

Cover

G protein-coupled receptors (GPCRs) form a large protein family that plays an important role in many physiological and pathophysiological processes. Since the sequencing of the human genome has revealed several hundred new members of this receptor family, many new opportunities for developing novel therapeutics have emerged. *In silico* approaches can considerably improve the efficiency of targeting GPCRs (pp. 2949–2956).

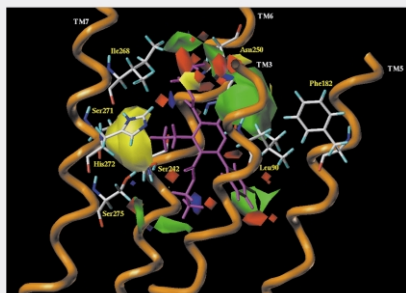


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contents

FEATURE ARTICLE

2949



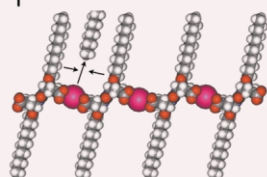
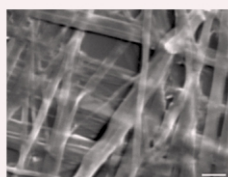
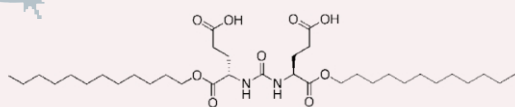
Demystifying the three dimensional structure of G protein-coupled receptors (GPCRs) with the aid of molecular modeling

Stefano Moro,* Francesca Deflorian, Giampiero Spalluto, Giorgia Pastorin, Barbara Cacciari, Soo-Kyung Kim and Kenneth A. Jacobson

GPCRs form a large protein family that plays an important role in many physiological and pathophysiological processes. Sequencing of the human genome has revealed several hundred new members of this receptor family, and many opportunities for developing novel therapeutics have emerged. Herein, we review our recent work on adenosine receptors.

COMMUNICATIONS

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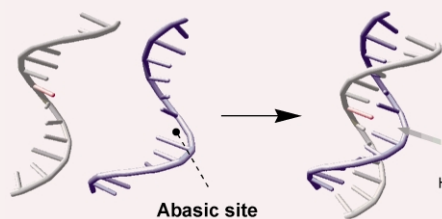


Fiber formation in water by a mono-urea dicarboxylic acid

Lara A. Estroff, Jessica S. Huang and Andrew D. Hamilton*

Monovalent cations trigger the formation of fibers by **1**. Using SEM, IR and XRD, a model of the molecular aggregation leading to fiber formation, as opposed to gelation, was developed.

2960



SNPs detection using an abasic site and pterin

Fluorescence detection of guanine–adenine transition by a hydrogen bond forming small compound

Keitaro Yoshimoto, Chun-Yan Xu, Seichi Nishizawa, Takanobu Haga, Hiroyuki Satake and Norio Teramae*

In combination with abasic site-containing oligodeoxynucleotides, 2-amino-4-oxopteridine (pterin) can selectively recognize guanine base over other nucleobases accompanied by fluorescence quenching, which allows clear detection of a guanine–adenine transition with the naked eye.

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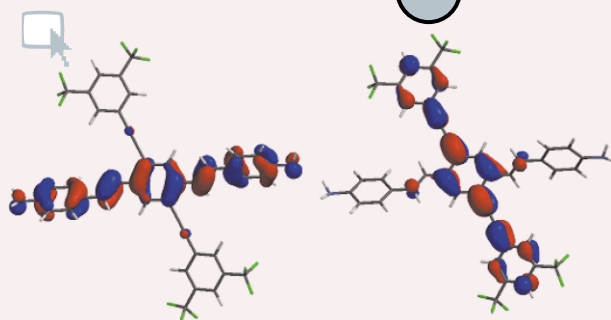
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Cruciform π -systems: hybrid phenylene-ethynylene/phenylene-vinylene oligomers

James N. Wilson, Mira Josowicz, Yiqing Wang and Uwe H. F. Bunz*

A series of distyryl(bisethynylphenyl) benzenes were prepared and their electronic properties were investigated. Correctly substituted, their LUMO is localized on the phenyleneethynylene branch, while the HOMO is localized on the distyrylbenzene branch. These cruciform π -systems are therefore electronically cross conjugated.

2964

High quality CdSeS nanocrystals synthesized by facile single injection process and their electroluminescence

Eunjoon Jang,* Shinae Jun and Lyongsun Pu

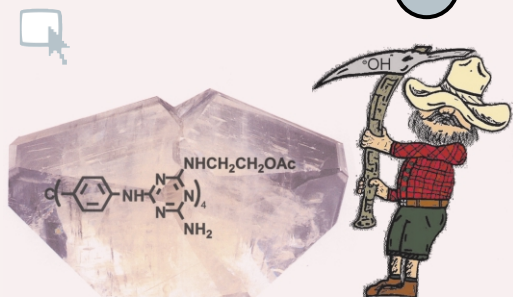


Highly luminescent CdSeS nanocrystals (quantum efficiency up to 85%), showing tunable luminescence properties from red to blue region with narrow band edge (FWHM = 34 nm), were synthesized by one-step addition of Se and S source mixture into the Cd precursor solution at elevated temperature.

