

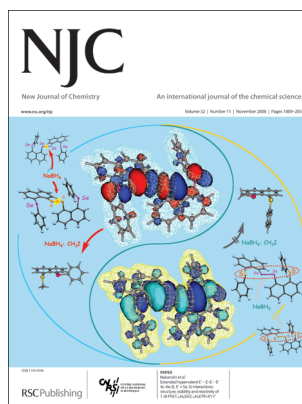
IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 32(11) 1809-2052 (2008)



Cover

See Sortino *et al.*, pp. 1899–1903.
Immobilization and release of single and double strand DNA is achieved by exploiting the light-controlled electrostatic interactions with the two-isomeric forms of a cationic azobenzene self-assembled on transparent platinum electrodes. Image reproduced by permission of Fiorella L. Callari, Salvatore Petralia, Sabrina Conoci and Salvatore Sortino from *New J. Chem.*, 2008, **32**, 1899.



Inside Cover

See Nakanishi *et al.*, pp. 1881–1889.
The reactivity of E–E in $\sigma(E_2E'_2 4c-6e)$ of 1-(8-PhE'C₁₀H₆)EE(C₁₀H₆ E'Ph-8')-1' is controlled by E': The E–E bonds are reduced by NaBH₄ when E' = Se but not if E' = S. Image reproduced by permission of Waro Nakanishi, Satoko Hayashi, Sayuri Morinaka, Takahiro Sasamori and Norihiro Tokitoh from *New J. Chem.*, 2008, **32**, 1881.

CHEMICAL SCIENCE

C81

Drawing together the research highlights and news from all RSC publications, *Chemical Science* provides a 'snapshot' of the latest developments across the chemical sciences, showcasing newsworthy articles and significant scientific advances.

Chemical Science

November 2008/Volume 5/Issue 11

www.rsc.org/chemicalscience

LETTER

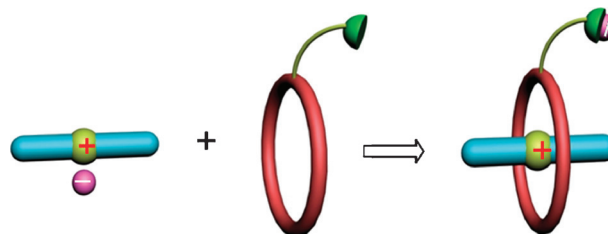


1827

Improved complexation between dibenzo-24-crown-8 derivatives and dibenzylammonium salts by ion-pair recognition

Kelong Zhu, Mingming Zhang, Feng Wang, Ning Li, Shijun Li and Feihe Huang*

The introduction of a urea-based anion binding site onto dibenzo-24-crown-8 can enhance the complexation between dibenzo-24-crown-8 derivatives and dibenzylammonium cation by ion-pair recognition.



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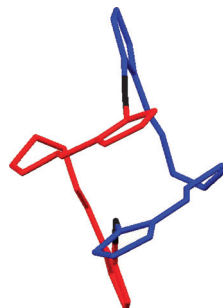
LETTERS

1831

Linking number analysis of a self-assembled lemniscular Möbius-metallamacrocycle

Senjuti De, Michael G. B. Drew,* Henry S. Rzepa* and Dipankar Datta*

By using the 1 : 2 condensate of benzil dihydrazone and 1-methyl-2-imidazole carboxaldehyde as an N donor ligand L, $[\text{Ag}_2\text{L}_2](\text{ClO}_4)_2 \cdot 0.5\text{H}_2\text{O}$ (**1**) is synthesized. **1** contains a 26 membered, 24π -electron metallamacrocycle which is revealed from a linking number analysis to be a double-twist Möbius cycle.

