

IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 34(3) 369–572 (2010)



Cover

See Nikolett B. Báthori *et al.*, pp. 405–413.
Partial isostructurality indicates why new crystals grow on specific faces of the mother prism. Nikolett B. Báthori, Petra Bombicz, Susan A. Bourne and Gerhard A. Venter, *New J. Chem.*, 2010, **34**, 405.

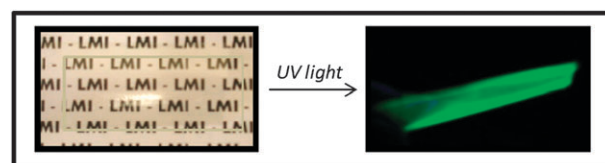
LETTERS

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A promising way to obtain large, luminescent and transparent thick films suitable for optical devices

Jérôme Deschamps,* Audrey Potdevin, Nathalie Caperaa, Geneviève Chadeyron, Sandrine Therias and Rachid Mahiou

A simple and general procedure for the elaboration of large, thick, transparent and self-standing films, consisting of well-dispersed phosphors embedded in a polymer matrix and applicable to optical devices, is reported.

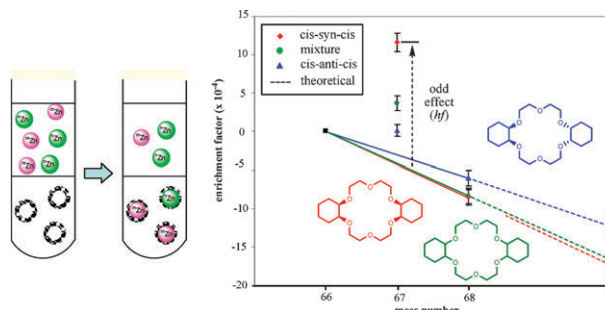


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Stereochemistry effect of dicyclohexano-18-crown-6 on zinc isotope separation

Yi Lin, Jeff Espinas, Stéphane Pellet-Rostaing,* Alain Favre-Régouillon and Marc Lemaire*

Zinc isotopes were fractionated using a liquid/liquid extraction with DCH18C6 and its pure *cis-syn-cis* and *cis-anti-cis* stereoisomers. The structures of the stereoisomers of DCH18C6 contribute to the enrichment of the Zn isotopes, with the best fractionation for the *cis-syn-cis* derivative.



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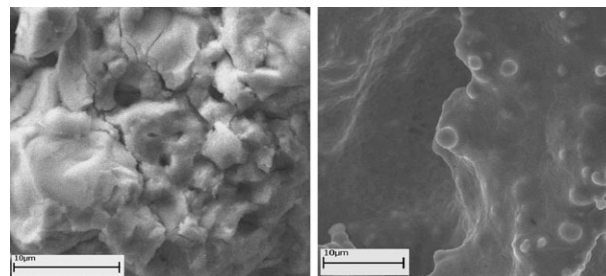
LETTERS

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The influence of a dc electric field on chemical interactions in “peroxide-metal” systems during combustion processes

Sergey M. Busurin, Maxim V. Kuznetsov,
Yury G. Morozov, Mariya L. Busurina and
Ivan P. Parkin*

The application of an external electric field to a self-propagating reaction changes the product microstructure.

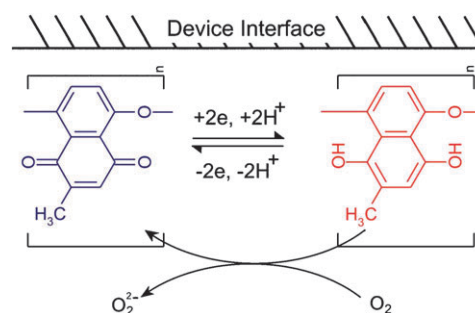


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Plumbagin: a natural product for smart materials?

Laura A. A. Newton, Emma Cowham, Duncan Sharp,
Ray Leslie and James Davis*

A quinone loaded film capable of on-demand production of reactive oxygen species.

