

IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 30(4) 493-656 (2006)



Cover

See Alain Chaumont and Georges Wipff, p. 537.

Molecular dynamics simulations predict that a tetrahedral macrotricyclic host with ammonium bridgeheads should capture halide anions in a room temperature "green" ionic liquid, and provide microscopic insights into the solvation of these species in the dry and humid forms of the liquid.

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CHEMICAL SCIENCE

C25

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, as well as the most significant scientific advances.

Chemical Science

April 2006/Volume 3/Issue 4

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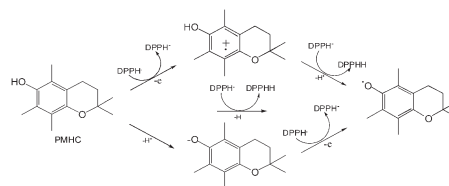
OPINION

503

How vitamin E scavenges DPPH radicals in polar protic media

Hong-Yu Zhang* and Hong-Fang Ji

H-Atom transfer and sequential proton-loss–electron-transfer rather than stepwise electron-transfer–proton-transfer are responsible for the 1,1-diphenyl-2-picrylhydrazyl radical scavenging of 2,2,5,7,8-pentamethyl-6-hydroxychroman, a vitamin E model, in polar protic solvent.



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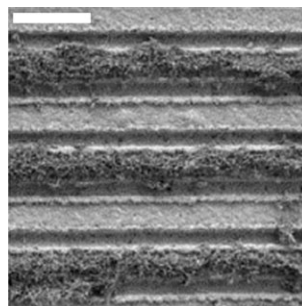


505

Chemical vapour deposition of titanium chalcogenides and pnictides and tungsten oxide thin films

Robert G. Palgrave and Ivan P. Parkin*

The microstructures of Ti-containing and tungsten oxide thin films prepared by CVD are precursor-dependent and have a direct influence on their functional properties.



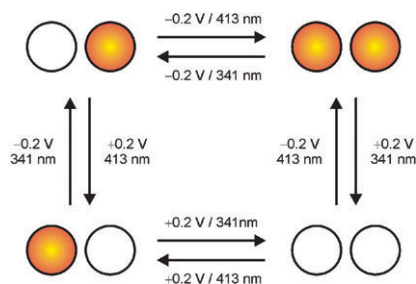
LETTERS

515

A multistate ensemble of molecular switches

Salvatore Sortino,* Salvatore Petralia, Santo Di Bella, Massimiliano Tomasulo and Francisco M. Raymo*

The four distinct states associated with a mixture of an electrochromic complex and a photochromic compound can be interconverted by operating the two molecular switches in parallel under the influence of electrical and optical inputs.

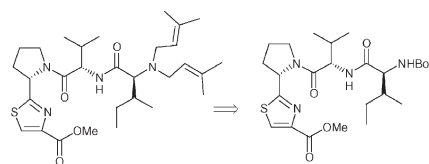


518

The first total synthesis of aeruginosamide

Zhiyong Chen and Tao Ye*

An efficient synthesis of the marine cyanobacterium metabolite aeruginosamide is presented.

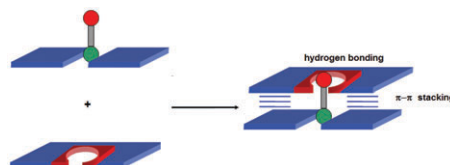


521

Metal complexes as second-sphere ligands

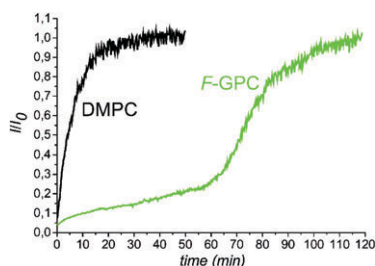
Augustin M. Madalan, Narcis Avarvari and Marius Andruh*

Novel supercomplexes are constructed from a mononuclear square planar Ni(II) or Pd(II) complex acting as a host receptor towards the aqua ligand from copper complexes.



LETTERS

524



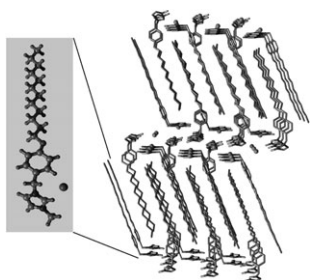
Microbubbles with exceptionally long life—synergy between shell and internal phase components

Frédéric Gerber, Marie Pierre Krafft,* Gilles Waton and Thierry F. Vandamme

Exceptionally long-lived microbubbles containing a fluorocarbon as part of their filling gas have been obtained by using a fluorinated phospholipid (*F*-GPC) instead of dimyristoylphosphatidylcholine (DMPC) as a shell component. An unexpected strong synergistic effect between the fluorocarbon gas and the fluorinated phospholipid has been observed.