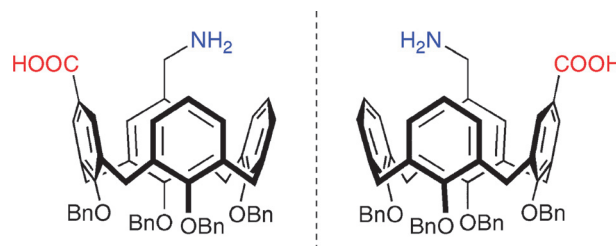


1835

Synthesis and optical resolution of an inherently chiral calix[4]arene amino acid

Seiji Shirakawa, Yuichi Tanaka, Takafumi Kobari and Shoichi Shimizu*

The first synthesis and optical resolution of an inherently chiral calix[4]arene amino acid has been achieved.

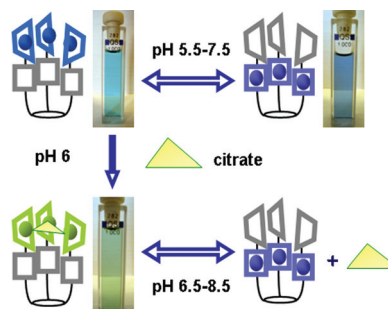


1839

The pH controlled uptake/release of citrate by a tri-copper(II) complex

Giacomo Dacarro, Piersandro Pallavicini and Angelo Taglietti*

The pH controlled movement of three copper ions inside a carefully designed receptor allows the recognition and uptake/release of citrate in aqueous solution in a manner that can be followed visually.

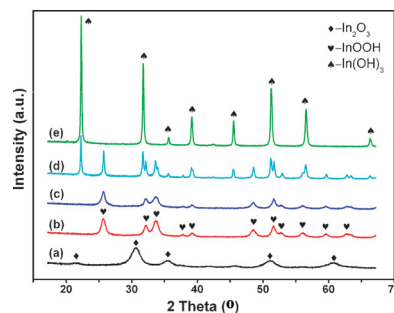


1843

Controlled preparation of In_2O_3 , InOOH and $\text{In}(\text{OH})_3$ via a one-pot aqueous solvothermal route

Tingjiang Yan, Xuxu Wang,* Jinlin Long, Huaxiang Lin, Rusheng Yuan, Wenxin Dai, Zhaozhui Li and Xianzhi Fu*

Pure cubic In_2O_3 , orthorhombic InOOH and cubic $\text{In}(\text{OH})_3$ nanocrystals were separately synthesized *via* a one-pot aqueous solvothermal route at low temperature by simply regulating the amount of water in the ternary system H_2O – DMF – $\text{In}(\text{NO}_3)_3 \cdot 4.5\text{H}_2\text{O}$.



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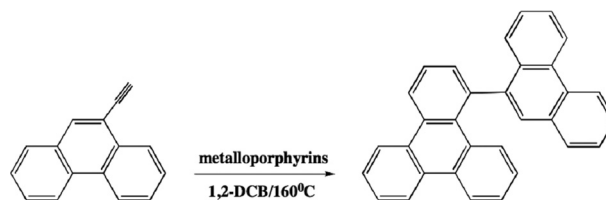


1847

Highly selective biaryl formation by the cyclooligomerization of arylethyne catalyzed by rhodium and ruthenium porphyrins

Pietro Tagliatesta,* Elfituri Elakkari, Alessandro Leoni, Angelo Lembo and Daniel Cicero

The formation of biaryl derivatives from arylethyne is catalyzed by rhodium or ruthenium porphyrins giving interesting derivatives in high yield and selectivity. The catalysts are resistant to the reaction conditions and can be reused for several synthesis with no change of activity.



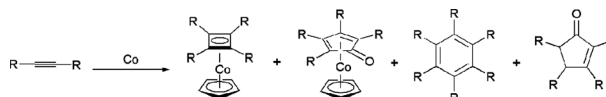
PERSPECTIVE

1850

Selected recent developments in organo-cobalt chemistry

Caroline J. Scheuermann née Taylor* and Benjamin D. Ward

Organometallic cobalt complexes are studied in fundamental organometallic and coordination chemistry, and are also widely used in the metal-mediated synthesis of organic compounds, including natural products. The exciting possibilities and new developments of this chemistry are described herein.



