**Cover**

The historical transformation of radical pair reactions from the proposal of the molecular "cage effect" in the 1930s (top), to the supramolecular "cage effect" (right), to the superdupermolecular "cage effect" (left). The lower right shows a ketone molecule in a zeolite supercage, showing several cations occupying space within the supercage.

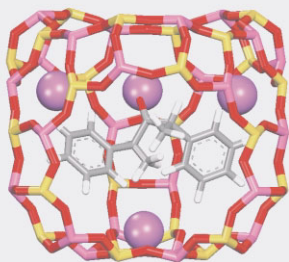


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contents

FEATURE ARTICLE

2279



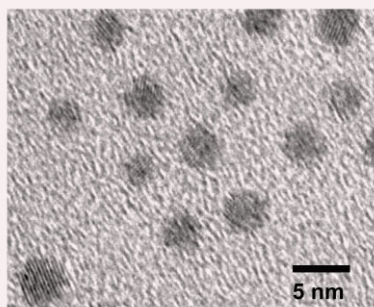
From molecular chemistry to supramolecular chemistry to superdupermolecular chemistry. Controlling covalent bond formation through non-covalent and magnetic interactions

Nicholas J. Turro

Controlling the selectivities of radical pair reactions can be accomplished by supramolecular effects; in addition, the selectivity of radical pair reactions in supramolecular systems are significantly influenced by the magnetic effects.

COMMUNICATIONS

2294

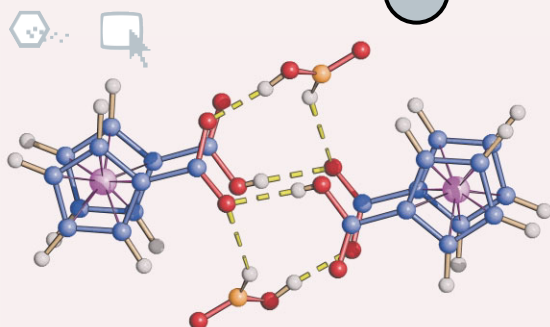


Thioalkylated tetraethylene glycol: a new ligand for water soluble monolayer protected gold clusters

Antonios G. Kanaras, Fadhil S. Kamounah, Kjeld Schaumburg, Christopher J. Kiely and Mathias Brust*

Ligand-stabilised, water-soluble gold nanoparticles of two different size ranges (2–4 and 5–8 nm) are readily prepared using monohydroxy (1-mercapto-11-yl) tetraethylene glycol as a novel capping agent.

2296

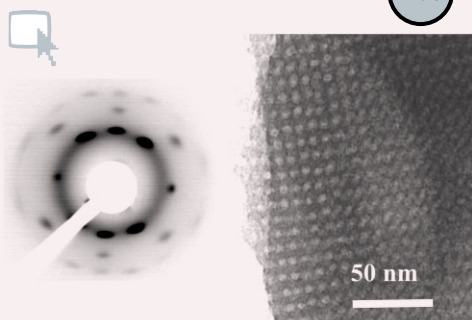


Supramolecular gas–solid reaction between formic acid vapours and solid $[\text{Co}^{\text{III}}(\eta^5\text{-C}_5\text{H}_4\text{COOH})(\eta^5\text{-C}_5\text{H}_4\text{COO})]$

Dario Braga,* Lucia Maini, Michele Mazzotti, Katia Rubini, Admir Masic, Roberto Gobetto and Fabrizia Grepioni*

Crystalline $[\text{Co}^{\text{III}}(\eta^5\text{-C}_5\text{H}_4\text{COOH})(\eta^5\text{-C}_5\text{H}_4\text{COO})]$ reversibly reacts with vapours of formic acid forming the co-crystal $[\text{Co}^{\text{III}}(\eta^5\text{-C}_5\text{H}_4\text{COOH})(\eta^5\text{-C}_5\text{H}_4\text{COO})][\text{HCOOH}]$ without proton transfer from formic acid to the deprotonated -COO^- group on the zwitterion.

2298



Structural control in self-standing mesostructured silica oriented membranes and xerogels

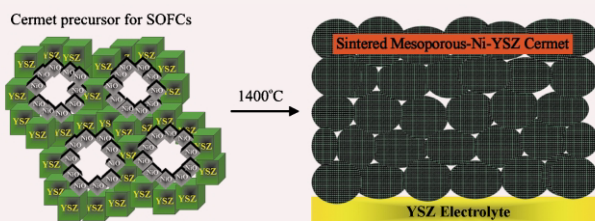
G. J. A. A. Soler-Illia, E. L. Crepaldi, D. Grosso, D. Durand and C. Sanchez*

The symmetry and orientation of large pore ($a = 150\text{--}200 \text{ \AA}$) mesostructured silica xerogels can be reproducibly tuned by an Evaporation-Induced Self Assembly (EISA) route. Mesostructure control was attained by changing the template (nonionic block copolymers P123 and F127) and water ($h = [\text{H}_2\text{O}]/[\text{Si}]$) ratio.

2300

Practical solid oxide fuel cells with anodes derived from self-assembled mesoporous-NiO-YSZ

Marc Mamak, Neil Coombs and Geoffrey A. Ozin*

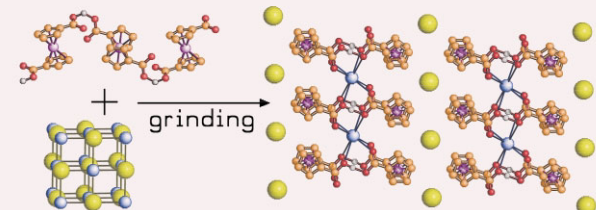


Solid oxide fuel cells comprised of an anode made from sintered and reduced mesoporous-NiO-YSZ are shown to provide stable current and power densities at the operating temperature of $800 \text{ }^\circ\text{C}$ and show better performance than cells with anode cermets made from mechanical mixtures of NiO and YSZ, attributable to the unique anode microstructure.

2302

Unexpected solid–solid reaction upon preparation of KBr pellets and its exploitation in supramolecular cation complexation

Dario Braga,* Lucia Maini, Marco Polito and Fabrizia Grepioni*

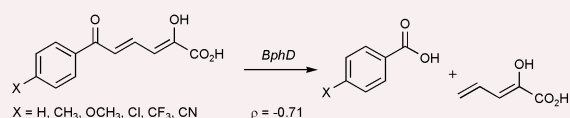


Pressing solid $[\text{Co}^{\text{III}}(\eta^5\text{-C}_5\text{H}_4\text{COOH})(\eta^5\text{-C}_5\text{H}_4\text{COO})]$ with KBr to prepare samples for IR spectroscopy leads to a profound solid state rearrangement with formation of the supramolecular complex $[\text{Co}^{\text{III}}(\eta^5\text{-C}_5\text{H}_4\text{COOH})(\eta^5\text{-C}_5\text{H}_4\text{COO})]_2 \cdot \text{K}^+\text{Br}^-$, which can also be obtained from solution crystallization.

2304

Hammett analysis of a C–C hydrolase-catalysed reaction using synthetic 6-aryl-2-hydroxy-6-ketohexa-2,4-dienoic acid substrates

Damian M. Speare, Petra Olf and Timothy D. H. Bugg*

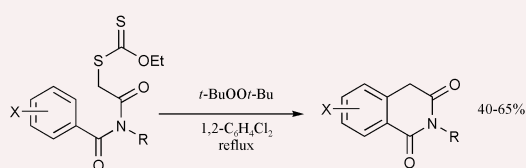


A Hammett plot ($\rho = -0.71$) has been measured for C–C hydrolase enzyme BphD, using six 6-aryl-2-hydroxy-6-ketohexa-2,4-dienoic acids synthesised by a Heck coupling strategy.

2306

An expedient synthesis of homophthalimides

Béatrice Quiclet-Sire* and Samir Z. Zard*

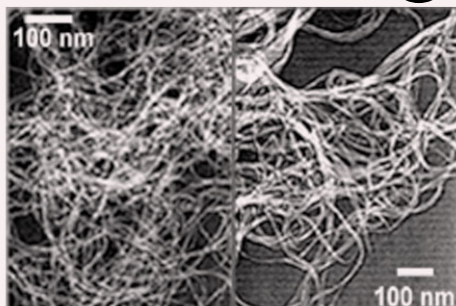


The six-membered heterocyclic subunit of homophthalimides can be obtained by a direct, hitherto unprecedented, radical cyclisation onto an aromatic ring starting from a xanthate precursor.

2308

Microwave-assisted purification of HIPCO carbon nanotubes

Ester Vázquez, Vasiliou Georgakilas and Maurizio Prato*

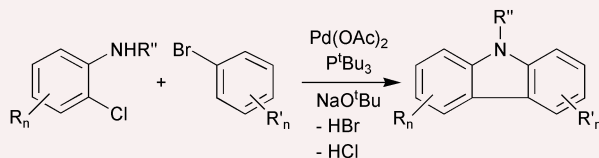


Selective microwave heating of iron particles in single-walled carbon nanotubes notably reduces the metal content.

