### **ChemComm**

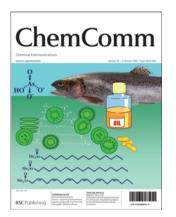
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#### IN THIS ISSUE

ISSN 1359-7345 CODEN CHCOFS (39) 4649-4844 (2008)



#### Cover

See Kevin A. Francesconi et al., pp. 4706–4707.
Arsenic-containing long-chain alkanes and alkenes, natural constituents of fish oil, are likely to be biosynthesised by phytoplankton and passed along the food chain.
Image reproduced by permission of Mojtaba S. Taleshi, Kenneth B. Jensen, Georg Raber, John S. Edmonds, Helga Gunnlaugsdottir and Kevin A. Francesconi from Chem. Commun., 2008, 4706.



#### Inside cover

See Leroy Cronin et al., pp. 4703-4705. Emerging from the sea of possibilities is a mixed polyoxomolybdenum/ vanadium-sulphite,  $[Mo^{VI}_{11}V^{V}_{5}V^{IV}_{2}O_{52}(\mu_{9}\text{-SO}_{3})]^{7}$ which was first identified using cryospray mass spectrometry. Image reproduced by permission of Haralampos N. Miras, Daniel J. Stone, Eric J. L. McInnes, Raphael G. Raptis, Peter Baran, George I. Chilas, Michael P. Sigalas, Themistoklis A. Kabanos and Lerov Cronin from Chem. Commun., 2008, 4703.

#### **CHEMICAL SCIENCE**

C73

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

### **Chemical Science**

October 2008/Volume 5/Issue 10

www.rsc.org/chemicalscience

#### **FEATURE ARTICLE**

4671

Computational and experimental tools in solving some mechanistic problems in the chemistry of Fischer carbene complexes

Miguel A. Sierra,\* Israel Fernández and Fernando P. Cossío

Combination of experimental and computational tools is exceedingly useful to unravel different thermal and photochemical transformations in Fischer carbene complexes and to foresee novel reaction pathways of these complexes.



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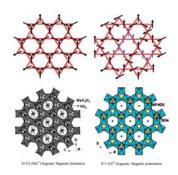
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#### Kagome network compounds and their novel magnetic properties

Swapan K. Pati\* and C. N. R. Rao\*

The structure and magnetic properties of Kagome network compounds are described and an attempt is made to provide an explanation for their varied properties on the basis of theoretical considerations.



#### **COMMUNICATIONS**

4694

#### Enantioselective organocatalytic conjugate addition of α-aminoketone to nitroolefins

Sébastien Belot, Sarah Sulzer-Mossé, Stefan Kehrli and Alexandre Alexakis\*

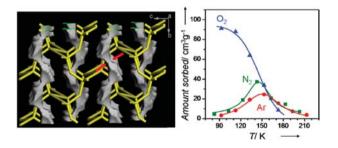
Asymmetric direct Michael addition of α-aminoketone to nitroolefins has been accomplished with good yields and selectivities using (S)-1-(2-Pyrrolidinylmethyl)pyrrolidine as organocatalyst and α-NH-Tosyl acetone as nucleophile source. This process provides synthetically useful 2-aryl-3-amino-disubstituted  $\gamma$ -acetyl nitro compounds.

4697

#### Temperature-triggered gate opening for gas adsorption in microporous manganese formate

Hyunuk Kim, Denis G. Samsonenko, Minyoung Yoon, Ji Woong Yoon, Young Kyu Hwang, Jong-San Chang\* and Kimoon Kim\*

Microporous manganese formate shows temperature-triggered gate opening for N<sub>2</sub> and Ar adsorption, which is not due to a structural change of the framework but due to dynamic opening of the pore aperture and/or sufficient kinetic energy of the adsorbates to overcome a barrier above a critical temperature.



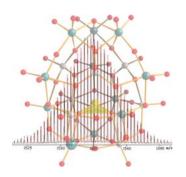
4700

#### Synergistic effects in gene delivery—a structure–activity approach to the optimisation of hybrid dendritic-lipidic transfection agents

Simon P. Jones, Nathan P. Gabrielson, Daniel W. Pack and David K. Smith\*

We report significant synergistic effects for gene delivery using hybrid mixed systems which combine aspects of both main classes of synthetic vectors, i.e., cationic polymers and cationic lipids.



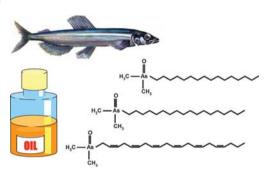


Solution identification and solid state characterisation of a heterometallic polyoxometalate {Mo $_{11}V_7$ }:  $[Mo_{-11}^{VI}V_5^VV_2^IO_{52}(\mu_9\text{-SO}_3)]^7-$ 

Haralampos N. Miras, Daniel J. Stone, Eric J. L. McInnes,\* Raphael G. Raptis, Peter Baran, George I. Chilas, Michael P. Sigalas, Themistoklis A. Kabanos\* and Leroy Cronin\*

A polyoxomolybdenum/vanadium-sulfite {M<sub>18</sub>} cluster-based compound,  $[Mo^{VI}_{11}V^{V}_{5}V^{IV}_{2}O_{52}(\mu_{9}-SO_{3})]^{7-}$ , is reported.

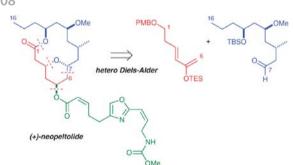
4706



Arsenic-containing hydrocarbons: natural compounds in oil from the fish capelin, Mallotus villosus

Mojtaba S. Taleshi, Kenneth B. Jensen, Georg Raber, John S. Edmonds, Helga Gunnlaugsdottir and Kevin A. Francesconi\*

Fish oils, rich sources of health-promoting compounds, also contain arsenic bound into hydrocarbons which raises intriguing questions about the biogenesis of these arsenicals and their metabolic fate.

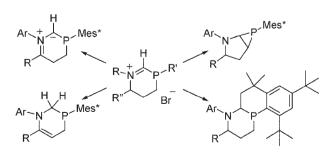


Total synthesis of the marine macrolide (+)-neopeltolide

Ian Paterson\* and Natalie A. Miller

A concise total synthesis of the antiproliferative macrolide (+)-neopeltolide has been completed, utilising a Jacobsen hetero Diels-Alder reaction to install the trisubstituted tetrahydropyran ring.

4711



A persistent P,N-heterocyclic carbene

Guido D. Frey, Maoying Song, Jean-Baptiste Bourg, Bruno Donnadieu, Michele Soleilhavoup and Guy Bertrand\*

Conjugate acids of cyclic (amino)(phosphino)carbenes (P-NHCs) have been prepared, and several different processes have been observed during their deprotonation, which include the formation of a metastable P-NHC, an azomethine ylide, and a bicyclic phosphirane.

#### Soluble precursors of 2,3-naphthalocyanine and phthalocyanine for use in thin film transistors

Atsuko Hirao, Taiji Akiyama, Tetsuo Okujima,\* Hiroko Yamada, Hidemitsu Uno, Yoshimasa Sakai, Shinji Aramaki\* and Noboru Ono\*

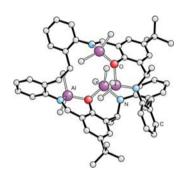
Soluble precursors of 2,3-naphthalocyanine (Nc) and phthalocvanine (Pc) were prepared and converted into insoluble semiconducting thin films of Pc and Nc.

#### 4717

#### Multinuclear alkylaluminium macrocyclic Schiff base complexes: influence of procatalyst structure on the ring opening polymerisation of ε-caprolactone

Abdessamad Arbaoui, Carl Redshaw\* and David L. Hughes

Two remote dialkylaluminium centres supported by a macrocyclic Schiff base ligand exhibited beneficial cooperative effects, whilst aluminoxane-type bonding proved to be detrimental to activity for the ring opening polymerisation of ε-caprolactone.