PAPERS

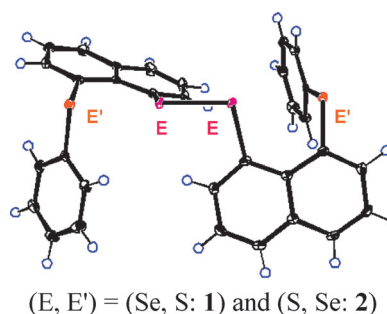


1881

Extended hypervalent E'...E-E...E' 4c-6e (E, E' = Se, S) interactions: structure, stability and reactivity of 1-(8-PhE'/C₁₀H₆)EE(C₁₀H₆E'/Ph-8')-1'

Waro Nakanishi,* Satoko Hayashi, Sayuri Morinaka, Takahiro Sasamori and Norihiro Tokitoh

Formation of E'...E-E...E' 4c-6e is confirmed for 1-(8-PhE'/C₁₀H₆)EE(C₁₀H₆E'/Ph-8')-1' [(E, E') = (Se, S: **1**) and (S, Se: **2**); the central S-S bond in **2** cleaves in the reduction with NaBH₄, whereas Se-Se in **1** does not, which are examined based on QC calculations.



1890

Synthesis and characterization of weakly coordinating anion salts of a new, stable carbocationic reagent, the dibenzosubereryl (dibenzotropylium) ion

Adina Cordoneanu, Mark J. Drewitt, Neda Bavarian and Michael C. Baird*

New compounds of the type [DBS][X] (DBS = dibenzosubereryl; X = weakly coordinating anions) have been synthesized and characterized and the chemistry of the planar, charge delocalized but highly electrophilic DBS⁺ carbocation has been studied.



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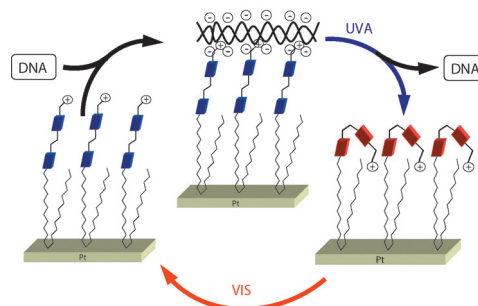
PAPERS

1899

Light-triggered DNA release by dynamic monolayer films

Fiorella L. Callari, Salvatore Petralia, Sabrina Conoci and Salvatore Sortino*

Immobilization and release of single and double strand DNA is achieved by exploiting the light-controlled electrostatic interactions with the two isomeric forms of a cationic azobenzene self-assembled on transparent platinum electrodes.

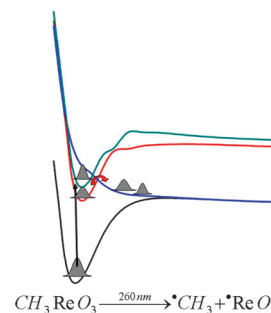


1904

Photoinduced bond cleavage in CH_3ReO_3 : excited state dynamics

Paulo Jorge Costa,* Maria José Calhorda, Sébastien Villaume and Chantal Daniel*

The rhenium–methyl bond cleavage in CH_3ReO_3 has been investigated by means of quantum chemical calculations: the spin–orbit coupling between the ^1E state and the $^3\text{A}_1$ dissociative state controls the radical formation $^{\bullet}\text{CH}_3 + ^{\bullet}\text{ReO}_3$ which occurs in 400 fs.

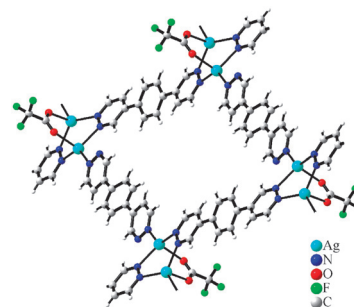


1910

Copper(I) and silver(I) coordination frameworks involving extended bipyridazine bridges

Anna S. Degtyarenko, Pavlo V. Solntsev, Harald Krautscheid, Eduard B. Rusanov, Alexander N. Chernega and Konstantin V. Domasevitch*

Novel 1,4-(pyridazin-4-yl)benzene ligand is an efficient polydentate N-donor towards silver(I) and copper(I) ions supporting structures of coordination frameworks based upon di- and tetranuclear metal/pyridazine clusters.