2310

A novel catalytic one-pot synthesis of carbazoles *via* consecutive amination and C–H activation

Robin B. Bedford* and Catherine S. J. Cazin

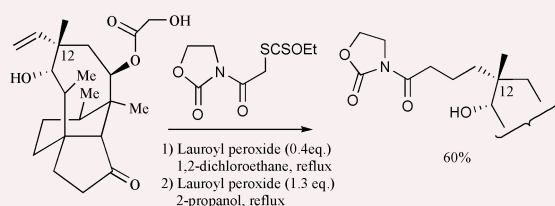


Catalytic amination of aryl bromides with 2-chloro-*N*-alkylated anilines is followed by C–H activation to give a novel synthesis of carbazoles in one pot.

2312

A flexible strategy for the divergent modification of pleuromutilin

Eric Bacqué, François Pautrat and Samir Z. Zard*

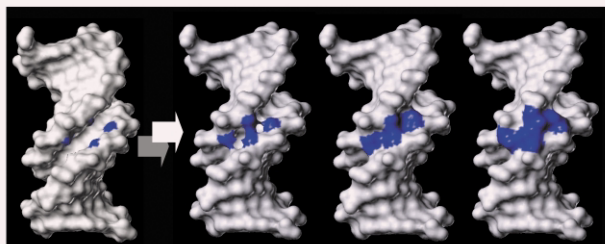


The complex antibacterial natural product, pleuromutilin, can be directly modified by the radical addition reaction of various xanthates to the unactivated terminal olefin present on C-12 followed by reductive removal of the xanthate group.

2314

DNA minor groove hydration probed with 4'-alkylated thymidines

Ilka Detmer, Daniel Summerer and Andreas Marx*

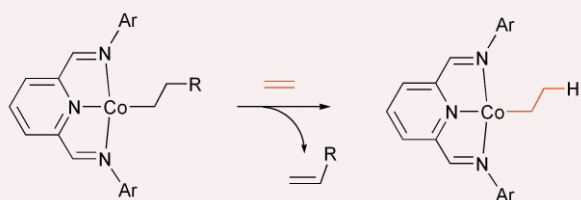


Employing 4'-alkylated oligonucleotides we investigated the involvement of DNA minor groove hydration on duplex stability and conformation. Our studies indicate that hydration is critical for DNA duplex stability.

2316

Bis(imino)pyridine cobalt alkyl complexes and their reactivity towards ethylene: a model system for β -hydrogen chain transfer

Vernon C. Gibson,* Kilian P. Tellmann, Martin J. Humphries and Duncan F. Wass

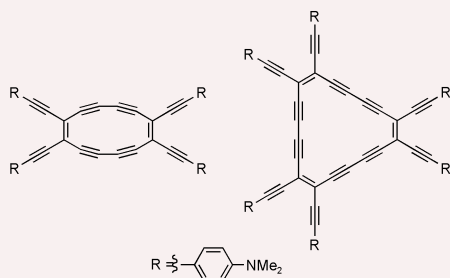


Bis(imino)pyridine cobalt(I) alkyl complexes react with ethylene *via* β -hydrogen transfer; mechanistic studies reveal a step-wise process rather than direct β -H transfer to ethylene.

2318

 π -Electron conjugation effects in antiaromatic dehydro[12]- and aromatic dehydro[18]-annulenes

Frieder Mitzel, Corinne Boudon, Jean-Paul Gisselbrecht, Maurice Gross and François Diederich*

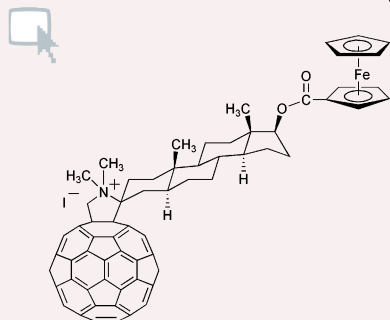


A novel photochemical route to *cis*-bisdeprotected tetraethynylethenes has enabled the synthesis of *N,N*-dimethylanilino-substituted perethynylated dehydro[12]- and dehydro[18]-annulenes. They feature strongly bathochromically shifted longest-wavelength absorption maxima due to efficient intramolecular charge-transfer between the peripheral electron donors and the electron-accepting acetylenic core.

2320

Small reorganisation energy and unique stabilisation of zwitterionic C_{60} -acceptor moieties

Dirk M. Guldi,* Chuping Luo, Tatiana Da Ros, Susanna Bosi and Maurizio Prato*

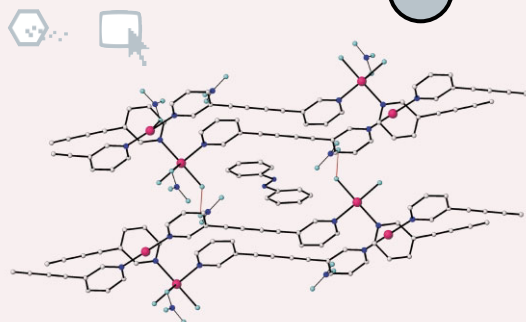


Fulleropyrrolidinium ions, namely, fullerene derivatives possessing a positive charge, exhibit smaller reorganization energies than neutral derivatives in photoinduced electron transfer, leading to accelerated charge separation and retarded charge recombination.

2322

Organic/inorganic supramolecular channel frameworks containing a photosensitive azobenzene molecule as an included guest

Md. Badruz Zaman, Konstantin Udachin, Md. Akhtaruzzaman, Yoshiro Yamashita and John A. Ripmeester*

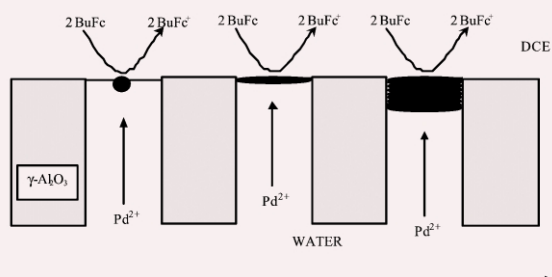


On the basis of specific local geometry and orientations of the nitrogen atoms in the ligands constructed, two novel porous coordination polymer host frameworks that can include azobenzene as guest are obtained.

2324

Controlled deposition of nanoparticles at the liquid–liquid interface

Mark Platt, Robert A. W. Dryfe* and Edward P. L. Roberts

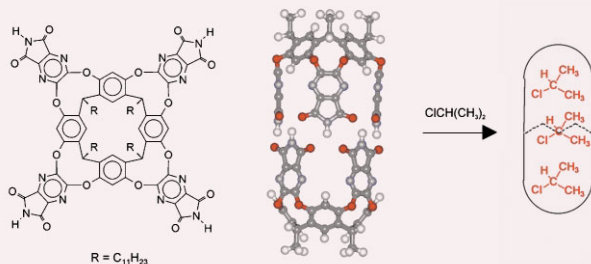


Palladium nanoparticles have been grown by applying a template-constrained method at the liquid–liquid interface. This novel method provides a simple route to the dispersion of well-defined palladium particles in γ -alumina.

2326

The inner solvation of a cylindrical capsule

Alexander Shivanyuk and Julius Rebek Jr.*



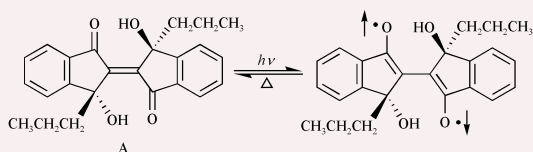
Typical solvents—not deuterated—can be used to evaluate the inner solvation of capsules by NMR. Solvents that occupy slightly more than half the space are readily encapsulated.

2328



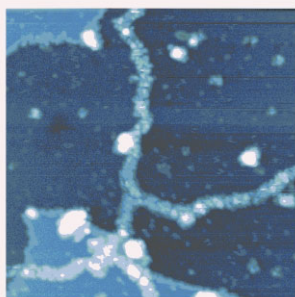
Photoinduced ground-state singlet biradical—novel insight into the photochromic compounds of biindenylidenediones

Lili Xu, Teruki Sugiyama, Huaming Huang, Zhiji Song, Jiben Meng* and Teruo Matsuura



The biindenylidenedione derivative (A) developed a biradical accompanied by the simultaneous photocolor development on UV or sunlight irradiation; the former of which showed antiferromagnetic behavior on account of the singlet ground state and a thermally accessible triplet state.

2330



Synthesis of long Poly(dA)·Poly(dT) DNA without structural defects using enzymatic reaction; Tailored ligated Poly(dA)·Poly(dT)

Shin-ichi Tanaka, Shinsuke Fujiwara, Hiroyuki Tanaka, Masateru Taniguchi, Hitoshi Tabata, Kiichi Fukui and Tomoji Kawai*

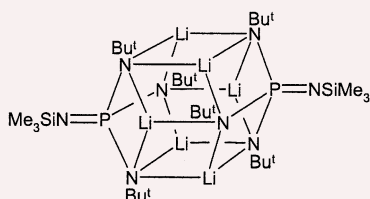
Poly(dA)·Poly(dT) molecules up to 1000 base pairs (bp) have been synthesized without defects in the duplex structure using enzymatic reaction.