#### 4720

#### Total syntheses of (+)-montanin A and (+)-teuscorolide

I-Chia Chen, Yen-Ku Wu, Hsing-Jang Liu\* and Jiang-Liang Zhu\*

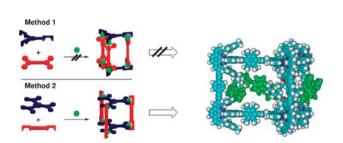
Herein, we describe the first total synthesis of  $(\pm)$ -montanin A and  $(\pm)$ -teuscorolide, two members of the *Teucrium* clerodane diterpenoid family. The synthesis of montanin A was first accomplished in 8 steps, from which teuscorolide was readily achieved in 2 steps.

#### 4723

#### Void and filled supramolecular nanoprisms—notable differences between seemingly identical construction principles

Michael Schmittel\* and Bice He

Void and filled supramolecular nanoprisms (void: 4900 Å<sup>3</sup>) were generated in quantitative yield, but only if units serving as pillars and panels in the self-assembly were optimised with regard to their kinetic behaviour.





### 42nd IUPAC CONGRESS Chemistry Solutions

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On behalf of IUPAC, the RSC is delighted to host the 42nd Congress (IUPAC 2009), the history of which goes back to 1894. RSC and IUPAC members, groups and networks have contributed a wealth of ideas to make this the biggest UK chemistry conference for several years.

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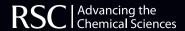
- Analysis & Detection
- Chemistry for Health
- Communication & Education
- Energy & Environment
- Industry & Innovation
- Materials
- Synthesis & Mechanisms

#### Plenary speakers

Peter G Bruce, University of St Andrews
Chris Dobson, University of Cambridge
Ben L Feringa, University of Groningen
Sir Harold Kroto, Florida State University
Klaus Müllen, Max-Planck Institute for Polymer Research
Sir J Fraser Stoddart, Northwestern University
Vivian W W Yam, The University of Hong Kong
Richard N Zare, Stanford University

For a detailed list of symposia, keynote speakers and to submit an abstract visit our website.







#### **COMMUNICATIONS**

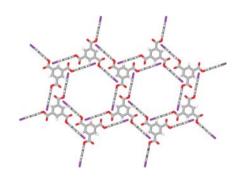


#### 4726

#### Hexagonal crystalline inclusion complexes of 4-iodophenoxy trimesoate

F. Christopher Pigge,\* Venu R. Vangala, Pradeep P. Kapadia, Dale C. Swenson and Nigam P. Rath

Bifurcated  $I \cdots \pi$  and  $I \cdots O = C$  halogen bonding interactions assist in formation of unique iodo-arene trimers leading to nanoscale channels in inclusion complexes of trimesic acid iodophenolate.

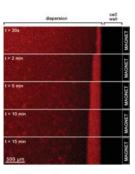




One-pot synthesis and characterizations of bi-functional phosphor-magnetic @SiO<sub>2</sub> nanoparticles: controlled and structured association of Mo<sub>6</sub> cluster units and γ-Fe<sub>2</sub>O<sub>3</sub> nanocrystals

F. Grasset,\* F. Dorson, Y. Molard, S. Cordier,\* V. Demange, C. Perrin, V. Marchi-Artzner and H. Haneda\*

Nanostructured silica coated bifunctional nanoparticles based on  $[Mo_6Br_{14}]^{2-}$  units as phosphorescent dye and magnetic maghemite γ-Fe<sub>2</sub>O<sub>3</sub> nanocrystals were synthesized and characterized.



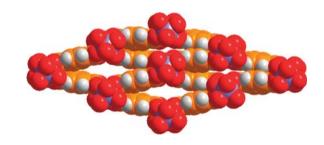


#### 4732

#### Effect of the nature of the metal on the breathing steps in MOFs with dynamic frameworks

Franck Millange,\* Nathalie Guillou, Richard I. Walton, Jean-Marc Grenèche, Irène Margiolaki and Gérard Férey

A highly distorted metastable phase is observed during the reversible dehydration of an iron(III) benzenedicarboxylate Metal-Organic Framework (MOF).

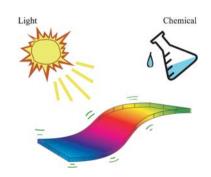


#### 4735

#### Chemical and optical control of peristaltic actuator based on self-oscillating porous gel

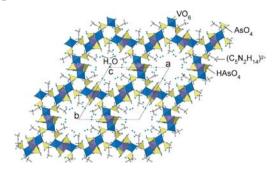
Shu-ichi Shinohara, Takahiro Seki, Takamasa Sakai, Ryo Yoshida and Yukikazu Takeoka\*

We demonstrate the chemical and optical control of the self-sustaining peristaltic motion of a structural colored porous hydrogel.



#### **COMMUNICATIONS**

4738

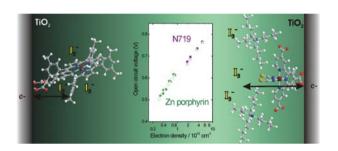


#### Microporous vanadyl-arsenate with the template incorporated exhibiting sorption and catalytic properties

Teresa Berrocal, José L. Mesa,\* José L. Pizarro. Begoña Bazán, Marta Iglesias, Andrés T. Aguayo, María I. Arriortua and Teófilo Rojo\*

 $(C_5H_{14}N_2)[(VO)_3(AsO_4)(HAsO_4)_2(OH)] \cdot 3H_2O$  behaves as a microporous organically templated compound, with reversible adsorption and desorption of N<sub>2</sub> at 77 K, and as an extremely efficient catalyst that catalyzes selective sulfoxide formation from organic sulfides, under mild conditions.

4741

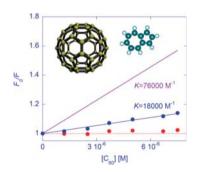


#### The origin of open circuit voltage of porphyrin-sensitised TiO<sub>2</sub> solar cells

Attila J. Mozer,\* Pawel Wagner, David L. Officer, Gordon G. Wallace, Wayne M. Campbell, Masanori Miyashita, Kenji Sunahara and Shogo Mori\*

The performance of porphyrin-sensitised TiO<sub>2</sub> solar cells is limited by their lower open circuit voltage compared to ruthenium complex-sensitised analogs, which is shown to arise from a reduced electron lifetime.

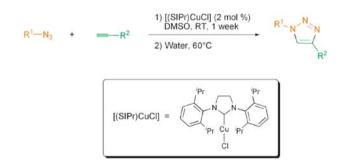
4744



A reassessment of the association between azulene and [60]fullerene. Possible pitfalls in the determination of binding constants through fluorescence spectroscopy

Lorenzo Stella,\* Agostina L. Capodilupo and Massimo Bietti\*

We show that the reported association between azulene and [60]fullerene is due to experimental artifacts, and suggest ways of avoiding such pitfalls.



#### A [(NHC)CuCl] complex as a latent Click catalyst

Silvia Díez-González,\* Edwin D. Stevens and Steven P. Nolan\*

A latent catalyst for the [3+2] cycloaddition reaction of azides and alkynes has been developed in accordance with the principles of Click chemistry

#### A general approach to triphenylenes and azatriphenylenes: total synthesis of dehydrotylophorine and tylophorine

Andrew McIver, Douglas D. Young and Alexander Deiters\*

A microwave-assisted [2+2+2] cyclotrimerization reaction was employed as the key step in the assembly of triphenylenes and azatriphenylenes. The developed approach was used in the total synthesis of phenantroindolizidine alkaloids.

$$\begin{array}{c}
R = X \\
\hline
 [2+2+2] \\
 cyclotrimerization \\
 X = CH \text{ or } N
\end{array}$$

4753

#### Selected regiocontrolled transformations applied to the synthesis of (1S)-cis-chrysanthemic acid from (1S)-3,4-epoxy-2,2,5,5-tetramethylcyclohexanol

Alain Krief,\* Humaira Y. Gondal and Adrian Kremer

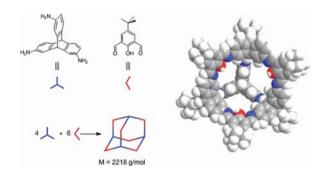
The enantioselective synthesis of (1R)-cis-chrysanthemic acid has been achieved in a few steps, avoiding the formation of byproducts.

