

ChemComm

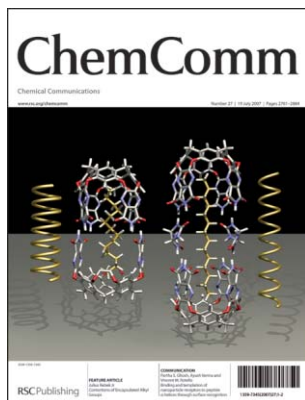
Chemical Communications

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IN THIS ISSUE

ISSN 1359-7345 CODEN CHCOFS (27) 2761–2884 (2007)



Cover

See Julius Rebek Jr, page 2777. A spring-loaded capsule: The cylindrical capsule on the left entices *n*-tetradecane inside where it assumes a helical conformation. This arrangement maximizes close contacts and loads the capsule with an alkane of compressed dimensions and high potential energy. The insertion of glycouril spacers gives the new extended capsule on the right, and liberates this energy as the alkane relaxes into an extended conformation. (Some atoms omitted for clarity.) Image by Dr. Michael Schramm and reproduced by permission of Julius Rebek Jr, *Chem. Commun.*, 2007, 2777.



Inside cover

See Stefano Zampolli, Paolo Betti, Ivan Elmi and Enrico Dalcanale, page 2790. A supramolecular approach to sub-ppb aromatic VOC detection in air. Image reproduced by permission of Stefano Zampolli, Paolo Betti, Ivan Elmi and Enrico Dalcanale, *Chem. Commun.*, 2007, 2790.

CHEMICAL SCIENCE

C49

Drawing together the research highlights and news from all RSC publications, *Chemical Science* provides a 'snapshot' of the latest developments across the chemical sciences showcasing newsworthy articles, as well as the most significant scientific advances.

Chemical Science

July 2007/Volume 4/Issue 7

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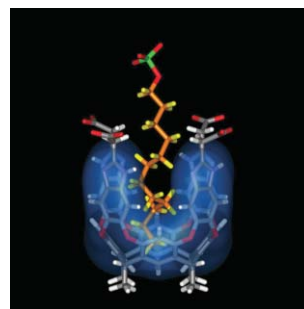
FEATURE ARTICLE

2777

Contortions of encapsulated alkyl groups

Julius Rebek, Jr.*

The binding of alkyl groups in cavitands or capsules follows a fluid model of recognition rather than lock-and-key or induced fit: the guest assumes the shape that best fills the available space, even if contortions to higher energy conformations are required.



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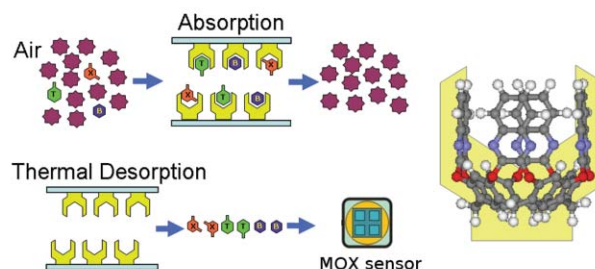
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2790

A supramolecular approach to sub-ppb aromatic VOC detection in air

Stefano Zampolli,* Paolo Betti, Ivan Elmi and Enrico Dalcanale*

A new sensing device for sub-ppb detection of aromatic volatile organic compounds (VOC) in air is reported, in which high selectivity and extremely low sensitivity are obtained by coupling a supramolecular concentration unit to a silicon-integrated Metal Oxide (MOX) detector.

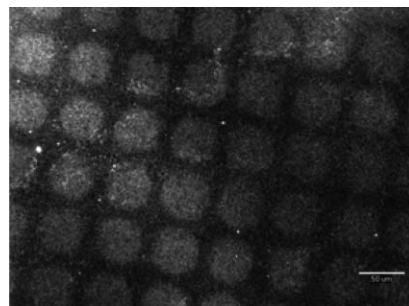


2793

Photografting and patterning of oligonucleotides on benzophenone-modified boron-doped diamond

Sabine Szunerits,* Naoto Shirahata, Paolo Actis, Jun Nakanishi and Rabah Boukherroub

Irradiation of a patterned benzophenone-terminated boron-doped diamond (BDD) surface with UV light ($\lambda = 350$ nm) in the presence of a 15^{mer} oligonucleotide resulted in the covalent linking of the DNA strand to the BDD interface.