2966

Excavations in molecular crystals

Erwan Le Fur, Eric Demers, Thierry Maris and James D. Wuest*

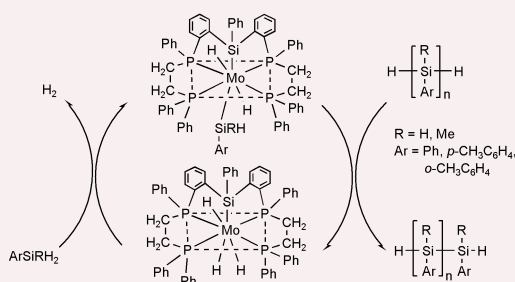


Single crystals built from porous molecular networks can react with agents that penetrate the crystals, cleave fragments from the network, and thereby increase the volume available for guests, all without loss of crystallinity.

2968

Dehydropolymerization of arylsilanes catalyzed by a novel silylmolybdenum complex

Makoto Minato,* Takaomi Matsumoto, Miyuki Ichikawa and Takashi Ito*

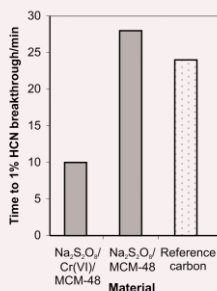


A complex $[\text{MoH}_3\{\text{Si}(\text{Ph})[\text{Ph}_2\text{PCH}_2\text{CH}_2\text{P}(\text{Ph})\text{C}_6\text{H}_4\text{-}o\}_2]$ can act as single-component catalyst for dehydrogenative polymerization of ArSiH_2R ($\text{Ar} = \text{Ph}$, p -tolyl, o -tolyl; $\text{R} = \text{H}$, Me) to $(\text{ArSiR})_n$.

2970

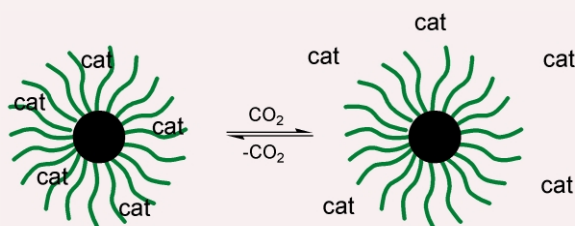
Peroxides in ordered nanoporous silicas: clean alternatives to transition metal oxidants for the removal of toxic gases

Michael J. Hudson,* Dominic B. Jackson, Jessica L. Ward and Matt J. Chinn



Ordered, nano-structured MCM-48 silica containing sodium peroxydisulfate is a novel, highly effective material for the decomposition of HCN under ambient conditions.

2972

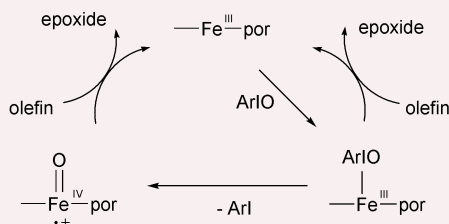


Use and recovery of a homogeneous catalyst with carbon dioxide as a solubility switch

Christopher D. Ablan, Jason P. Hallett, Kevin N. West, Rebecca S. Jones, Charles A. Eckert, Charles L. Liotta and Philip G. Jessop*

A method for fluorosilica catalysis is described, in which application of CO₂ gas causes the reversible release of the catalyst from fluorosilica.

2974

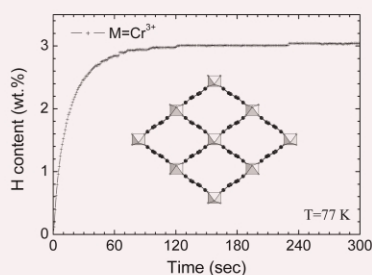


Multiple active oxidants in competitive epoxidations catalyzed by porphyrins and corroles

James P. Collman,* Li Zeng and Richard A. Decréau

We demonstrate the existence of multiple active oxygenating species in porphyrin and corrole-catalyzed competitive epoxidations of styrene and *cis*-cyclooctene.

2976

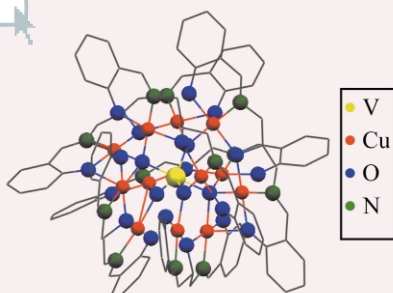


Hydrogen adsorption in the nanoporous metal-benzenedicarboxylate M(OH)(O₂C-C₆H₄-CO₂) (M = Al³⁺, Cr³⁺), MIL-53

G rard F rey,* Michel Latroche, Christian Serre, Franck Millange, Thierry Loiseau and Annick Percheron-Gu egan

The nanoporous metal-benzenedicarboxylates M(OH)(O₂C-C₆H₄-CO₂) show a hydrogen storage capacity of 3.1 and 3.8 wt.% for M = Cr³⁺ and Al³⁺, respectively when loaded at 77K under 1.6 MPa.

2978

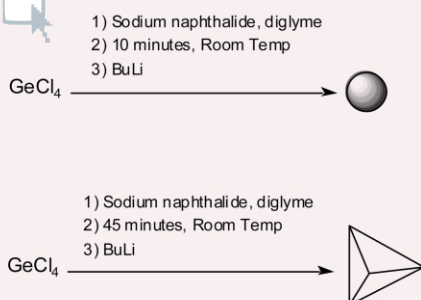


Encapsulation of paramagnetic 3d¹-vanadium(IV) in an antiferromagnetically coupled dodecanuclear copper(II) cage

Arindam Mukherjee, Munirathinam Nethaji and Akhil R. Chakravarty*

Encapsulation of vanadium(IV) in the Schiff base complex [Cu₁₂VO₅L₆] shows antiferromagnetically coupled dodecanuclear copper(II) cage which becomes essentially diamagnetic below 40 K in the presence of the paramagnetic vanadium(IV).