4756

#### One-pot synthesis of a shape-persistent endo-functionalised nano-sized adamantoid compound

Michael Mastalerz

By a reversible twelve-fold imine condensation of a rigid  $C_3$ -symmetric triamine and a salicyldialdehyde a highly symmetric cage compound bearing functional groups in the interior is accessible.

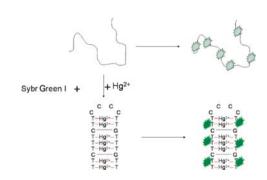


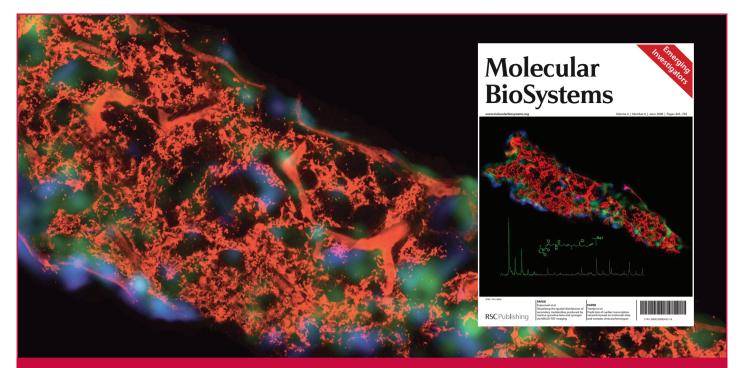
4759

#### Highly sensitive and selective detection of Hg<sup>2+</sup> in aqueous solution with mercury-specific DNA and Sybr Green I

Jing Wang and Bin Liu\*

Sybr Green I efficiently discriminates mercury-specific DNA and mercury-specific DNA/Hg<sup>2+</sup> complex, which provides a label-free, fast, fluorescence turn on assay for Hg<sup>2+</sup> detection with high sensitivity and selectivity.





## **Emerging Investigators theme issue**

*Molecular BioSystems* issue 6, 2008, devoted to outstanding young scientists at the chemical- and systems-biology interfaces, features novel methods to visualise and manipulate protein function in living cells, the development of chemical techniques to monitor specific protein post-translational modifications, new insights into metabolomics and much, much more!

#### Papers include:

Visualization of phosphatase activity in living cells with a FRET-based calcineurin activity sensor Robert H. Newman and Jin Zhang

Conformation and the sodium ion condensation on DNA and RNA structures in the presence of a neutral cosolute as a mimic of the intracellular media

Shu-ichi Nakano, Lei Wu, Hirohito Oka, Hisae Tateishi Karimata, Toshimasa Kirihata, Yuichi Sato, Satoshi Fujii, Hiroshi Sakai, Masayuki Kuwahara, Hiroaki Sawai and Naoki Sugimoto

A quantitative study of the recruitment potential of all intracellular tyrosine residues on EGFR, FGFR1 and IGF1R Alexis Kaushansky, Andrew Gordus, Bryan Chang, John Rush and Gavin MacBeath

**Direct printing of trichlorosilanes on glass for selective protein adsorption and cell growth** Dawn M. Yanker and Joshua A. Maurer

A chemical approach for detecting sulfenic acid-modified proteins in living cells Khalilah G. Reddie, Young Ho Seo, Wilson B. Muse III, Stephen E. Leonard and Kate S. Carroll

#### See also:

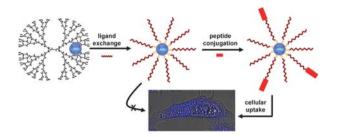
Chem Soc Rev issue 7, 2008 - Chemistry-Biology Interface theme issue For more details visit www.rsc.org/chemsocrev/cbi



Ligand exchanged photoluminescent gold quantum dots functionalized with leading peptides for nuclear targeting and intracellular imaging

Shu-Yi Lin, Nai-Tzu Chen, Shu-Pin Sum, Leu-Wei Lo\* and Chung-Shi Yang\*

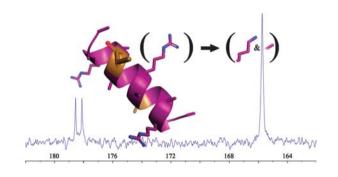
Ligand exchanged gold quantum dots conjugated with cell-penetrating peptides are a new class of photoluminescent probes for nuclear targeting and intracellular imaging.



#### 4765

Lysine and arginine residues do not increase the helicity of alanine-rich peptide helices

James M. Stewart, Jasper C. Lin and Niels H. Andersen\* Residue-specific <sup>13</sup>C=O NMR data establish that substituting a central helical alanine with either Arg or Lys decreases helicity. This parameter,  $\delta(^{13}C')$ , is validated as a helicity measure.

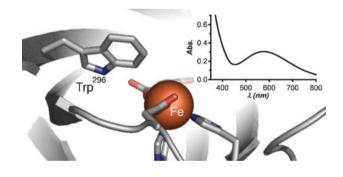


#### 4768

Auto-hydroxylation of FIH-1: an Fe(II), α-ketoglutarate-dependent human hypoxia sensor

Yuan-Han Chen, Lindsay M. Comeaux, Stephen J. Eyles and Michael J. Knapp\*

HIF-asparaginyl hydroxylase (FIH-1) normally couples  $O_2\text{-activation}$  to hydroxylation of  $Asn^{803}$  on the  $\alpha\text{-subunit}$ of the hypoxia-inducible factor (HIFα), a key step in  $pO_2$  sensing. In the absence of HIF $\alpha$ ,  $O_2$ -activation becomes uncoupled, leading to self-hydroxylation at Trp<sup>296</sup> and a purple Fe(III)–O–Trp chromophore.



#### 4771

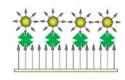
Microgravimetric lectin biosensor based on signal amplification using carbohydrate-stabilized gold nanoparticles

Young-Ku Lyu, Kyung-Rae Lim, Bo Young Lee, Kwan Soo Kim and Won-Yong Lee\*

A highly sensitive microgravimetric lectin Con A biosensor has been developed using mannose-stabilized Au nanoparticles as a signal amplifier.







#### **COMMUNICATIONS**

$$\begin{array}{c} C_{12}H_{25}OOC \\ C_{12}H_{25}OOC \\ OH \end{array}$$

$$\begin{array}{c} H^+ \\ - H^+ \end{array}$$

$$\begin{array}{c} C_{12}H_{25}OOC \\ C_{12}H_{25}OOC \\ O--H \end{array}$$

#### trans-2-Aminocyclohexanol as a pH-sensitive conformational switch in lipid amphiphiles

Barbora Brazdova, Ningrong Zhang, Vyacheslav V. Samoshin\* and Xin Guo\*

Protonation-induced conformational change of lipid tails is reported as a novel strategy to render pH-sensitive lipid amphiphiles and lipid colloids.

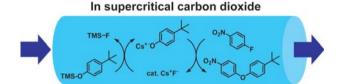
In CH<sub>2</sub>Cl<sub>2</sub> solution:  $\lambda_{abs} = 575 \text{ nm}, \ \lambda_{em} = 610 \text{ nm}$  $\lambda_{em} = 620 \text{ nm CIE } (0.65, 0.34)$ In EL device:

Bulky 4-tritylphenylethynyl substituted boradiazaindacene: pure red emission, relatively large Stokes shift and inhibition of self-quenching

Dakui Zhang, Yugeng Wen, Yi Xiao,\* Gui Yu,\* Yunqi Liu and Xuhong Qian\*

Bulky 4-tritylphenylethynyl substituted boradiazaindacene with pure red emission, relatively large Stokes shift, high fluorescence quantum yield, and low self-quenching was efficiently synthesized and qualified as a potential EL dopant.