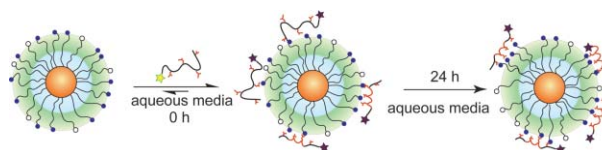


2796

Binding and templation of nanoparticle receptors to peptide α -helices through surface recognition

Partha S. Ghosh, Ayush Verma and Vincent M. Rotello*

Nanoparticles featuring highly flexible chains provide templateable surfaces for recognition of peptides.

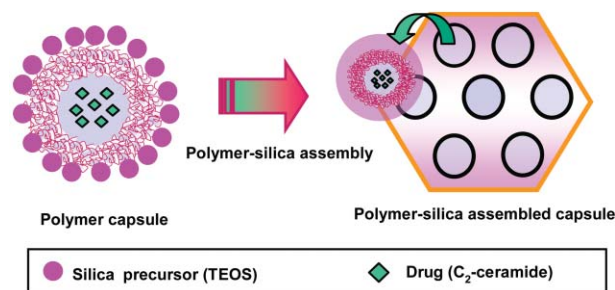


2799

One-pot synthetic route to polymer-silica assembled capsule encased with nonionic drug molecule

You-Hwan Son, Man park, Young Bin Choy, Hye Ryung Choi, Dong Seok Kim, Kyoung Chan Park and Jin-Ho Choy*

A novel combinational drug delivery system (DDS) of soft (polymer) and hard (inorganic) vehicles was prepared *via* a simple one-pot synthesis, which showed an improved chemotherapeutic efficacy of a model drug.



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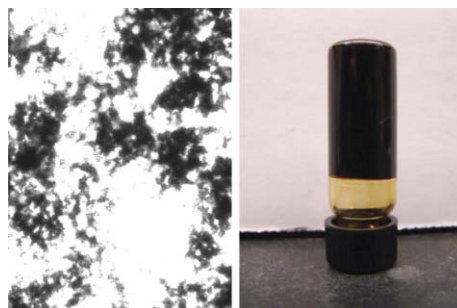
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2802

Coordination polymer gels: synthesis, structure and mechanical properties of amorphous coordination polymers

Brian S. Luisi, Kevin D. Rowland and Brian Moulton*

Ligand exchange reactions between Mn_{12} -single molecule magnets and poly-carboxylate ligands yield amorphous, highly porous coordination polymer gels, a new class of coordination polymer based materials that exhibit ligand dependent mechanical properties.

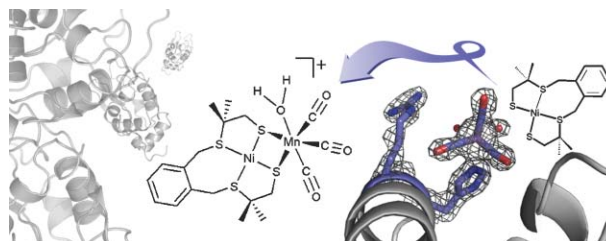


2805

Tricarbonylmanganese(I)-lysozyme complex: a structurally characterized organometallic protein

Mathieu Razavet, Vincent Artero,* Christine Cavazza,* Yohan Oudart, Colette Lebrun, Juan Carlos Fontecilla-Camps and Marc Fontecave

The reaction of the new and structurally characterized covalent $\{Mn(CO)_3(H_2O)_2\}^+$ -lysozyme adduct with NiS_4 and NiN_2S_2 complexes generates binuclear Ni-Mn complexes.

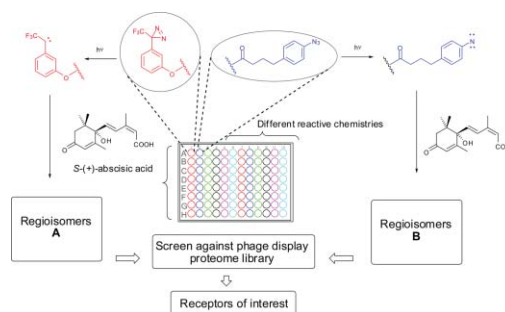


2808

A photoimmobilisation strategy that maximises exploration of chemical space in small molecule affinity selection and target discovery

Suzanne J. Dilly, Matthew J. Bell, Andrew J. Clark, Andrew Marsh,* Richard M. Napier, Martin J. Sergeant, Andrew J. Thompson and Paul C. Taylor*

The authors show that the use of multiple photochemistries is necessary to ensure diverse immobilisation of small molecules for selective binding of polypeptides using phage display and antibody libraries.