2332



Syntheses and structures of an unsolvated tetrakisimidophosphate $\{Li_3[P(NBu^t)_3(NSiMe_3)]\}_2$ and the face-sharing double-cubane $\{Li_2(THF)[P(O)(NBu^t)_2(NHBU^t)]\}_2$

Andrea Armstrong, Tristram Chivers,* Mark Krahn, Masood Parvez and Gabriele Schatte



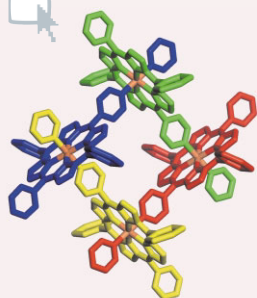
A rational synthesis and the X-ray structures of the first unsolvated trillithium tetrakisimidophosphate and, for comparison, the related oxoamidobis(imido)phosphate system are described.

2334



Unique 2D metalloporphyrin networks constructed from iron(II) and meso-tetra(4-pyridyl)porphyrin

Long Pan, Sean Kelly, Xiaoying Huang and Jing Li*



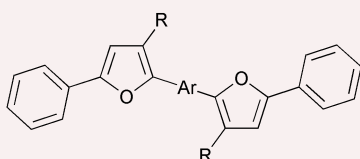
Two novel extended network structures of metalloporphyrin FeTPyP have been synthesized and characterized. Both structures contain alternately perpendicular porphyrin molecules that give rise to an unprecedented two-dimensional paddle-wheel-like pattern (4^4 topology) with a different packing sequence, namely $\dots ABAB \dots$ and $\dots ABCDABCD \dots$.

2336



Non-amine-based furan-containing oligoaryls as efficient hole transporting materials

Ling-Zhi Zhang, Chieh-Wei Chen, Chin-Fa Lee, Chung-Chih Wu* and Tien-Yau Luh*

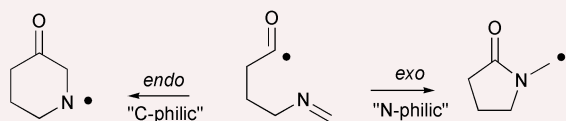


A new class of highly stable furan-based hole transporting oligomeric materials, synthesized from the corresponding propargylic dithioacetals, serve as efficient hole transporting materials in electroluminescent devices.

2338

5-Azahexenoyl radicals cyclize *via* nucleophilic addition to the acyl carbon rather than 5-*exo* homolytic addition at the imine

Chantal T. Falzon, Ilhyong Ryu and Carl H. Schiesser*



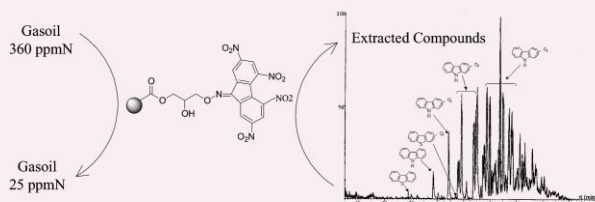
CCSD(T)/cc-pVDZ//BHLYP/cc-pVDZ

Molecular orbital calculations predict that the 5-azahexenoyl radical ring closes *via* nucleophilic addition to the acyl carbon to afford the 5-*exo* product.

2340

A new material for selective removal of nitrogen compounds from gasoils towards more efficient HDS processes

Mathieu Macaud, Emmanuelle Schulz, Michel Vrinat and Marc Lemaire*

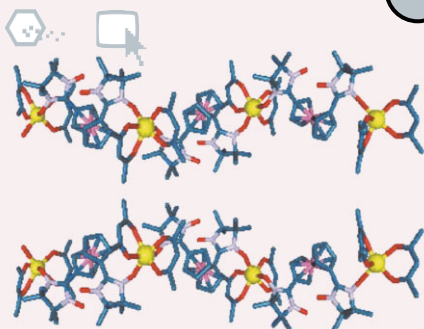


A selective removal of nitrogen compounds from gasoils is proposed, using a new recyclable material capable of forming charge-transfer complexes. The selective elimination of nitrogen species strongly improves the HDS of denitrogenated feed.

2342

Spontaneous resolution and absolute configuration of a coordination polymer formed by Mn^{II} and a ferrocene-based bisnitronyl nitroxide radical

Christian Sporer, Klaus Wurst, David B. Amabilino, Daniel Ruiz-Molina, Holger Kopacka, Peter Jaitner* and Jaume Veciana*

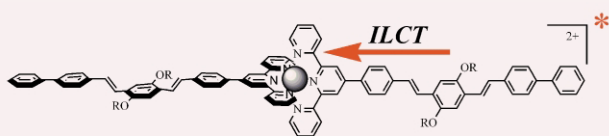


The enantiomers of a coordination polymer containing metallic and organic open-shell units with seven sources of chirality condense in different crystals forming a conglomerate, as proven by X-ray crystallography and solid state CD.

2344

Preferential solvation of an ILCT excited state in bis(terpyridine–phenylene–vinylene) Zn(II) complexes

Xian-yong Wang, André Del Guerzo and Russell H. Schmechl*

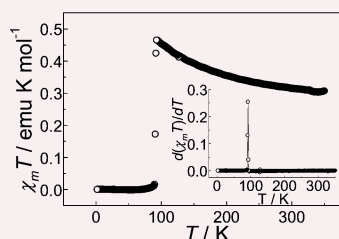


The excited state of terpyridine derivatives of phenylene–vinylene fragments chelating Zn(II) show strong solvatochromism (up to 56 nm) upon preferential solvation by polar solvents of an intraligand charge transfer state.

2346

Peculiar magnetic behavior in ion-pair complex [1-(4'-fluorobenzyl)pyridinium][Ni(mnt)₂] (mnt²⁻ = maleonitriledithiolate)

Jingli Xie, Xiaoming Ren, You Song, Wenwei Zhang, Wenlong Liu, Cheng He and Qingjin Meng*

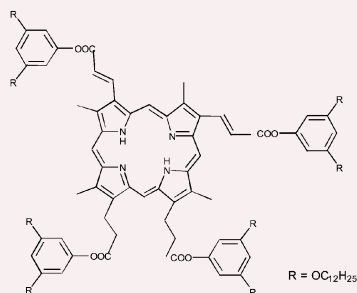


An ion-pair complex, [FBzPy][Ni(mnt)₂], forms a discrete stacking column and shows a peculiar magnetic transition from paramagnetic to diamagnetic around 90 K.

2348

The first asymmetrically β -polysubstituted porphyrin-based hexagonal columnar liquid crystal

M. Castella, F. López-Calahorra, D. Velasco* and H. Finkelmann

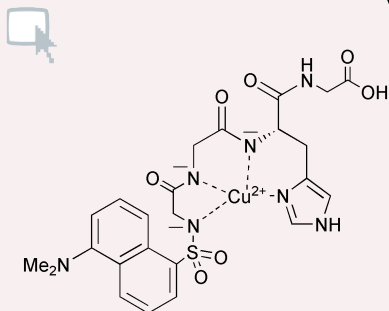


The first asymmetrically β -polysubstituted porphyrin from commercially available hemin-IX through a short synthesis is reported to present hexagonal columnar liquid crystal order over a wide range of temperatures including room temperature.

2350

A dansylated peptide for the selective detection of copper ions

Yujun Zheng, Kerim M. Gattás-Asfura, Veeranjanyulu Konka and Roger M. Leblanc*

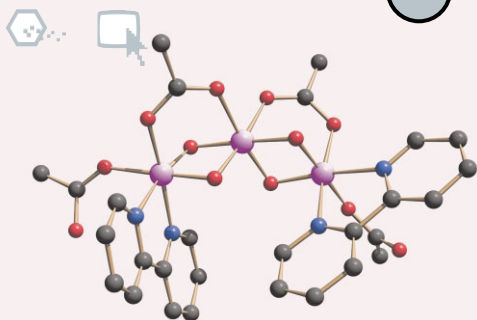


A dansyl labeled tetrapeptide, *i.e.* dansyl-gly-gly-his-gly, was synthesized and investigated as a new fluorescent chemosensor for the selective detection of copper ions in aqueous solution.

2352

Towards a synthetic model of the photosynthetic water oxidizing complex: $[Mn_3O_4(O_2CMe)_4(bpy)_2]$ containing the $[Mn^{IV}_3(\mu-O)_4]^{4+}$ core

Sumit Bhaduri, Maren Pink and George Christou*

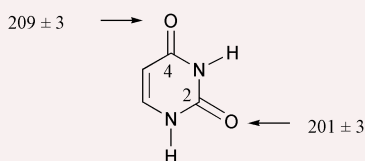


A trinuclear Mn^{IV} complex has been prepared that contains the $[Mn(\mu-O)_2Mn(\mu-O)_2Mn]^{4+}$ V-shaped core thought to occur, attached to a fourth Mn, in the photosynthetic water oxidizing complex. Magnetochemical studies establish an $S = 3/2$ ground state.