4780



Diarvl ether synthesis in supercritical carbon dioxide in batch and continuous flow modes

Jin-Kyun Lee, Matthew J. Fuchter, Rachel M. Williamson, Gary A. Leeke, Edward J. Bush, Ian F. McConvey, Simon Saubern, John H. Ryan and Andrew B. Holmes\*

Diaryl ethers have been prepared with high conversions in batch and continuous flow mode in scCO2 using a fluoride-initiated S<sub>N</sub>Ar reaction.

organics Hydrophilic zeolite Hydrophobic zeolite organics -OH (TEFS)

Fabrication of hydrophobic zeolites using triethoxyfluorosilane and their application as supports for TiO<sub>2</sub> photocatalysts

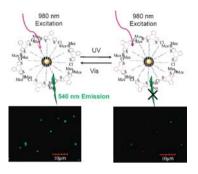
Yasutaka Kuwahara, Takashi Kamegawa, Kohsuke Mori and Hiromi Yamashita\*

Hydrophobically modified Y-zeolites were prepared by simple modification with triethoxyfluorosilane (TEFS). These zeolites, used as supports, enhanced the efficiency of deposited TiO2 for the photocatalytic degradation of organics diluted in water.

#### Up-conversion luminescent switch based on photochromic diarylethene and rare-earth nanophosphors

Zhiguo Zhou, He Hu, Hong Yang, Tao Yi,\* Kewei Huang, Mengxiao Yu, Fuyou Li\* and Chunhui Huang

A novel and unique route to a highly efficient luminescent switch with nondestructive readout capability by utilizing photochromic diarylethene and up-conversion LaF<sub>3</sub>:Yb,Ho nanophosphors was developed.



#### 4789

Self-assembling squares with amino acid-decorated bipyridines: heterochiral self-sorting of dynamically interconverting diastereomers

Alexander Rang, Martin Nieger, Marianne Engeser, Arne Lützen and Christoph A. Schalley\*

Heterochiral self-sorting into only one stereoisomer is observed when metallo-supramolecular squares self-assemble from amino acid-substituted, dynamically interconverting bipyridine stereoisomers and  $dpppM(OTf)_2$  corners (M = Pd, Pt).

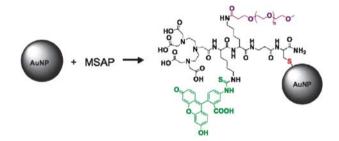


#### 4792

#### Simplified syntheses of complex multifunctional nanomaterials

Elisabeth Garanger, Elena Aikawa, Fred Reynolds, Ralph Weissleder and Lee Josephson\*

A nanomaterial, such as a gold nanoparticle, can be reacted with a trifunctional, single-attachment-point reagent to obtain a multifunctional probe in a single step.

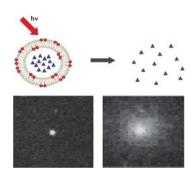


#### 4795

#### Spectrally tunable uncaging of biological stimuli from nanocapsules

Kimberly A. Dendramis, Peter B. Allen, Philip J. Reid and Daniel T. Chiu\*

This paper describes the uncaging of the cellular stimuli in the far red, which is based on the photolysis of nanocapsules whose shells have been photosensitized with highly absorptive chromophores.





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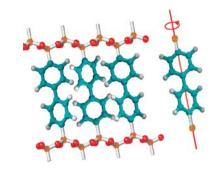
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#### Molecular rotors in hierarchically ordered mesoporous organosilica frameworks

Silvia Bracco, Angiolina Comotti,\* Patrizia Valsesia. Bradley F. Chmelka and Piero Sozzani

Periodic mesoporous organosilicas show a mobility of the diphenylene rotors with correlation times as short as a few nanoseconds, realizing an amphidynamic hybrid material. The structure and dynamics were elucidated by multinuclear solid state NMR from 30 to 500 MHz.

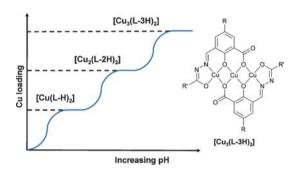


#### 4801

#### Polyacidic multiloading metal extractants

Ross J. Gordon, John Campbell, David K. Henderson, Dorothy C. R. Henry, Ronald M. Swart, Peter A. Tasker,\* Fraser J. White, Jenny L. Wood and Lesley J. Yellowlees

Polynucleating di- and tri-acidic ligands can substantially increase the molar and mass transport efficiencies for the recovery of base metals by solvent extraction.

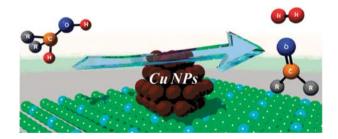


#### 4804

#### Copper nanoparticles on hydrotalcite as a heterogeneous catalyst for oxidant-free dehydrogenation of alcohols

Takato Mitsudome, Yusuke Mikami, Kaori Ebata, Tomoo Mizugaki, Koichiro Jitsukawa and Kiyotomi Kaneda\*

We developed a highly efficient heterogeneous catalytic system using hydrotalcite-supported Cu nanoparticles (Cu/HT) that can successfully promote the oxidant-free dehydrogenation of various alcohols under liquid-phase conditions.

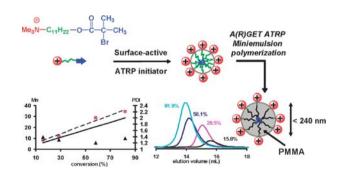


#### 4807

#### Use of a simple surface-active initiator in controlled/living free-radical miniemulsion polymerization under AGET and **ARGET ATRP conditions**

François Stoffelbach,\* Nebewia Griffete, Chuong Bui and Bernadette Charleux\*

This communication describes the first example of the efficient use of a simple amphiphilic molecule as both a surfactant and an initiator in the miniemulsion polymerization of methyl methacrylate under AGET and ARGET ATRP conditions.



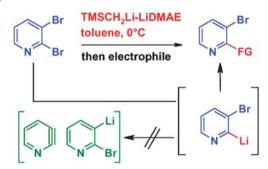
Q

4810

Gold-catalyzed efficient tandem assembly of terminal alkynes and arynes: synthesis of alkynylated biphenyl derivatives

Chunsong Xie, Yuhong Zhang\* and Yuzhu Yang Gold catalysts have been found to catalyze the tandem assembly of arynes and terminal alkynes efficiently in the presence of CuI under mild reaction conditions to provide useful alkynylated biphenyl derivatives.

4813



 $\label{eq:Bromine-lithium} Bromine-lithium\ exchange\ under\ non-cryogenic\ conditions: \\ TMSCH_2Li-LiDMAE\ promoted\ C-2\ lithiation\ of\ 2,3-dibromopyridine$ 

Philippe C. Gros\* and Fatima Elaachbouni

The first fully C-2 selective bromine–lithium exchange in 2,3-dibromopyridine was performed at 0  $^{\circ}$ C in toluene using the TMSCH<sub>2</sub>Li–LiDMAE reagent (LiDMAE = Me<sub>2</sub>N(CH<sub>2</sub>)<sub>2</sub>OLi). The reaction occurred without isomerization of the lithio intermediate while preventing elimination into pyridyne.

4816

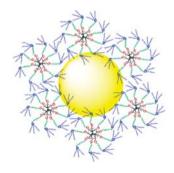


Synthesis of highly phenylene substituted *p*-phenylene oligomers from pyrylium salts

Christian Mahler, Ute Müller, Walter M. Müller, Volker Enkelmann, Chulsoon Moon, Gunther Brunklaus,\* Herbert Zimmermann and Sigurd Höger\*

A simple route towards functionalized *p*-phenylene oligomers is described that does not use metal-mediated cross-coupling reactions.

