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IN THIS ISSUE

ISSN 1359-7345 CODEN CHCOFS (19) 1989-2080 (2006)



Cover

See Nikos S. Hatzakis, Hans Engelkamp, Kelly Velonia, Johan Hofkens, Peter C. M. Christianen, Allan Svendsen, Shamkantr A. Patkar, Jesper Vind, Jan C. Maan, Alan E. Rowan and Roeland J. M. Nolte, page 2012, Single enzyme kinetics of a TLL-BSA hetero-dimer, in which the BSA acts as a protein foot, was measured using confocal fluorescent microscopy. Image reproduced by permission of Alan E. Rowan and Roeland J. M. Nolte et al. from Chem. Commun., 2006, 2012.



Inside cover

See Kana M. Sureshan, Melanie Trusselle, Stephen C. Tovey, Colin W. Taylor and Barry V. L. Potter, page 2015. A synthetic glyconucleotide binds to a second messenger receptor core releasing Ca2+ more effectively than the natural ligand; cells loaded with fluorescent dye in 96-wells facilitate determination of the dose-response curve (yellow). Image reproduced by permission of Barry V. L. Potter et al. from Chem. Commun., 2006, 2015.

CHEMICAL SCIENCE

C33

In this issue...

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

May 2006/Volume 3/Issue 5 www.rsc.org/chemicalscience

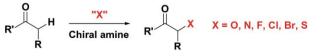
FEATURE ARTICLE

2001

Organocatalytic direct asymmetric α-heteroatom functionalization of aldehydes and ketones

Mauro Marigo and Karl Anker Jørgensen*

The organocatalytic enantioselective amination, oxygenation, fluorination, chlorination, bromination and sulfenylation of aldehydes and ketones, using chiral amines as the catalysts, leading to optically active compounds of significant importance for *e.g.* the life-science industry are presented. Furthermore, some other transformations are also outlined, as well as their scope, potential and application.



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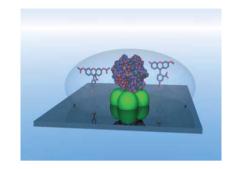
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2012



Synthesis and single enzyme activity of a clicked lipase–BSA hetero-dimer

Nikos S. Hatzakis, Hans Engelkamp, Kelly Velonia, Johan Hofkens, Peter C. M. Christianen, Allan Svendsen, Shamkantr A. Patkar, Jesper Vind, Jan C. Maan, Alan E. Rowan* and Roeland J. M. Nolte*

A novel clicked TLL–BSA heterodimer is found to be more active compared to native TLL. Single molecule studies reveal that the anchored TLL remains active for more than 40 000 turnovers and slowly fluctuates between different conformations each with its own catalytic activity.

2015

Guanophostin A: Synthesis and evaluation of a high affinity agonist of the D-myo-inositol 1,4,5-trisphosphate receptor

Kana M. Sureshan, Melanie Trusselle, Stephen C. Tovey, Colin W. Taylor and Barry V. L. Potter*

Guanophostin A is the most potent synthetic adenophostin A-like agonist at the $Ins(1,4,5)P_3$ receptor; multiple interactions of the guanine moiety with the receptor binding core are proposed.

2018

Solvent-free selective photocatalytic oxidation of benzyl alcohol to benzaldehyde by molecular oxygen using 9-phenyl-10-methylacridinium

Kei Ohkubo, Kyou Suga and Shunichi Fukuzumi*

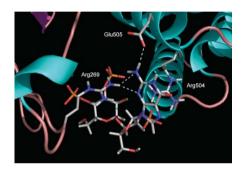
9-Phenyl-10-methylacridinium ion acts as an effective photocatalyst for solvent free selective photocatalytic oxidation of benzyl alcohol to benzaldehyde under visible light irradiation *via* photoinduced electron transfer.

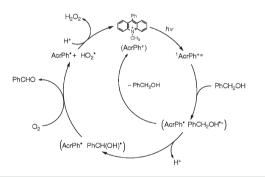
2021

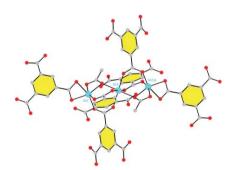
Microwave-assisted synthesis of anionic metal-organic frameworks under ionothermal conditions

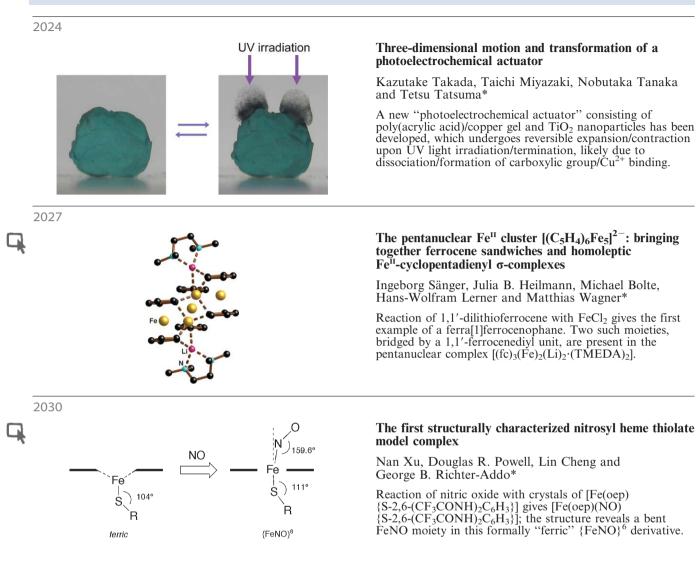
Zhuojia Lin, David S. Wragg and Russell E. Morris*