2980



Time dependent size and shape control of germanium nanocrystals

Louisa J. Hope-Weeks

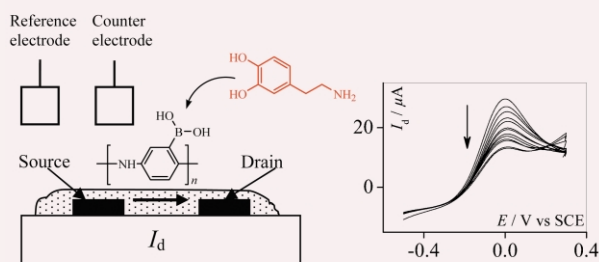
Preparation of germanium nanocrystals at room temperature has been examined by means of varying the growth time. By varying the growth time period, it is possible to control sizes and shapes of nanocrystals formed.

2982

Poly(aniline boronic acid)-based conductimetric sensor of dopamine

Bruno Fabre* and Laurent Taillebois

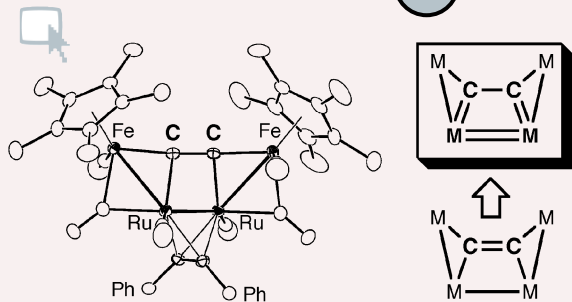
Poly(aniline boronic acid)-coated interdigitated microelectrodes show specific dopamine-induced changes in resistance at pH 7.4.



2984

 μ_4 -Dicarbyne complex with a dimetallacyclobutatriene core: A new binding mode of C_2 species

Masako Terada, Gou Higashihara, Akiko Inagaki and Munetaka Akita*

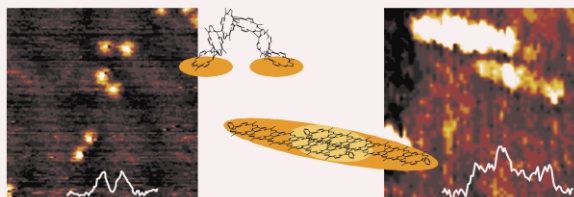
Reaction of a permetalated ethene, $(\mu_4-C=C)Fe_2Ru_2Cp^*_2(CO)_{10}$, with diphenylacetylene affords the adduct with a new C_2 -binding mode, a μ_4 -dicarbyne complex, $(\mu_4-C-C)Fe_2Ru_2Cp^*_2(CO)_6(\mu-Ph-C\equiv C-Ph)$, containing a dimetallacyclobutatriene core.

2986

STM images of individual porphyrin hexamers; *meso-meso* singly linked orthogonal hexamer and *meso-meso*, β - β , β - β triply-linked planar hexamer on Cu(100) surface

Akihiko Takagi, Yoshiki Yanagawa, Akihiko Tsuda, Naoki Aratani, Takuya Matsumoto,* Atsuhiko Osuka* and Tomoji Kawai*

STM observation of chain porphyrin arrays on Cu(100): a bridge-like structure for a singly linked hexamer, whereas a rigid planar and one-dimensional stacked structure for a triply linked hexamer.

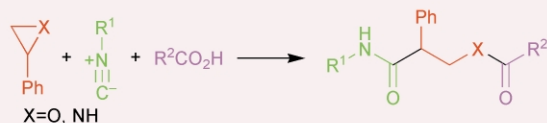


2988

A novel isocyanide based three component reaction

Oliver T. Kern and William B. Motherwell*

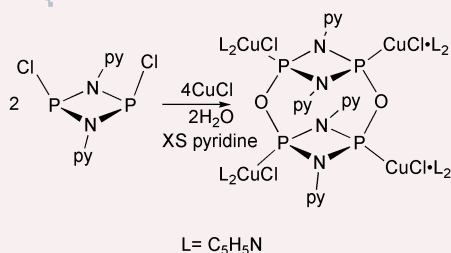
A three component reaction involving an isocyanide, a carboxylic acid and an epoxide or aziridine as the electrophile is described.



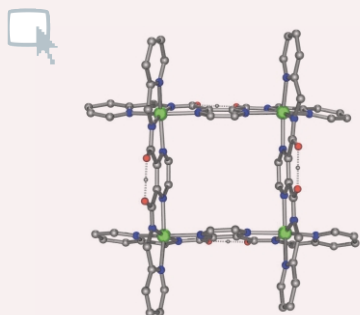
2990

***Exo*-metal coordination by a tricyclic $\{[P(\mu-N-2-NC_5H_4)]_2(\mu-O)]_2$ dimer in $\{[P(\mu-N-2-NC_5H_4)]_2(\mu-O)]_2\{CuCl\cdot(C_5H_5N)_2\}_4$ $\{2-NC_5H_4 = 2$ -pyridyl, $C_5H_5N =$ pyridine)**

Andrew D. Bond, Emma L. Doyle, Felipe García, Richard A. Kowenicki, Mary McPartlin, Lucía Riera and Dominic S. Wright*

Reaction of $[ClP(\mu-N-2-NC_5H_4)]_2$ with CuCl in the presence of C_5H_5N and H_2 gives the new cyclic ligand $\{[P(\mu-N-2-NC_5H_4)]_2(\mu-O)]_2$.