528

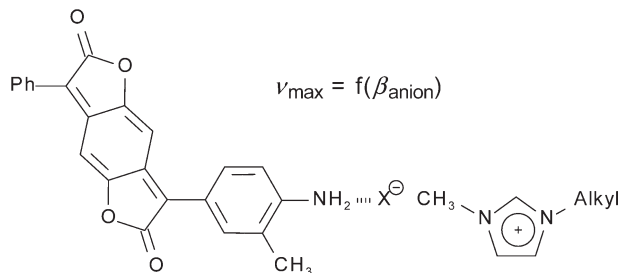


New ionic liquid crystals based on imidazolium salts

William Dobbs, Laurent Douce,* Lionel Allouche, Alain Louati, François Malbosc and Richard Welter

1-(4-Dodecyloxybenzyl)-3-methyl-1*H*-imidazol-3-ium salts with different anions (Br^- , BF_4^- , SCN^- , PF_6^- , CF_3SO_3^- , $(\text{CF}_3\text{SO}_2)_2\text{N}^-$) have been prepared in order to investigate their mesomorphic behavior and electrochemical properties.

533



New aspects on polarity of 1-alkyl-3-methylimidazolium salts as measured by solvatochromic probes

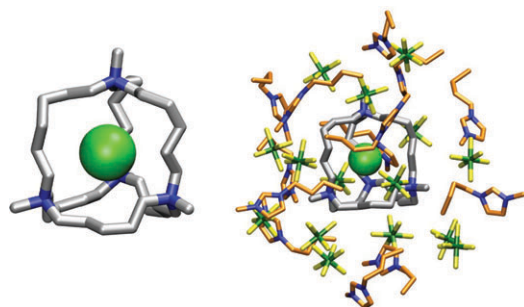
Alexander Oehlke, Katja Hofmann and Stefan Spange*

Kamlet–Taft solvatochromic polarity parameters β and π^* of ionic liquids with 1-alkyl-3-methylimidazolium cations are determined in two ways by the counter anion X^- : the β value represents the hydrogen bond basicity and the π^* value depends on the polarizability of X^- .

PAPERS



537



Halide anion solvation and recognition by a macrotricyclic tetraammonium host in an ionic liquid: a molecular dynamics study

Alain Chaumont and Georges Wipff*

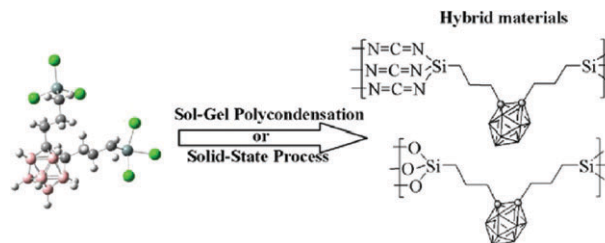
The solvation of halide X^- anions and of their $\text{X}^- \subset \text{L}^{4+}$ complexes is described in the dry and humid forms of the [BMI][PF₆] ionic liquid. A selectivity is predicted for F^- in the dry liquid.

PAPERS

546

Synthetic approaches to the preparation of hybrid network materials incorporating carborane clustersArántzazu González-Campo, Rosario Núñez,*
Clara Viñas and Bruno Boury

Hybrid organic–inorganic class II materials with carborane units were prepared from a single trichlorosilylcarborane-containing precursor and polymerised *via* different processes, giving rise to structurally significantly different materials.

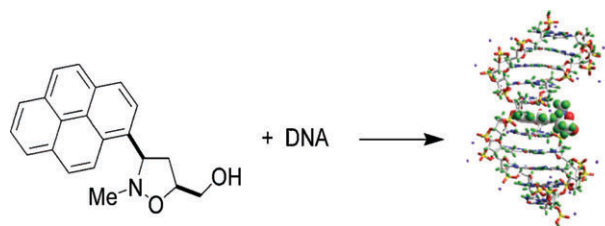


554

Binding of a non-ionic pyrenylisoxazolidine derivative to double-stranded polynucleotides: spectroscopic and molecular modelling studies

Antonio Rescifina,* Ugo Chiacchio, Anna Piperno and Salvatore Sortino*

It is demonstrated that a pyrenylisoxazolidine derivative with potential anticancer activity binds to DNA. The presence of the isoxazolidine substituent plays a key role in determining some preference for alternating AT rather than for GC sequences.

