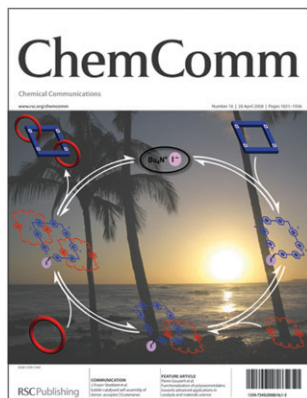


IN THIS ISSUE

ISSN 1359-7345 CODEN CHCOFS (16) 1821-1936 (2008)



Cover

See J. Fraser Stoddart *et al.*, pp. 1853–1855. Although the sun is now setting on catenanes at UCLA, NU horizons beckon for polycatenanes in Evanston. Image reproduced by permission of Kaushik Patel, Ognjen Š. Miljanić and J. Fraser Stoddart from *Chem. Commun.*, 2008, 1853.

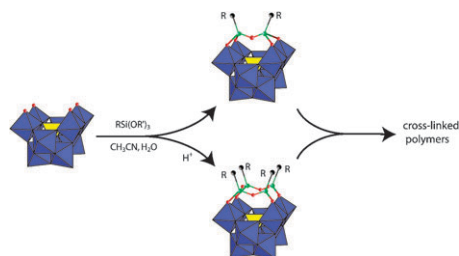
FEATURE ARTICLE

1837

Functionalization of polyoxometalates: towards advanced applications in catalysis and materials science

Anna Proust,* René Thouvenot* and Pierre Gouzerh*

Covalent derivatization as well as self-assembly play an outstanding role in the development of new applications of polyoxometalates in catalysis and materials science. Both aspects are considered in this feature article, with special attention to organonitrogen, organosilyl and organophosphonyl derivatives and to multifunctional nanosized polyoxomolybdates.



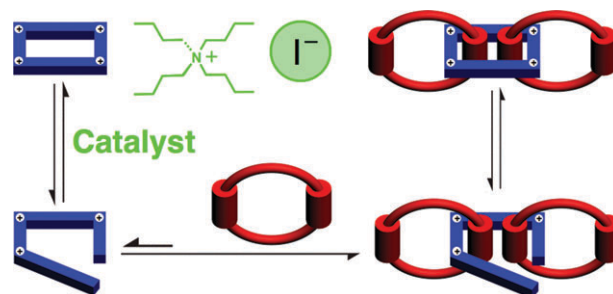
COMMUNICATIONS

1853

Iodide-catalysed self-assembly of donor-acceptor [3]catenanes

Kaushik Patel, Ognjen Š. Miljanić and J. Fraser Stoddart*

Charged donor-acceptor [3]catenanes comprising the π -accepting cyclobis(paraquat-4,4'-biphenylene) and π -donating aromatic crown ether macrocycles have been prepared in high yields using thermodynamically controlled dynamic nucleophilic substitution.



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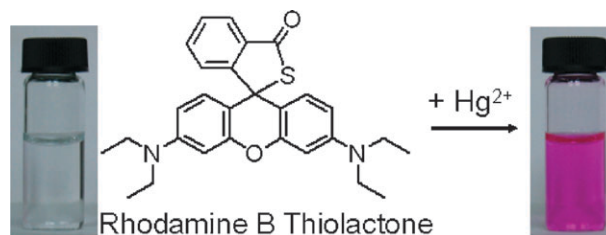
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1856

Rhodamine B thiolactone: a simple chemosensor for Hg^{2+} in aqueous media

Wen Shi and Huimin Ma*

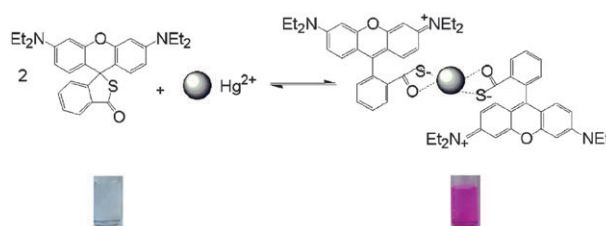
Rhodamine B thiolactone is developed as a simple chemosensor towards Hg^{2+} in neutral aqueous solution with high selectivity.



