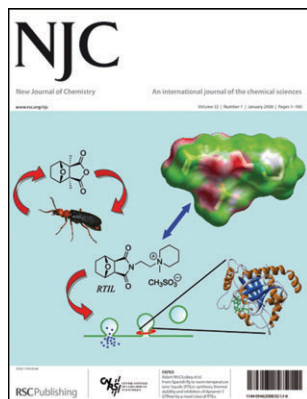


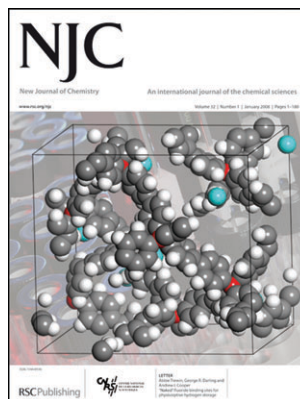
## IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 32(1) 1-180 (2008)



### Cover

See Adam McCluskey *et al.*, p. 28. The scaffold from blister beetle, cantharidin, is modified to a bulky cation with associated anion—an ionic liquid. Surprisingly, it blocks the GTPase activity of the endocytosis protein dynamin. Reproduced with permission from Adam McCluskey from *New J. Chem.*, 2008, **32**, 28.



### Inside Cover

See Andrew I. Cooper *et al.*, p. 17. Proposed model structure for a hypothetical porous polymer where “naked fluoride” moieties are site isolated and available for H<sub>2</sub> physisorption. Reproduced with permission from Andrew Cooper from *New J. Chem.*, 2008, **32**, 17.

## CHEMICAL SCIENCE

### C1

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.

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January 2008/Volume 5/Issue 1

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### 15

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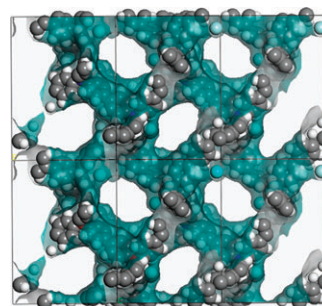
## LETTERS

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**“Naked” fluoride binding sites for physisorptive hydrogen storage**

Abbie Trewin, George R. Darling\* and Andrew I. Cooper\*

Models suggest that charge separated ammonium fluorides may have enhanced binding affinities with molecular hydrogen and that such “naked” fluoride moieties might be incorporated in microporous polymers.

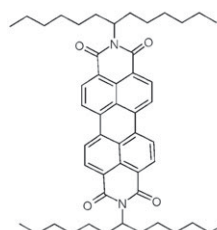


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**Brightly shining nanoparticles: lipophilic perylene bisimides in aqueous phase**

Heinz Langhals\*

The dispersion of lipophilic perylene bisimides into nanosized particles opens the aqueous phase to these highly fluorescent, water insoluble materials.



## PAPERS

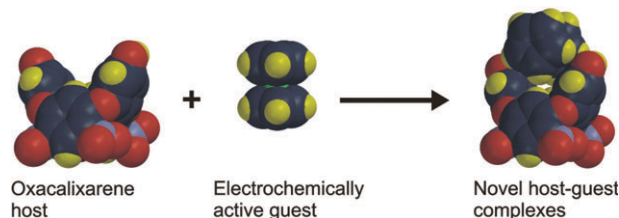


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**Inclusion of electrochemically active guests by novel oxacalixarene hosts**

David Sobransingh, Mahender B. Dewal, Jacob Hiller, Mark D. Smith and Linda S. Shimizu\*

The first exploration of the host–guest properties of an oxacalixarene host with the electrochemically active guests ferrocene, cobaltocenium and their oxidized and reduced forms is reported. This host shows a significant thermodynamic (85 fold) preference for positively charged guests over the neutral species.

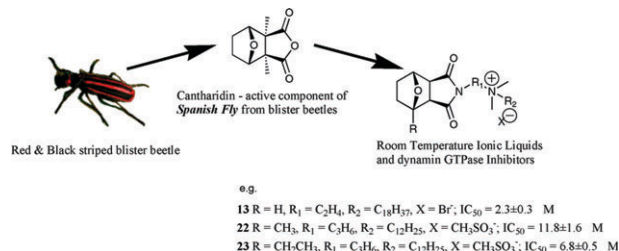


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**From Spanish fly to room-temperature ionic liquids (RTILs): synthesis, thermal stability and inhibition of dynamin 1 GTPase by a novel class of RTILs**

Jie Zhang, Geoffrey A. Lawrance, Ngoc Chau, Phillip J. Robinson and Adam McCluskey\*

In a series of simple synthetic manipulations the active component of the aphrodisiac Spanish fly has resulted in the generation of a new family of room temperature ionic liquids that are also dynamin inhibitors.