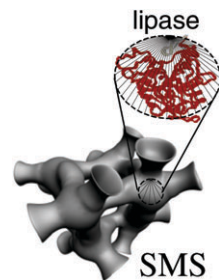


562

Immobilization of lipase on silicas. Relevance of textural and interfacial properties on activity and selectivity

Anne Galarneau,* Mihaela Mureseanu, Sophie Atger, Gilbert Renard and François Fajula

Lipases encapsulated in Sponge Mesoporous Silica change their typoselectivity and are very active for short chain esters hydrolysis.

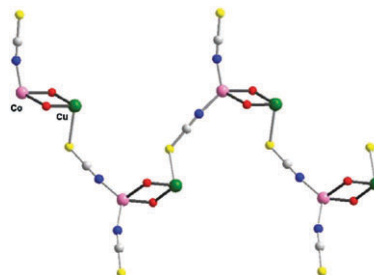


572

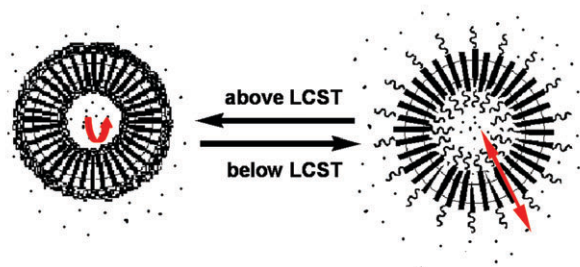
An original 1D Cu–Co heterometallic compound: synthesis, structure and magnetic properties

Jean-Pierre Costes,* Ruxandra Gheorghe, Marius Andruh,* Sergiu Shova and Juan-Modesto Clemente Juan

A copper–cobalt heterodinuclear complex behaves as a one-dimensional alternating zig-zag chain-like structure with a strong antiferromagnetic Cu–Co exchange interaction through the phenoxo bridges and a weak ferromagnetic Cu–Co interaction through the thiocyanato bridge.



577

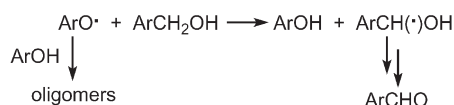


Thermosensitive cross-linked polymer vesicles for controlled release system

Xiangrong Chen, Xiaobin Ding,* Zhaohui Zheng and Yuxing Peng

Schematic illustration of the controlled loading and releasing principle of the thermosensitive cross-linked polymer vesicles.

583



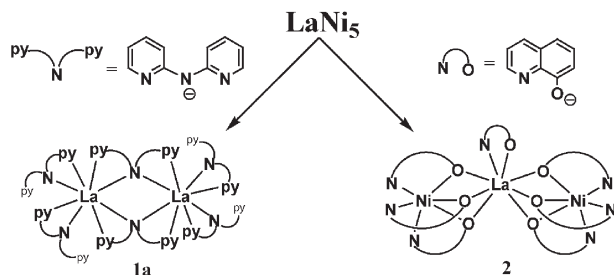
Mechanistic and steric issues in the oxidation of phenolic and non-phenolic compounds by laccase or laccase-mediator systems. The case of bifunctional substrates

Francesca d'Acunzo, Carlo Galli,* Patrizia Gentili* and Federica Sergi

Phenoxyl radicals from lignin could act as natural mediators of laccase, thus underlining the central role of this enzyme in biodelignification.



592

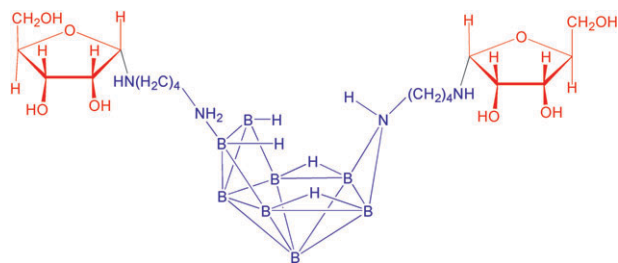


A rare earth alloy as a synthetic reagent: contrasting homometallic rare earth and heterobimetallic outcomes

Glen B. Deacon,* Craig M. Forsyth, Peter C. Junk and Stuart G. Leary

Rare earth alloy LaNi_5 reacts with 2,2'-dipyridylamine (HNpy_2) giving a homometallic lanthanum complex $[\text{La}(\text{Npy}_2)_3]_2$ which exists in two linkage isomers, or with 8-hydroxyquinoline (HOQ) giving a bimetallic La–Ni complex $[\text{Ni}_2\text{La}(\text{OQ})_7]$ having a bent Ni–La–Ni array held by six O-bridged OQ ligands.