1859

Rhodamine thiospirolactone. Highly selective and sensitive reversible sensing of $\text{Hg}(\text{II})$ Xin-Qi Zhan, Zhen-Hua Qian, Hong Zheng,*
Bing-Yuan Su, Zhi Lan and Jin-Gou Xu*

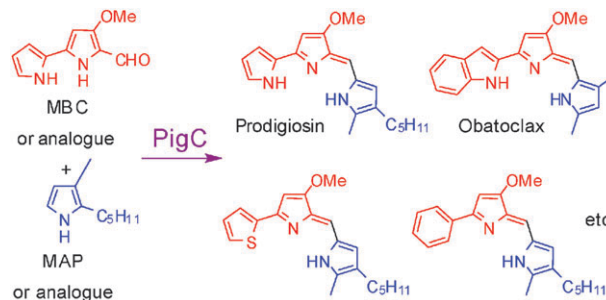
A novel rhodamine thiospirolactone chemosensor **1** was found to develop prominent absorbance and fluorescence enhancements in the presence of Hg^{2+} in aqueous solution and this was suggested to result from the thiospiro ring opening induced by Hg^{2+} binding.



1862

Chemoenzymatic synthesis of prodigiosin analogues—exploring the substrate specificity of PigCSuresh R. Chawrai, Neil R. Williamson,
George P. C. Salmond* and Finian J. Leeper*

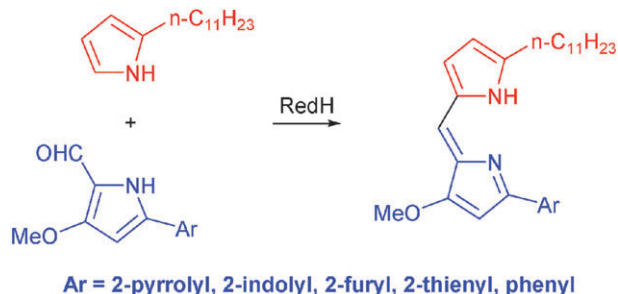
Analogues of prodigiosin, a tripyrrolic pigment with potent immunosuppressive and anticancer activities, have been produced by feeding synthetic analogues of the normal precursor MBC to mutants of *Serratia*.




1865

Role and substrate specificity of the *Streptomyces coelicolor* RedH enzyme in undecylprodiginine biosynthesisStuart W. Haynes, Paulina K. Sydor, Anna E. Stanley,
Lijiang Song and Gregory L. Challis*

The broadened substrate specificity of the *Streptomyces coelicolor* RedH enzyme has been exploited to generate several analogues of the antibiotic undecylprodiginine via mutasynthesis utilising synthetic analogues of the key biosynthetic intermediate MBC (in blue).





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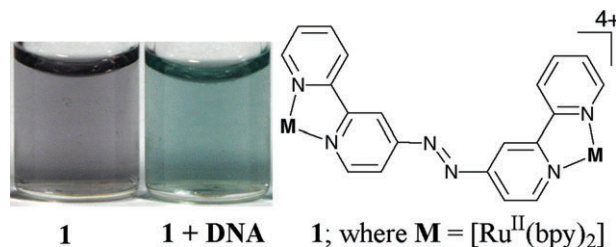
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1868

A dinuclear ruthenium(II) complex that functions as a label-free colorimetric sensor for DNA

Veronica Gonzalez, Tom Wilson, Izumi Kurihara, Arata Imai, Jim A. Thomas* and Joe Otsuki*

A dinuclear ruthenium(II) complex that incorporates an azo-based bridging ligand groove binds to DNA. This interaction results in distinctive purple-to-green color changes that are dependent on both DNA sequence and structure.

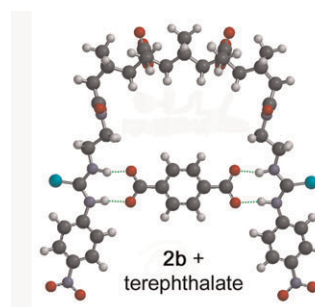


1871

Size matters—strong binding of the terephthalate dianion by thiourea functionalised fused [n]polynorbornane hosts

Adam J. Lowe and Frederick M. Pfeffer*

Remarkably strong binding of the new [5]polynorbornane based host **2b** to the terephthalate dianion is based on size complementarity of the preorganised binding cleft with the rigid dicarboxylate guest.