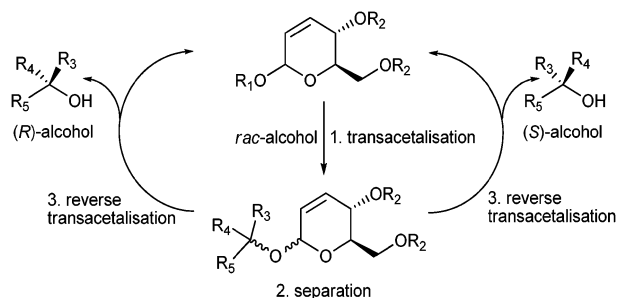


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Toward preparative resolution of chiral alcohols by an organic chemical method

Nino Malic, Cornelis Moorhoff, Valerie Sage, Dilek Saylik,
Euneace Teoh, Janet L. Scott and Christopher R. Strauss*

Asymmetric alcohols were resolved as predominantly α -*O*-glycosides of 2,3-unsaturated hexoses and the enantiomers recovered by a transglycosylation process that could allow the auxiliary to be recycled.

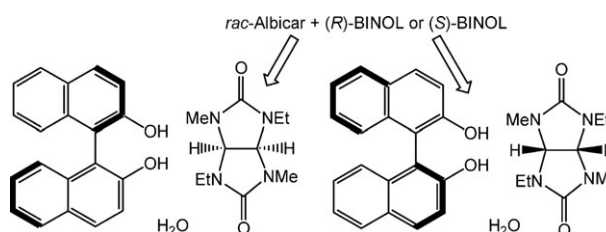


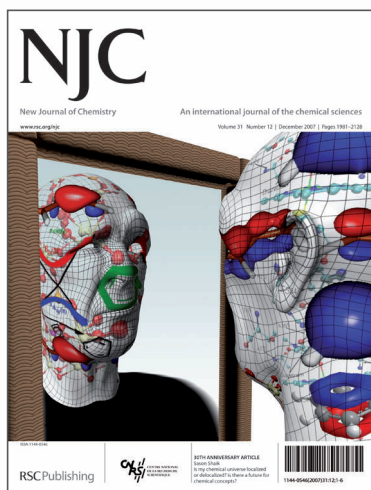
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The chiral drug Albicar: resolution of its racemate *via* complexation with BINOL

Denis A. Lenev,* Konstantin A. Lyssenko and
Remir G. Kostyanovsky*

Both enantiomers of the chiral drug Albicar were prepared from their complexes with (*R*)- and (*S*)-BINOL.





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New J. Chem., 2009, **33**, (1), 186-195

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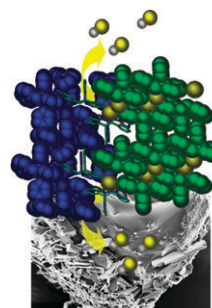
PAPERS

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Investigation of sublimation with and without dissociation in the chloride and nitrate salts of 4-(1-hydroxy-1,2-diphenylethyl)pyridine

Nikoletta B. Báthori,* Petra Bombicz, Susan A. Bourne* and Gerhard A. Venter

Both $1\text{H}^+ \cdot \text{Cl}^-$ and $1\text{H}^+ \cdot \text{NO}_3^-$ sublime and recrystallize on heating, the former with dissociation and loss of HCl. The two salts are isostructural, but Hirschfeld surface analysis shows significant differences between the intermolecular interactions.

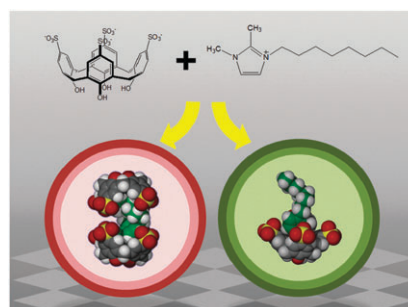


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Multi-component bi-layers featuring [1-octyl-2,3-dimethylimidazolium] \cap *p*-sulfonatocalix[4]arene] supermolecules

Irene Ling, Yatimah Alias,* Alexandre N. Sobolev and Colin L. Raston*

1-Octyl-2,3-dimethylimidazolium cations are confined in the anionic *p*-sulfonatocalix[4]arene cavity, essentially forming 'molecular capsules', or with the *n*-octyl chain penetrating the adjacent bi-layer in multi-component solid state structures.