4819



Gold nanoparticles synthesis and stabilization *via* new "clicked" polyethyleneglycol dendrimers

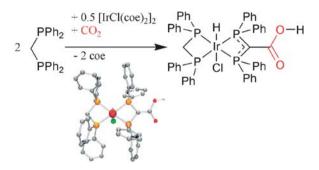
Elodie Boisselier, Abdou K. Diallo, Lionel Salmon, Jaime Ruiz and Didier Astruc\*

Whereas "click" dendrimers with non-polyethylene glycol tethers do not stabilize gold nanoparticles (AuNPs), new "click" dendrimers with tetraethylene glycol and triethylene glycol (TEG) tethers stabilize small AuNPs (1.9 nm) inside the dendrimers of first and second generations (resp. 81 and 243 TEG tethers) and larger AuNPs (4.1 nm) outside the dendrimers of generation zero (27 TEG tethers).

## A C-H activation-CO<sub>2</sub>-carboxylation reaction sequence mediated by an 'Iridium(dppm)' species. Formation of the anionic ligand (Ph<sub>2</sub>P)<sub>2</sub>C-COOH

Jens Langer,\* María José Fabra, Pilar García-Orduña, Fernando J. Lahoz and Luis A. Oro\*

The selective carboxylation of dppm with CO<sub>2</sub> under mild conditions, mediated by iridium, yields an organometallic analogue of carbodiphosphorane CO<sub>2</sub> adducts.

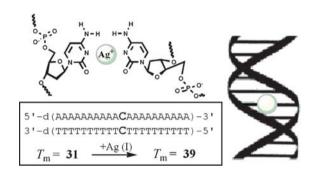


4825

### Specific interactions between silver(1) ions and cytosine-cytosine pairs in DNA duplexes

Akira Ono,\* Shiqi Cao, Humika Togashi, Mitsuru Tashiro, Takashi Fujimoto, Tomoya Machinami, Shuji Oda, Yoko Miyake, Itaru Okamoto and Yoshiyuki Tanaka

Specific binding of Ag(1) cations significantly stabilizes the cytosine–cytosine base pair mismatches in DNA duplexes.

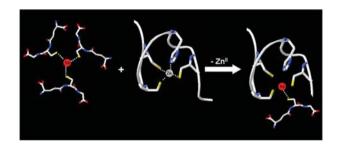


4828

## Interaction of trivalent antimony with a CCHC zinc finger domain: potential relevance to the mechanism of action of antimonial drugs

Cynthia Demicheli,\* Frédéric Frézard, John B. Mangrum and Nicholas P. Farrell\*

Sb<sup>III</sup> competes with Zn<sup>II</sup> for its binding to the CCHC zinc finger domain of the NCp7 protein of HIV-1, indicating that zinc finger proteins may be targets for antimony-based drugs.

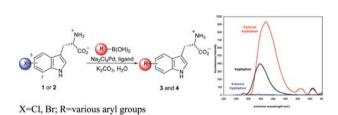


4831

## Development of fluorescent aryltryptophans by Pd mediated cross-coupling of unprotected halotryptophans in water

Abhijeet Deb Roy, Rebecca J. M. Goss,\* Gerd K. Wagner\* and Michael Winn

A convenient and high yielding procedure for the Suzuki–Miyaura cross-coupling of unprotected halotryptophans in water is reported. The fluorescent properties of tryptophan can be tuned by the installation of various aromatic substituents on the indole ring.



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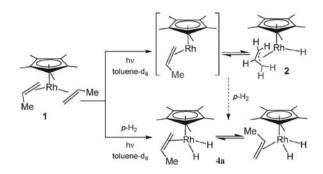
Professor Mehmet Toner, Harvard Medical School, Boston, USA

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#### Utilisation of an η<sup>3</sup>-allyl hydride complex, formed by UV irradiation, as a controlled source of 16-electron $(\eta^5-C_5Me_5)Rh(CH_2=CHMe)$

Catherine J. Sexton, Joaquín López-Serrano, Agustí Lledós and Simon B. Duckett\*

Low temperature UV irradiation of solutions of  $(\eta^5-C_5Me_5)Rh(CH_2=CHMe)_2$  yields  $(\eta^5-C_5Me_5)Rh(\eta^3-CH_2CHCH_2)(H)$ , which provides controlled access to the 16-electron fragment  $(\eta^5-C_5Me_5)Rh(CH_2=CHMe).$ 



#### 4837

#### Metal-catalyzed reaction of N-(2-indolyl)methyl, N-bis(trimethylsilyl)methyl diazoamides: an entry into the β-carboline ring system

Bao Zhang and Andrew G. H. Wee\*

The intramolecular metallocarbenoid reaction of 2-indolyl N-BTMSM diazoamides proceeded efficiently with high conformational control and chemoselectivity to form cyclopropyl intermediates that rearranged to give tetrahydro-β-carboline derivatives.

R = Me, MOM,  $RSO_2$ ;  $R' = CH_2(TMS)_2$ , R'' = H,  $CH_2OMOM$ ; R''' = H or  $CO_2R$ 

#### 4840

#### A catalytic highly enantioselective direct synthesis of 2-bromo-2-nitroalkan-1-ols through a Henry reaction

Gonzalo Blay,\* Victor Hernández-Olmos and José R. Pedro\*

Highly enantiomerically enriched 2-bromo-2-nitroalkan-1-ols are prepared by direct condensation of aliphatic and aromatic aldehydes with bromonitromethane in the presence of a catalytic amount of copper(II) acetate and a  $C_1$ -symmetric camphor-derived amino pyridine ligand.

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# Chemical Science

An environmentally-friendly route to an industrial chemical is unveiled

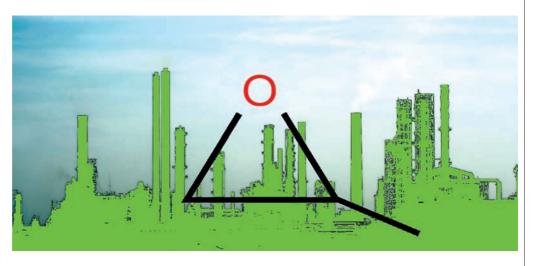
## Propylene oxide gets a green makeover

US chemists have developed a greener, higher yielding and more selective route to propylene oxide, an important industrial chemical that is manufactured worldwide on a million tonne scale.

Propylene oxide is a vital building block for making many other compounds and materials, such as surfactants and foams. However, the two routes used to manufacture it in bulk involve environmentally unfriendly peroxides and chlorinated materials to oxidise propylene, and produce undesirable waste products.

Qunlai Chen and Eric Beckman at the University of Pittsburgh have devised a one-pot route that uses a titanium-modified zeolite catalyst to prepare the oxidant hydrogen peroxide in situ from hydrogen and oxygen. Additionally the reaction solvent is environmentally benign liquid- or supercritical-carbon dioxide containing small quantities of methanol and water.

According to Beckman, many of the common side reactions of



the process (such as propylene hydrogenation or propylene oxide hydrolysis) can be effectively suppressed by using an ammonium acetate additive to neutralise the surface acidity of the catalyst.

Propylene conversion rates are normally limited to less than 10% in order to maintain the required product selectivity. Using the onepot route, Beckman obtains yields Propylene oxide is manufactured annually on a million tonne scale

#### Reference

Q Chen and E J Beckman, Green Chem., 2008, **10**, 934 (DOI: 10.1039/b803847c) of over 21% with an 82% selectivity for the first time.