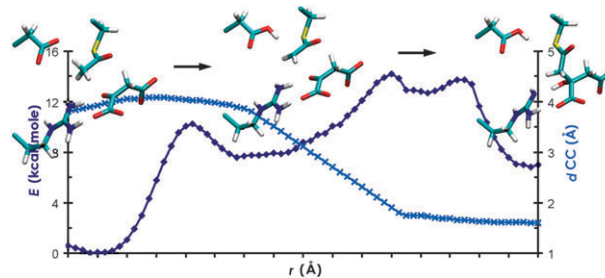


1874

High-level QM/MM modelling predicts an arginine as the acid in the condensation reaction catalysed by citrate synthase

Marc W. van der Kamp, Francesca Perruccio and Adrian J. Mulholland*

High-level *ab initio* quantum mechanical/molecular mechanical (QM/MM) modelling of citryl-CoA formation in citrate synthase reveals that an arginine residue acts as the proton donor.

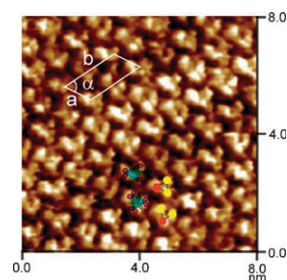


1877

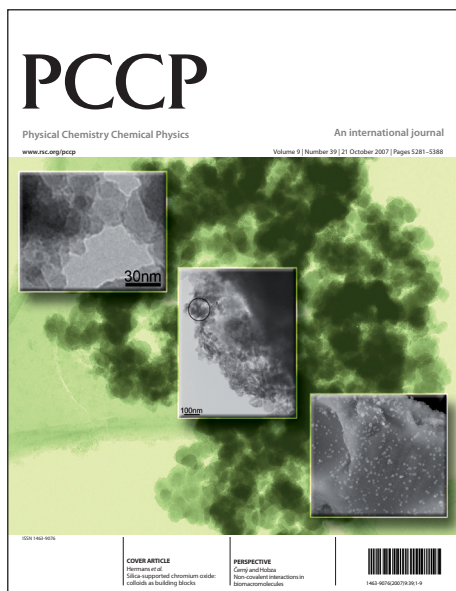
TNT adsorption on Au(111): electrochemistry and adlayer structure

Rui Wen, Hong-Xia Zhang, Cun-Ji Yan, Hui-Juan Yan, Ge-Bo Pan and Li-Jun Wan*

Cyclic voltammetry of Au(111) in a HClO₄ solution containing TNT showed three well-defined cathodic peaks. STM observations reveal that TNT molecules can form a well-ordered adlayer with a (2√3 × 4√3) structure on Au(111) in a flat-lying orientation.



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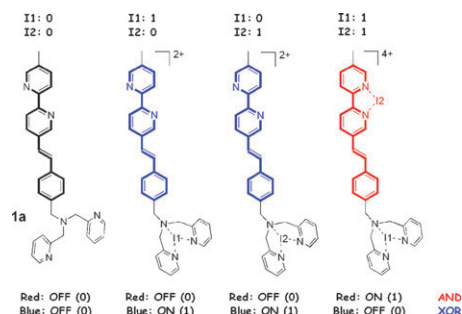
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1880

Unimolecular binary half-adders with orthogonal chemical inputs

Lu Zhang, Wesley A. Whitfield and Lei Zhu*

Unimolecular half-adders based upon an arylvinyl-bipyridyl fluorophore platform were demonstrated where all the chemical input combinations were fully processed by half-adder molecules to generate the arithmetic results of the entire truth table.

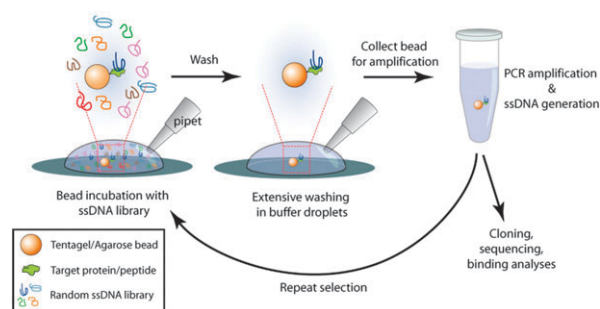


1883

Single microbead SELEX for efficient ssDNA aptamer generation against botulinum neurotoxin

Jeffrey B.-H. Tok* and Nicholas O. Fischer

An efficient and easy-to-execute single microbead SELEX approach is developed to generate high affinity ssDNA aptamers against botulinum neurotoxin.

