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### IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 31(4) 461-600 (2007)



### Cover

See Musiri M. Balakrishnarajan, Pattath D. Pancharatna and Roald Hoffmann, New J. Chem., 2007, 31, 473. View of Nice from Mount Boron. Image reproduced by permission of Patrick Murris, http://www.alpix.com/nice/

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### C25

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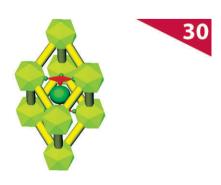
### **PAPER**

### 473

### Structure and bonding in boron carbide: The invincibility of imperfections

Musiri M. Balakrishnarajan, Pattath D. Pancharatna and Roald Hoffmann\*

30th Anniversary article: Electronic structure studies on boron carbide show that the origin of electron deficiency arising from the variation in carbon concentration is an attempt to reduce the antibonding interaction (indicated in red) between C-B-C chains and the B<sub>12</sub> unit.



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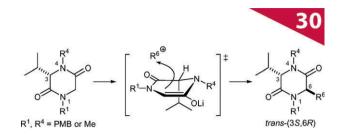
### **PAPER**

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### On the origins of diastereoselectivity in the alkylation of diketopiperazine enolates

Steven D. Bull, Stephen G. Davies,\* A. Christopher Garner, Alastair L. Parkes, Paul M. Roberts, Thomas G. R. Sellers, Andrew D. Smith, Juan A. Tamayo, James E. Thomson and Richard J. Vickers

**30th Anniversary article:** Minimisation of 1,2-torsional strain results in high diastereoselectivity in the alkylations of diketopiperazine enolates.



### **PERSPECTIVE**

496

### The chemistry of Bodipy: A new El Dorado for fluorescence tools

Raymond Ziessel,\* Gilles Ulrich and Anthony Harriman New advances in the field of highly fluorescent Bodipy dyes are reviewed with special emphasis on Cascatelle Dyes for which highly efficient intramolecular energy-transfer accounts for high

Supplementary functions 
$$X = C$$
,  $N$ 
 $R_8$ 
 $R_{6,7}$ 
 $R_8$ 
 $R_{1,2}$ 
 $R_{1,3}$  &  $R_{5,7}$ 

extension of delocalisation and/or functional groups

Stokes' shift enhancement and/or functional groups

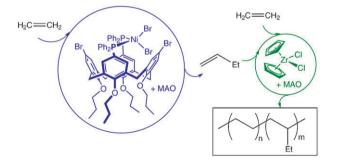
### **LETTER**

Stokes' shifts.

502

### Calix[4]arene-derived nickel diphosphine complexes for LLDPE synthesis via orthogonal tandem and one-pot catalysis

David Sémeril,\* Manuel Lejeune and Dominique Matt\* LLDPE containing only ethyl branches was obtained from ethylene by orthogonal tandem and one-pot catalysis (up to 2.7%) by combining a calixarene-diphosphine nickel complex and [Cp2ZrCl2].



### **PAPER**

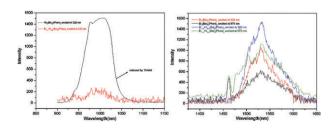


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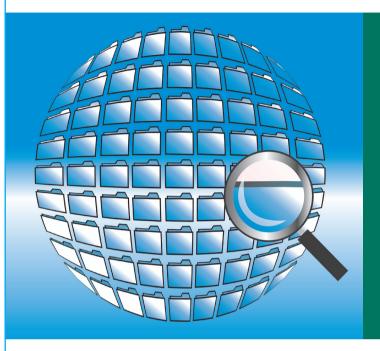
### Crystal structure and near-infrared luminescence properties of novel binuclear erbium and erbium-ytterbium cocrystalline complexes

Limei Song, Qi Wang, Daihua Tang, Xinhou Liu and Zhen Zhen\*

The NIR photoluminescent properties of three binuclear complexes of erbium and ytterbium, Er<sub>2</sub>(Ba)<sub>6</sub>(Phen)<sub>2</sub>, Yb<sub>2</sub>(Ba)<sub>6</sub>  $(Phen)_2$  and  $Er_{1.4}Yb_{0.6}(Ba)_6(Phen)_2$  (Ba = benzoate, Phen =1,10-phenanthroline), were investigated, and their luminescent mechanisms were proposed for the sensitization process.