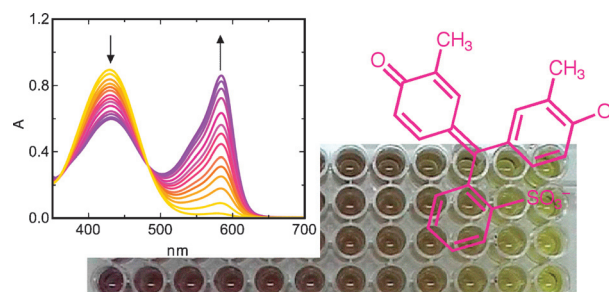


1919

Selective sensing of competitive anions by non-selective hosts: the case of sulfate and phosphate in water

M. Neus Piña, Bartomeu Soberats, Carmen Rotger, Pablo Ballester, Pere M. Deyà and Antoni Costa*

The combination of the acid–base indicators Cresol Red or Bromocresol Green with a squaramide based host gives two IDA sensing ensembles that allow the quantification of sulfate and phosphate anions in water samples. The new colorimetric method is demonstrated on a microplate reader.





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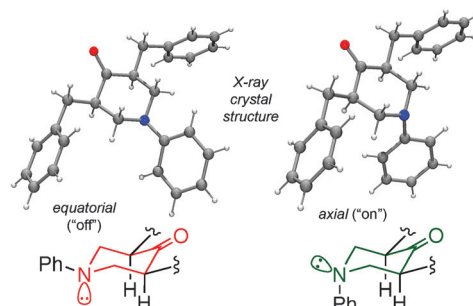


1924

Links between through-bond interactions and assembly structure in simple piperidones

Ling Yuan, Bobby G. Sumpter, Khalil A. Abboud and Ronald K. Castellano*

Both the axial and equatorial configurations of a simple piperidone are represented in the solid state based on refined values of occupancy factors. The experimental result is complemented by calculations that expose the links between molecular/supramolecular structure and through-bond (hyperconjugative) interactions in donor- σ -acceptor molecules.

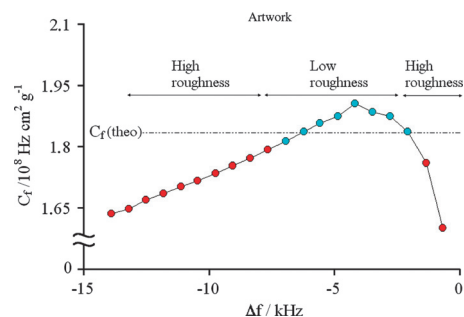


1935

Effect of the thickness of thallium deposits on the values of EQCM sensitivity constant

Ana-Laura Donjuan-Medrano and Antonio Montes-Rojas*

Relation between morphology of thallium films and sensitivity constant C_f values at low and high roughness.

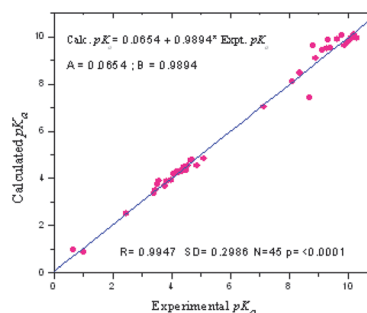


1945

Acidity of *meta*- and *para*-substituted aromatic acids: a conceptual DFT study

Kartick Gupta, Santanab Giri and Pratim K. Chattaraj*

The pK_a values of the aromatic acids may be estimated reasonably well in terms of the electrophilicity based charge transfer index, fractional number of electrons transferred, or group charge.