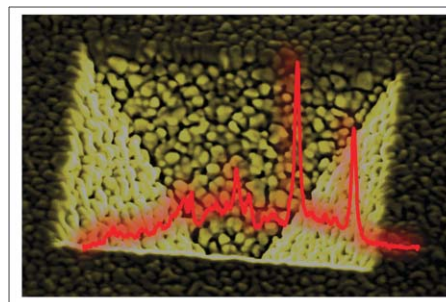


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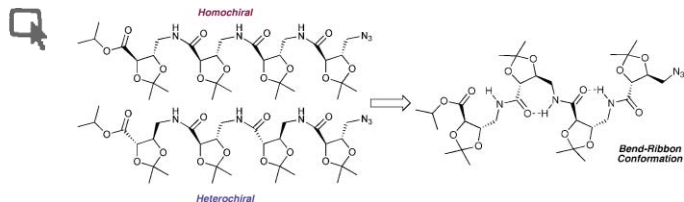
Highly sensitive detection of dye-labelled DNA using nanostructured gold surfaces

Robert J. Stokes, Alexandra Macaskill, Jennifer A. Dougan, Philip G. Hargreaves, Helen M. Stanford, W. Ewen Smith, Karen Faulds and Duncan Graham*

Careful control of surface chemistry results in a strong SERRS response from dye-labelled oligonucleotides assembled on nanostructured gold surfaces.



2814

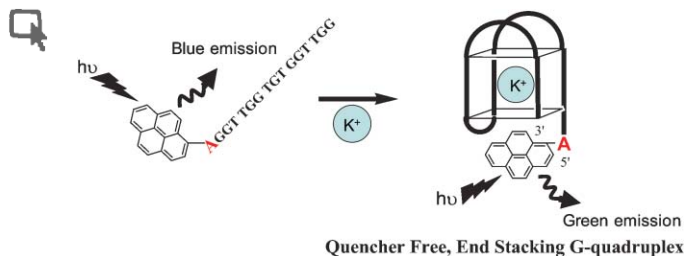


Bend-ribbon forming γ -peptides

Abhishek Kothari, M. Khurram N. Qureshi, Elizabeth M. Beck and Martin D. Smith*

Homo- and heterochiral tetrameric γ -peptide derivatives in which the backbone is constrained by a five-membered ring populate a bend-ribbon conformation in solution stabilized by intramolecular hydrogen bonds.

2817

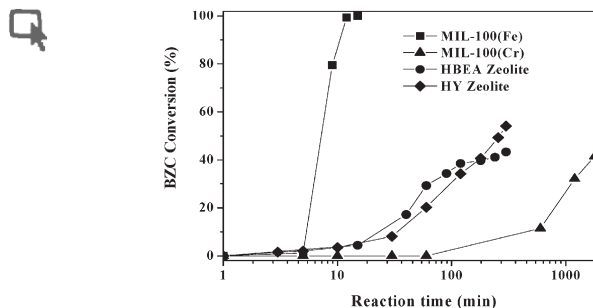


Probing the stable G-quadruplex transition using quencher-free end-stacking ethynyl pyrene-adenosine

Young Jun Seo, Il Joon Lee, Jeong Wu Yi and Byeang Hyeon Kim*

Pyrene-modified adenosines in the dangling positions of G-rich oligodeoxynucleotides undergo π -stacking in their G-quadruplex formation, but not in their single strands, which can be characterized by fluorescence λ_{\max} changes that occur on stacking.

2820



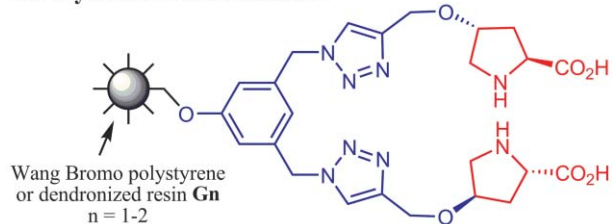
Synthesis and catalytic properties of MIL-100(Fe), an iron(III) carboxylate with large pores

Patricia Horcajada, Suzy Surblé, Christian Serre,* Do-Young Hong, You-Kyong Seo, Jong-San Chang, Jean-Marc Grenèche, Irene Margiolaki and Gérard Férey

The large-pore iron(III) carboxylate MIL-100(Fe) has been isolated and its structure solved from X-ray powder diffraction data. Friedel-Crafts benzylation catalytic tests indicate a high activity and selectivity for MIL-100(Fe).