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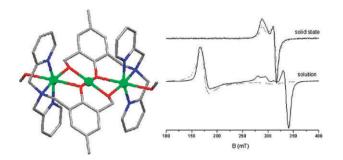
### **PAPERS**

### 512

### Changes in magnetic properties from solid state to solution in a trinuclear linear copper(II) complex

Iryna A. Koval, Hilda Akhideno, Stefania Tanase, Catherine Belle.\* Carole Duboc. Eric Saint-Aman. Patrick Gamez, Duncan M. Tooke, Anthony L. Spek, Jean-Louis Pierre and Jan Reedijk\*

The nature of exchange coupling between the metal centers in the linear trinuclear copper(II) complex changes from antiferromagnetic in the solid state to ferromagnetic in solution.

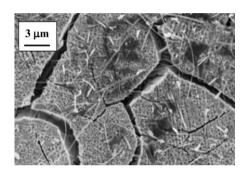


### 519

### Nanowires of molecule-based charge-transfer salts

Jean-Philippe Savy, Dominique de Caro,\* Christophe Faulmann, Lydie Valade, Manuel Almeida, Tadahiro Koike, Hideki Fujiwara, Toyonari Sugimoto, Jordi Fraxedas, Thierry Ondarçuhu and Claude Pasquier

Nanowires and nanofibres of molecule-based conductors are prepared using an adsorption in organic solution method or an electrodeposition technique on various substrates, such as stainless steel conversion coatings or silicon wafers.

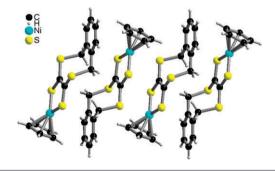


### 528

### The contrasted structural and magnetic behaviour of two single-component paramagnetic dithiolene complexes

Mitsushiro Nomura and Marc Fourmigué\*

Two neutral, formally  $Ni^{III}$  (S = 1/2) [CpNi(dithiolene)] complexes with eight-membered fused rings crystallize into uniform spin chains or inversion-centred dyads.

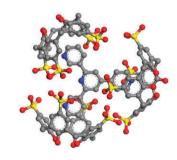


### 535

### Solution and solid state interplay of isomeric 4'-(pyridyl)-3,2':6',3''-terpyridines with p-sulfonatocalix[4]arene

Christopher B. Smith, Mohamed Makha,\* Colin L. Raston\* and Alexandre N. Sobolev

Solution and solid state interplay of isomeric 4'-(pyridyl)-3,2':6',3''-terpyridines with *p*-sulfonatocalix[4]arene.



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0303



### **PAPERS**



543

### A novel photochromic liquid crystal system based on biindenvlidenedione derivatives

J. Han,\* Y.-X. Li, M.-L. Pang, K.-G. Cheng, Y.-M. Wang, Y.-X. Ma and J.-B. Meng\*

A novel series of photochromic liquid crystals derived from the biindenylidene system were designed and prepared, which simultaneously undergo photochromism in the crystalline state as well as the generation of radicals, and some of them displayed monotropic smectic mesophase. These novel compounds might be used as potential multi-functional organic materials.

$$\begin{array}{c} C_nH_{2n+1} \\ \\ O \\ OH \\ O \\ \end{array}$$



549

### Chemoselectivity in $\sigma$ bond activation by lanthanocene complexes from a DFT perspective: reactions of Cp2LnR $(R = CH_3, H, SiH_3)$ with $SiH_4$ and $CH_3-SiH_3$

Lionel Perrin, Odile Eisenstein\* and Laurent Maron\*

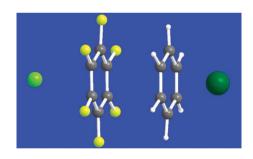
The selectivity of the  $\sigma$  bond metathesis between silicon containing molecules and lanthanocene derivatives have been studied with DFT calculations.

