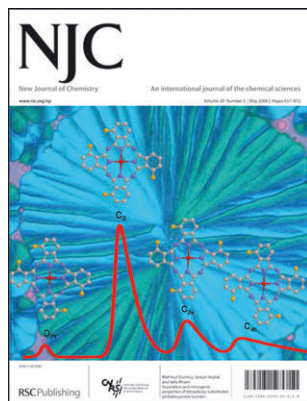


IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 30(5) 657-812 (2006)



Cover

See Vefa Ahsen *et al.*, page 675.

The cover exhibits the HPLC chromatogram and molecular structure of four isomers of non-peripheral substituted nickel(II) phthalocyanine. It is found out that non-peripheral substituted phthalocyanine isomers D_{2h} , C_{2v} and C_s are liquid at room temperature whereas, C_{4h} isomer exhibits liquid-crystalline properties at the same temperature. The background shows the polarized microscope picture of this isomer.

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CHEMICAL SCIENCE

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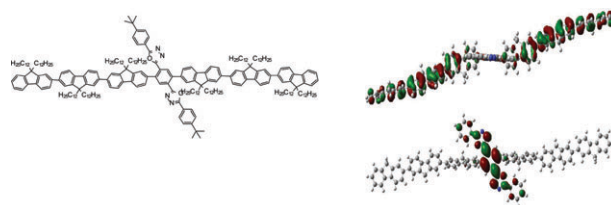
LETTERS

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Cruciform p-n diblock conjugated oligomers for electroluminescent applications

Hong-Yu Wang, Jia-Chun Feng, Gui-An Wen, Hong-Ji Jiang, Jun-Hua Wan, Rui Zhu, Chuan-Ming Wang, Wei Wei and Wei Huang*

The optoelectronic properties of the cruciform p-n diblock oligomers can be independently tuned by the oligofluorene and oxadiazole branches to increase the charge mobility.



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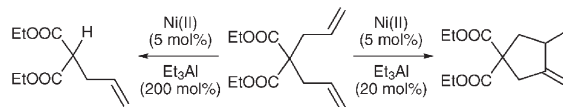
LETTERS

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Nickel-catalyzed cyclization of α,ω -dienes: formation vs. cleavage of C–C bonds

David Nečas,* Matyáš Turský, Iva Tišlerová and Martin Kotora*

The course of the reaction of 1,7-heptadienes catalyzed by a Ni(II)–organoaluminium system, *i.e.* C–C bond formation (cyclization) or C–C bond cleavage (deallylation), can be controlled by the amount of organoaluminium used.



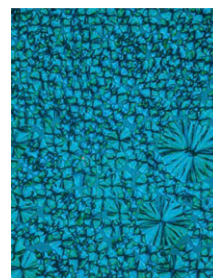
PAPERS

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Separation and mesogenic properties of tetraalkoxy-substituted phthalocyanine isomers

Mahmut Durmuş, Serkan Yeşilot and Vefa Ahsen*

The separation and properties of four possible structural isomers of non-peripherally substituted nickel(II) phthalocyanine were studied. The mesogenic properties of pure isomer C_{4h} were described.

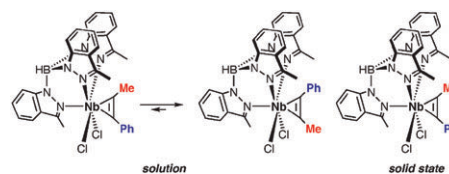


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Aromatic interactions in hydrotris(3-methylindazolyl) borate organoniobium complexes: control of an alkyne ligand orientation in the crystal

Pascal Oulié, Johannes Teichert, Laure Vendier, Céline Dablemont and Michel Etienne*

Aromatic interactions between an hydrotris(3-methylindazolyl) borate and an alkyne phenyl ring control the orientation of a phenylpropyne ligand in the solid state. This alkyne rotamer is the less abundant in solution.