2354

The gas phase proton affinity of uracil: measuring multiple basic sites and implications for the enzyme mechanism of orotidine 5'-monophosphate decarboxylase

Mary Ann Kurinovich, Linda M. Phillips, Seema Sharma and Jeehiun K. Lee*

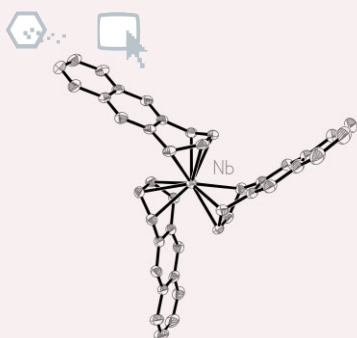


It has been shown for the first time experimentally that the O2 and O4 sites of uracil have different proton affinities, and as implied in previous computational studies, the O4 is more basic and would be energetically preferred in an orotate ribose 5'-monophosphate decarboxylase catalysis mechanism involving proton transfer to oxygen.

2356

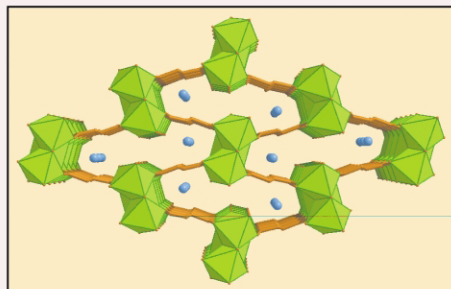
Tris(1-4- η^4 -anthracene)niobate(1-), the first polyaromatic hydrocarbon complex of niobium

William W. Brennessel, John E. Ellis,* Sergey N. Roush, Brian R. Strandberg, Oliver E. Woissetschläger and Victor G. Young Jr.



The title compound is the first isolable synthon for atomic niobium anion and promises to be a useful reagent for the general exploration of low-valent niobium chemistry.

2358



The first 3-D ferrimagnetic nickel fumarate with an open framework: $[\text{Ni}_3(\text{OH})_2(\text{O}_2\text{C}-\text{C}_2\text{H}_2-\text{CO}_2)(\text{H}_2\text{O})_4]\cdot 2\text{H}_2\text{O}$

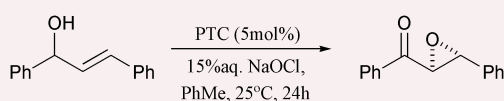
Nathalie Guillou, Sybille Pastre, Carine Livage* and Gérard Férey

This ferrimagnetic compound is the first example of an organised three-dimensional fumarate of a transition metal. It belongs to a new family of very promising co-ordination polymers which associates a 3-D iono-covalent framework and 3D magnetic interactions.

2360

Asymmetric epoxidation *via* phase-transfer catalysis: direct conversion of allylic alcohols into α,β -epoxyketones

Barry Lygo* and Daniel C. M. To

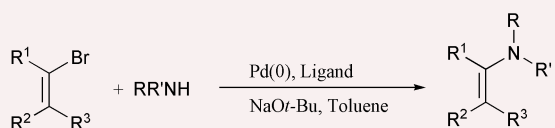


The direct oxidation of allylic alcohols to α,β -epoxyketones can be achieved with high levels of enantiomeric excess *via* chiral phase-transfer catalysts.

2362

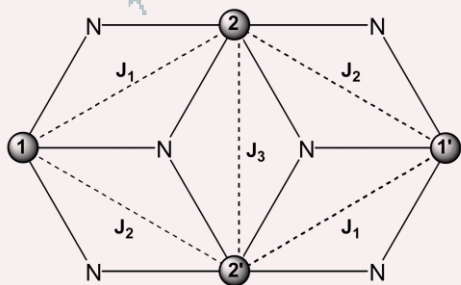
Novel method for the synthesis of enamines by palladium catalyzed amination of alkenyl bromides

José Barluenga,* M. Alejandro Fernández, Fernando Aznar and Carlos Valdés



The intermolecular palladium catalyzed cross-coupling reaction between secondary amines and alkenyl bromides is described for the first time and gives rise to enamines with very high yields and regioselectivity.

2364

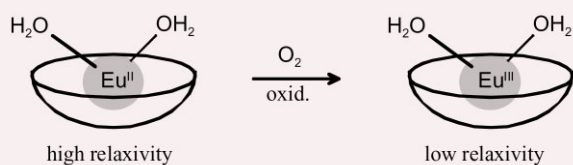


Synthesis, structure and magnetism of a new dicubane-like ferromagnetic tetranuclear nickel cluster containing versatile azido-only bridges and a bis(bidentate) Schiff base blocker

Tapan K. Karmakar, Swapan K. Chandra, Joan Ribas,* Golam Mostafa, Tian H. Lu and Barindra K. Ghosh*

A one-pot reaction of Ni(II) nitrate, sodium azide and a bis(bidentate) Schiff base results in a new dicubane-like Ni_4 cluster where versatility of azide is revealed through coordination as terminal μ_3 - and μ_2 -bridgings and global ferromagnetic exchange.

2366



Eu^{II} -cryptate with optimal water exchange and electronic relaxation: a synthon for potential pO_2 responsive macromolecular MRI contrast agents

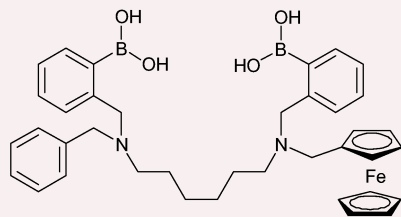
László Burai, Rosario Scopelliti and Éva Tóth*

The cryptate $[\text{Eu}^{\text{II}}(2.2.2)(\text{H}_2\text{O})_2]^{2+}$ has two inner sphere waters, optimal water exchange and electronic relaxation rates, which, together with its relative redox stability, make it a candidate for pO_2 responsive MRI contrast agent applications.

2368

A modular electrochemical sensor for saccharides

Susumu Arimori, Shin Ushiroda, Laurence M. Peter, A. Toby A. Jenkins and Tony D. James*

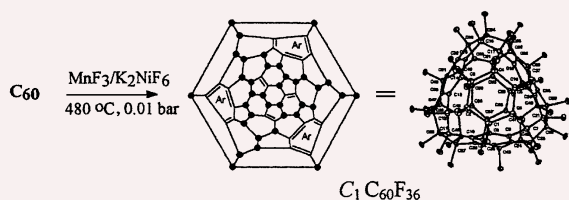


An electrochemical sensor for D-glucose has been prepared using ferrocene, two boronic acid groups and hexamethylene linker.

2370

C₆₀F₃₆: there is a third isomer and it has C₁ symmetry

Anthony G. Avent, Brian W. Clare, Peter B. Hitchcock, David L. Kepert and Roger Taylor*

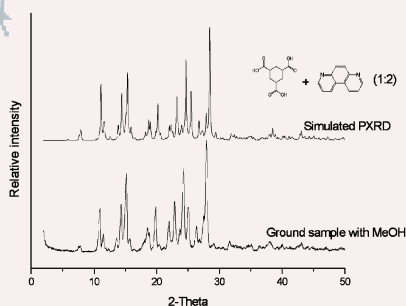


From fluorination of [60]fullerene with MnF₃/K₂NiF₆ at 480 °C we have isolated and characterised by both ¹⁹F NMR spectrum and single crystal X-ray analysis, a C₁ isomer of C₆₀F₃₆; it has three planar delocalised aromatic rings, three short C=C bonds (due to compression from the adjacent fluorines), the longest FC–CF bond (1.684 Å) yet found in a fluorofullerene, and its stability is predicted by calculations.

2372

Mechanochemistry and co-crystal formation: effect of solvent on reaction kinetics

Ning Shan, Fumio Toda and William Jones*

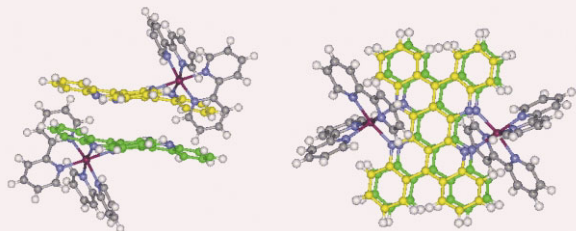


We demonstrate that significant improvements in kinetics of co-crystal formation by grinding can be achieved by the addition of minor amounts of appropriate solvent.

2374

Dibenzoeilatin: a novel ligand exhibiting remarkable complementary π–π stacking interactions

Sheba D. Bergman, Dvora Reshef, Stanislav Groysman, Israel Goldberg and Moshe Kol*

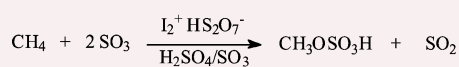


Even though dibenzoeilatin is substantially distorted from planarity, its ruthenium complex [Ru(bpy)₂(dbneil)][PF₆]₂ forms discrete dimers held by strong π–π stacking interactions due to the perfect complementarity between the stacking dibenzoeilatin moieties.