2823

Heterogeneous catalyst for asymmetric aldol reaction



Polymer-supported proline-decorated dendrons: dendritic effect in asymmetric aldol reaction

Tzofit Kehat and Moshe Portnoy*

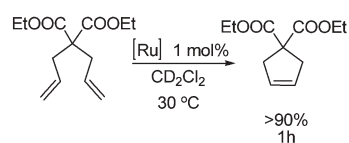
A dendritic/branched interface between a solid support and catalytic proline units remarkably enhances the activity and enantioselectivity of the catalytic system in asymmetric aldol reaction.

2826

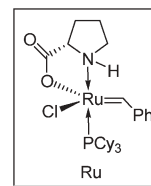
Bidentate *N,O*-prolinate ruthenium benzylidene catalyst highly active in RCM of disubstituted dienes

Joseph S. M. Samec and Robert H. Grubbs*

Catalyst shows high activity in ring-closing metathesis of functionalized disubstituted dienes.



Catalyst shows high activity in ring-closing metathesis of functionalized disubstituted dienes

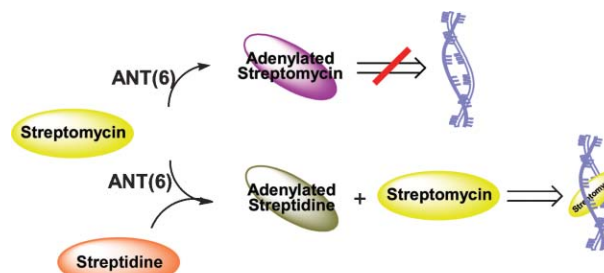


2829

Rescue of the streptomycin antibiotic activity by using streptidine as a “decoy acceptor” for the aminoglycoside-inactivating enzyme adenyl transferase

Montserrat Latorre, Pablo Peñalver, Julia Revuelta, Juan Luis Asensio, Eduardo García-Junceda* and Agatha Bastida*

The use of streptidine as a “decoy acceptor” allows the antibiotic activity of streptomycin to recover against the *E. coli* strain overexpressing the aminoglycoside-modifying enzyme 6-O-adenyl transferase from *Bacillus subtilis*.

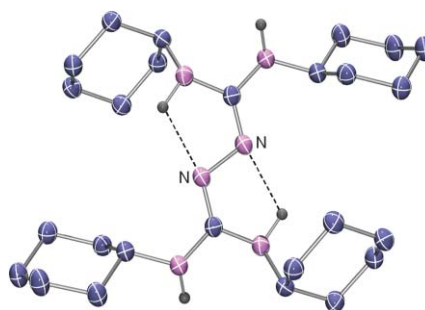


2832

The first urea azine molecule and its coordination to uranium in the first actinide guanidinate complexes

Claude Villiers, Pierre Thuéry and Michel Ephritikhine*

The urea azine molecule $(\text{CyNH})_2\text{C}=\text{N}-\text{N}=\text{C}(\text{HNCy})_2$ (**1**) was prepared by reaction of the carbodiimide $\text{CyN}=\text{C}=\text{NCy}$ and H_2NNH_2 ; this novel type of bis-guanidine proved useful for the building of polynuclear compounds, as illustrated by the synthesis of the tetra- and hexanuclear uranium guanidinate complexes $[(\text{THF})_2\text{Li}(\mu\text{-Cl})_2\text{UCl}(\mu\text{-L})_2]$ and $[\text{UCl}(\mu\text{-L})_2\text{UCl}_2(\mu\text{-Cl})_2\text{UCl}(\mu\text{-L})_2]$ ($\text{L} = \mathbf{1} - \mathbf{2H}$).

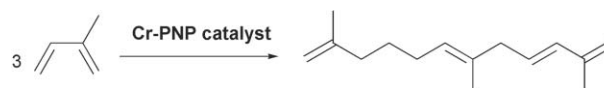


2835

The selective trimerisation of isoprene with chromium *N,N*-bis(diarylphosphino)amine catalysts

Lucy E. Bowen, Manutsavin Charernsuk and Duncan F. Wass*

Chromium catalysts supported by *N,N*-bis(diarylphosphino)amine ligands, on activation with methyl aluminoxane (MAO), selectively trimerise isoprene to predominantly linear materials.