2992

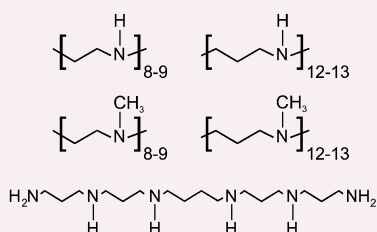


Control of molecular architecture by the degree of deprotonation: self-assembled di- and tetranuclear copper(II) complexes of *N,N'*-bis(2-pyridylmethyl)pyrazine-2,3-dicarboxamide

Julia Hausmann, Geoffrey B. Jameson and Sally Brooker*

Reaction of bis-terdentate pyrazine diamide ligand H_2L with Cu^{II} results in a navy-blue dimer $[Cu^{II}(H_2L)(MeCN)]_2(BF_4)_4$ or, in the presence of base, a grass-green $[2 \times 2]$ grid $[Cu^{II}(HL)]_4(BF_4)_4$

2994

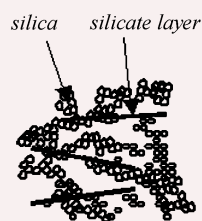


Chemical properties of polyamines with relevance to the biomineralization of silica

Henning Menzel,* Sandra Horstmann, Peter Behrens,* Petra Bärnreuther, Ilka Krueger and Michael Jahns

Polyamines mimicking substances which occur naturally in biosilicas have been synthesized and show an accelerating effect on silica condensation, which depends on the chemical nature, the architecture (linear or branched), and the degree of polymerization.

2996



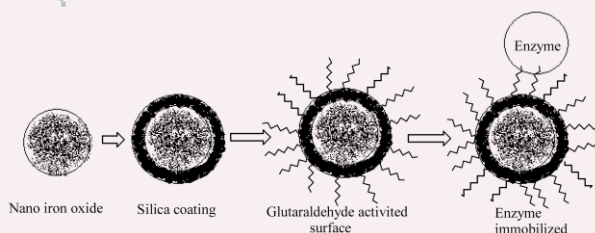
Silica-clay nanocomposite

Silica-clay nanocomposites

Sadok Letaief and Eduardo Ruiz-Hitzky*

New silica-clay porous nanocomposite materials have been prepared by a sol-gel procedure using alkoxy silanes and organoclays that involves the delamination of the layered solids. These solids could be transformed into organic-inorganic bipolar functional materials.

2998

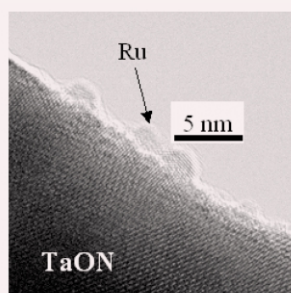


Colloidal stable silica encapsulated nano-magnetic composite as a novel bio-catalyst carrier

Xin Gao, K. M. Kerry Yu, Kin Y. Tam and Shik Chi Tsang*

A colloidal stable silica-encapsulated magnetic nano-composite is employed to carry β -lactamase, which allows site (enzyme) isolation, accessibility as good as the free enzyme and reusability upon application of magnetic separation.

3000



Unusual enhancement of H_2 evolution by Ru on TaON photocatalyst under visible light irradiation

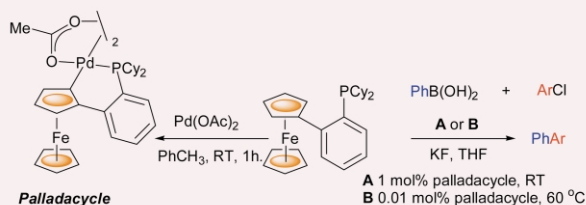
Michikazu Hara, Jun Nunoshige, Tsuyoshi Takata, Junko N. Kondo and Kazunari Domen

H_2 evolution on TaON photocatalyst under visible light irradiation ($420 \text{ nm} \leq \lambda \leq 500 \text{ nm}$) in an aqueous methanol solution is found to be remarkably enhanced by adding Ru as a noble-metal co-catalyst

3002

A ferrocene based palladacyclic precatalyst for the Suzuki cross-coupling of aryl chlorides

Francesc X. Roca and Christopher J. Richards*

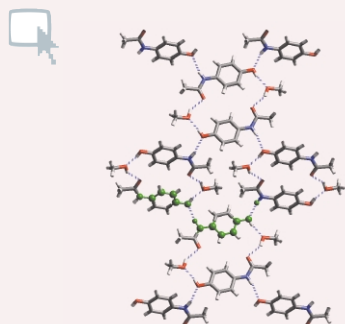


Addition of palladium acetate to 2-(dicyclohexylphosphino)phenylferrocene gave a palladacycle that is a very effective precatalyst for the Suzuki cross-coupling of aryl chlorides.