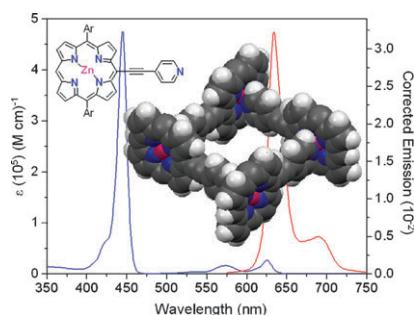


1886

Fast energy transfer within a self-assembled cyclic porphyrin tetramer

Rebecca A. Jensen, Richard F. Kelley, Suk Joong Lee, Michael R. Wasielewski,* Joseph T. Hupp* and David M. Tiede

Rapid energy transfer is observed within a tetrameric cyclic self-assembly of ethynylpyridyl-functionalized Zn(II)-porphyrin. The assembly structure is established by solution-phase X-ray scattering and diffraction and the directionality of energy transfer is assessed using femtosecond transient absorption and anisotropy spectroscopies.

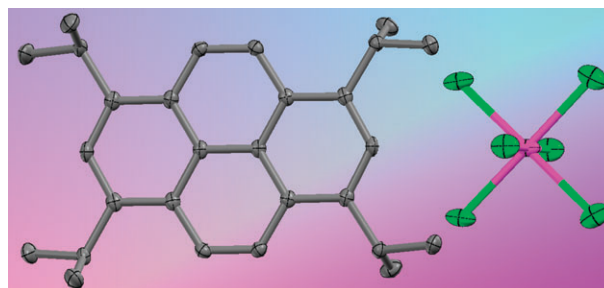


1889

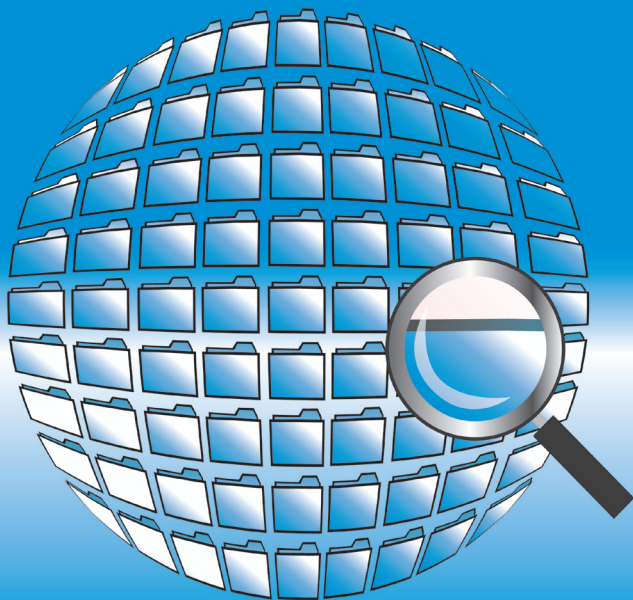
Isolation and X-ray structural characterization of tetraisopropylpyrene cation radical

Moloy Banerjee, Vijay S. Vyas, Sergey V. Lindeman and Rajendra Rathore*

X-Ray crystallographic structural characterization of the monomeric cation-radical salt of 1,3,6,8-tetraisopropylpyrene provided unequivocal experimental evidence that a hole (or polaron) causes the elongation of the bonds on which the HOMO resides.



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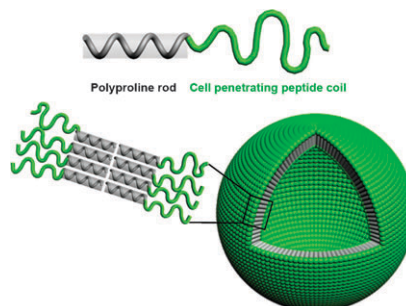
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1892

Self-assembly of a peptide rod–coil: a polyproline rod and a cell-penetrating peptide Tat coil

You-Rim Yoon, Yong-beom Lim, Eunji Lee and Myongsoo Lee*

Peptide rod–coil molecules, composed of a stiff polyproline rod and a hydrophilic cell-penetrating peptide Tat coil, self-assemble into nanocapsules and mediate efficient intracellular delivery of entrapped hydrophilic molecules.