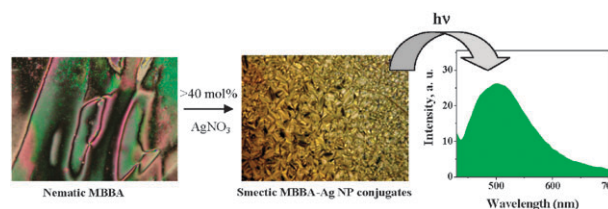


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Nematic to smectic texture transformation in MBBA by *in situ* synthesis of silver nanoparticles

P. K. Sudhadevi Antharjanam* and Edamana Prasad*

Nanoparticle-induced texture transformation: *In situ* synthesis of silver nanoparticles in MBBA liquid crystal induces a texture change for the mesogenic material. The resulting organic-inorganic conjugate forms a glassy liquid crystalline phase upon rapid cooling and emits light at 500 nm upon photo-excitation.

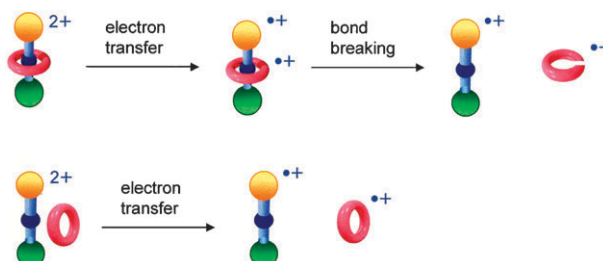


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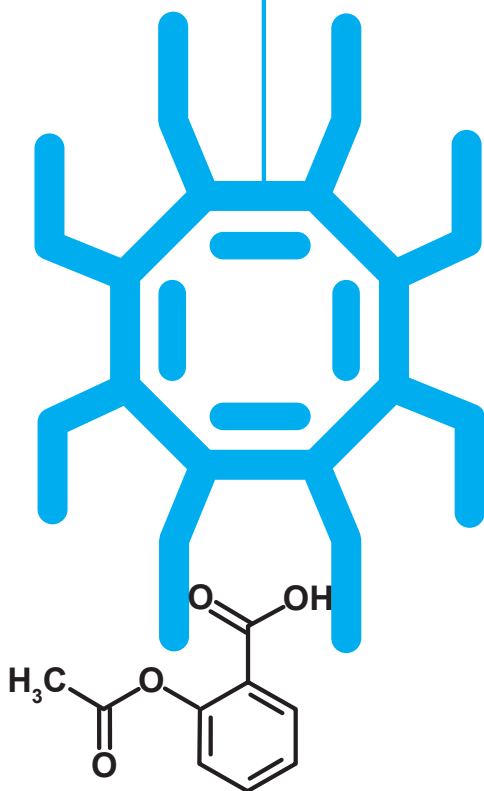
Electron transfer from wheel to axle in a rotaxane. A mass spectrometric investigation

Sara Pasquale, Stefano Di Stefano* and Bernardo Masci*

Electron transfer processes from the anthracene-based wheel to the viologen-based axle have been investigated in a new rotaxane and in related unthreaded and pseudo-rotaxanic adducts by a MS/MS CID technique.



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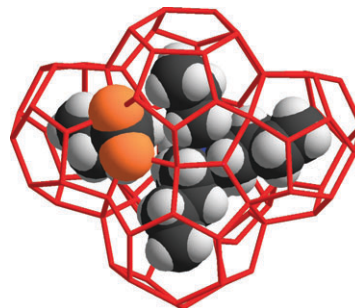
PAPERS

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The structure of the ionic clathrate hydrate of tetrabutylammonium valerate $(C_4H_9)_4NC_4H_9CO_2 \cdot 39.8H_2O$

Tatyana Rodionova,* Vladislav Komarov,
Janusz Lipkowski and Natalia Kuratieva

The detailed crystal structure of the ionic clathrate hydrate of tetrabutylammonium valerate $(C_4H_9)_4NC_4H_9CO_2 \cdot 39.8H_2O$ has been determined by single crystal X-ray analysis. Special features of the crystal structures of ionic clathrate hydrates of tetraalkylammonium carboxylates are discussed.