2376

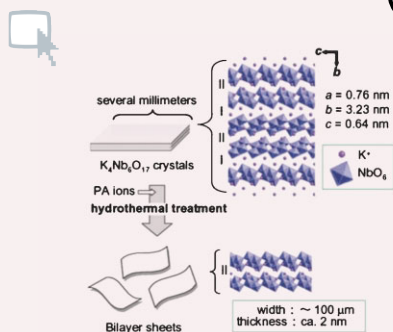
High yield conversion of methane to methyl bisulfate catalyzed by iodine cations

Roy A. Periana,* Oleg Mirinov, Douglas J. Taube and Scott Gamble



Iodine in 2% oleum is an efficient catalyst for the selective oxidation of methane to methyl bisulfate in 40% yield.

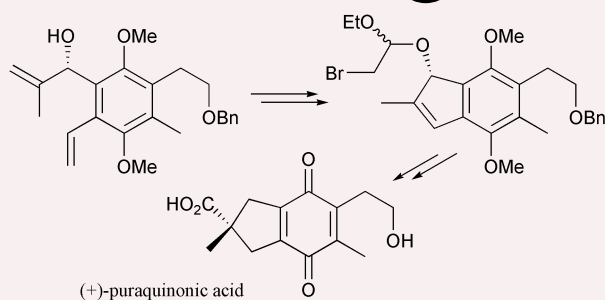
2378

**Formation of extraordinarily large nanosheets from $K_4Nb_6O_{17}$ crystals**

Nobuyoshi Miyamoto, Hisao Yamamoto, Ryozo Kaito and Kazuyuki Kuroda*

Exfoliated $K_4Nb_6O_{17}$ bilayer nanosheets in extraordinarily large size (ca. $100 \mu m$) were prepared by the direct reaction of $K_4Nb_6O_{17} \cdot 3H_2O$ crystals with an aqueous solution of propylamine; the size was extremely larger than that of exfoliated nanosheets (several μm) reported previously.

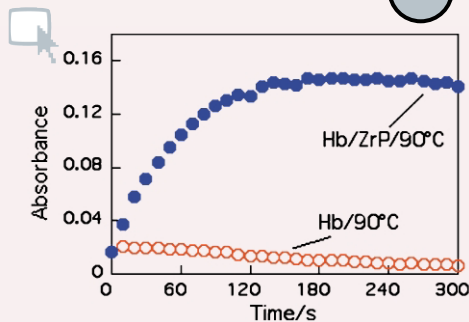
2380

**Synthesis of (+)-puraquinonic acid**

Derrick L. J. Clive* and Maolin Yu

An asymmetric aldol reaction is used to make the starting alcohol shown; the hydroxy controls the absolute stereochemistry of the quaternary center, and is then removed, leading ultimately to (+)-puraquinonic acid, enantiomeric with natural material.

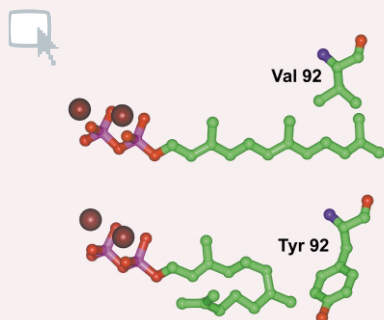
2382

**High temperature peroxidase activities of HRP and hemoglobin in the galleries of layered Zr(IV)phosphate**

C. V. Kumar* and A. Chaudhari

High temperature peroxidase-like activity of hemoglobin intercalated in the galleries of alpha-Zr(IV) phosphate.

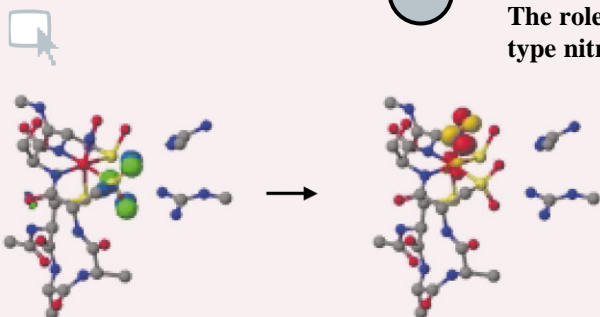
2384

**Tyrosine 92 of aristolochene synthase directs cyclisation of farnesyl pyrophosphate**

Melanie J. Calvert, Susan E. Taylor and Rudolf K. Allemann*

The bulkiness of Tyr 92 of Aristolochene Synthase is critical for cyclisation of farnesyl pyrophosphate and the prevention of β -(E)-farnesene formation.

2386

**The role of post-translational modification in the photoregulation of Fe-type nitrile hydratase**

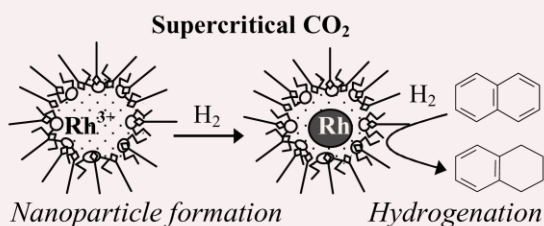
Shannon N. Greene, Christopher H. Chang and Nigel G. J. Richards*

DFT and INDO/S calculations are consistent with the hypothesis that post-translational modifications in Fe-type nitrile hydratase play a key role in the photoregulation of the enzyme by nitric oxide.

2388

Catalytic hydrogenation of arenes with rhodium nanoparticles in a water-in-supercritical CO₂ microemulsion

Mariko Ohde, Hiroyuki Ohde and Chien M. Wai*

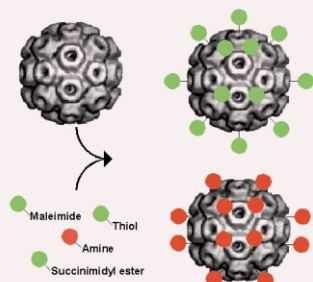


Rhodium nanoparticles dispersed by a CO₂ microemulsion are effective catalysts for rapid hydrogenation of arenes in supercritical CO₂.

2390

Chemical modification of a viral cage for multivalent presentation

Eric Gillitzer, Debbie Willits, Mark Young* and Trevor Douglas*

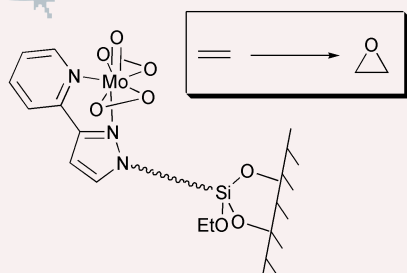


Here we present methods exploiting the chemistry of engineered, or native, exposed functional groups for modifying the surface of a viral protein cage.

2392

Oxidiperoxo molybdenum modified mesoporous MCM-41 materials for the catalytic epoxidation of cyclooctene

Mingjun Jia and Werner R. Thiel*

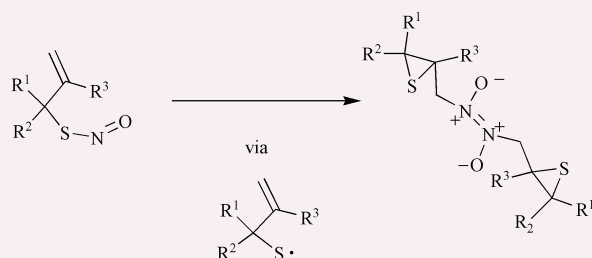


MCM-41 grafted oxidiperoxo molybdenum complexes are highly active heterogeneous catalysts for cyclooctene epoxidation and show no leaching into the liquid-phase.

2394

Thioepoxide formation by ring closure of allylthiyl radicals—a novel rearrangement of allylic thionitrites

Marta Cavero, William B. Motherwell,* Pierre Potier and Jean-Marc Weibel

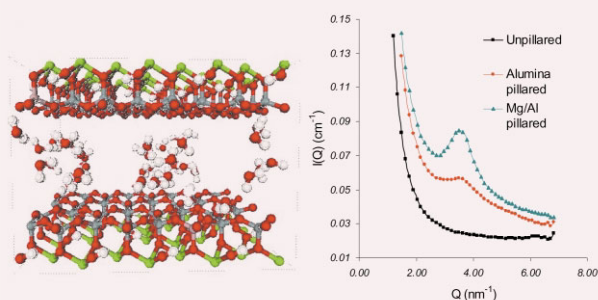


The first examples involving ring closure of an allylthiyl radical to a thioepoxide are described.