597



The first synthesis of azanoborane-containing sugars, possible boron carriers for neutron capture therapy

Mohamed E. El-Zaria,* Afaf R. Genady and Detlef Gabel

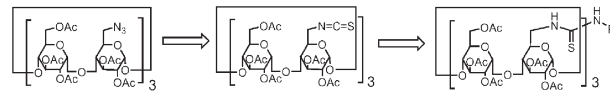
Synthesis, characterization, and *in vitro* toxicity of azanoborane-containing monosaccharide unit clusters as delivery agents for boron neutron capture therapy.

603

New synthetic approach to per-*O*-acetyl-isocyanates, isothiocyanates and thioureas in the disaccharide and cyclodextrin series

Stephane Menuel, Stanislaw Porwanski and Alain Marsura*

Pure cyclodextrin or disaccharide isocyanates and isothiocyanates are readily prepared at a scale-up level by the phosphine imide strategy. The first syntheses of ^{ACE}tris-isocyanato- and ^{ACE}tris-isothiocyanato-per-*O*-acetyl- α -cyclodextrins and direct conversion of the latter into thioureido-cyclodextrin derivatives are reported.



609

New tools for the analysis of refractive index measurements in liquid mixtures. Application to 2-diethylaminoethanol + water mixtures from 283.15 to 303.15 K

Isabel M. S. Lampreia,* Ângela F. S. S. Mendonça, Sara M. A. Dias and João Carlos R. Reis

Apparent and partial molar refractions of mixing are introduced and shown to be interesting new tools to probe the complex process of mixing amphiphiles with water.

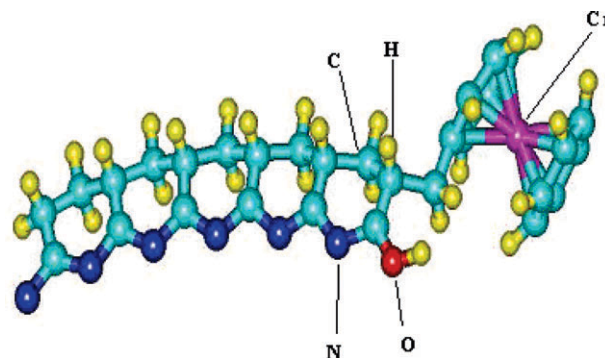


615

Chromium-containing organometallic nanomaterials for non-linear optics

Larisa G. Klapshina,* Ilya S. Grigoryev, Tatyana I. Lopatina, Vladimir V. Semenov, Georgy A. Domrachev, William E. Douglas, Boris A. Bushuk, Sergei B. Bushuk, Andrey Yu. Lukianov, Andrey V. Afanas'ev, Robert E. Benfield and Alexey I. Korytin

Novel non-linear optical polymeric film-producing nanocomposites based on bis(arene)chromium complexes incorporated into a CN-containing matrix have been developed.

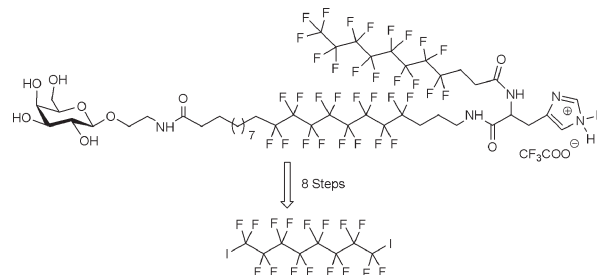


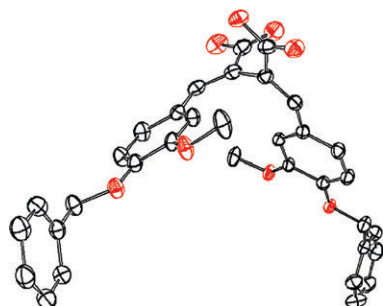
629

Synthesis and preliminary biological studies of hemifluorinated bifunctional bolaamphiphiles designed for gene delivery

S  verine Denoyelle, Ange Polidori,* M  lanie Brunelle, Pascal Y. Vuillaume, Sylvette Laurent, Yousef ElAzhary and Bernard Pucci*

The multistep synthesis and the preliminary DNA transfection results of a new series of bifunctional hemifluorocarbon bolaamphiphiles are described.