3004

Pressure-induced formation of a solvate of paracetamol

Francesca P. A. Fabbiani, David R. Allan, Alice Dawson, William I. F. David, Pamela A. McGregor, Iain D. H. Oswald, Simon Parsons and Colin R. Pulham*

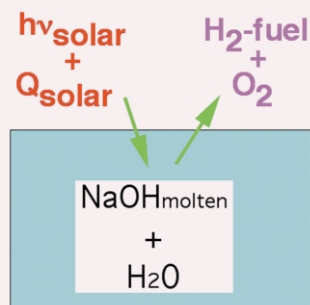


Recrystallisation of paracetamol from a solution in methanol contained in a diamond-anvil cell at a pressure of 0.62 GPa resulted in the formation of a 1 : 1 solvate that was characterised *in situ* by spectroscopic and diffraction methods.

3006

Electrochemical potential tuned solar water splitting

Stuart Licht,* Leonid Halperin, Michael Kalina, Martina Zidman and Nadezhda Halperin



Efficient solar hydrogen fuel formation is accomplished by tuning the water splitting potential, rather than the photosensitizer bandgap. This permits semiconductors such as Si to drive water cleavage from molten NaOH.

3008

Flexible dye sensitised nanocrystalline semiconductor solar cells

Saif A. Haque, Emilio Palomares, Hari M. Upadhyaya, Lucy Otley, Robert J. Potter, Andrew B. Holmes and James R. Durrant*

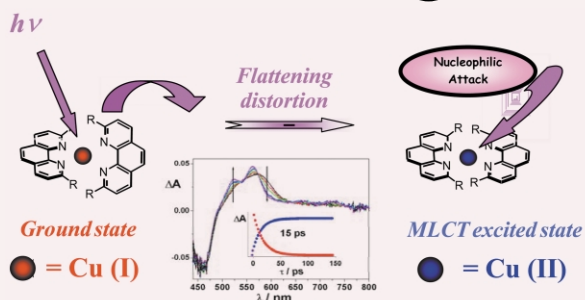


We report here flexible solid-state solar cells based upon dye-sensitized nanocrystalline Al_2O_3 coated TiO_2 films and an I_2/NaI doped solid-state polymer electrolyte. Such devices show remarkably high solar-light to electrical energy conversion efficiencies of $\sim 5.3\%$ under 10 mW cm^{-2} AM1.5 illumination.

3010

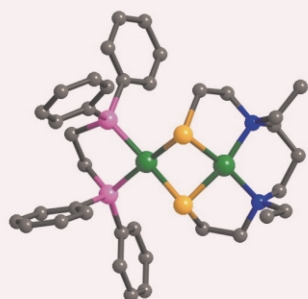
Ultrafast dynamics of Cu(I)-phenanthrolines in dichloromethane

Tissa Gunaratne, Michael A. J. Rodgers,* Delphine Felder, Jean-François Nierengarten,* Gianluca Accorsi and Nicola Armaroli*



Transient absorption spectrometry of Cu(I)-phenanthrolines in CH_2Cl_2 reveals ligand-independent dynamic processes lasting 15 ps, which are associated with the peculiar structural rearrangements occurring for this class of compounds upon photoexcitation.

3012

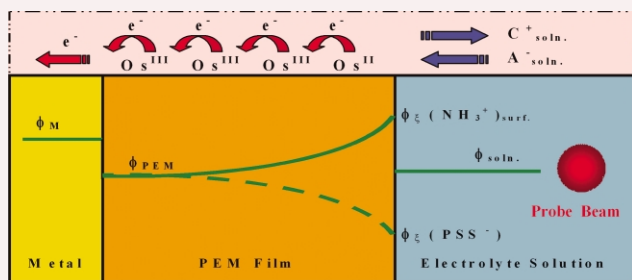


Structure and electronic properties of an asymmetric thiolate-bridged binuclear complex: a model for the active site of acetyl CoA synthase

Qiang Wang, Alexander J. Blake, E. Stephen Davies, Eric J. L. McInnes, Claire Wilson and Martin Schröder*

The binuclear Ni(II) complex $[(\text{dppe})\text{Ni}(\mu\text{-}^{\prime}\text{S},\text{S}^{\prime})\text{Ni}(\text{L})](\text{PF}_6)_2$ [$\text{L} = (N,N'$ -diethyl-3,7-diazanonane-1,9-dithiolato) $^{2-}$] shows a reversible one-electron reduction to afford a mixed-valent Ni(II)-Ni(I) species; the reduced complex mimics the redox properties of the Ni_p site in the active A-cluster of acetyl coenzyme A synthase.

3014

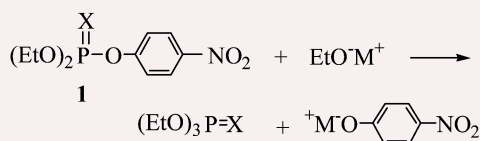


Probe beam deflection study of ion exchange in self-assembled redox polyelectrolyte thin films

Doris E. Grumelli, Alejandro Wolosiuk, Erica Forzani, Gabriel A. Planes, César Barbero and Ernesto J. Calvo*

Probe beam deflection during chronoamperometric oxidation–reduction of osmium complex in layer-by-layer self-assembled redox active polyelectrolyte multilayers.

3016



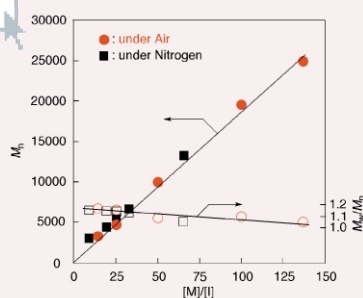
X = O (**1a**), X = S (**1b**): M = Li, Na, K

Significant and differential acceleration of dephosphorylation of the insecticides, paraoxon and parathion, caused by alkali metal ethoxides

Ik-Hwan Um,* Sang-Eun Jeon, Mi-Hwa Baek and Hye-Ran Park

1a is *ca.* 20–30 times more reactive than **1b** toward dissociated EtO^- but *ca.* 2×10^3 times more reactive toward ion-paired EtO^-Li^+ in anhydrous EtOH.