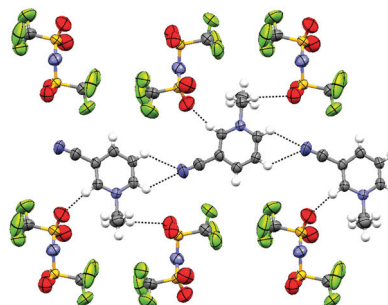


1953

Ionic liquid characteristics of 1-alkyl-*n*-cyanopyridinium and 1-alkyl-*n*-(trifluoromethyl)pyridinium salts

Christopher Hardacre, John D. Holbrey,* Claire L. Mullan, Mark Nieuwenhuyzen, W. Matthew Reichert, Kenneth R. Seddon and Simon J. Teat

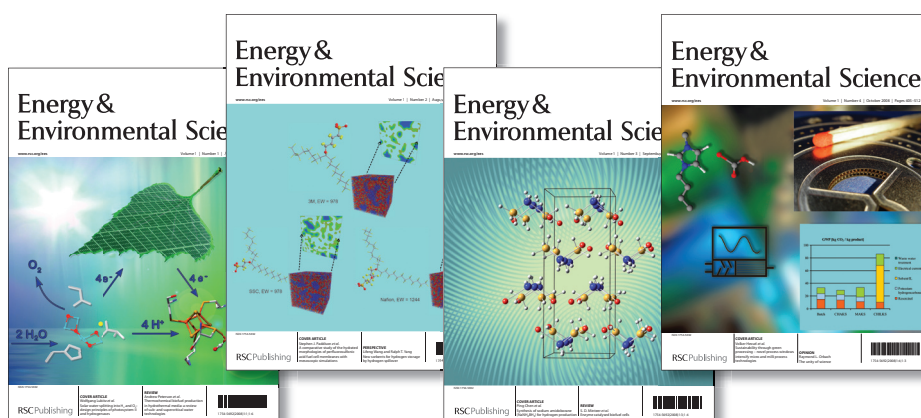
The presence of electron withdrawing groups on pyridinium cations leads to strong cation-cation hydrogen-bonding in the solid state; however, ionic liquids were also formed with the appropriate selection of counter ion.



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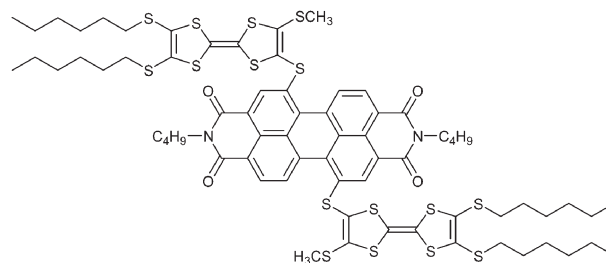
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PAPERS

1968

Synthesis and properties of a tetrathiafulvalene–perylene tetracarboxylic diimide–tetrathiafulvalene dyadYu Zhang, Liang-Zhen Cai, Cheng-Yun Wang,*
Guo-Qiao Lai and Yong-Jia Shen*

A tetrathiafulvalene–perylene tetracarboxylic diimide–tetrathiafulvalene dyad has been synthesized and its cyclic voltammetric, absorption spectroscopic and fluorescence spectroscopic data described.

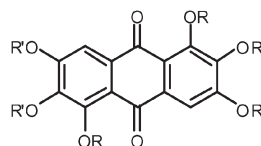


1974

Room-temperature electron-deficient discotic liquid crystals: facile synthesis and mesophase characterization

Hari Krishna Bisoyi and Sandeep Kumar*

Two novel series of rufigallol-based room-temperature discotic liquid crystals having very wide mesophase range have been designed and synthesized using microwave dielectric heating within a few minutes in good yield.