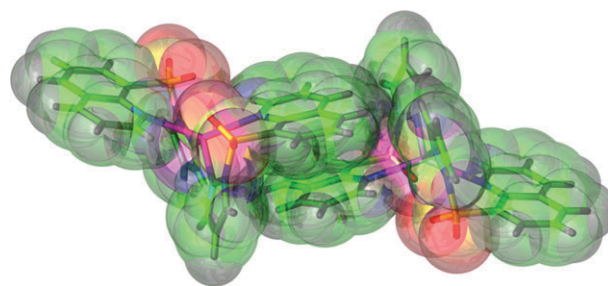


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8-Quinoline based ligands and their metallic derivatives: A structural and statistical investigation of quinoline π - π stacking interactions

Radu F. Semeniuc,* Thomas J. Reamer and
Mark D. Smith

The ligand 8-sulfonyl-(1-pyrazolyl)-quinoline coordinates to silver (I) centers to form supramolecular structures based on concerted π - π stacking/ $C-H \cdots \pi$ interactions. A statistical analysis of these interactions showed that they are common for metal complexes of quinoline based ligands.

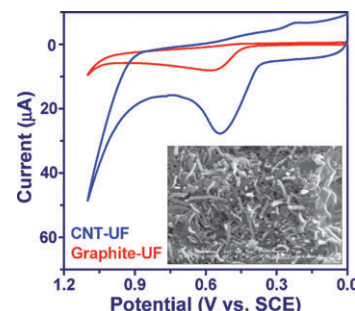


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A multi-walled carbon nanotube/poly(urea-formaldehyde) composite prepared by *in situ* polycondensation for enhanced electrochemical sensing

Bangguo Wei, Luyan Zhang and Gang Chen*

A novel multi-walled carbon nanotube/poly(urea-formaldehyde) composite was prepared for enhanced electrochemical sensing based on *in situ* polycondensation.

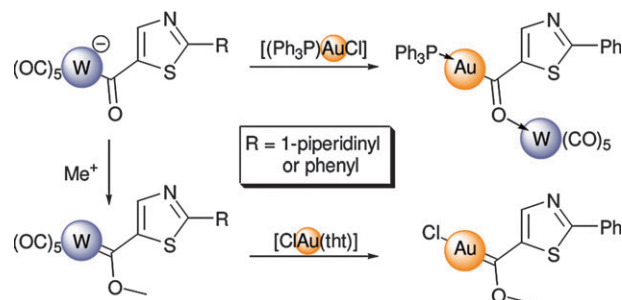


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Fischer-type tungsten acyl (carbeniate), carbene and carbyne complexes bearing C5-attached thiazolyl substituents: interaction with gold(I) fragments

Christoph E. Strasser, Stephanie Cronje and
Helgard G. Raubenheimer*

Carbeniate (acyl), carbene and carbyne complexes of tungsten prepared from 5-deprotonated thiazoles and tungsten hexacarbonyl react with gold(I) complexes by ligand transfer and/or adduct formation.



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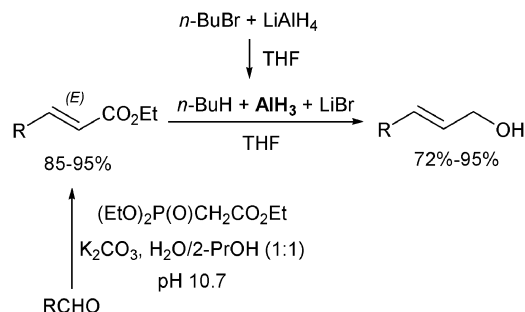
PAPERS

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An improved two-step synthetic route to primary allylic alcohols from aldehydes

Zheng Liu, Yaqiong Gong, Hoe-Sup Byun and Robert Bittman*

A convenient protocol to prepare AlH_3 in THF from LiAlH_4 and $n\text{-BuBr}$ has been developed. AlH_3 was used for the 1,2-reduction of (*E*)- α,β -unsaturated esters *in situ*, affording allylic alcohols in high yields (72–95%). To prepare the (*E*)- α,β -unsaturated esters, a modified Horner–Wadsworth–Emmons reaction in the presence of K_2CO_3 in H_2O –2-PrOH (1 : 1) was employed.