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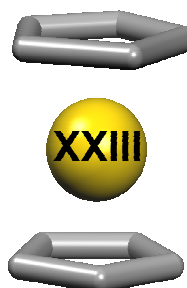
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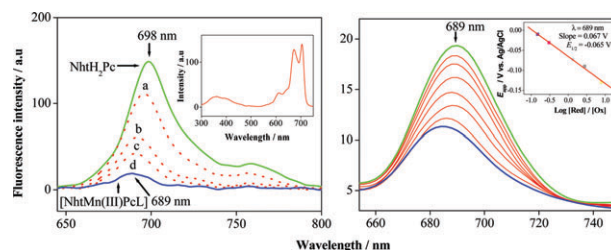


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### ***In situ* monitoring of metallation of metal-free phthalocyanine via UV-Vis and steady-state fluorescence techniques. Thin-layer UV-Vis and fluorescence spectroelectrochemistry of a new non-aggregating and electrochromic manganese(3+) phthalocyanine**

Ismail Yilmaz\*

[NhtMn(3+)PcL] was synthesized and characterized with spectroelectrochemistry, and monitored by *in situ* UV-Vis and fluorescence techniques.

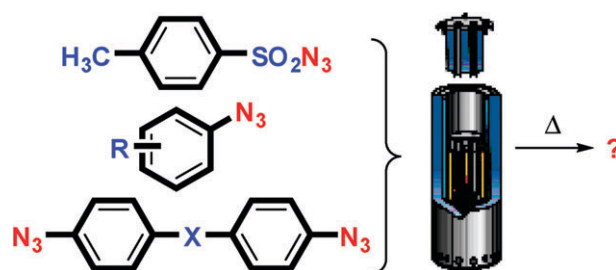


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### **Hazardous N-containing system: thermochemical and computational evaluation of the intrinsic molecular reactivity of some aryl azides and diazides**

Paolo Cardillo, Lucia Gigante, Angelo Lunghi, Alessandro Fraleoni-Morgera and Paolo Zanirato\*

The exothermic decompositions of some aryl azides were studied experimentally using DSC, weight loss TGA-FTIR and C80-FTIR techniques, and theoretically using the CHETAH and T1 software.

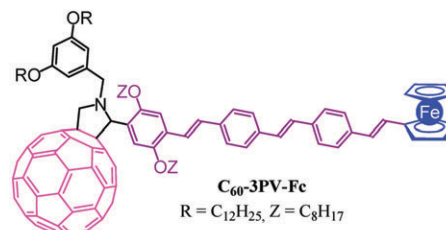


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### **Synthesis and electronic properties of fullerene derivatives substituted with oligophenylenevinylene-ferrocene conjugates**

Teresa M. Figueira-Duarte, Yannick Rio, Andrea Listorti, Béatrice Delavaux-Nicot, Michel Holler, Filippo Marchioni, Paola Ceroni,\* Nicola Armaroli\* and Jean-François Nierengarten\*

The synthesis and electronic properties of C<sub>60</sub>-bridge-Fc arrays are described.

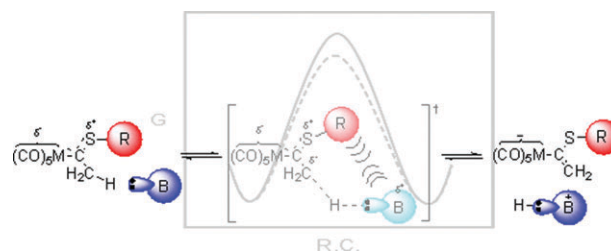


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### **Effects of the alkyl substituent in the $\pi$ -donor heteroatom on the kinetic and thermodynamic acidities of Fischer thiocarbene complexes**

Martin Eduardo Zoloff Michoff, Diego Marcelo Andrada, Alejandro Manuel Granados\* and Rita Hoyos de Rossi\*

The proton transfer reaction from a series of *S*-alkyl Fischer thiocarbene complexes to OH<sup>-</sup> and a series of primary and secondary amines was studied, finding that the thermodynamic acidity is mainly governed by the hydrophobicity of the substituent; whereas the kinetic acidity is more sensible to its steric effect.