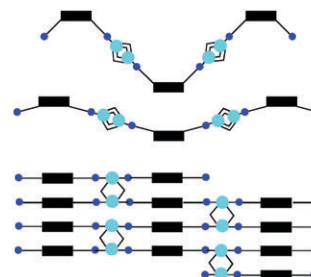


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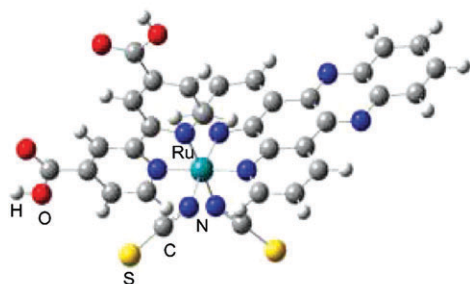
Molecular tectonics: generation of 1- and 2-D copper coordination networks by positional isomeric tectons based on a phenylenediamine backbone bearing two isonicotinoyl moieties

Jérôme Pansanel, Abdelaziz Jouaiti, Sylvie Ferlay, Mir Wais Hosseini,* Jean-Marc Planeix and Nathalie Kyritsakas

1-D and 2-D coordination networks generated upon interconnection of organic tectons with two different types of copper dimers.



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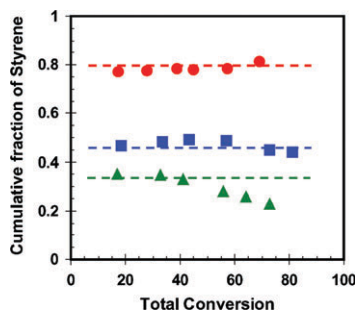


Molecular and electronic ground and excited structures of heteroleptic ruthenium polypyridyl dyes for nanocrystalline TiO₂ solar cells

Nobuko Onozawa-Komatsuzaki, Osamu Kitao,*
Masatoshi Yanagida, Yuichiro Himeda, Hideki Sugihara
and Kazuyuki Kasuga*

Novel ruthenium complexes having 1,10-phenanthroline or dipyrrodo[3,2-*a*:2',3'-*c*]phenazine (dppz) ligands were synthesized and used as sensitizers for dye-sensitized solar cells.

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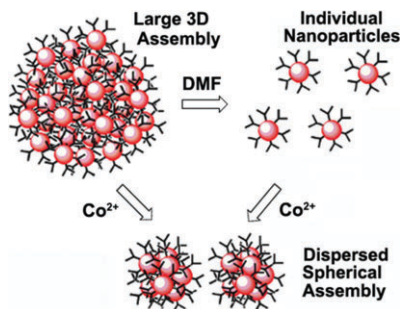


Gradient or statistical copolymers by batch nitroxide mediated polymerization: effect of styrene/methyl acrylate feed

Khaled Karky, Eve Péré, Claude Pouchan, Hélène Garay,
Abdel Khoukh, Jeanne François, Jacques Desbrières and
Laurent Billon*

First gradient copolymers by batch nitroxide mediated polymerization.

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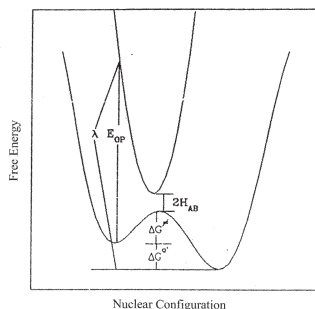


From large 3D assembly to highly dispersed spherical assembly: weak and strong coordination mediated self-aggregation of Au colloids

Xuanjun Zhang, Dan Li* and Xiao-Ping Zhou

Distinctly different 3D assemblies of Au nanoparticles are constructed. Large 3D aggregates formed *via* weak-coordination can be directly transferred into dispersed 3D spherical assemblies *via* strong coordination.

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Estimation of the reorganization and reaction free energies for electron transfer processes from optical and thermal data. An application to the reaction $[\text{Fe}^{\text{II}}(\text{CN})_5\text{pzCo}^{\text{III}}(\text{NH}_3)_5] \rightarrow [\text{Fe}^{\text{III}}(\text{CN})_5\text{pzCo}^{\text{II}}(\text{NH}_3)_5]$

F. Muriel, R. Jiménez, P. Pérez-Tejeda, P. López-Cornejo,
G. López-Pérez and F. Sánchez*

An increase in the electronic coupling between donor and acceptor centres does not necessarily produce an increase in the rate of the electron transfer reactions.

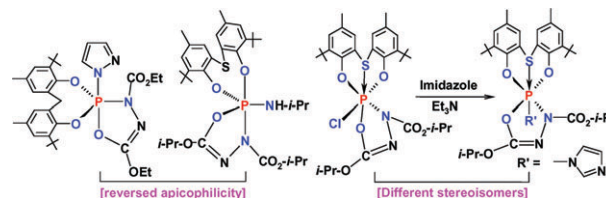
PAPERS

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Structurally diverse penta- and hexacoordinate phosphorus compounds from the reaction of diethyl or diisopropyl azodicarboxylates with phosphorus(III) compounds

K. V. P. Pavan Kumar, N. Satish Kumar and K. C. Kumara Swamy*

New pentacoordinate phosphorus compounds that exhibit the 'reverse apicophilicity' phenomenon and violate Bent's rule in trigonal bipyramidal geometry are described.