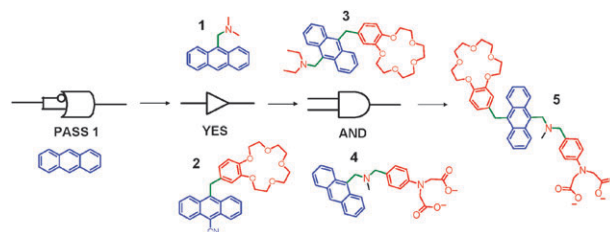


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From PASS 1 to YES to AND logic: building parallel processing into molecular logic gates by sequential addition of receptors

David C. Magri* and A. Prasanna de Silva

The molecular logic gate **4** detects the proton and zinc concentrations in an aqueous solution based on AND and INH logic; collectively **1**–**5** provide insight into the rational design of future logic gates with built-in orthogonality and cooperativity.

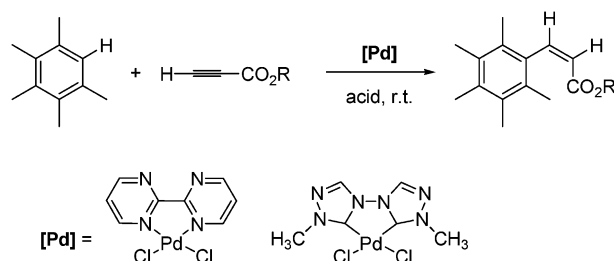


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Alkyne hydroarylation with palladium(II) complexes bearing chelating N-heterocyclic ligands: effect of non-coordinated nitrogens on catalyst efficiency

Luca Gazzola, Cristina Tubaro,* Andrea Biffis and Marino Basato

Palladium(II) complexes with chelating ligands bearing nitrogen atoms not involved in the coordination to the metal display a good catalytic activity in the hydroarylation of alkynes, giving selectively products of formal *trans*-hydroarylation of the triple bond.

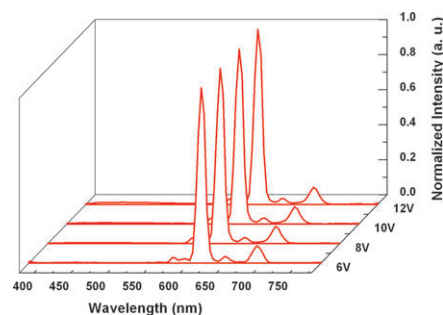


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Synthesis and electroluminescent property of novel europium complexes with oxadiazole substituted 1,10-phenanthroline and 2,2'-bipyridine ligands

Zhuqi Chen, Fei Ding, Feng Hao, Ming Guan, Zuqiang Bian,* Bei Ding and Chunhui Huang

Several europium complexes, with oxadiazole moieties incorporated into the neutral ligand, show improved thermal stabilities for vapor deposition, highly efficient photoluminescence, and remarkable electroluminescence performance.





Drawing disciplines together

Introducing Professor Peter Junk

Associate Editor

Peter Junk graduated from the University of Western Australia in 1984 obtaining a Bachelor of Science with first class honours in physical and inorganic chemistry, and completed his PhD in organometallic chemistry under the supervision of Professor Colin Raston in 1988. He currently holds a position of Professor of Chemistry and is the Head of the School of Chemistry at Monash University, Australia.

His main research interests are in rare earth and main group organometallic, organoamido and aryloxo chemistry, but has applied interests in X-ray imaging and corrosion inhibition. To date, he has published more than of 250 publications and reviews.

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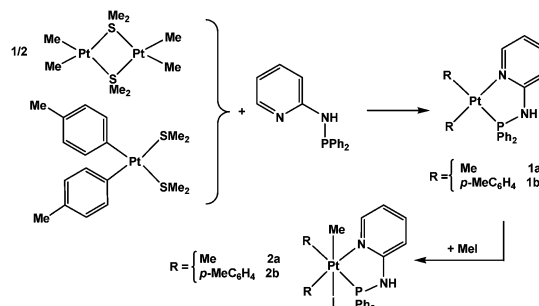
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Diorganoplatinum(II) complexes with chelating PN ligand 2-(diphenylphosphinoamino)pyridine; synthesis and kinetics of the reaction with MeI

S. Masoud Nabavizadeh,* Elham S. Tabei, Fatemeh Niroomand Hosseini, Niloofar Keshavarz, Sirous Jamali and Mehdi Rashidi*

New organoplatinum(II) complexes were synthesized and characterized by multinuclear NMR spectroscopy. The kinetics and mechanism of oxidative addition of MeI to these complexes was studied by UV-Vis spectrophotometry.