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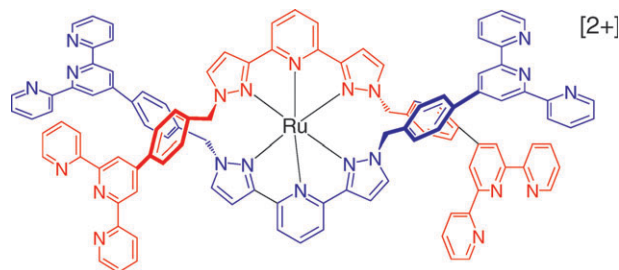
## PAPERS

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**Post-coordination functionalisation of pyrazolyl-based ligands as a route to polynuclear complexes based on an inert  $\text{Ru}^{\text{II}}\text{N}_6$  core**

Qiao-Hua Wei, Stephen P. Argent, Harry Adams and Michael D. Ward\*

Alkylation of the four pyrazolyl NH groups of the  $\text{Ru}(\text{II})$  complex of 2,6-bis(pyrazol-3-yl)pyridine allows vacant bipyridyl or terpyridyl binding sites to be added to the central kinetically inert core; this process allows stepwise assembly of polynuclear assemblies.

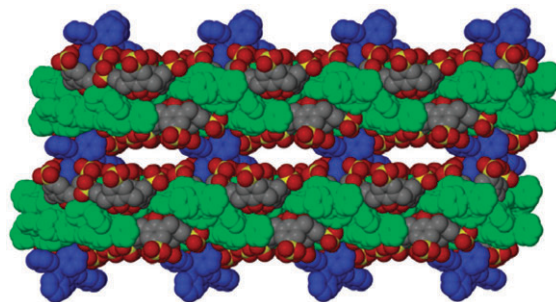


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**Nanoporous materials based on heteroleptic bilayers built up from bisphosphonium, *p*-sulfonatocalix[4]arene ions**

Mohamed Makha,\* Yatimah Alias, Colin L. Raston\* and Alexandre N. Sobolev

A systematic study of molecular interactions of bisphosphonium cations with *p*-sulfonatocalix[4]arene in the presence of lanthanide metal cations reveals diverse supramolecular architectures with in some cases nanoporosity within the bilayer arrangement.

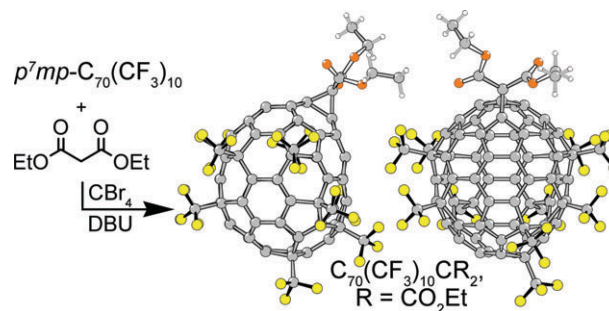


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**Regioselective synthesis and crystal structure of  $\text{C}_{70}(\text{CF}_3)_{10}[\text{C}(\text{CO}_2\text{Et})_2]$** 

Nataliya S. Ovchinnikova, Daria V. Ignat'eva, Nadezhda B. Tamm, Stanislav M. Avdoshenko, Alexey A. Goryunkov,\* Ilya N. Ioffe, Vitaliy Yu. Markov, Sergey I. Troyanov, Lev N. Sidorov, Marina A. Yurovskaya and Erhard Kemnitz

Fullerene  $p^7mp\text{-C}_{70}(\text{CF}_3)_{10}$  is prone to enter a standard Bingel reaction with diethyl bromomalonate to afford a single isomer of  $\text{C}_{70}(\text{CF}_3)_{10}[\text{C}(\text{CO}_2\text{Et})_2]$ .