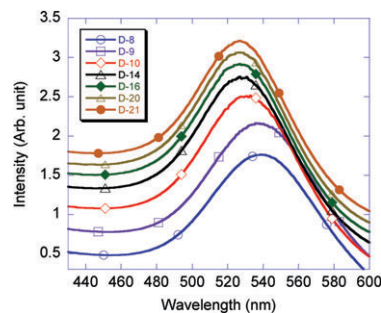


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Evolution study of photo-synthesized gold nanoparticles by spectral deconvolution model: a quantitative approach

Chung-Sung Yang,* Mong-Shian Shih and Fang-Yi Chang

During the monitoring of the evolution of Au nanoparticles photo-synthesized *via* a conventional UV-visible irradiation ($200\text{ nm} < \lambda < 600\text{ nm}$), two independent growth progresses of nanocrystals were observed.

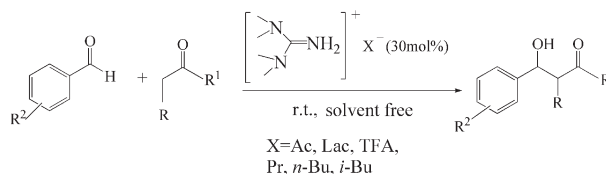


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Study on guanidine-based task-specific ionic liquids as catalysts for direct aldol reactions without solvent

Anlian Zhu, Tao Jiang,* Buxing Han,* Jun Huang, Jicheng Zhang and Xiumin Ma

The effect of anions on the catalytic activity was believed to operate through their interaction with the cation and the regioselectivity was believed to come from the special structure of the tetramethylguanidine-based enamine.

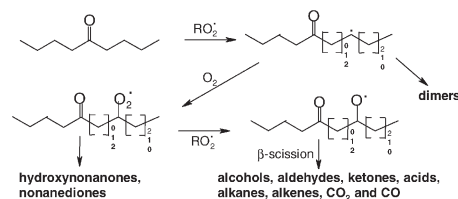


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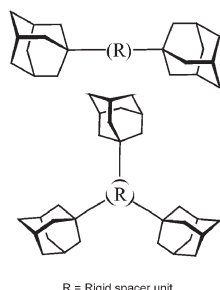
A mechanistic study of the liquid phase autoxidation of nonan-5-one

Christopher J. Hammond, John R. Lindsay Smith,* Eiji Nagatomi, Moray S. Stark and David J. Waddington*

Mechanisms are described to account for the large range of products from the liquid phase autoxidation of nonan-5-one.



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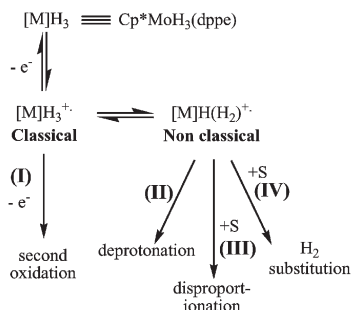


Synthesis, crystalline inclusion and structural study of bulkily stoppered and rigid framework molecular constructions

Torsten Müller, Wilhelm Seichter and Edwin Weber*

A series of compounds featuring a structure composed of linear or trigonal ethynyl and aryl containing rigid construction elements (R) with attached terminal adamantyl stoppers were synthesized to study their structures and enclathrating properties.

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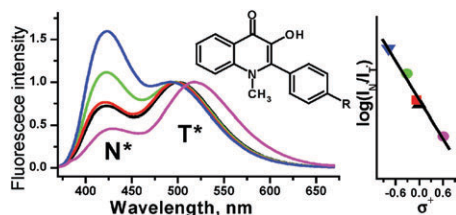


Electrochemical and DFT studies of the oxidative decomposition of the trihydride complexes Cp*M(dppe)H₃ (M = Mo, W) in acetonitrile

Rinaldo Poli,* Miguel Baya, Rita Meunier-Prest and Suzanne Raveau

A comprehensive electrochemical investigation of the oxidation of Cp*MoH₃(dppe) in acetonitrile by cyclic voltammetry, backed up by DFT calculations, reveals a new way in which oxidation leads to decomposition and clarifies the mechanism of the oxidatively induced H₂ reductive elimination.