Structural and conformational study of two solvates of a fulgenic acid derivative

Valerio Giannellini, Massimo Bambagiotti-Alberti,*
Bruno Bruni and Massimo Di Vaira*

The solid state structures of two solvates and the results of a conformational study are reported for an essential intermediate of the synthesis of a cancer-protective agent which also belongs to a class of compounds with interesting photochromic properties.

AUTHOR INDEX

- | | | | |
|-----------------------------------|--------------------------------|--------------------------------|------------------------------|
| Afanas'ev, Andrey V., 615 | Di Vaira, Massimo, 647 | Junk, Peter C., 592 | Porwanski, Stanislaw, 603 |
| Allouche, Lionel, 528 | Dias, Sara M. A., 609 | Klapshina, Larisa G., 615 | Pucci, Bernard, 629 |
| Andruh, Marius, 521, 572 | Ding, Xiaobin, 577 | Korytin, Alexey I., 615 | Raymo, Francisco M., 515 |
| Atger, Sophie, 562 | Dobbs, William, 528 | Krafft, Marie Pierre, 524 | Reis, João Carlos R., 609 |
| Avarvari, Narcis, 521 | Domrachev, Georgy A., 615 | Lampreia, Isabel M. S., 609 | Renard, Gilbert, 562 |
| Bambagiotti-Alberti, Massimo, 647 | Douce, Laurent, 528 | Laurent, Sylvette, 629 | Rescifina, Antonio, 554 |
| Benfield, Robert E., 615 | Douglas, William E., 615 | Leary, Stuart G., 592 | Semenov, Vladimir V., 615 |
| Boury, Bruno, 546 | ElAzhary, Yousef, 629 | Lopatina, Tatyana I., 615 | Sergi, Federica, 583 |
| Brunelle, Mélanie, 629 | El-Zaria, Mohamed E., 597 | Louati, Alain, 528 | Shova, Sergiu, 572 |
| Bruni, Bruno, 647 | Fajula, François, 562 | Lukianov, Andrey Yu., 615 | Sortino, Salvatore, 515, 554 |
| Bushuk, Boris A., 615 | Forsyth, Craig M., 592 | Madalan, Augustin M., 521 | Spange, Stefan, 533 |
| Bushuk, Sergei B., 615 | Gabel, Detlef, 597 | Malbosc, François, 528 | Tomasulo, Massimiliano, 515 |
| Chaumont, Alain, 537 | Galarneau, Anne, 562 | Marsura, Alain, 603 | Vandamme, Thierry F., 524 |
| Chen, Xiangrong, 577 | Galli, Carlo, 583 | Mendonça, Ângela F. S. S., 609 | Viñas, Clara, 546 |
| Chen, Zhiyong, 518 | Genady, Afaf R., 597 | Menuel, Stephane, 603 | Vuillaume, Pascal Y., 629 |
| Chiacchio, Ugo, 554 | Gentili, Patrizia, 583 | Mureseanu, Mihaela, 562 | Waton, Gilles, 524 |
| Clemente Juan, Juan-Modesto, 572 | Gerber, Frédéric, 524 | Núñez, Rosario, 546 | Welter, Richard, 528 |
| Costes, Jean-Pierre, 572 | Gheorghe, Ruxandra, 572 | Oehlke, Alexander, 533 | Wipff, Georges, 537 |
| d'Acunzo, Francesca, 583 | Giannellini, Valerio, 647 | Palgrave, Robert G., 505 | Ye, Tao, 518 |
| Deacon, Glen B., 592 | González-Campo, Arántzazu, 546 | Parkin, Ivan P., 505 | Zhang, Hong-Yu, 503 |
| Denoyelle, Séverine, 629 | Grigoryev, Ilya S., 615 | Peng, Yuxing, 577 | Zheng, Zhaohui, 577 |
| Di Bella, Santo Di, 515 | Hofmann, Katja, 533 | Petralia, Salvatore, 515 | |
| | Ji, Hong-Fang, 503 | Piperno, Anna, 554 | |
| | | Polidori, Ange, 629 | |

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