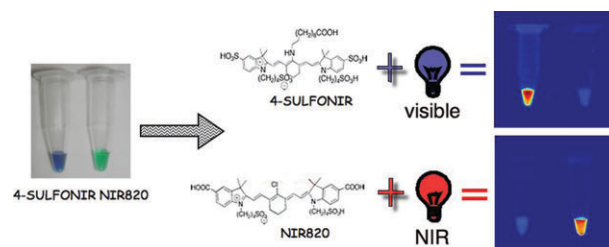


1895

A near-infrared dye for multichannel imaging

Wellington Pham,* Lauren Cassell, Amelie Gillman, Dmitry Koktysh and John C. Gore

A large Stokes shift dye, composed of water-solubility and near-infrared feature, was developed for multichannel imaging applications.

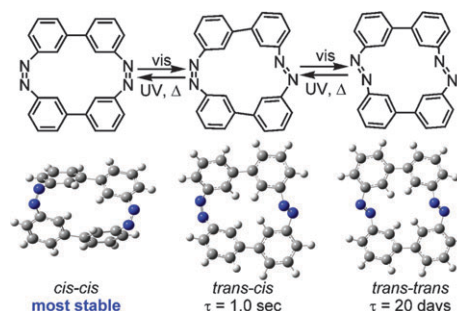


1898

Unconventional thermodynamically stable *cis* isomer and *trans* to *cis* thermal isomerization in reversibly photoresponsive [0.0](3,3′)-azobenzenophane

Yasuo Norikane,* Ryuzi Katoh and Nobuyuki Tamaoki*

Sterically hindered [0.0](3,3′)-azobenzenophane exhibits thermal *trans*-to-*cis* isomerization to the thermodynamically stable *cis*-*cis* isomer, and reversible photochemical isomerization with good fatigue resistance.

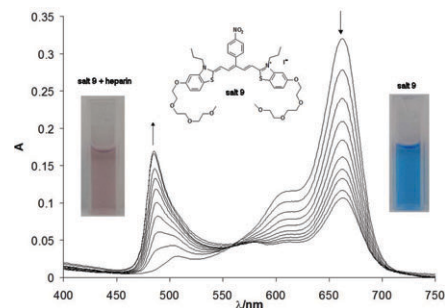


1901

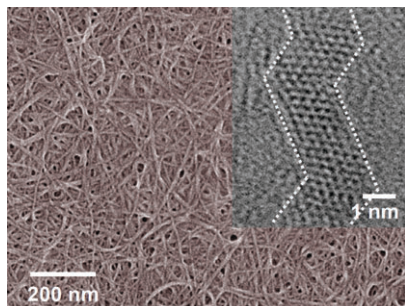
Optical sensing of sulfate by polymethinium salt receptors: colorimetric sensor for heparin

Tomáš Bříza,* Zdeněk Kejík, Ivana Císařová, Jarmila Králová, Pavel Martásek and Vladimír Král*

Polymethinium salt **9** with PEG substitution showed high selectivity for sulfate anions and heparin at physiological conditions. Intracellular imaging of heparin-rich subcellular compartments was achieved with polymethinium receptor **9** for cancer cells lines.



1904

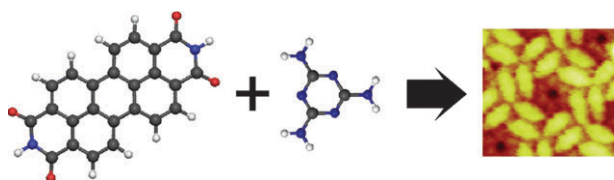


Time-dependent growth of zinc hydroxide nanostrands and their crystal structure

Xinsheng Peng, Jian Jin, Noriko Kobayashi, Wolfgang Schmitt and Izumi Ichinose*

Positively-charged crystalline zinc hydroxide nanostrands with a diameter of 2 nm and a length of a few micrometres rapidly grew in a dilute aqueous solution of zinc nitrate and aminoethanol. The nanostrands were composed of hexagonal clusters of $[Zn_{61}(OH)_{116}(H_2O)_n]^{6+}$.