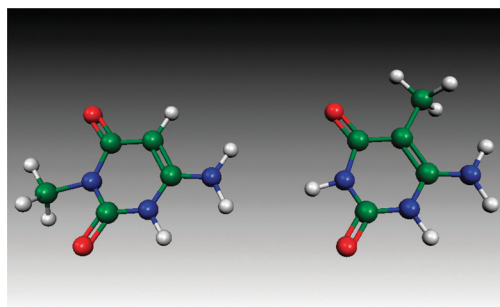
R, R' = Combinations of

C_nH_{2n+1} and 

1981

Hydrogen bonding of 3- and 5-methyl-6-aminouracil with natural DNA basesGábor Paragi,* Emília Szájli, Ferenc Bogár, Lajos Kovács,
Célia Fonseca Guerra and F. Matthias Bickelhaupt*

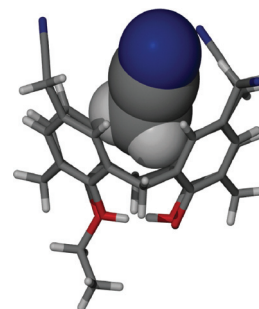
Theoretical investigation of hydrogen bonding of 3- and 5-methyl-6-aminouracil with natural DNA bases using density functional theory at BP86/TZ2P level.

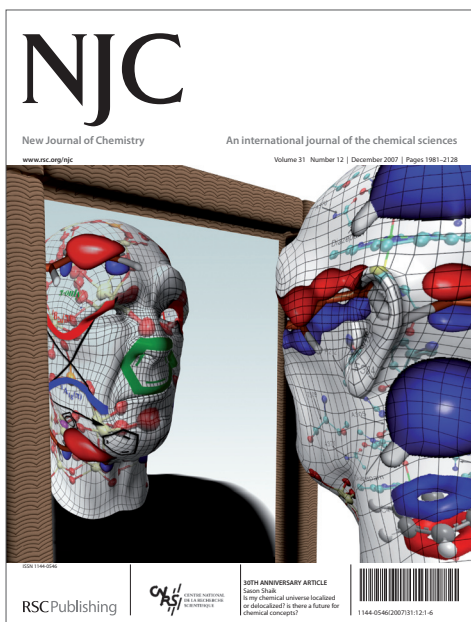


1988

Trianionic calix[4]arene monoalkoxy derivatives: synthesis, solid-state structures and self-assembly propertiesKinga Suwinska, Oleksandr Shkurenko, Cyrille Mbemba,
Antoine Leydier, Said Jebors, Anthony W. Coleman,*
Rima Matar and Pierre Falson

Novel trianionic monoalkyl-calix[4]arenes show CMC values in the range 0.1 to 1.6 mM. The structures of the intermediate trinitrile compounds are 1-D inclusion polymers.





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Associate Editor for the Americas

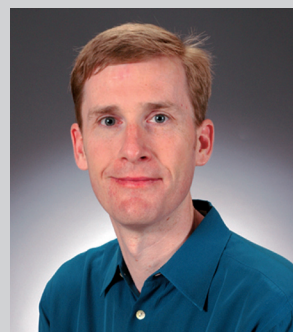
Michael is an associate professor in the Department of Chemistry and the director for the Center for Catalysis at the University of Florida in Gainesville, Florida. He is a fellow of both the Alfred P. Sloan Foundation and the Royal Society of Chemistry. His research interests focus on the design of ligands and metal complexes for the selective recognition and sequestration of cations and anions and for biomimetic catalysis.

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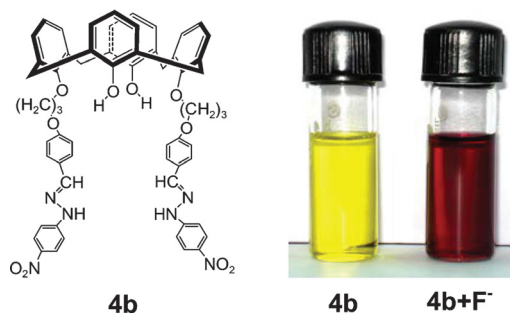


1999

A new class of functionalized calix[4]arenes as neutral receptors for colorimetric detection of fluoride ions

Har Mohindra Chawla,* Rahul Shrivastava and Satya Narayan Sahu

The molecular receptor **4b** selectively recognizes fluoride ions *via* H-bonds and subsequent deprotonation to elicit a distinct colour change from yellow to dark purple.