2396

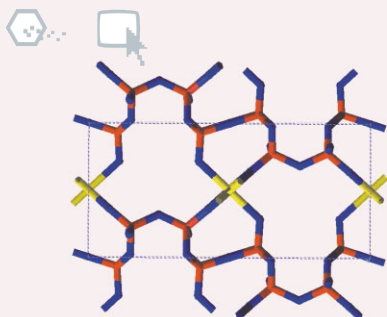
Characterisation of pillared clays by contrast-matching small-angle neutron scattering

Th. A. Steriotis,* K. L. Stefanopoulos, U. Keiderling, A. De Stefanis and A. A. G. Tomlinson



Contrast matching SANS has been applied to independently resolve the structure of each phase in alumina PILCs. Interpillar distances in montmorillonite PILCs differ compared with beidellite PILCs

2398

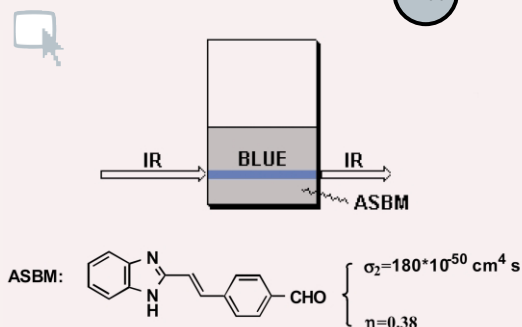


Synthesis of a new open framework cerium silicate and its structure determination by single crystal X-ray diffraction

Hae-Kwon Jeong, Annamalai Chandrasekaran and Michael Tsapatsis*

Framework structure of a new cerium silicate (red: silicon, blue: oxygen, yellow: cerium).

2400

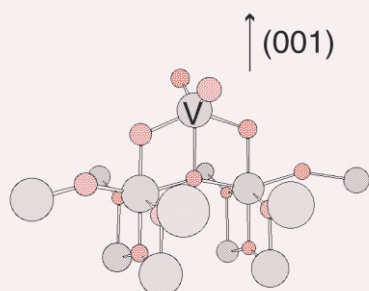


Two-photon induced blue fluorescent emission of heterocycle-based organic molecule

Z. L. Huang, N. Li, H. Lei, Z. R. Qiu, H. Z. Wang,* Z. P. Zhong and Z. H. Zhou

An organic molecule based on a heterocycle acceptor has been found to exhibit an intensive two-photon induced blue emission ($\eta = 0.38$) and a large two-photon absorption cross section ($\sigma_2 = 180 \times 10^{-50} \text{ cm}^4 \text{ s}$ at 780 nm), which implies that the molecule is a promising candidate for an application such as multi-channel two-photon microscopy.

2402

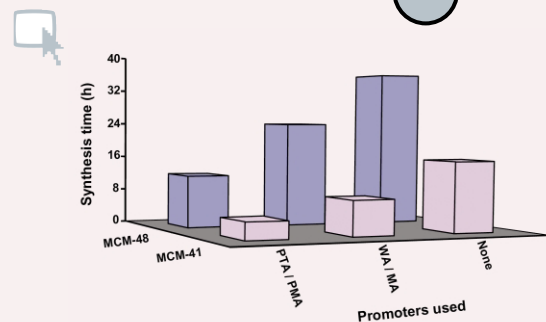


Structure of low concentrations of vanadium on TiO₂ determined by XANES and *ab initio* calculations

Yasuo Izumi,* Fumitaka Kiyotaki, Hideaki Yoshitake, Ken-ichi Aika, Tae Sugihara, Takashi Tatsumi, Yasuhiro Tanizawa, Takafumi Shido and Yasuhiro Iwasawa

The major local structure of low concentrations (1–3 wt% V) of vanadium on TiO₂ was determined to have two terminal oxo groups and in total five oxygen coordination by XANES combined with fluorescence spectrometry and *ab initio* calculations of XANES spectra.

2404

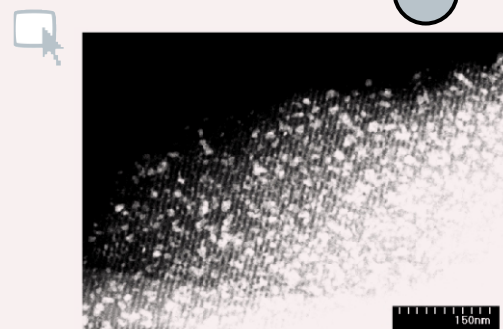


Heteropolyacids aided rapid and convenient syntheses of highly ordered MCM-41 and MCM-48: exploring the accelerated process by ²⁹Si MAS NMR and powder X-ray diffraction studies

Kausik Mukhopadhyay,* Anirban Ghosh and Rajiv Kumar*

A rapid and convenient route is reported for the synthesis of highly ordered Si-MCM-41 and Si-MCM-48, wherein catalytic amounts of heteropolyacids reduce the syntheses times by 3 to 4 fold.

2406



Uniform formation of uranium oxide nanocrystals inside ordered mesoporous hosts and their potential applications as oxidative catalysts

Z. T. Zhang, M. Konduru, S. Dai* and S. H. Overbury*

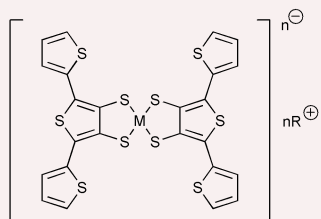
Highly dispersed uranium oxide nanocrystal catalysts supported on ordered mesoporous silica matrixes with large surface areas and porosities have been synthesized *via* a co-assembly methodology.

2408

A new family of conjugated metallopolymer from electropolymerised bis[(terthiophene)dithiolene] complexes

Cristina Pozo-Gonzalo, Rory Berridge, Peter J. Skabara,* Elena Cerrada, Mariano Laguna, Simon J. Coles and Michael B. Hursthouse

M = Ni(II), R = Bu_nN, n = 2
 M = Pd(II), R = Et_nN, n = 2
 M = Au(III), R = PPN, n = 1
 M = Au(III), R = Bu_nN, n = 1

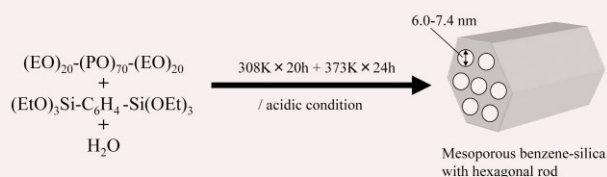


A novel series of bis(dithiolene) metal complexes incorporating fused terthiophene units have been prepared. All new complexes can be polymerised electrochemically and the nickel analogue affords a low bandgap material with very broad absorption characteristics.

2410

Synthesis of large-pore phenylene-bridged mesoporous organosilica using triblock copolymer surfactant

Yasutomo Goto and Shinji Inagaki*

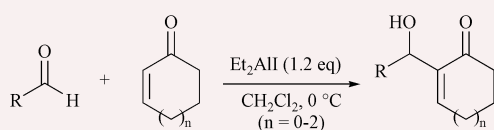


Periodic mesoporous benzene-silicas with large pores of 6.0 to 7.4 nm in diameter are synthesized using triblock copolymer as a template. These mesoporous materials have a well-defined hexagonal rod morphology and high thermal stability up to 823 K in air.

2412

The Baylis–Hillman condensation of α,β -conjugate cycloketones with aldehydes using diethylaluminum iodide alone as the promoter

Wei Pei, Han-Xun Wei and Guigen Li*

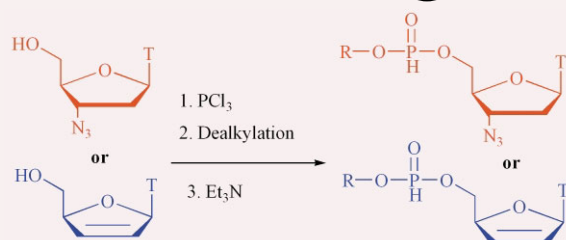


Effective Baylis–Hillman-type reaction of α,β -conjugate cycloketones with aldehydes proceeded in the presence of Et₂AlI as the promoter without the direct use of any Lewis bases (53–72% yields, 7 examples).

2414

One-pot synthesis of hydrogen phosphonate derivatives of d4T and AZT

Xiao Bin Sun, Jian Xun Kang and Yu Fen Zhao*



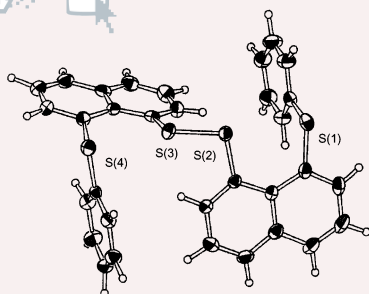
T = thymine R = ethyl, isopropyl, t-butyl, cyclohexyl, benzyl

A simple and one-pot route for the synthesis of d4T or AZT hydrogen phosphonate derivatives *via* reaction of d4T or AZT with phosphorus trichloride, then alcoholysis and dealkylation in the presence of the corresponding alcohol is described.