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TOF: >500 h⁻¹

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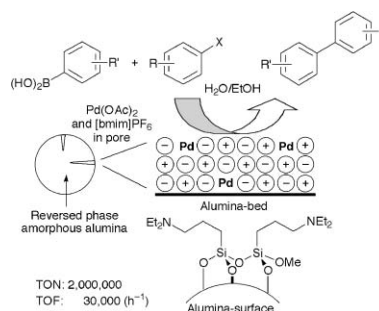
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2838

Supported ionic liquid catalyst (Pd-SILC) for highly efficient and recyclable Suzuki–Miyaura reaction

Hisahiro Hagiwara,* Keon Hyeok Ko, Takashi Hoshi and Toshio Suzuki

Palladium acetate immobilized on reversed phase alumina with the aid of [bmim]PF₆, was highly efficient to promote the Suzuki–Miyaura reaction in aqueous EtOH without a ligand up to a 5th re-use in 95% average yield with TON and TOF of 2×10^6 and 3×10^4 (h⁻¹), respectively.

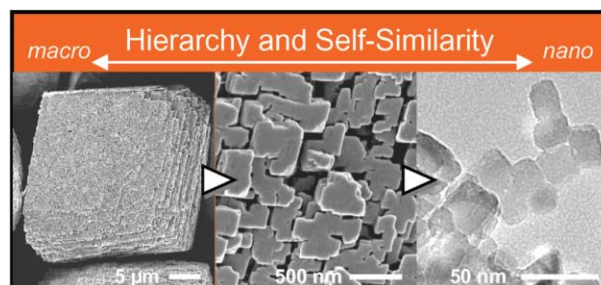


2841

A hierarchical self-similar structure of oriented calcite with association of an agar gel matrix: inheritance of crystal habit from nanoscale

Yuya Oaki, Shinichiro Hayashi and Hiroaki Imai*

Calcite crystals grown with association of an organic gel matrix led to the generation of a hierarchical, self-similar architecture possessing rhombohedral habit under ambient conditions.

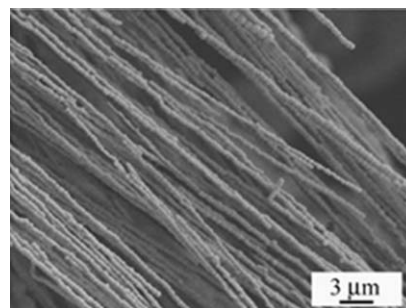


2844

Formation of one-dimensional nickel wires by chemical reduction of nickel ions under magnetic fields

Lixia Sun, Qianwang Chen,* Yan Tang and Ying Xiong

The magnetic fields applied during the chemical reduction of nickel ions can synchronously influence both the nucleation and the parallel growth of nickel.

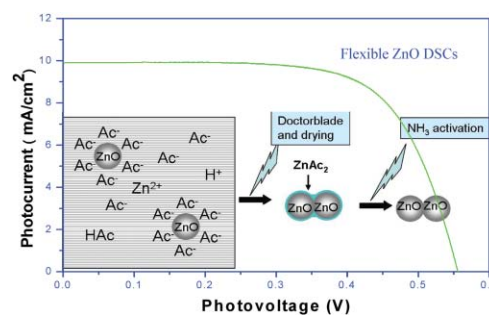


2847

Room temperature fabrication of porous ZnO photoelectrodes for flexible dye-sensitized solar cells

Xizhe Liu, Yanhong Luo, Hong Li, Yuzun Fan, Zhexiong Yu, Yuan Lin, Liquan Chen and Qingbo Meng*

The authors fabricated ZnO photoelectrodes at room temperature by doctor-blading ZnO gel; the adequate interparticle connection and the effective ammonia activation process improved the flexible DSC's efficiency to 3.8% (under 100 mW cm⁻²).





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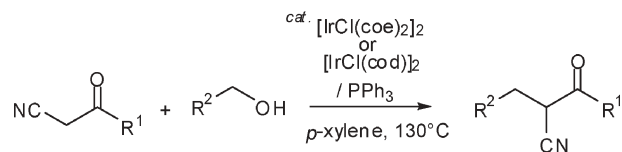
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2850

Alkylation of active methylene compounds with alcohols catalyzed by an iridium complex

Masao Morita, Yasushi Obora and Yasutaka Ishii*

Base-free direct catalytic α -alkylation of active methylene compounds with primary alcohols was successfully achieved using an $[\text{IrCl}(\text{cod})]_2$ complex in the presence of PPh_3 to afford the corresponding saturated α -alkylated products in good yields.