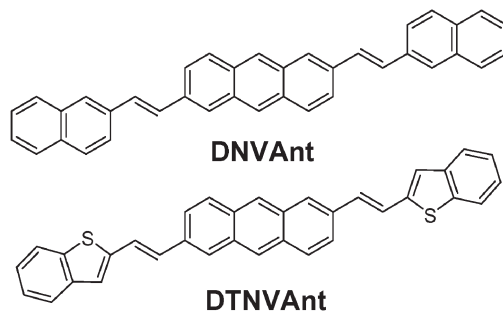


2006

Organic thin-film transistors based on 2,6-bis(2-arylvinyl)anthracene: high-performance organic semiconductors

Myoung-Chul Um, Junhyuk Jang, Jung-Pyo Hong, Jihoon Kang, Do Yeung Yoon, Seong Hoon Lee, Jang-Joo Kim* and Jong-In Hong*

Two novel organic semiconductors based on arylvinylanthracene have exhibited good electrical performance (up to $0.2 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$) on SiO_2/Si at a low substrate deposition temperature and can be easily synthesized in large quantities.

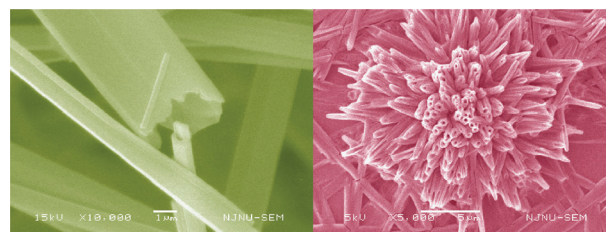


2011

Uncommon hexagonal microtubule based gel from a simple trimesic amide

Naïen Shi, Gui Yin, Hongbian Li, Min Han and Zheng Xu*

A small molecule of *N,N',N''*-tris(3-methylpyridyl)-trimesic amide was assembled into a novel hexagonal microtubule through intermolecular hydrogen bonds, and simultaneously formed a gel in H_2O –THF mixed solvent.

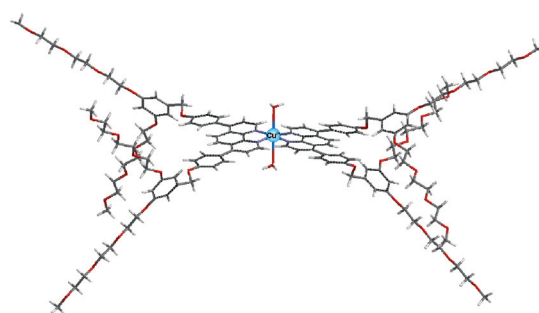


2016

Hydrophilic oxybathophenanthroline ligands: synthesis and copper(II) complexation

Holger Stephan,* Stefanie Juran, Karin Born, Peter Comba, Gerhard Geipel, Uwe Hahn, Nicole Werner and Fritz Vögtle*