2416

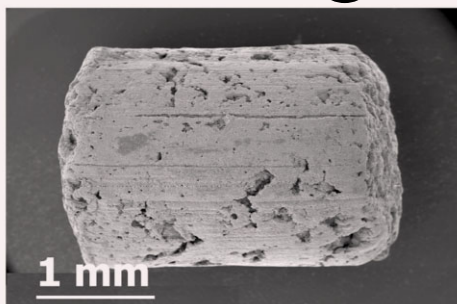
Linear alignment of four sulfur atoms in bis[(8-phenylthio)naphthyl] disulfide: contribution of linear S₄ hypervalent four-centre six-electron bond to the structure

Warô Nakanishi,* Satoko Hayashi and Takamitsu Arai



The four sulfur atoms in bis[8-(phenylthio)naphthyl]-1,1'-disulfide are demonstrated to align linearly by X-ray crystallographic analysis, where the linear S₄ alignment is stabilized by the nonbonded four-centre six-electron interaction.

2418



Beta zeolite supported on a macroscopic pre-shaped SiC as a high performance catalyst for liquid-phase benzoylation

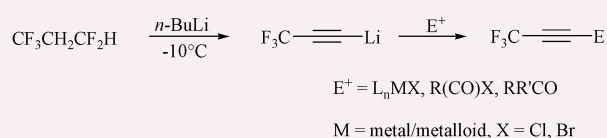
G. Winé, J. P. Tessonnier, C. Pham-Huu* and M. J. Ledoux

Preparation and characterisation of a highly active and stable beta zeolite supported on a pre-shaped silicon carbide catalyst for the benzoylation reaction in liquid phase.

2420

Hydrofluorocarbon 245fa: a versatile new synthon in alkyne chemistry

Alan K. Brisdon* and Ian R. Crossley

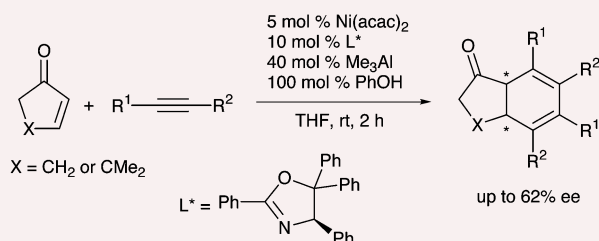


A novel synthetic route to organic, inorganic and organometallic systems containing the trifluoropropynyl group utilises hydrofluorocarbon 245fa (1,1,1,3,3-pentafluoropropane, $\text{CF}_3\text{CH}_2\text{CF}_2\text{H}$) as a convenient synthon. Mild conditions are employed in an expedient and economical one-pot procedure, based on the intermediacy of trifluoropropynyllithium.

2422

Catalytic enantioselective intermolecular [2 + 2 + 2] cycloaddition of an alkene and two alkynes

Shin-ichi Ikeda,* Hirokazu Kondo, Taro Arie and Kazunori Odashima

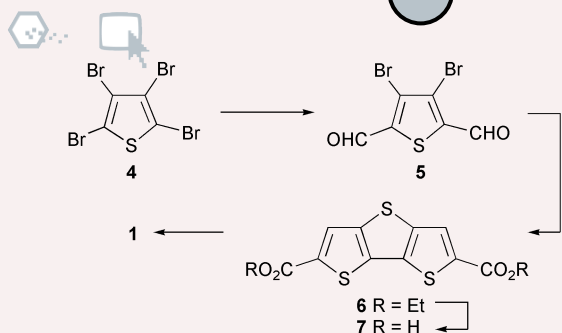


The first catalytic enantioselective *intermolecular* [2 + 2 + 2] cycloaddition of an alkene and two alkynes was developed in the presence of a nickel complex modified by monodentate oxazolines and an aluminium phenoxide.

2424

Improved synthesis of dithieno[3,2-*b*:2',3'-*d*]thiophene (DTT) and derivatives for cross coupling

Joseph Frey,* Andrew D. Bond and Andrew B. Holmes*

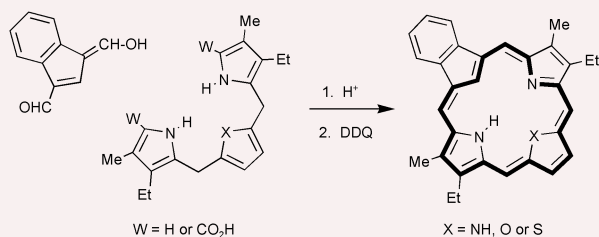


Improved synthesis of dithieno[3,2-*b*:2',3'-*d*]thiophene (DTT) and derivatives for cross coupling.

2426

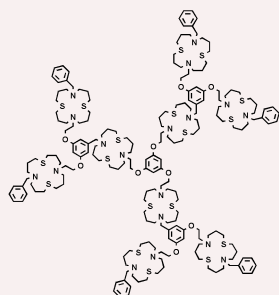
Synthesis, spectroscopy and metallation of mixed carbaporphyrinoid systems

Dachun Liu and Timothy D. Lash*



Modified tripyrranes were shown to condense with pyridine, benzene and indene dialdehydes to give a series of aromatic porphyrinoids, including oxa- and thia-carbaporphyrins; the former was readily converted into the corresponding nickel(II) and palladium(II) organometallic derivatives.

2428

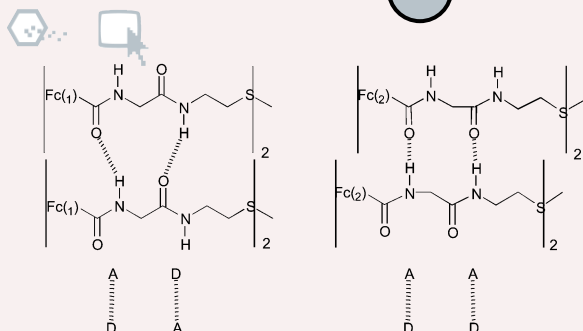
A second generation dendrimer incorporating nine S₂N₂-donor macrocycles and its palladium(II) complexIan M. Atkinson, Jy D. Chartres, Andrew M. Groth, Leonard F. Lindoy,*
Mark P. Lowe and George V. Meehan*

A new second generation dendrimer incorporating nine S₂N₂-donor macrocyclic units has been synthesised and demonstrated to coordinate to a total of nine Pd(II) cations.

2430

Ferrocenoyl glycylycystamine: organization into a supramolecular helicate structure

Irene Bediako-Amoa, Roberta Silerova and Heinz-Bernhard Kraatz*

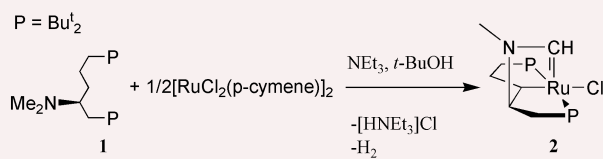


The synthesis of a ferrocene-peptide conjugate is reported, which exhibits intermolecular hydrogen bonding between adjacent peptide chains leading to the formation of an unprecedented supramolecular double helicate having two different H-bonding patterns.

2432

Triple C–H activation of 1,5-bis(di-*tert*-butylphosphino)-2-(*S*)-dimethylaminopentane on ruthenium gives a chiral carbene complex

Vladimir F. Kuznetsov, Alan J. Lough and Dmitry G. Gusev*

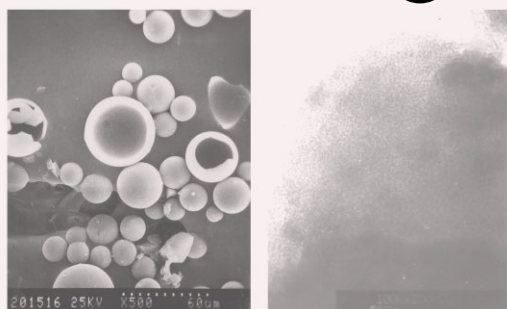


This communication reports the preparation of a novel *trans*-chelating diphosphine, 1,5-bis(di-*tert*-butylphosphino)-2-(*S*)-dimethylaminopentane (**1**), that undergoes triple C–H activation in reaction with [RuCl₂(*p*-cymene)]₂ to give a chiral square-pyramidal 16-electron carbene complex **2**.

2434

Synthesis of stable hollow silica microspheres with mesoporous shell in nonionic W/O emulsion

Wenjiang Li, Xiaoxiang Sha, Wenjun Dong and Zichen Wang*

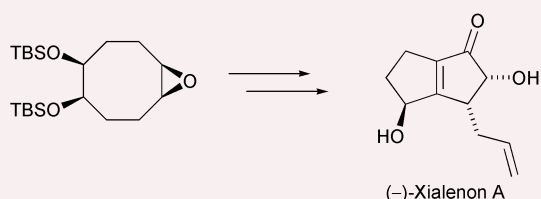


Stable hollow silica microspheres were synthesized by a sol-gel method in nonionic W/O emulsion. The mesoporous shell wall of the spheres could have potential applications as controlled release capsules for drugs, dyes, cosmetics and inks, artificial cells, catalysts, and fillers.