1907

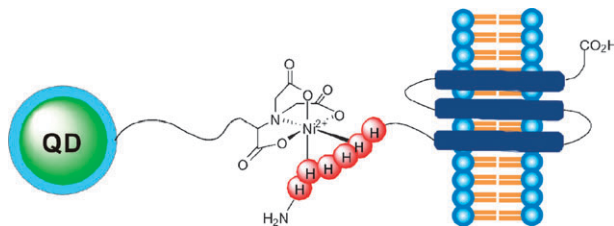


A chiral pinwheel supramolecular network driven by the assembly of PTCDI and melamine

Fabien Silly,* Adam Q. Shaw, Martin R. Castell and G. A. D. Briggs

PTCDI molecules form grid domains, whereas melamine molecules form chiral hexagonal domains on an Au(111) surface. We show that mixing of PTCDI and melamine in a ratio of 3 : 4 leads to the formation of a chiral “pinwheel” structure.

1910

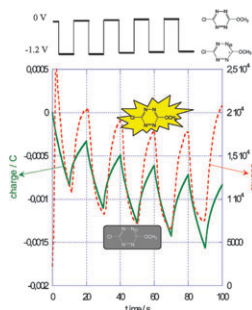


Ni-nitrilotriacetic acid-modified quantum dots as a site-specific labeling agent of histidine-tagged proteins in live cells

Junwon Kim, Hye-Young Park, Jaeseung Kim, Jiyoung Ryu, Do Yoon Kwon, Regis Grailhe and Rita Song*

Ni-nitrilotriacetic acid (NTA) functionalized quantum dots (QDs) were exploited as a site-specific labeling agent of histidine-tagged proteins in live cells. The Ni-NTA modified QDs were found to be water-soluble, aggregation free and stable for several months.

1913



Fluorescence microscopy coupled to electrochemistry: a powerful tool for the controlled electrochemical switch of fluorescent molecules

Fabien Miomandre,* Rachel Meallet-Renault, Jean-Jacques Vachon, Robert Bernard Pansu and Pierre Audebert*

The coupling of fluorescence microscopy with three-electrode cell electrochemistry is used to evidence the reversible switch of a tetrazine derivative between their fluorescent oxidized and non-emissive reduced forms.

1916

Preparation of silyl substituted crotylzinc reagents and their highly diastereoselective addition to carbonyl compounds

Matthew D. Helm, Peter Mayer and Paul Knochel*

Readily prepared β -silyl substituted crotylzinc reagents undergo highly selective allylation of carbonyl compounds leading to *syn*-homoallylic alcohols.

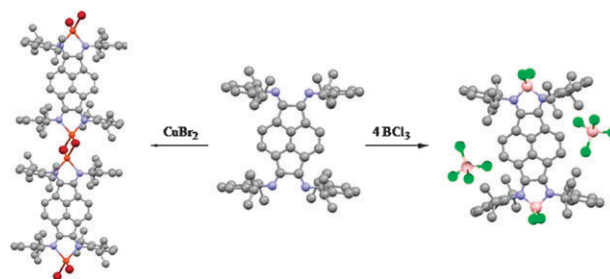


1918

Synthesis and reactivity of tetrakis(imino)pyracene (TIP) ligands; bifunctional analogues of the BIAN ligand class

Kalyan V. Vasudevan, Michael Findlater and Alan H. Cowley*

The first two examples of a new class of bifunctional BIAN-type ligand have been prepared, structurally characterized, and used for the support of a diboron dication and a CuBr polymer.

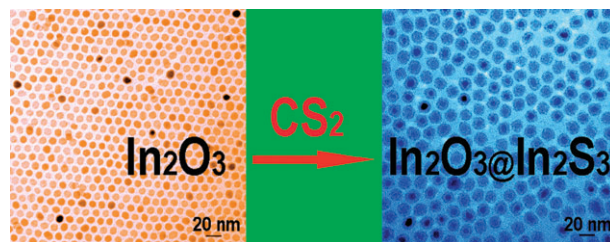


1920

One-pot synthesis of reverse type-I $\text{In}_2\text{O}_3@ \text{In}_2\text{S}_3$ core-shell nanoparticles

Zhaoyong Sun, Amar Kumbhar, Kai Sun, Qingsheng Liu and Jiye Fang*

A novel method to one-pot-synthesize high-quality $\text{In}_2\text{O}_3@ \text{In}_2\text{S}_3$ core-shell nanoparticles, consisting of a step of reducing In_2O_3 core surface into a layer of active indium metal in high-temperature organic solution and a step of converting this layer to In_2S_3 using CS_2 , has been developed.