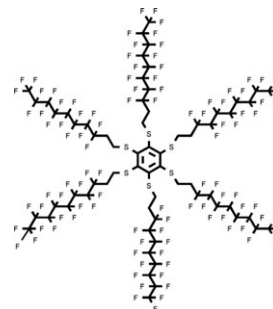


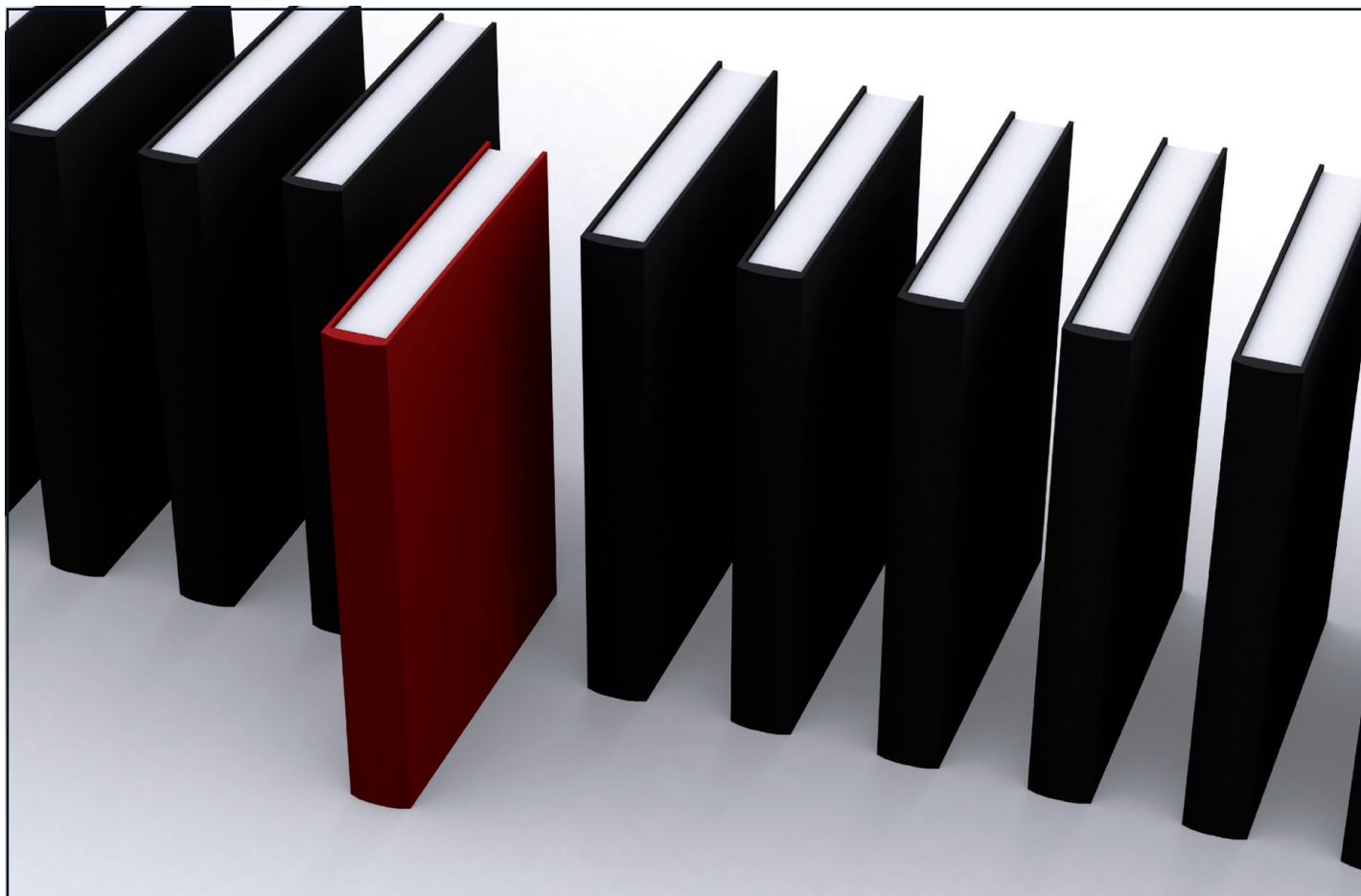
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**Star-shaped heavily fluorinated aromatic sulfurs: stabilization of palladium nanoparticles active as catalysts in cross-coupling reactions**

Sandra Niembro, Adelina Vallribera\* and Marcial Moreno-Mañas

Star-shaped heavily fluorinated compounds have been prepared and used as stabilizers of palladium nanoparticles. These materials are useful and reusable catalysts in Mizoroki–Heck, Suzuki and Sonogashira cross-couplings.