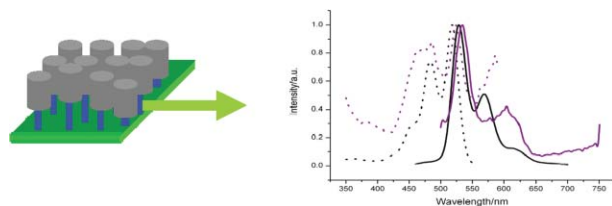


2853

Fabrication of oriented zeolite L monolayers employing luminescent perylene-3,4,9,10-tetracarboxylic diimide-bridged silsesquioxane precursor as the covalent linker

Huanrong Li,* Yige Wang, Wenjun Zhang, Binyuan Liu and Gion Calzaferri

Oriented zeolite L monolayers with dense packing and high coverage degree have been obtained by using a luminescent perylene-3,4,9,10-tetracarboxylic diimide-bridged silsesquioxane precursor as the novel molecular binder.

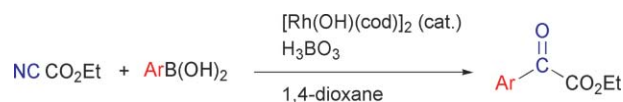


2855

Synthesis of α -keto esters by the rhodium-catalysed reaction of cyanoformate with arylboronic acids

Hirosi Shimizu and Masahiro Murakami*

An arylrhodium(I) species selectively reacts with the cyano group of ethyl cyanoformate to afford the corresponding α -keto ester in good yield. This result is in sharp contrast to the reactivity of arylmagnesium bromide and aryllithiums, which attack at the ester group.

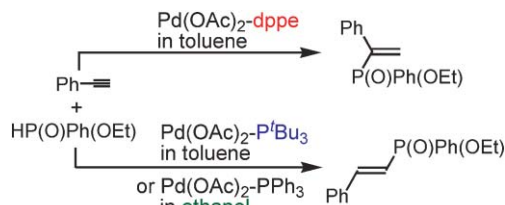


2858

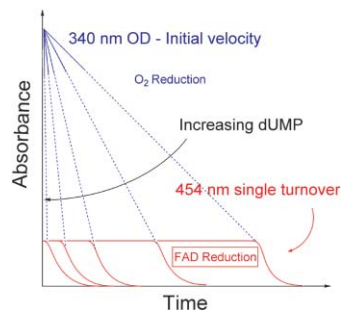
Palladium-catalysed regioselective addition reaction of ethyl phenylphosphinate with terminal acetylenes: ligand- and solvent-dependent regioselectivity

Satish Kumar Nune and Masato Tanaka*

Palladium-1,2-bis(diphenylphosphino)ethane complex catalyses regioselective Markovnikov addition of ethyl phenylphosphinate to terminal alkynes in toluene, while the use of tri-*tert*-butylphosphine as the ligand or ethanol as the solvent leads to regioselectivity reversal.



2861

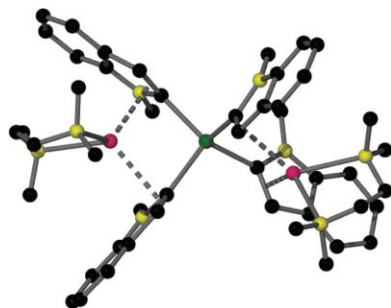


The relationships between oxidase and synthase activities of flavin dependent thymidylate synthase (FDTS)

Anatoly Chernyshev, Todd Fleischmann, Eric M. Koehn, Scott A. Lesley and Amnon Kohen*

New findings lead to a revised understanding of the substrates' binding order, the role of the substrate as an activator, and the observed lag phase in the FDTS catalyzed reaction.

2864

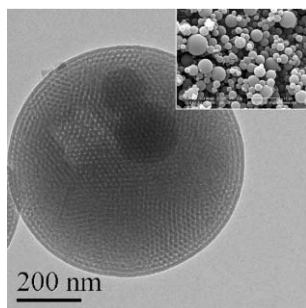


Structurally-defined direct C-magnesiation and C-zincation of N-heterocyclic aromatic compounds using alkali-metal-mediated metallation

Ben Conway, Eva Hevia,* Alan R. Kennedy and Robert E. Mulvey*

Direct C-magnesiation of 1-methylindole is achieved by the synergic action of a disodium tetraalkylmagnesiato base to generate a disodium tetraindol-2-yl complex.