3018

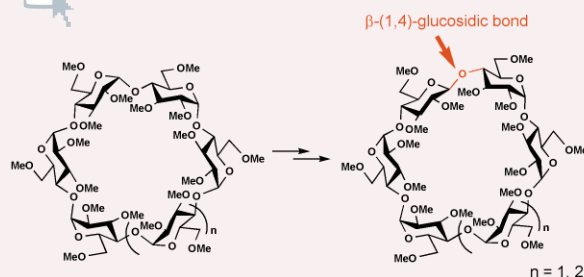


Living cationic ring-opening polymerization by water-stable initiator: synthesis of a well-defined optically active polythiourethane

Atsushi Nagai, Bungo Ochiai and Takeshi Endo*

Living cationic polymerization of a cyclic thiourethane under air and water was achieved using a well-defined water-resistant cationic initiator in non-distilled CH_2Cl_2 at mild temperature.

3020



A facile synthesis of novel cyclodextrin derivatives incorporating one β -(1,4)-glucosidic bond and their unique inclusion ability

Toshiyuki Kida, Akira Kikuzawa, Yohji Nakatsuji and Mitsuru Akashi*

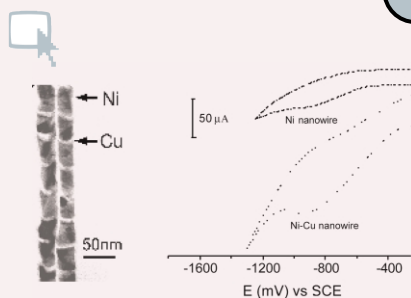
Novel types of cyclodextrin derivatives incorporating one β -(1,4)-glucosidic bond were easily synthesized in three steps from permethylated α - and β -cyclodextrins.

3022

Novel electrocatalytic activity in layered Ni–Cu nanowire arrays

Hui-Min Zhang, Yu-Guo Guo, Li-Jun Wan* and Chun-Li Bai*

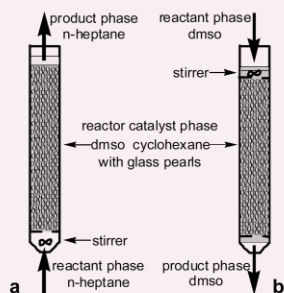
Composite Ni–Cu nanowire arrays show high electrocatalytic activity for the reduction of hydrogen peroxide



3024

Continuous biphasic catalysis: palladium catalyzed cross coupling reactions

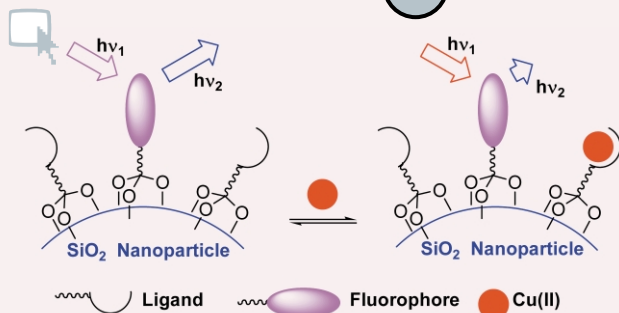
Jens Hillerich and Herbert Plenio*

A homogeneous catalyst immobilized with a polar phase tag in dmsO solution and a reactant/product carrying solvent *n*-heptane flowing through this reactor can be used to continuously produce aryl acetylenes *via* Pd-mediated C–C coupling reactions.

3026

A fluorescence nanosensor for Cu²⁺ on silica particles

Elena Brasola, Fabrizio Mancin, Enrico Rampazzo, Paolo Tecilla* and Umberto Tonellato*

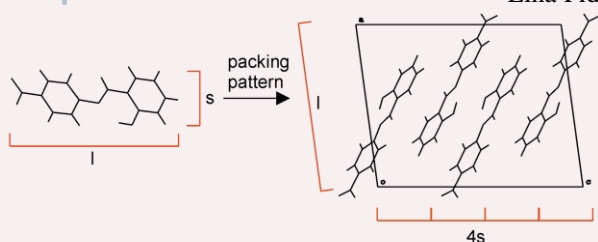
A fluorescence nanosensor for Cu²⁺ ions has been obtained by surface functionalization of silica particles with trialkoxysilane derivatized ligand and fluorescent dye.

3028

A new model of crystal packing

Elna Pidcock* and W. D. Sam Motherwell

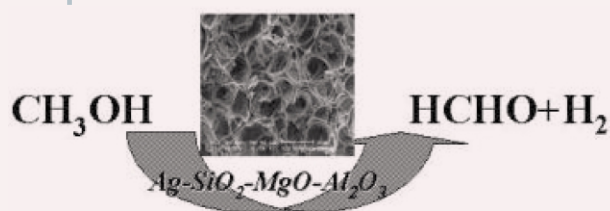
A new, conceptually simple model of crystal packing is proposed which uses “packing patterns” to describe unit cells in terms of molecular building blocks.