Yasutaka Ishii, an expert in hydrocarbon oxidation reactions using hydrogen peroxide, based at Kansai University, Osaka, Japan, considers this method to be a very interesting green route for making propylene oxide, pointing out that no harmful waste is produced. David Parker

### In this issue

#### **Sweet smell of success**

Ionic liquids assist the synthesis of a lemon scented chemical

#### **Natural product hybrids fight cancer**

A potent hybrid of two anticancer natural products has been designed and synthesised

#### **Instant insight: Lovely bubbly**

Gérard Liger-Belair, University of Reims Champagne-Ardenne, France, celebrates what gives champagne its sparkle

#### **Instant insight: Tasting the chemistry**

Susan Ebeler, University of California, Davis, US, reveals the science behind the flavour in everyone's favourite tipple









A snapshot of the latest developments from across the chemical sciences

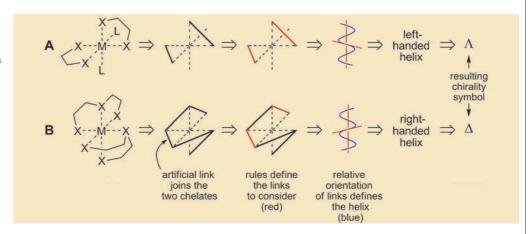
## **Research highlights**

A new proposal for defining the chirality of octahedral complexes is put forward

## Getting to grips with complex chirality

Naming inorganic compounds is usually a routine operation, but one problem has long defied solution – how to define the chirality of certain octahedral complexes containing chelates (ligands with more than one point of attachment). Santiago Herrero from the Complutense University of Madrid, Spain, and his colleague have now proposed a way of doing this.

The general idea when defining the chirality of such complexes is to ignore the identity of the donor atoms on the ligands and any chiral centres on the chelates, as this can be dealt with by standard stereochemical symbols. Instead. the focus is the topology of the chelate network. This is how the six atoms attached to the central metal atom – the vertices of the octahedron - are joined together. The chelates are first drawn as straight lines joining the vertices. These lines are then compared, and the complex assigned as  $\Lambda$  (lambda) if they define a left-handed helix, and  $\Delta$  (delta) if they define a righthanded helix. This is fine in simple complexes such as A (see image),



but things get difficult in cases like **B**, because there is more than one possible pair of lines to compare. Herrero and Usón have now devised a heirarchy of rules that enable such systems to be dealt with.

The new system works by first (if necessary) artificially linking the chelates together so that the resulting line has the greatest number of changes of plane. A set of rules then allows you to pick a pair of links that you can use to define the complex as  $\Delta$  or  $\Lambda$ . Further rules,

Defining the chirality of chelate-containing complexes is a longstanding problem

Reference

S Herrero and M A Usón, *Dalton Trans*, 2008, 4993 (DOI: 10.1039/b806050a) involving consideration of all the vertices that are not directly joined, allow the designation of chirality in even stranger complexes.

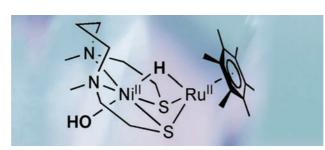
Although the chirality symbols in several cases are different under the new system, says Herrero, there are fewer rules to contend with. In conclusion, he says that their method 'could be useful for keeping and searching precise structural information about octahedral compounds'. David Barden

Water-soluble organometallics may aid the development of new types of catalysts

## **Energy from model enzymes**

Mimicking enzymes with inorganic complexes could offer a new route to catalysing hydrogen fuel cells, claim Japanese scientists.

In nature, hydrogenases are enzymes that catalyse the splitting of hydrogen in its H2 form into two separate protons and two electrons. However, there has been some controversy over the mechanism by which the enzyme operates, with mechanistic studies contradicting experimental data. Now, a group led by Seiji Ogo at Kyushu University, Fukuoka, have solved this problem by making a nickel-ruthenium complex that acts as a model of the enzyme. They say this complex could be used to develop new cathode catalysts for hydrogen fuel cells.



Described by Chris Pickett, an energy expert from University of East Anglia, Norwich, UK, as 'an elegant chemical precedent', the complex is water-soluble like natural hydrogenases, and so allows the first study of a model in the hydrogenases' natural environment.

Ogo explains that that understanding the exact

Impersonating nature could offer access to new types of catalysts for fuel cells

#### Reference

B Kure et al, Dalton Trans., 2008, 4747 (DOI: 10.1039/ b807555g) mechanism of the hydrogenase will allow scientists to progress research into new types of catalysts for hydrogen fuel cells. The group studied how the complex reacts and showed that the generation of single and double exchange products is simultaneous, just as observed for the naturally occurring enzymes. Ogo is now looking forward to further studies on this model that should uncover more details of the reaction

Water soluble organometallics like these have become more and more interesting for both life and materials sciences. Ogo hopes that technology for the extraction of electrons from hydrogen, using his new complexes can now be developed. *Laura Howes* 

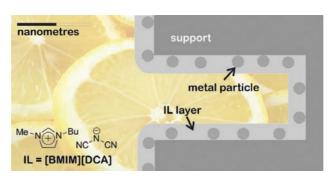
### Ionic liquids improve the synthesis of a lemon scented chemical

### **Sweetsmell of success**

Scientists from Germany have used ionic liquids to improve the performance of a catalyst that produces citronellal from citral - two compounds that are commonly used as a flavouring and in the perfumery industry, both having a sweet lemon

The hydrogenation of citral is usually performed with a palladiumcarbon catalyst. Unfortunately, this reaction does not selectively stop at citronellal, often hydrogenating further to make other products.

Peter Claus and colleagues from the Technical University of Darmstadt have been looking for a catalyst that would produce citronellal selectively. 'This is very important to the chemical industry, where consecutive hydrogenations must very often be prevented,' says Claus



Ionic liquids are salts in liquid form, and are frequently used as non-volatile solvents and stabilisers in chemical reactions. Claus found that by impregnating an already known Pd/SiO<sub>2</sub> catalyst with an ionic liquid (called butylmethylimidazolium dicyanamide) an almost 100 per cent yield of citronellal

The ionic liquid (IL) coating improves the hydrogenation catalyst's performance

Reference

J Arras et al. Chem. Commun. 2008, 4058 (DOI: 10.1039/ b810291k)

is obtained, and very little further hydrogenation occurred.

What's more, by using the ionic liquid as a coating on the catalyst, rather than a bulk solvent, the production cost decreased, and there was no need to separate out the product at the end of the reaction, making the process one step shorter.

Douglas MacFarlane from the ionic liquids group at Monash University, Australia, says this development opens up new areas for catalyst applications. 'This is a fascinating piece of work that shows how effective an ionic liquid layer can be in controlling the selectivity of a conventional solid phase catalyst,' he says. Rebecca Brodie

Potent combination of two anticancer molecules synthesised

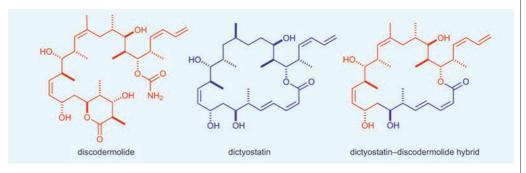
## **Natural product hybrid fights cancer**

A potent hybrid of two anticancer natural products has been designed and synthesised by UK chemists.

Developing analogues of natural products with improved biological activity is an area of great current interest. Ian Paterson and colleagues at the University of Cambridge have now made a natural product analogue with anticancer activity using a combination of rational design and state-of-the-art synthesis.

Discodermolide is a natural product from marine sponges with high activity against cancer cells. It is currently in clinical trials, but the search is always on for more active analogues. Paterson compared the structure of discodermolide with that of dictyostatin, a more potent but less studied natural product. Using knowledge of the protein binding site involved in the anticancer activity of both molecules, they improved the potency of discodermolide by replacing a part of its structure with a fragment from dictyostatin.

Both natural products are only available in minute quantities, so



A hybrid of discodermolide (red) and dictyostatin (blue) has been assembled

Reference I Paterson, G J Naylor and A E Wright, Chem. Commun.. 2008, DOI: 10.1039/b811575c the group made their hybrid from scratch. Paterson says that this proved challenging, but that they were able to exploit boron aldol methodology and other synthetic methods to develop 'an efficient and scalable route' to the hybrid.

