour of novel thiosemicarbazone drug candidates with potential antiviral activity

Romina J. Glisoni, Diego A. Chiappetta, Liliana M. Finkielstein, Albertina G. Moglioni and Alejandro Sosnik*

(A, B) TEM micrographs of 7.5 μM 5,6-dimethoxy-1-indanone TSC aggregates in water-DMSO (98:2) stained with 2% phosphotungstic acid. (A) day 0 and (B) day 30. Scale bar = 100 nm. (C) Optical microscope micrograph of 150 μM 5,6-dimethoxy-1-indanone TSC aggregates in water-DMSO (98:2) at day 0. Scale bar = 10 μm.

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