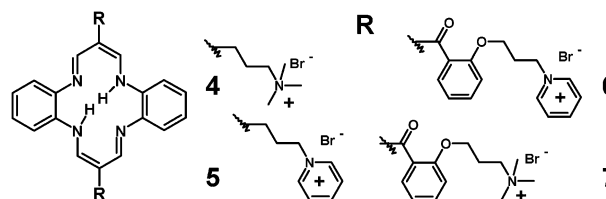


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Cationic side-chains control DNA/RNA binding properties and antiproliferative activity of dicationic dibenzotetraaza[14]annulene derivatives

Marijana Radić Stojković, Marko Marjanović, Dariusz Pawlica, Lukasz Dudek, Julita Eilmes, Marijeta Kralj and Ivo Piantanida*

Studied DBTAA derivatives efficiently differentiated between DNA and RNA as well as between A–T(U) and G–C basepair composition and demonstrated pronounced antiproliferative activity.

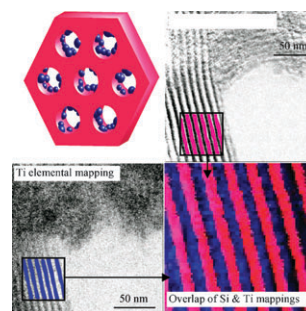


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Insight into the structure and localization of the titania overlayer in TiO₂-coated SBA-15 materials

Fuxiang Zhang, Xavier Carrier, Jean-Marc Krafft, Yuji Yoshimura and Juliette Blanchard*

EELS (Energy-Filtered TEM) images of a TiO₂/SBA-15 showing the localisation of the grafted TiO₂ particles.

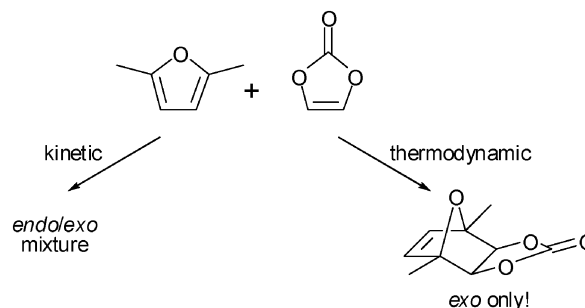


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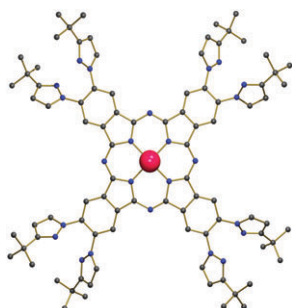
Diels–Alder reaction of vinylene carbonate and 2,5-dimethylfuran: kinetic vs. thermodynamic control

Céline Taffin, Glenda Kreutler, Damien Bourgeois,* Eric Clot and Christian Périgaud

Thermal Diels–Alder reaction: prolonged heating, and, instead of a black tar, obtain the *exo* adduct cleanly! The reaction between 2,5-dimethyl furan and vinylene carbonate was studied from experimental and computational points of view, to demonstrate the shift from kinetic to thermodynamic control.



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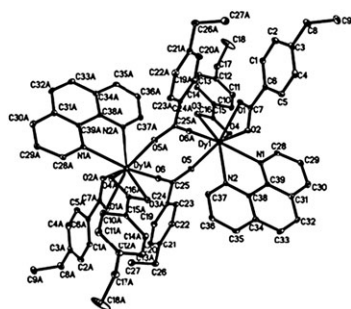


Novel pyrazole functionalized phthalocyanines and their first row transition metal complexes

Daniel Dehe, Christian Lothschütz and Werner R. Thiel*

Well soluble octapyrazolyl functionalized phthalodinitriles and their transition metal complexes were obtained by electrophilic aromatic substitution of dichlorophthalonitrile with pyrazoles bearing alkyl side chains.