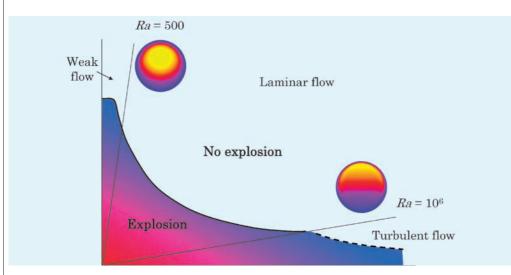
The hybrid was then tested on four cancer cell lines, and was found to be more potent than discodermolide for all of them. The group also found that deactivating the two hydroxyl groups at the bottom left of the molecule, by tying them up in a ring, resulted in a large drop in activity. This indicates, says Paterson, that one or both of

these hydroxyls 'play a key role' in the activity of dictyostatin and discodermolide.

Dennis Curran, from the University of Pittsburgh, US, finds the work very exciting: 'the Paterson group has a flair for analogue design and efficient synthesis, and it looks like they have hit gold with the testing results on this one'. Future work, says Paterson, will involve 'further probing the pharmacophore and anticancer profiles of these fascinating marine natural products and their hybrids'.

Is your reaction mixture going to explode? Why not ask a theoretical chemist...

## When convection goes without a bang



UK researchers have been investigating how to predict whether a reacting mixture will explode.

Silvana Cardoso and colleagues, at the University of Cambridge, have worked out how to separate the different effects that remove heat from the reaction and hence prevent explosions. These effects are conduction, where the heat flows through material, and convection,

where hot material rises away from the reaction site. 'To date', says Cardoso, 'these effects have been analysed in a coupled form. Previously they have been taken into account either in an empirical way, by modifying simpler solutions valid when only heat conduction is present, or in a complex, numerical calculation. Our new treatment allows us to grasp a whole landscape of explosion phenomena which

Theoretical chemists have improved our understanding of why things explode

#### Reference

T.-Y. Liu *et al*, *Phys. Chem. Chem. Phys.*, 2008, **10**, 5521 (DOI: 10.1039/b808222g)

seemed to be unrelated before.'

Cardoso says 'this project aims to develop a more comprehensive theory of explosion, in which the effects of natural convection, as well as those of forced fluid flow, such as by a pump or a stirrer, may be quantified in an explicit manner.' Vitaly Volpert, a mathematician at the University of Lyon, France, identifies the key contribution of the research: 'The interest of the work is that the authors compare the numerical simulations with experimental results, and consider a spherical geometry, which has not been done before.'

Volpert identifies two directions this research could take next, 'If we are talking about fire safety, and this is an important issue, I would say a systematic experimental and theoretical investigation of fuel tanks and so on is needed.' From a theoretical point of view, however, he would like to see a systematic investigation of complex nonlinear dynamics, for example the transition of the behaviour of the combusting system to chaos and chaotic heat explosions. *Colin Batchelor* 

### Researchers step closer to explaining hydrocarbon formation in space

### **A T**itan discovery

The chemistry used to make a rare argon–carbene cation may hold the key to hydrocarbon formation on Saturn's largest moon, claim European researchers.

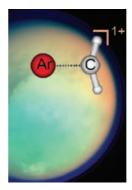
Detlef Schröder from the Academy of Sciences in Prague, Czech Republic, and co-workers have made a noblegas compound by colliding argon with dications. Using experimental and theoretical studies they showed that bromomethane (CH<sub>3</sub>Br) can be ionised to the molecular dication CH<sub>3</sub>Br<sup>2+</sup> – that can rearrange to the tautomer CH<sub>2</sub>BrH<sup>2+</sup>. The reaction of this dication with argon leads to the argon–carbene cation (ArCH<sub>2</sub><sup>+</sup>). <sup>1</sup> Schröder also made the corresponding carbene cation for other noble gases, including krypton

and xenon.

Their work could shed light on the mysteries of the upper part of Titan's atmosphere – the ionosphere – that is known to consist of complex hydrocarbons. Previously scientists have struggled to explain how these are formed.

Stephen Price, from University College London, UK, agrees saying that 'in recent years the bondforming chemistry of molecular doubly-charged ions has been implicated in environments as varied as the interstellar medium and planetary ionospheres.' And Schröder has shown before that dications are involved in the growth of hydrocarbons on Titan.<sup>2</sup>

Compounds containing noble-



Hydrocarbon formation in space is poorly understood

gases are rare because they are notoriously difficult to make, with most needing to contain highly electronegative elements – such as fluorine, iodine, oxygen – that are capable of attacking the closed-shell configuration of electrons of the noble gas atoms.

Price adds that, 'the synthesis of argon-carbon bonds using doubly-charged molecular reagents, further extends the range of fields in which the chemistry of gas-phase dications is potentially important.'

Emma Shiells

#### References

1 D Ascenzi et al, Chem. Commun., 2008, 4055 (D0I:10.1039/b811115d) 2 C L. Ricketts et al, Chem. Eur. J., 2008, **16**, 4770

## **Instant insight**

# Lovely bubbly

Gérard Liger-Belair, University of Reims Champagne-Ardenne, France, celebrates what gives champagne its sparkle

Since the time of the Benedictine monk Dom Pierre Perignon (1638–1715) champagne is the wine of celebration. With its image inextricably linked to the elegance of its effervescence - the small bubbles it emits.

In champagne and sparkling wines, carbon dioxide molecules form in excess during a unique second fermentation process. And once opened, champagne in a typical 0.75 litre bottle releases approximately five litres of CO<sub>2</sub>. This equates to a huge 20 million bubbles formed per bottle.

Bubbles do not just appear as champagne is poured, the dissolved CO<sub>2</sub> molecules must be able to group together and push their way through the liquid molecules. Energetically this is not easy, and close inspection of glasses filled with champagne shows that most of the bubble nucleation (growth) sites are preexisting gas cavities on the surface of the glass. These gas cavities are trapped inside cellulose fibres on the surface of the glass, that come from the surrounding air or from wiping the glass with a cloth before use.

Recent calculations have linked the final bubbles' size with a combination of their growth rate, the speed with which they ascend and other parameters. The amount of dissolved carbon dioxide content is important: a reduction by a factor of two - which is approximately the factor between champagne and beer - decreases the average bubble size by about 40 %. This is the main reason why, contrary to popular belief, beer bubbles are significantly smaller than those in champagne. The bubble size is also strongly gravity and pressure dependent. On the Moon for example, where the

gravity acceleration is only a sixth of that on Earth, bubbles would be about three times larger in volume. And if you could enjoy a glass of champagne on the top of Mount Everest, where the overall pressure is only about 30 per cent of the pressure at the sea level, bubbles would increase by a factor of almost four in volume. This is basically the same phenomenon that is responsible for gas embolism in divers who have breathed high pressure air under water, if they resurface too quickly.

Once formed, bubbles rise toward the liquid surface due to their own buoyancy. While rising, they continue to grow in size by continuously absorbing carbon dioxide molecules dissolved into the champagne. Bubbles therefore continuously accelerate along their way through the champagne. This continuous acceleration can be watched using high speed photographs, where the continuously increasing spacing between the successive bubbles in a given bubble train can be seen. Contrary to popular belief however, champagne bubbles rise at a relatively slow pace (0.5 kilometres per hour), comparable to that of a turtle. That said, when opening a bottle of champagne the release of CO<sub>2</sub> means an uncontrolled cork can reach speeds of 50-60 kilometres per hour!

Without bubbles champagne would be unrecognisable, sparkling wines and beers would be flat. However, the role of effervescence is suspected to go far beyond the sole aesthetical point of view. Bubbles bursting at the liquid surface radiate hundreds of tiny liquid jets which quickly break up into a multitude of tiny droplets every second. Those tiny droplets, ejected up to



A standard bottle of champagne releases 20 million bubbles

Reference G Liger-Belair, Chem. Soc. Rev., 2008, DOI: 10.1039/ several centimetres above the liquid surface, partly evaporate, thus accelerating the transfer of volatile organic compounds and enhancing the flavour profile of the wine.