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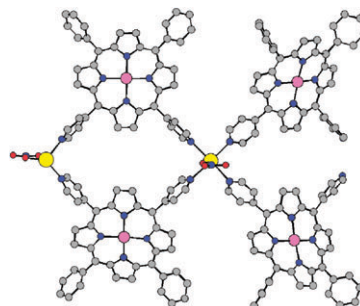
## PAPERS

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**Molecular tectonics: ribbon type coordination networks based on porphyrins bearing two pyridine or two pyridine *N*-oxide units**

Emmanuel Deiters, Véronique Bulach\* and Mir Wais Hosseini\*

The combination of two metallaporphyrin based tectons bearing two pyridyl or pyridyl *N*-oxide groups with  $\text{Cd}^{2+}$  or  $\text{Cu}^{2+}$  cations leads in the crystalline phase to the formation of either homo- or hetero-metallic ribbon-type 1-D coordination networks.

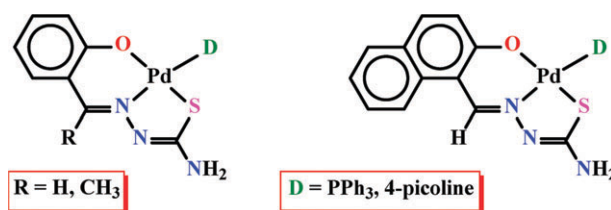


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**Synthesis, structure, spectroscopic properties and cytotoxic effect of some thiosemicarbazone complexes of palladium**

Sarmistha Halder, Shie-Ming Peng, Gene-Hsiang Lee, Tanmay Chatterjee, Asama Mukherjee, Sushanta Dutta, Utpal Sanyal and Samareesh Bhattacharya\*

A group of palladium thiosemicarbazone complexes have shown remarkable cytotoxicity towards HL-60 and U-937 cell lines.

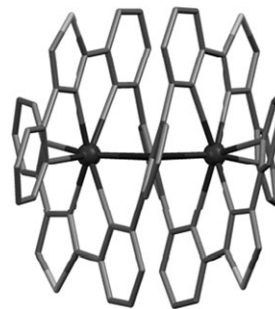


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**Synthesis and X-ray structures of cadmium-containing dinuclear double helicates derived from ligands containing *N*-oxide units**

Georgios Bokolinis, T. Riis-Johannessen, John C. Jeffery and Craig R. Rice\*

Two novel ligands that contain both *N*-oxide units and a polydentate pyridyl-thiazolyl ligand chain have been synthesized and reaction of either of these ligands with  $\text{Cd}^{2+}$  results in the formation of a dinuclear double helicate.

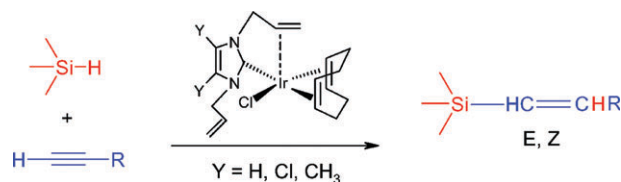


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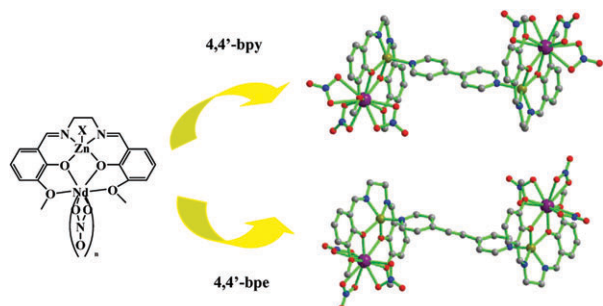
**Alkenyl-functionalized NHC iridium-based catalysts for hydrosilylation**

Alessandro Zanardi, Eduardo Peris and Jose A. Mata\*

The coordination of a series of bis-alkenyl-NHC ligands to Ir(I) is reported. The catalytic activity of the resulting complexes towards the hydrosilylation of alkynes is described.



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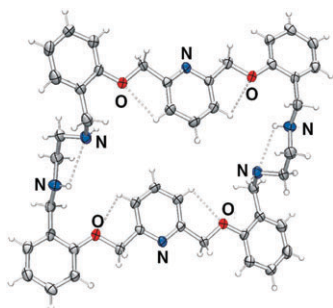


### Tetranuclear NIR luminescent Schiff-base Zn–Nd complexes

Xingqiang Lü,\* Weiyu Bi, Wenli Chai, Jirong Song, Jianxin Meng, Wai-Yeung Wong, Wai-Kwok Wong\* and Richard A. Jones

Tetranuclear luminescent  $[\text{Zn}_2\text{Nd}_2\text{L}_2(4,4'\text{-bpy})(\text{NO}_3)_6] \cdot \text{Et}_2\text{O}$  (**2**) and  $[\text{Zn}_2\text{Nd}_2\text{L}_2(4,4'\text{-bpe})] \cdot 2\text{H}_2\text{O}$  (**3**) (4,4'-bpy = 4,4'-bipyridine, 4,4'-bpe = *trans*-bis(4-pyridyl)ethylene) complexes are formed from 4,4'-bipyridyl bidentate linkers to a dinuclear Zn–Nd architecture unit.