Ionothermal synthesis—the use of an ionic liquid as both solvent and template in the synthesis of materials—has been used to prepare, in combination with microwave heating, an anionic metal–organic framework. The ionic liquid cation is occluded in the structure to balance the charge on the framework.









2033

 $SnCl_4 \cdot 5H_2O + H_3PO_4 = \frac{S}{2}$

Solvothermal treatment 180 °C, in ethanol



One-pot synthesis of spring-like superstructures consisting of layered tin(IV) hydrogen phosphate nanodisks

Hui Qiao, Falong Jia, Zhihui Ai, Zhaosheng Li and Lizhi Zhang*

One-pot solvothermal treatment of tin tetrachloride and phosphoric acid in ethanol produced spring-like superstructures consisting of layered tin(IV) hydrogen phosphate nanodisks.

COMMUNICATIONS

2036

Hybrid bidentate ligand for functional recognition: an application to regioselective C=C double bond hydrogenation

Frédéric Goettmann, Pascal Le Floch* and Clément Sanchez*

High regioselectivities can be obtained in heterogeneously catalysed hydrogenation by using the supporting material as a functional recognition agent.

2039

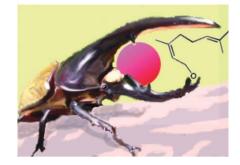
The cationic cluster Grignard $[{MgCl(thf)_2}_3(\mu_3-C_3H_5)_2]^+$

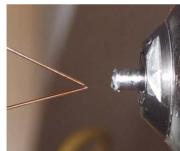
Richard A. Layfield,* Thomas H. Bullock, Felipe García, Simon M. Humphrey and Peter Schüler

The reaction of allylmagnesium chloride with methylaluminium dichloride in thf solvent unexpectedly affords the ion-separated complex $[{MgCl(thf)_2}_3(\mu_3-C_3H_5)_2]_2[Mg(C_3H_5)_4]$, which contains both a cluster Grignard and a tetraorganomagnesiate dianion.

Extractive electrospray ionization for direct analysis of undiluted urine, milk and other complex mixtures without

Huanwen Chen, Andre Venter and R. Graham Cooks* On-line droplet–droplet extraction and electrospray ionization for direct, continual analysis by mass spectrometry of trace components in complex samples such as raw undiluted urine.







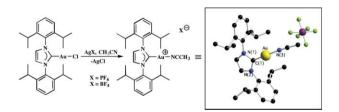
2042

sample preparation

Synthesis, isolation and characterization of cationic gold(I) *N*-heterocyclic carbene (NHC) complexes

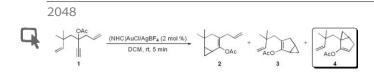
Pierre de Frémont, Edwin D. Stevens, Manuel R. Fructos, M. Mar Díaz-Requejo, Pedro J. Pérez and Steven P. Nolan*

A number of cationic gold(I) complexes have been synthesized and found to be stabilized by the use of *N*-heterocyclic carbene ligands.





COMMUNICATIONS



Au¹-catalyzed cycloisomerization of 1,5-enynes bearing a propargylic acetate: formation of unexpected bicyclo[3.1.0]hexene

Nicolas Marion, Pierre de Frémont, Gilles Lemière, Edwin D. Stevens, Louis Fensterbank, Max Malacria and Steven P. Nolan*

The use of *N*-heterocyclic carbene (NHC) as a ligand in the gold(I)-catalyzed cycloisomerization of enyne results in the assembly of a new carbocyclic product.

A molecular tool kit for the variable design of logic operations (NOR, INH, EnNOR)

Miguel de Sousa, Baltazar de Castro, Sergio Abad, Miguel A. Miranda and Uwe Pischel*

A phthalimide–terbium(III)-based system for the variable design of optical molecular logic gates (*NOR*, *INH*, *EnNOR*) is described.

Synthesis and excited state properties of a [60]fullerene derivative bearing a star-shaped multi-photon absorption chromophore

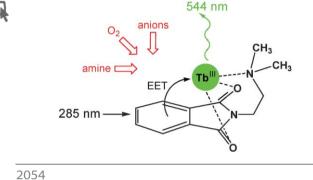
Teresa M. Figueira-Duarte, John Clifford, Vincenzo Amendola, Aline Gégout, Jean Olivier, François Cardinali, Moreno Meneghetti,* Nicola Armaroli* and Jean-François Nierengarten*

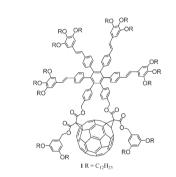
The synthesis and excited state properties of a compound assembling C_{60} with a new multi-photon absorption chromophore are reported.