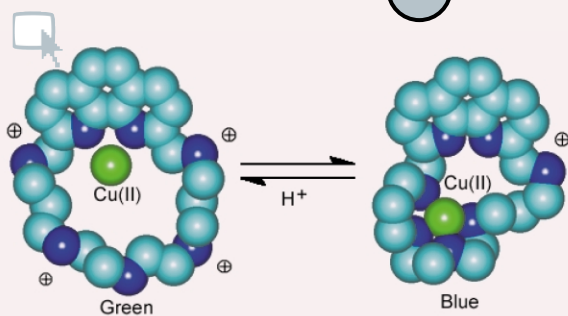
3030

First observation of highly efficient dehydrogenation of methanol to anhydrous formaldehyde over novel Ag–SiO₂–MgO–Al₂O₃ catalyst

Li-Ping Ren, Wei-Lin Dai,* Yong Cao, Hexing Li and Kangnian Fan*

Novel beautiful flower-like Ag–SiO₂–MgO–Al₂O₃ catalyst prepared by sol–gel method showed extremely high activity and selectivity (both equal to 100%) in the direct dehydrogenation of methanol to anhydrous formaldehyde.

3032



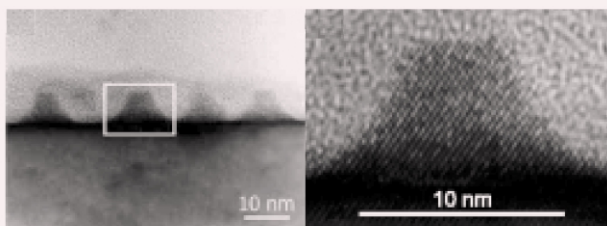
Hydrogen-ion driven molecular motions in Cu²⁺-complexes of a ditopic phenanthrolinephane ligand

Angel Mendoza, Juan Aguilar, Manuel G. Basallote,* Laura Gil, Juan C. Hernández, M. Angeles Máñez, Enrique García-España,* Lena Ruiz-Ramírez, Conxa Soriano and Begoña Verdejo

One of the first reports on a proton-driven metal ion interchange between the two sites of a ditopic phenanthrolinephane receptor characterised by spectroscopic and stopped-flow techniques is presented.

3034

Facile fabrication of 2-dimensional arrays of sub-10 nm single crystalline Si nanopillars using nanoparticle masks



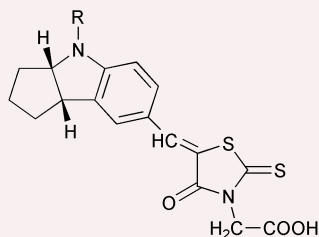
Young-Kyu Hong, Jae Ho Bahng, Geunseop Lee, Hanchul Kim, Wondong Kim, Sekyung Lee, Ja-Yong Koo,* Jong-Il Park, Woo-ran Lee and Jinwoo Cheon*

A simple procedure for the fabrication of sub-10 nm scale Si nanopillars in a 2-D array using reactive ion etching with 8 nm Co nanoparticles as etch masks is demonstrated.

3036

Highly-efficient metal-free organic dyes for dye-sensitized solar cells

Tamotsu Horiuchi,* Hidetoshi Miura and Satoshi Uchida

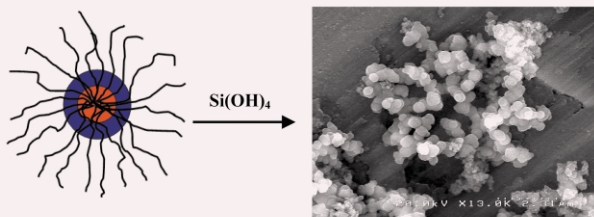


A solar-to-electric conversion efficiency of 6.1% is achieved with this new indoline dye. Furthermore, indoline dyes are shown to be highly stable to photoredox processes by cyclic voltammogram

3038

Functional analysis of the biomimetic silica precipitating activity of the R5 peptide from *Cylindrotheca fusiformis*

Marc R. Knecht and David W. Wright*

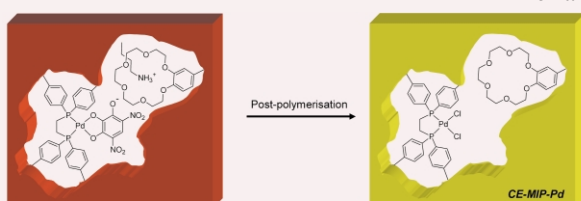


A synthetic site-directed mutagenesis study of the non post-translationally modified silica precipitating R5 peptide reveals that the RRIL motif is critical in the formation of active silica precipitating assemblies.

3040

Crown-ether functionalised second coordination sphere palladium catalysts by molecular imprinting

Florian Viton, Peter S. White and Michel R. Gagné*



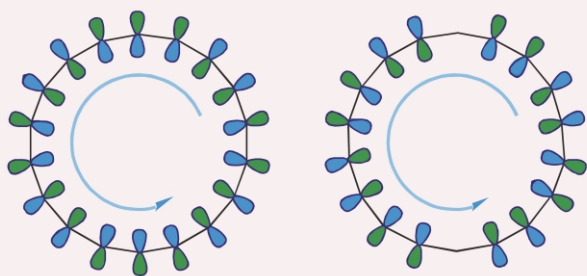
Functionalisation of the second coordination sphere of a molecularly imprinted Pd complex was achieved by localising within the polymeric cavity a crown-ether receptor capable of altering the catalytic activity of the reactive site.