556

### MP2 study of cooperative effects between cation- $\pi$ , anion- $\pi$ and $\pi$ - $\pi$ interactions

Antonio Frontera,\* David Quiñonero, Antoni Costa, Pablo Ballester and Pere M. Deyà\*

Important cooperativity effects exist between cation $-\pi$ , anion $-\pi$ and  $\pi$ – $\pi$  interactions.

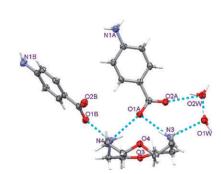




### Supramolecular associates of para-aminobenzoic acid with N- and N,O-heterocyclic molecules

Brian Moulton, Brian S. Luisi, Marina S. Fonari,\* Stepan S. Basok, Eduard V. Ganin and Victor Ch. Kravtsov

PABA molecule illustrates its ability to achieve a suitable balance between the driving force to coordinate to aminia binding sites of cyclic molecules and its tendency to self-assemble via supramolecular heterosynthons in the crystalline multicomponent complexes.



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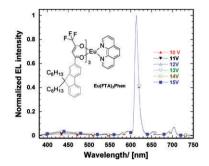


### 569

### Bright red light-emitting devices based on a novel europium complex doped into polyvinylcarbazole

Yong Zhang, Chun Li, Huahong Shi, Bin Du, Wei Yang and Yong Cao\*

The complex (1,10-phenanthroline)tris[4,4,4-trifluoro-1-(9,9-dihexylfluoren-2-yl)-1,3-butanedione] europium(III) was synthesized. Devices based on the complex doped into a PVK:PBD host as emitter showed a maximum EOE of 4.28% and luminance efficiency of 4.60 cd A

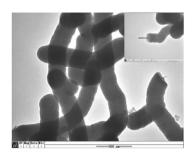


### 575

### A novel hybrid nanostructure based on SiO<sub>2</sub>@carbon nanotube coaxial nanocable

Shaojun Guo, Lijian Huang and Erkang Wang\*

We present a simple, generally applicable procedure for obtaining diameter-controlled SiO<sub>2</sub>@ carbon nanotubes (CNTs) coaxial nanocables. These coaxial nanocables with high solubility in polar solvent, have been used as functional templates for assembling CNTs/Au nanorods heterogeneous nanostructures to form multifunctional assembly system. These hybrid nanostructures may find applications in nanoelectronics, photonics, and nanodevices.

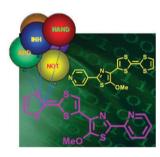


### 580

### New TTF derivatives: several molecular logic gates based on their switchable fluorescent emissions

Chen-Jie Fang, Zhi Zhu, Wei Sun, Chun-Hu Xu and Chun-Hua Yan\*

New redox-fluorescence dependent TTF derivatives were used to construct logic gates by purposely selecting the initial state, by virtue of the peculiar redox property of TTF.

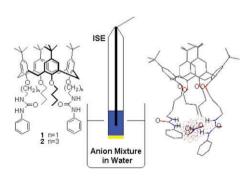


### 587

### Improved nitrate sensing using ion selective electrodes based on urea-calixarene ionophores

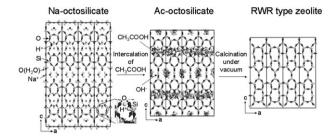
Benjamin Schazmann\* and Dermot Diamond\*

Improving the selectivity of nitrate over chloride in water-based anion sensing with the aid of urea-calix[4] arene ionophores.



### **PAPER**

593



## Convenient conversion of crystalline layered silicate octosilicate into RWR-type zeolite by acetic acid intercalation

Yasunori Oumi,\* Takeshi Takeoka, Takuji Ikeda, Toshiro Yokoyama and Tsuneji Sano

Acetic acid intercalated octosilicate (Ac-octosilicate) was successfully prepared and converted into the highly crystalline RWR-type zeolite by the dehydration—condensation of silanol groups of the interlayer.

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