¹³C NMR spectroscopic study of scandium dimetallofullerene, Sc₂@C₈₄ vs. Sc₂C₂@C₈₂

Yuko Iiduka, Takatsugu Wakahara, Koji Nakajima, Takahiro Tsuchiya, Tsukasa Nakahodo, Yutaka Maeda, Takeshi Akasaka,* Naomi Mizorogi and Shigeru Nagase

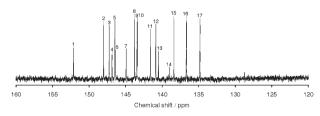
Although Sc₂C₈₄ has been widely believed to have the form Sc₂@C₈₄, the present ¹³C NMR study reveals that it is a scandium carbide metallofullerene, Sc₂C₂@C₈₂, which has a C₈₂(C_{3v}) cage.





2057

2051



2060

Three-dimensional networks of lanthanide 1,2,4-triazolates: ³/₂[Yb(Tz)₃] and ³/₂[Eu₂(Tz)₅(TzH)₂], the first 4f networks with complete nitrogen coordination

Klaus Müller-Buschbaum* and Yassin Mokaddem

The solvent-free melt reaction of Eu and Yb metals with the N-heterocycle 1,2,4-triazole gives the first three-dimensional networks of the lanthanides with complete nitrogen coordination spheres.

2063

Organic solvent nanofiltration in asymmetric hydrogenation: enhancement of enantioselectivity and catalyst stability by ionic liquids

Hau-To Wong, Yoong Hsiang See-Toh, Frederico Castelo Ferreira, Robert Crook and Andrew G. Livingston*

Ionic liquids demonstrate enhancements on enantiomeric excess and catalyst stability in asymmetric hydrogenation reactions; nanofiltration demonstrates a straightforward method for separating and recycling ionic liquid and catalyst.

2066

DyI₂ initiated mild and highly selective silyl radicalcatalyzed cyclotrimerization of terminal alkynes and polymerization of MMA

Zhenyu Zhu, Chuanfeng Wang, Xu Xiang, Chengfu Pi and Xigeng Zhou*

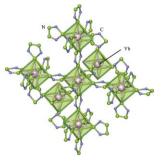
An efficient method for the formation of silyl radicals by the reaction of chlorosilanes with DyI_2 has been established, demonstrating for the first time the potential of DyI_2 as a catalytic and initiating reagent in organic synthesis and suggesting that the presence of lanthanide ions can improve the selectivity of some silyl radical-catalyzed reactions.

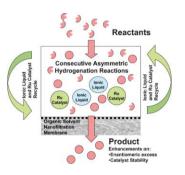
2069

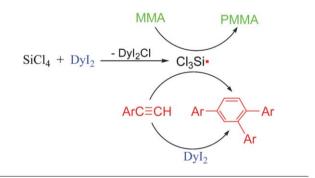
Synthetic studies directed toward the proposed structure for heteroscyphic acid A

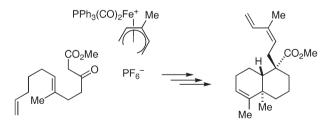
Subhabrata Chaudhury, Shukun Li and William A. Donaldson*

A route to the carbon skeleton of the proposed structure for heteroscyphic acid A was developed utilizing a Mn(III)/Cu(II) mediated oxidative free-radical cyclization and nucleophilic addition to (3-methylpentadienyl)iron(1+) cation.

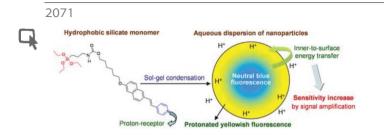








COMMUNICATIONS



1/2 02

X-ray

Dye-concentrated organically modified silica nanoparticles as a ratiometric fluorescent pH probe by one- and two-photon excitation

Sehoon Kim, Haridas E. Pudavar and Paras N. Prasad*

Basic dye-concentrated nanoparticles (~ 33 nm in diameter) show fluorescence-based ratiometric pH response, by one- and two-photon excitations, with improved proton sensing ability (p $K_a \sim 6.4$) through nanoscopic intraparticle energy transfer.

Oxidative N-dealkylation in cobalt–bispidine– H_2O_2 systems

Peter Comba,* Shigemasa Kuwata, Gerald Linti, Hans Pritzkow, Máté Tarnai and Hubert Wadepohl

The reaction of the Co^{II} complex with the rigid bispidine ligand L¹ with two tertiary amine and two pyridine donors, $[Co^{II}(L^1)(OH_2)_2]^{2+}$, with H_2O_2 and O_2 produces $[Co^{II}(L^2)(OH_2)_2]^{3+}$, where L² is demethylated at one of the amine donors, and CH₂O.

ADDITION AND CORRECTION

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X-ray

Q

Zhimou Yang, Gaolin Liang and Bing Xu

DFT

Supramolecular hydrogels based on β -amino acid derivatives

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