3042

A diatropic ring current in a fluorofullerene trannulene

Glenn A Burley, Patrick W Fowler, Alessandro Soncini, John P B Sandall and Roger Taylor

Current-density maps reveal a diamagnetic ring current in the [18]*trans*-annulene substructure of $C_{60}F_{15}X_3$, dominated by the contribution of the four electrons in the doubly degenerate HOMO (shown), as in a classical aromatic ($4n + 2$) annulene.

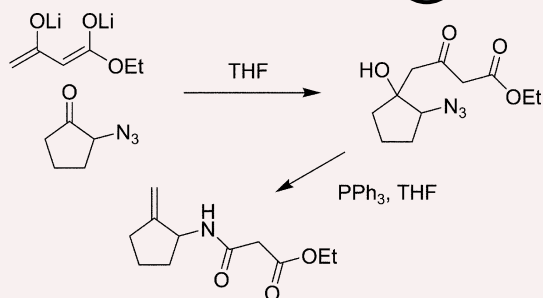


3044

Domino ‘Staudinger–aza-Wittig–1,5-phosphonium-rearrangement–fragmentation’ reactions of 1-azido-2-hydroxy-4,6-dioxohexanes

Peter Langer,* Ilia Freifeld and Heydar Shojaei

The domino ‘Staudinger–aza-Wittig–1,5-phosphonium-rearrangement–fragmentation’ reaction of 1-azido-2-hydroxy-4,6-dioxohexanes allows a convenient synthesis of functionalized 1-acetamido-2-alkylidenecyclopentanes.

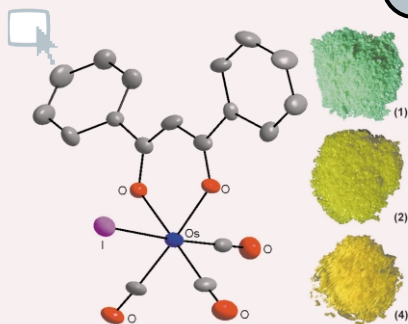


3046

Synthesis and characterization of luminescent osmium(II) carbonyl complexes based on chelating dibenzoylmethanate and halide ligands

Yao-Lun Chen, Chittaranjan Sinha, I-Chia Chen, Kuan-Lin Liu, Yun Chi,* Jen-Kan Yu, Pi-Tai Chou* and Tian-Huey Lu

A new series of dibenzoylmethanate Os(II) complexes **1–5** have been synthesized, showing remarkable phosphorescence with extended lifetimes of 29–64 μ s in room-temperature fluid solution.

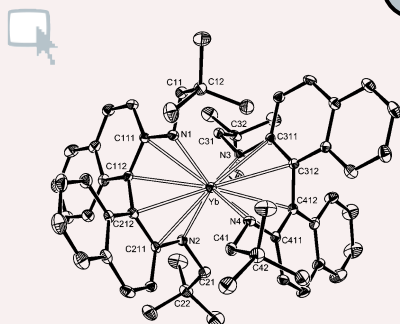


3048

Lanthanide complexes derived from (*R*)-1,1'-binaphthyl-2,2'-bis(neopentylamine) – {Li(THF)₄}{Ln[(*R*)-C₂₀H₁₂N₂(C₁₀H₂₂)₂]} (Ln = Sm, Yb) – novel catalysts for enantioselective intramolecular hydroamination

Jacqueline Collin,* Jean-Claude Daran, Emmanuelle Schulz and Alexander Trifonov*

The complexes {Li(THF)₄}{Ln[(*R*)-C₂₀H₁₂N₂(C₁₀H₂₂)₂]} (Ln = Sm, Yb) have been synthesized, fully characterized and found to be efficient and enantioselective catalysts for intramolecular hydroamination of 1-(aminomethyl)-1-allylcyclohexane.

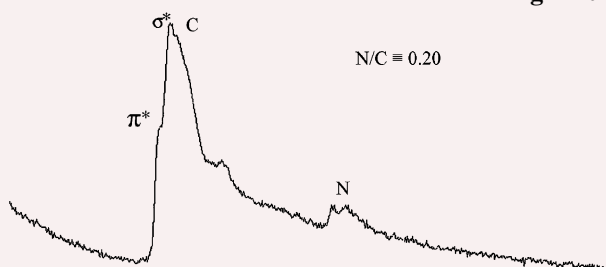


3050

Synthesis and field emission of carbon nanotubular fibers doped with high nitrogen content

Chengchun Tang,* Dmitri Golberg, Yoshio Bando, FangFang Xu and Baodan Liu

Nitrogen-doped carbon nanotubular fibers with a very high nitrogen concentration (~20 at.%) were synthesized through the aerosol-assisted decomposition of dimethylformamide in the presence of catalyst. The synthesized fibers possess a novel ‘‘pearl necklace-like’’ morphology and exhibit an excellent field emission performance.



ADDITIONS AND CORRECTIONS

3052

Yan Li, Jie-Sheng Huang, Zhong-Yuan Zhou and Chi-Ming Che*

Oxo-bridge metal carbene complexes. Synthesis, structure and reactivities of $\{[\text{Os}(\text{Por})(\text{CPh}_2)_2\text{O}]\}$ (Por = porphyrinato dianion)

3052

Michael Deligny, François Carreaux, Bertrand Carboni, Loïc Toupet and Gilles Dujardin

A novel diastereoselective route to α -hydroxyalkyl dihydropyrans using a hetero Diels–Alder/allylboration sequence

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NOTE: An asterisk in the heading of each paper indicates the author who is to receive any correspondence.