2867

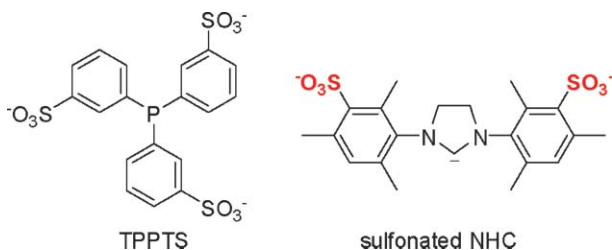


One-step synthesis of ordered mesoporous carbonaceous spheres by an aerosol-assisted self-assembly

Yan Yan, Fuqiang Zhang, Yan Meng, Bo Tu and Dongyuan Zhao*

Ordered mesoporous carbonaceous spheres with variable structures have been successfully prepared by using phenolic resols as a carbon precursor and amphiphilic triblock copolymers as a template *via* a one-step aerosol-assisted organic-organic self-assembly method.

2870



Sulfonated N-heterocyclic carbenes for Suzuki coupling in water

Christoph Fleckenstein, Sutapa Roy, Steffen Leuthäuser and Herbert Plenio*

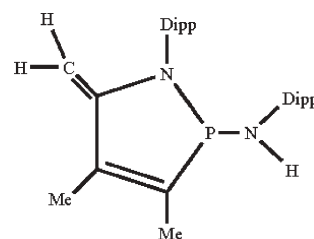
Tri(*m*-sulfonyl)triphenylphosphine is the prototypical water-soluble phosphine. We have now synthesized various 3- and 4-sulfonated imidazolium and imidazolinium salts to enable the aqueous organometallic chemistry of NHC metal complexes.

2873

Valence isomer of a β -diketiminato-supported phosphinidene: a case of C–H activation and ring contraction

Zheng Lu, Michael Findlater and Alan H. Cowley*

Reduction of a β -diketiminato-supported chlorophosphenium cation results in a valence isomer of the corresponding phosphinidene.

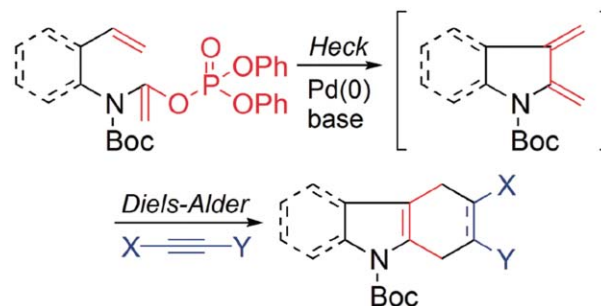


2876

A new method for the generation of indole-2,3-quinodimethanes and 2-(*N*-alkoxycarbonylamino)-1,3-dienes. Intramolecular Heck/Diels–Alder cycloaddition cascade starting from acyclic α -phosphono enecarbamates

Haruhiko Fuwa* and Makoto Sasaki*

An intramolecular Heck/Diels–Alder cycloaddition cascade starting from acyclic α -phosphono enecarbamate has been developed, which allows for the generation of various nitrogen heterocycles in a rapid and efficient manner.

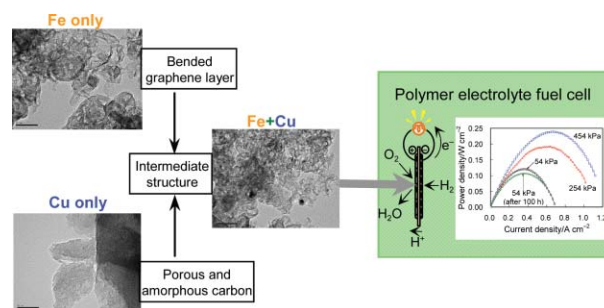


2879

Structure control of a carbon-based noble-metal-free fuel cell cathode catalyst leading to high power output

Jun Maruyama* and Ikuo Abe

Controllability of carbon structure was demonstrated and applied to a carbon-based fuel cell cathode catalyst, causing the highest level of power output among noble-metal-free cathode type polymer electrolyte fuel cells.




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