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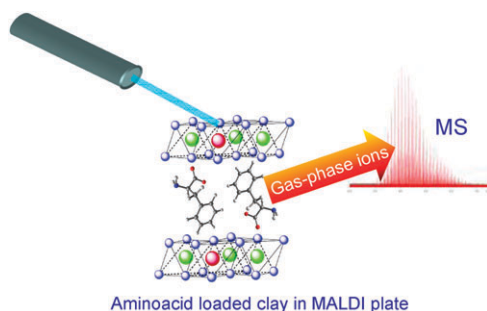


Crystal structures, luminescent and thermal properties of a new series of lanthanide complexes with 4-ethylbenzoic acid

Hong-Mei Ye, Ning Ren, Jian-Jun Zhang,* Shu-Jing Sun and Juan-Fen Wang

A series of lanthanide complexes with the 4-ethylbenzoic acid ligand (4-eba), $[Ln(4-eba)_3(phen)]_2$ ($Ln = Nd, Sm, Eu, Tb, Dy$ and Ho ; phen = 1,10-phenanthroline), have been synthesized and structurally characterized by single-crystal X-ray diffraction.

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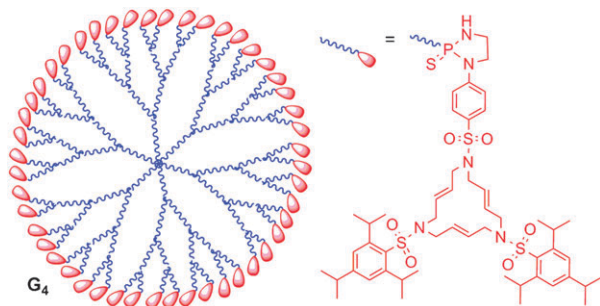


A new role for layered double hydroxides hybrid materials—uptake and delivery of small molecules into the gas phase

Pedro D. Vaz* and Carla D. Nunes

Gas-phase ions can be produced directly from composite clay materials holding guest species inside its intragallery spacing in MALDI experiments. This approach leads to the analysis of low molecular weight analytes with interference-free signals from the matrix.

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An efficient synthesis combining phosphorus dendrimers and 15-membered triolefinic azamacrocycles: towards the stabilization of platinum nanoparticles

Grégory Franc, Elena Badetti, Carine Duhayon, Yannick Coppel, Cédric-Olivier Turrin, Jean-Pierre Majoral,* Rosa-María Sebastián* and Anne-Marie Caminade*

Triazatriolefinic macrocycles grafted as terminal groups of phosphorus dendrimers allow the obtaining of Pt nanoparticle networks.

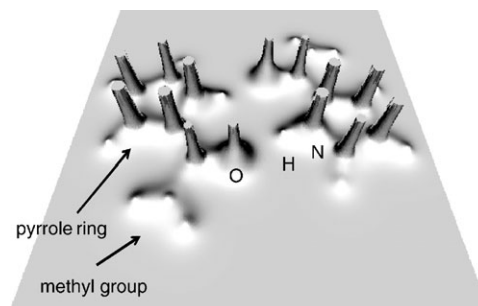
PAPERS

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Spectroscopic and theoretical studies on some new pyrrol-2-yl-chloromethyl ketones

Alina T. Dubis,* Małgorzata Domagała and Sławomir J. Grabowski*

A novel series of pyrrole-2-yl chloromethyl ketones were synthesized and studied by FT-IR, ^1H , ^{13}C NMR spectroscopy and DFT calculations at B3LYP/6-311++G(d,p) level of approximation.

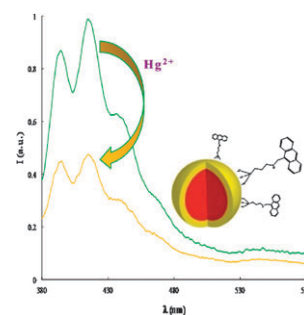


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Preparation of Hg^{2+} selective fluorescent chemosensors based on surface modified core-shell aluminosilicate nanoparticles

Estefanía Delgado-Pinar, Noemí Montoya, Maite Galiana, M. Teresa Albelda, Juan C. Frias, Hermás R. Jiménez, Enrique García-España* and Javier Alarcón*

A synthetic procedure for the preparation of functional structured hybrid materials containing boehmite-silica core-shell nanoparticles and anthracene-containing amines is reported.



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