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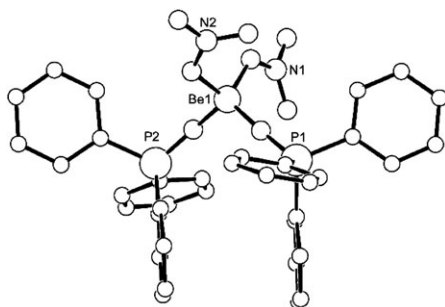


2-Aryl-3-hydroxyquinolones, a new class of dyes with solvent dependent dual emission due to excited state intramolecular proton transfer

Dmytro A. Yushchenko,* Volodymyr V. Shvadchak, Andrey S. Klymchenko, Guy Duportail, Yves Mély and Vasyly G. Pivovarenko*

The presently studied dyes appear as new prospective polarity-sensitive probes, with fluorescence properties that can be tuned by the substituents at the 2-aryl ring and nitrogen heteroatom.

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Synthesis, spectroscopic studies and structural systematics of phosphine oxide complexes with Group II metal (beryllium–barium) nitrates

Martin F. Davis, William Levason,* Raju Ratnani,* Gillian Reid* and Michael Webster

Phosphine oxide complexes of the nitrates of Be, Mg, Ca, Sr and Ba have been prepared and characterised, and the structures of four examples determined. The solution speciation has been probed by a combination of ¹H, ³¹P{¹H} and ⁹Be NMR spectroscopy.

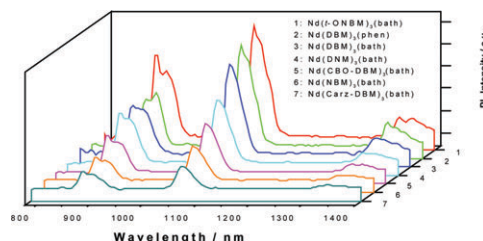
PAPERS

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Promoting near-infrared emission of neodymium complexes by tuning the singlet and triplet energy levels of β -diketonates

Lifen Yang, Zeliang Gong, Daobo Nie, Bin Lou, Zuqiang Bian, Min Guan, Chunhui Huang,* Hyun Joo Lee and Woo Phil Baik

The near infrared emissions of neodymium complexes can be promoted by modifying the ligand and consequently tuning the singlet and triplet energy levels.

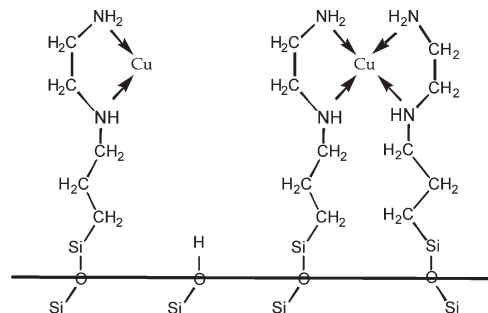


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Characterisation of the grafting of (3-aminoethyl)aminopropyltrimethoxy silane on precipitated silica

Sophie de Monredon, Agnès Pottier, Jocelyne Maquet, Florence Babonneau* and Clément Sanchez

This study investigates the reaction between AEPTS and a precipitated silica. The spatial distribution of the grafted species was studied by ESR and UV-visible spectroscopies after complexation of Cu(II) ions.

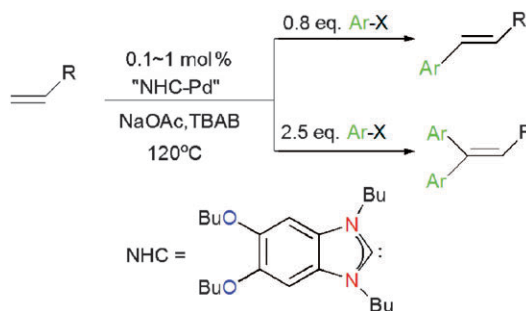


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Heck reaction catalysed by palladium supported with an electron-rich benzimidazolylidene generated *in situ*: remarkable ligand electronic effects and controllable mono- and di-arylation

Gang Zou,* Wen Huang, Yuanjing Xiao and Jie Tang

Controllable mono- and di-arylation of terminal olefins with aryl halides *via* the Heck reaction catalysed by palladium supported with an electron-rich N-heterocyclic carbene in molten tetrabutylammonium bromide.



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