The close observation of bubbles collapsing at the surface of a glass filled with champagne reveals another unexpected and lovely phenomenon. A few seconds after pouring, and after the collapse of the foamy head, the surface of a champagne flute is covered with a layer of bubbles - a kind of bubble raft. Here each bubble is surrounded by approximately six neighbouring bubbles. These bubbles arrange themselves in a hexagonal pattern, resembling those in beeswax. Due to capillary forces, when a bubble

bursts and leaves an open cavity at the champagne surface, adjacent bubbles are sucked towards this empty cavity and creating short-lived flower-shaped structures, invisible to the naked eye.

Who would have imagined that a flute of champagne is such a fantastic playground for a chemical physicist in love with microphotography, or for a champagne lover with the time and knowledge to reflect on what is happening right under his nose?

Read Gérard Liger-Belair's critical review 'Recent advances in the science of champagne bubbles' in issue 11, 2008 of Chemical Society Reviews.





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## **Instant insight**

# **Tasting the chemistry**

Susan Ebeler, University of California, Davis, US, reveals the science behind the flavour in everyone's favourite tipple

As you sit down to quaff a glass of wine after work, do you ever pause to notice the faint aroma of boxwood, violets or paraffin? Your perception of wine flavour mainly involves four of the five senses - vision, touch, taste and smell. And it is our nose that gives the greatest contribution to the flavour by detecting the aroma of hundreds of volatile chemical compounds in the wine. The compounds responsible for the smells above are - at low concentrations - typically present in popular grape varieties such as Sauvignon blanc, Pinot noir and Riesling.

As you reach the end of the bottle do you ever start to ponder about the people who make your wine? It may surprise you to learn that science - including analytical chemistry, sensory science, genetics and molecular biology - plays a large part in providing much of the information needed by wineries to make their wine as appealing as possible to our senses. This includes knowledge of the chemical compounds that contribute to wine flavour, how this flavour is formed during grape growth and the winemaking process, how humans perceive flavour compounds and how human genetics can influence individual perception of smells.

Over 1000 different aroma compounds in grapes and wines have now been identified using various analytical tools. Gas chromatography, one of the most powerful tools for separating complex mixtures into individual components, has been widely used for this purpose since the 1950s. However, sensitivity to aromas varies significantly from person to person, so not all volatile compounds that are identified using analytical tools will actually contribute to what you smell. Conversely, sometimes our sensitivity far exceeds that of the analytical chemist's tools.



We have scientists to thank for the delicious taste of both fruity red and crisp white wine

The aroma of the compound that contributes to bell pepper aroma in many Sauvignon blanc and Cabernet Sauvignon wines for example can be sensed by humans at concentrations as low as 2 ng per litre - that's equivalent to two drops mixed into 20 Olympic size swimming pools - far below what any analytical technique can currently sense without special sampling or extraction techniques. New methods for preparing and extracting samples are now allowing scientists to push the limits of analytical detection without requiring litres and litres of sample. Additionally by combining gas chromatography with the human sense of smell, in a technique called gas chromatography-olfactometry, scientists can now isolate the 15-20 chemical compounds that contribute the most to wine aroma from the hundreds or thousands of compounds identified in a specific wine.

Wine aroma is further complicated by interactions between volatile

Reference P Polášková et al, Chem. Soc. Rev., 2008, DOI: 10.1039/

aroma, and non-aroma, compounds. The interactions mean that two aroma compounds may smell differently when mixed together. Additionally a strong fruity aroma can also mask a weaker vegetable aroma in a wine.

Using a combination of sensory and analytical tools, and an improved understanding of the genetics, physiology and neurobiology of how humans perceive smells, scientists are ever improving our knowledge of the factors that contribute to overall wine aroma perception.

Molecular biologists are also studying how plant and yeast genes impact aroma formation in the grape and during fermentation, improving our understanding of the biochemical processes involved in flavour formation.

Armed with this knowledge, viticulturists and winemakers can study how vineyard practices - such as soil conditions, irrigation and fertilisation - and winemaking processes – such as choice of yeast strain, fermentation temperature, yeast nutrients, oxygen exposure impact the chemical composition and sensory properties of their wine. All this information allows winemakers to identify grape varieties, yeast strains, and fermentation conditions that will yield desired flavour properties for specific wine styles and consumer preferences.

I suspect you didn't realise the chemistry in a glass of wine is quite so complex. So, the next time you enjoy a glass of fine wine take time to toast the chemists, plant scientists, viticulturists and winemakers who've used the latest scientific tools to ensure that it tastes and smells the way you know and love.

Read Pavla Polášková, Julian Herszage and Susan Ebeler's critical review Wine flavor: chemistry in a glass' in issue 11, 2008 of Chemical Society Reviews

# **Essential elements**

## **Engineering success**

CrystEngComm celebrated its tenth year of publication in style on 28 August with a lunch reception held at the XXI Congress and General Assembly of the International Union of Crystallography in Osaka, Japan. As part of the celebrations, the journal also awarded five poster prizes at the meeting.

Since its launch in 1999, *CrystEngComm* has gone from strength to strength, growing in size by more than a factor of ten. The journal now boasts the fastest publication times and highest immediacy index for a crystal engineering journal, plus an impressive impact factor of 3.47. In his welcome speech, CrystEngComm editor Jamie Humphrey outlined the successes of the past decade and extended his thanks: 'This success has been possible only through the support that you and other members of the crystal



engineering community have given the journal – your support as authors, referees, readers and in some cases editorial and advisory board members.'

Regular CrystEngComm author Pierangelo Metrangolo of Milan, Italy, who attended the lunch reception, cites the journal as one of his favourites for publication of his research. 'In particular,' he says, 'I appreciate the speed at which papers are processed and the very kind co-operation of the editorial staff. What else to say: Happy Birthday *CrystEngComm...*, and keep up the good work!'

A decade since launch and the future for *CrystEngComm* has never looked so bright. Celebrations will continue later this year with an anniversary theme issue, including articles by editorial and advisory board members, and the journal is also heavily involved in the organisation of a crystal engineering symposium as part of the IUPAC Congress next year in Glasgow.

Visit www.crystengcomm.org for updates on these and other exciting events.

### **Facebook fans**

Enjoyed reading the first few issues of RSC Publishing's newest journal, Energy & Environmental Science (EES)? Then become a Facebook fan by visiting the *EES* Facebook page and joining in. Fans can see summaries and link to the latest *EES* articles published online, view and share relevant videos, images, events and news. Use the page to find out about upcoming events where you can meet the editors or contribute to a discussion and connect with fellow fans. Fans will see stories in their News Feed when their friends become fans or engage with the EES Facebook page in a variety of ways. You can find the EES Facebook page by searching for Energy & Environmental Science using the Quick Search bar on any Facebook page or by going to the main search page. Or paste the following URL into

Or paste the following URL into your browser: www.facebook.com/pages/Energy-Environmental-Science/24375018213. See you there!

### Awarm reception in Philadelphia

The atmosphere inside the Philadelphia Marriott mirrored the sunny blue sky outside as guests gathered at the RSC Reception. Held on 17 August, it coincided with the 236th American Chemical Society National Meeting and Exposition taking place at the Pennsylvania Convention Center.

Around 200 people listened to RSC president Dave Garner as he welcomed guests, including Nobel prize winner Bob Grubbs from Caltech,

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Left to right: Jonathan Sessler (U Texas at Austin), Kate Sear (deputy editor ChemComm, RSC), Kevin Burgess (Texas A&M), Peter Wipf (Pittsburgh)

a variety of eminent and emerging researchers, plus university librarians and local RSC members. The incoming

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president of the ACS, Tom Lane, was also there with a number of his society colleagues, indicating the continuing warm friendship

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between the two chemical societies

Guests enjoyed refreshments while catching up with friends old and new, and RSC staff were on hand to describe the latest RSC initiatives, including the hot topics of *Energy & Environmental Science, Integrative Biology* and *Metallomics*, the three newest RSC journals.

At the end of a genial evening, everyone was looking forward to meeting again – so see you all in Salt Lake City in spring 2009!

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### **RSC** Publishing