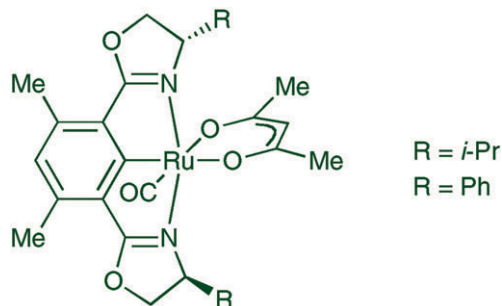


1923

A new NCN pincer ruthenium complex and its catalytic activity for enantioselective hydrogenation of ketones

Jun-ichi Ito, Satoshi Ujii and Hisao Nishiyama*

(Phebox-R)Ru(CO)(acac) complexes were synthesized by C-H bond activation with $\text{RuCl}_3 \cdot 3\text{H}_2\text{O}$ and were applied for enantioselective hydrogenation of ketones.



1926

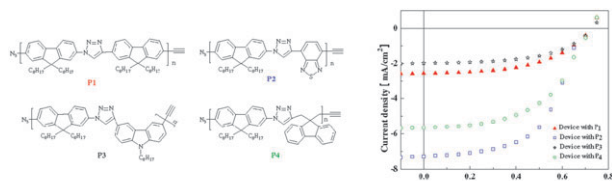


An unusual dianion equivalent from acylsilanes for the synthesis of substituted β -keto esters

Chris V. Galliford and Karl A. Scheidt*

The addition of lithiated diazo esters to acylsilanes provides unprecedented access to β -silyloxy allenolates, unusual dianion equivalents. The proposed reaction pathway proceeds by a 1,2-Brook rearrangement followed by loss of nitrogen gas. The addition of two electrophiles to this *in situ* generated nucleophile results in a multicomponent synthesis of substituted β -keto esters in high yield.

1929

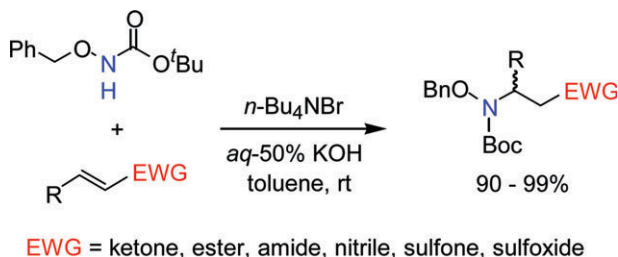


Novel fluorene-based functional 'click polymers' for quasi-solid-state dye-sensitized solar cells

Md. Anwarul Karim, Young-Rae Cho, Jin Su Park, Sung Chul Kim, Hee Joo Kim, Jae Wook Lee,* Yeong-Soon Gal and Sung-Ho Jin*

Quasi-solid-state dye-sensitized solar cells with configuration of $\text{SnO}_2:\text{F}/\text{TiO}_2/\text{N}_3$ dye/quasi-solid-state electrolyte/Pt devices using click polymers have been fabricated; the maximum power conversion efficiency was 2.80%.

1932



Phase-transfer catalytic aza-Michael addition of *tert*-butyl benzyloxycarbamate to electron-deficient olefins

Jihoon Lee, Mi-hyun Kim, Sang-sup Jew, Hyeung-geun Park* and Byeong-Seon Jeong*

A highly efficient aza-Michael addition of *tert*-butyl benzyloxycarbamate to a wide range of electron-deficient olefins (ketone, ester, amide, nitrile, sulfone, sulfoxide) under phase-transfer catalytic reaction conditions is presented (90–99%).

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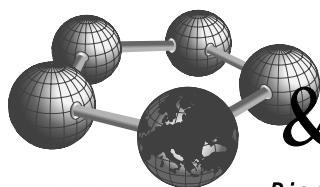
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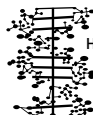
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