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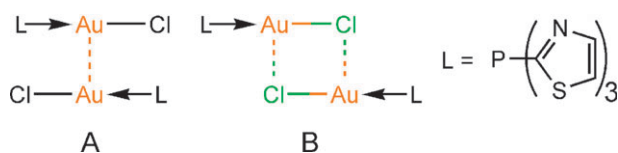


### A new 34-membered $\text{N}_6\text{O}_4$ -donor macrocycle: synthetic, X-ray and solvent extraction studies

Marco Wenzel, Kerstin Gloe, Karsten Gloe,\* Gert Bernhard, Jack K. Clegg, Xue-Kui Ji and Leonard F. Lindoy\*

Use of a new  $\text{N}_6\text{O}_4$ -donor macrocycle for cation ( $\text{Ag}^+$ ,  $\text{Zn}^{2+}$ ) and anion ( $\text{I}^-$ ,  $\text{CrO}_4^{2-}$ ) extraction as well as for metal salt extraction in association with a tripodal thiourea co-extractant is reported.

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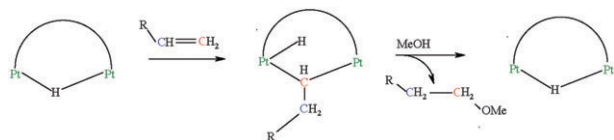


### Preparation of tris(azolyl)phosphine gold(i) complexes: digold(i) coordination and variation in solid state intermolecular interactions

C. E. Strasser, W. F. Gabrielli, C. Esterhuysen, O. B. Schuster, S. D. Nogai, S. Cronje and H. G. Raubenheimer\*

Amongst the rich structural chemistry of tris(azol-2-yl)-phosphine complexes of chlorogold(i) the first example of a compound that exhibits both  $\text{Au} \cdots \text{Au}$  (A) and  $\text{Au} \cdots \text{Cl}$  (B) interactions of very similar energy (DFT calculations), albeit in two crystal modifications, was discovered.

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### Studies towards the catalytic anti-Markovnikov functionalisation of alkenes

Christian J. Richard and Adrian W. Parkins\*

Evidence is presented that the catalytic anti-Markovnikov functionalisation of terminal alkenes proceeds *via* a di- or trinuclear cluster complex of platinum. The presence of peroxides in the alkene led to complications which are explained by a Hock rearrangement.

## PAPERS

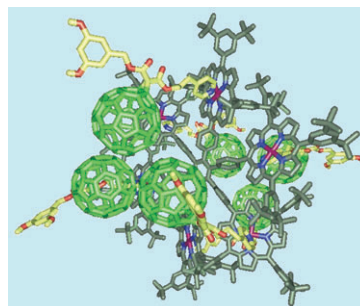


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### Large photoactive supramolecular ensembles prepared from C<sub>60</sub>–pyridine substrates and multi-Zn(II)–porphyrin receptors

Ali Trabolsi, Maxence Urbani, Juan Luis Delgado, Fettah Ajamaa, Mourad Elhabiri, Nathalie Solladié,\* Jean-François Nierengarten\* and Anne-Marie Albrecht-Gary\*

Getting bigger, getting better; increased stability has been evidenced by increasing the number of components.

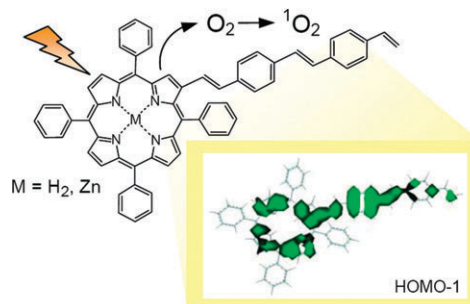


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### Extending the porphyrin core: synthesis and photophysical characterization of porphyrins with $\pi$ -conjugated $\beta$ -substituents

Barbara Ventura,\* Lucia Flamigni, Giancarlo Marconi, Fabio Lodato and David L. Officer\*

Vinyl or *p*-phenylene vinylene  $\beta$  substituted free-base and Zn-porphyrins have been studied: both spectroscopic and photophysical data show peculiar and interesting properties.





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