2436

Enantioselective total synthesis of (–)-xialenon A

David M. Hodgson,* Jean-Marie Galano and Martin Christlieb

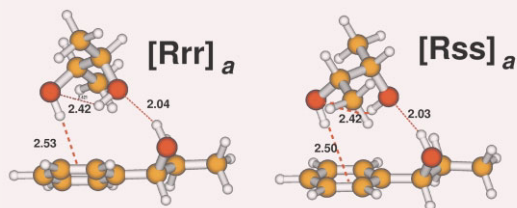


(–)-Xialenon A is synthesised *via* enantioselective transannular desymmetrisation of a substituted cyclooctene epoxide.

2438

Chiral discrimination of 2,3-butanediols by laser spectroscopy

D. Scuderi, A. Paladini, S. Piccirillo, M. Satta, D. Catone, A. Giardini, A. Filippi and M. Speranza*

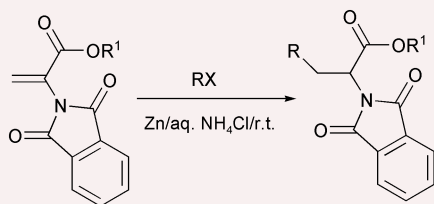


The 1cR2PI/TOF technique has been applied for the first time to structurally discriminate all the isomers—diastereomers and enantiomers—of 2,3-butanediol through the spectroscopic analysis of their supersonically expanded van der Waals complexes with a chiral chromophore, *i.e.* *R*-(+)-1-phenyl-1-propanol. It has been shown that the spectral signatures of these isomeric complexes critically depend upon conformation and the configuration of the diol moiety.

2440

Synthesis of α -amino acid derivatives and amines *via* activation of simple alkyl halides by zinc in water

Taisheng Huang, Charlene C. K. Keh and Chao-Jun Li*

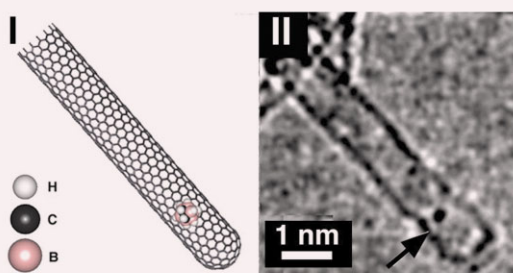


A simple synthesis of α -amino acids and amines is developed *via* Zn-mediated addition of alkyl iodides and bromides to enamides and imines in aqueous NH_4Cl .

2442

Direct imaging of *o*-carborane molecules within single walled carbon nanotubes

David A. Morgan, Jeremy Sloan* and Malcolm L. H. Green*

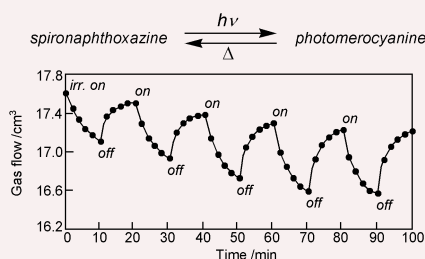


Treatment of single walled carbon nanotubes (SWNTs) with *o*-carborane at 350 °C results in the encapsulation of discrete molecules (I and II) and 'zig-zag' chains which may be directly imaged by transmission electron microscopy.

2444

Light-controlled gas permeability of mesoporous silica glass bearing photochromic spironaphthoxazine on its surface

Shigeyuki Yagi,* Naemi Minami, Junpei Fujita, Yutaka Hyodo, Hiroyuki Nakazumi,* Tetsuo Yazawa, Tetsuro Kami and Aliyar Hyder Ali

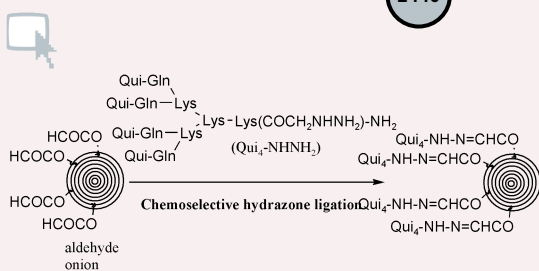


The gas permeability of photochromic spironaphthoxazine-appended mesoporous silica glass was controlled by photo-irradiation.

2446

Grafting of synthetic mannose receptor-ligands onto onion vectors for human dendritic cells targeting

Pascale Chenevier,* Cyrille Grandjean, Estelle Loing, Frédéric Malingue, Gerhild Angyalosi, Hélène Gras-Masse, Didier Roux, Oleg Melnyk and Line Bourel-Bonnet

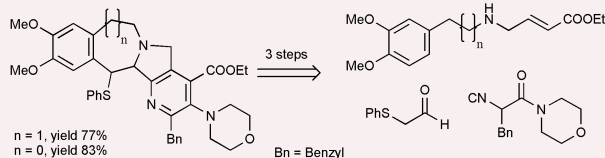


The first successful grafting of molecular addresses onto the surface of an onion vector has been realized adopting a hydrazone chemoselective ligation.

2448

Rapid access to tetracyclic ring system of lennoxamine type natural product by combined use of a novel three-component reaction and Pummerer cyclization

Rocio Gámez Montaña and Jieping Zhu*

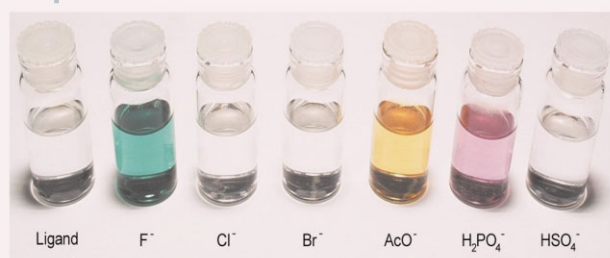


A three-step synthesis of tetracyclic compounds from readily available starting materials is reported.

2450

A selective colorimetric anion sensor based on an amide group containing macrocycle

Piotr Piątek and Janusz Jurczak*

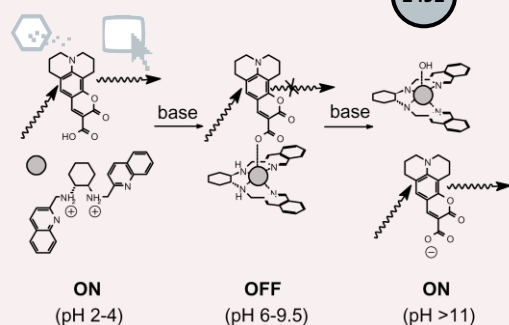


A new colorimetric pendant-arm macrocyclic anion sensor allows for selective 'naked-eye' differentiation of F^- , AcO^- and $H_2PO_4^-$ with similar basicity.

2452

'On-off-on' fluorescent indicators of pH windows based on three separated components

Piersandro Pallavicini,* Valeria Amendola, Chiara Massera, Etienne Mundum and Angelo Taglietti

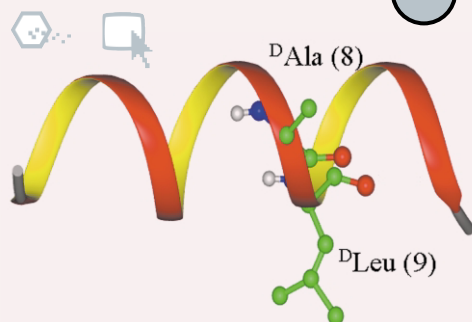


New 'on-off-on' fluorescent indicators for pH windows are obtained with ternary systems in which the three separated components are Cu^{2+} , a tetraaza ligand and the fluorophore Coumarin 343.

2454

A right handed peptide helix containing a central double D-amino acid segment

Subrayashastry Aravinda, Narayanaswamy Shamala,* Shrilakshmi Desiraju and Padmanabhan Balaram*

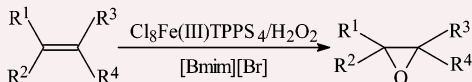


The crystal structure of the 13 residue peptide Boc-Leu-Aib-Val-Ala-Leu-Aib-Val- $DAla$ - $DLeu$ -Aib-Leu-Aib-Val-OMe reveals a continuous right handed helix, despite the centrally positioned double D-segment.

2456

Epoxidation of alkenes with hydrogen peroxide catalyzed by iron(III) porphyrins in ionic liquids

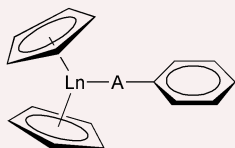
K. A. Srinivas, Anil Kumar and S. M. S Chauhan*



An efficient procedure is described for catalyst recycling and easy product isolation in alkene epoxidation with hydrogen peroxide catalyzed by water-soluble iron(III) porphyrin in environmentally benign and ambient temperature ionic liquids.

Are metal alkoxides linear owing to electrostatic repulsion?

Maria Rosa Russo, Nikolas Kaltsoyannis* and Andrea Sella



Density functional calculations have been used to probe the electronic and geometric structures of $[\text{LnCp}_2\text{APh}]$ ($\text{Ln} = \text{La}, \text{Lu}$; $\text{Cp} = \eta^5\text{-C}_5\text{H}_5$; $\text{A} = \text{O}, \text{S}$; $\text{Ph} = \text{C}_6\text{H}_5$) and suggest that the linearity of the Ln-O-Ph vector may have an unusually simple origin.

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