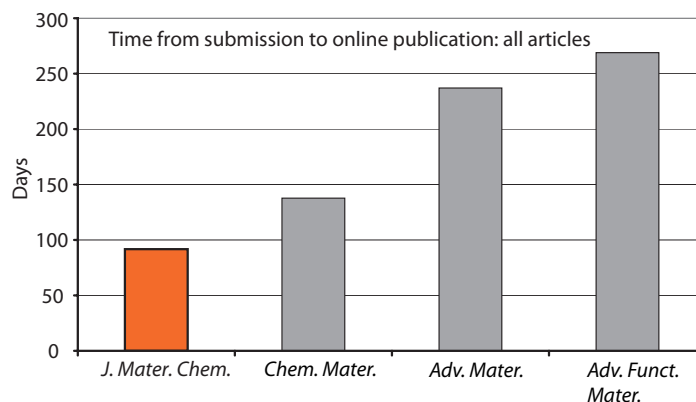
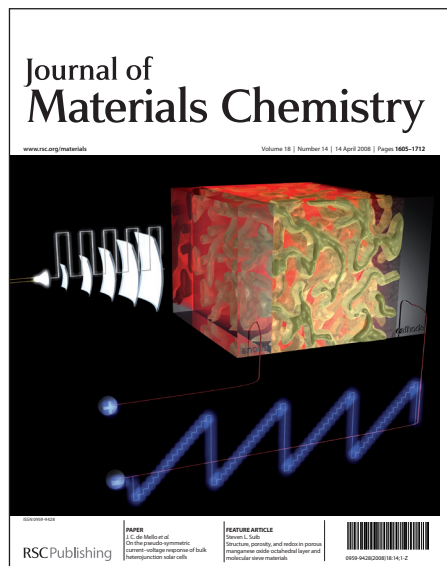
Water-soluble bathophenanthroline-derived ligands were employed in the complexation of copper(II), revealing the rapid formation of stable $[\text{Cu}(\text{L})_2(\text{OH}_2)_2]^{2+}$ -type (L = ligand) species.



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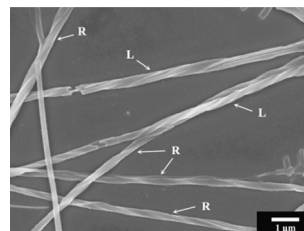


2023

Helical ribbons tuned by alkoxy chains in achiral twin-tapered dihydrazide derivatives

Songnan Qu, Haitao Wang, Zhixin Yu, Binglian Bai and Min Li*

Achiral twin-tapered dihydrazide derivatives effectively gel ethanol in which both left- and right-handed helical ribbons were generated by tuning the length of the alkoxy side chains.

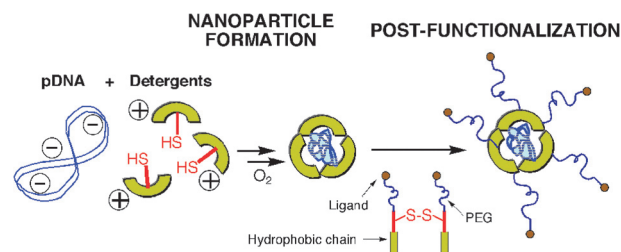


2027

Formulation of PEG–folic acid coated nanometric DNA particles from perfluoroalkylated cationic dimerizable detergents and *in vitro* folate-targeted intracellular delivery

Loïc Le Gourriérec, Christophe Di Giorgio, Jacques Greiner and Pierre Vierling*

Perfluoroalkylated thiol detergents containing an amino polar head and their use for condensing DNA into virus-sized monomolecular DNA nanoparticles are reported. These particles were very efficient transfection systems and were further post-labeled with PEG–folic acid conjugate.

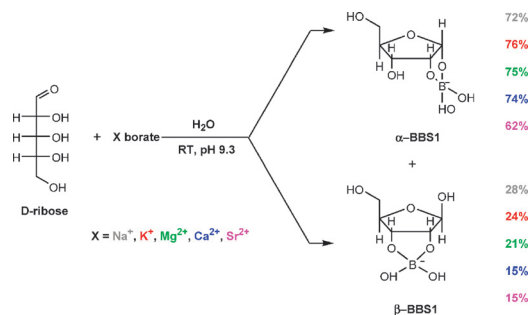


2043

Interactions of D-ribose with polyatomic anions, and alkaline and alkaline-earth cations: possible clues to environmental synthesis conditions in the pre-RNA world

Ana F. Amaral, M. Matilde Marques, José A. L. da Silva* and João J. R. Fraústo da Silva

The effect of cations on borate–ribose-bound species was studied, and it was found that the cations affect the relative amounts of ribopyranose/ribofuranose isomers in solution.



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