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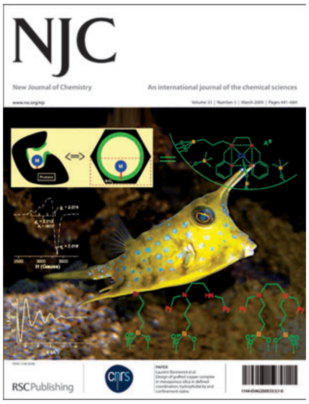
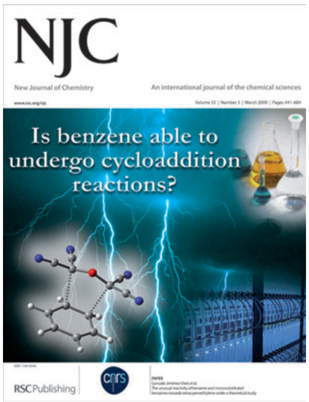


Cover
See Laurent Bonneviot *et al.*, pp. 484–496.
This fish has hexagonal patterned skin reminiscent of the 2D hexagonal silicas used in our article. The schemes are superimposed on a picture of a *Lactoria cornuta*.
Image reproduced with permission of the Aquarium Grand Lyon, La Mulatière, (www.aquariumlyon.fr); Sébastien Abry, Aurore Thibon, Belén Albela, Pierre Delichère, Fréderic Banse and Laurent Bonneviot, *New J. Chem.*, 2009, **33**, 484.



Inside Cover
See Gonzalo Jiménez-Osés *et al.*, pp. 471–478.
Experimental and computational studies demonstrate the ability of benzene derivatives, the prototypical aromatic compounds, to experience cycloaddition reactions towards tetracyanoethylene oxide to give synthetically valuable tetrahydroisobenzofuranes and arylmalononitriles.
Image reproduced by permission of Gonzalo Jiménez-Osés, José Elguero and José I. García from *New J. Chem.*, 2009, **33**, 471.

CHEMICAL SCIENCE

C17

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
March 2009/Volume 6/Issue 3
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LETTERS

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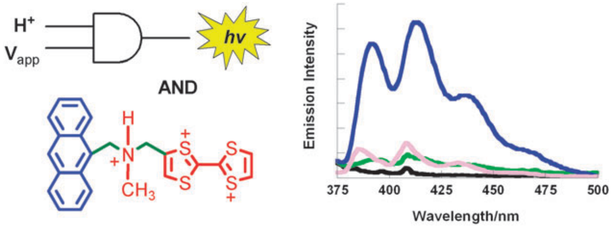
A fluorescent AND logic gate driven by electrons and protons

David C. Magri*

A molecular logic gate displays a fluorescence output after oxidation in acidic media according to an AND logic algorithm.



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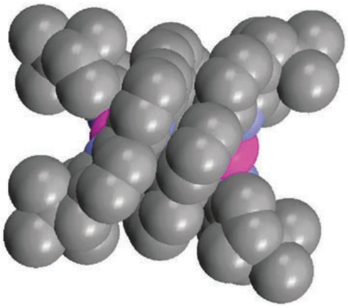
LETTERS

462

Diastereoselective preparation of Cu(I) and Ag(I) double helices by the use of chiral bis-bipyridine ligands

Laure-Emmanuelle Perret-Aebi,* Alexander von Zelewsky* and Antonia Neels*

Formation through self-assembly reaction of highly diastereoselective double helices with copper(I) and silver(I) as coordination centers.



PAPERS

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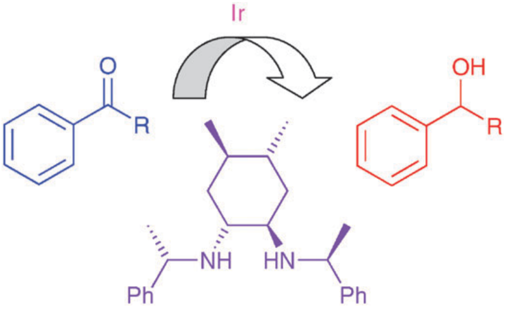
Iridium complexes of chiral diamines containing carbon and nitrogen stereocentres: synthesis, structure and evaluation as transfer hydrogenation catalysts

José A. Fuentes,* Marcia B. France, Alexandra M. Z. Slawin and Matthew L. Clarke

Ir(III) complexes of a chiral diamine ligand have been synthesised, and found to be active in the asymmetric transfer hydrogenation of bulky ketones, giving excellent conversions and moderate enantioselectivities.



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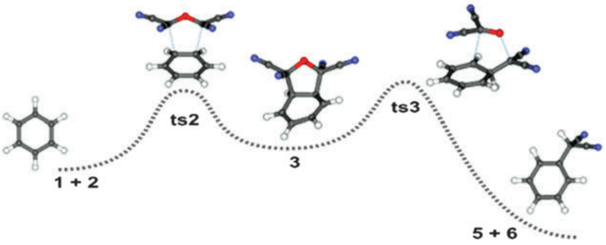
The unusual reactivity of benzene and monosubstituted benzenes towards tetracyanoethylene oxide: a theoretical study

Gonzalo Jiménez-Osés,* José Elguero and José I. García

The cycloaddition of tetracyanoethylene oxide with benzene derivatives, and the subsequent evolution of the corresponding cycloadducts are theoretically investigated using DFT and highly correlated *ab initio* calculations.



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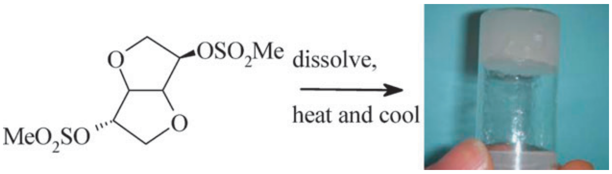
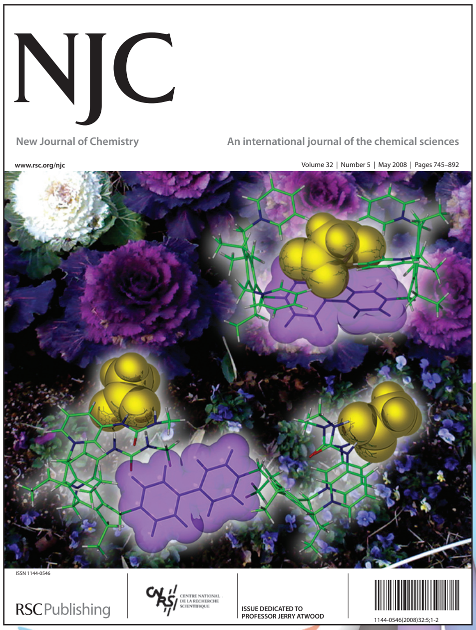
A low molecular weight hydro and organogelator derived from an isohexide and sol–gel transcription of the alcogel

Steven J. Craythorne, Ciara L. Pollock, Alexander J. Blake, Mark Nieuwenhuyzen, Andrew C. Marr and Patricia C. Marr*

The bis-dimethyl sulfonyl derivative of isosorbide has been shown to gel a range of solvents. This low Mwt organogelator has been structurally characterised by single X-ray crystallography. The organogels have been used to transcribe silica by a sol–gel process.





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Drawing disciplines together

Introducing Professor Peter Junk

Associate Editor

Peter Junk graduated from the University of Western Australia in 1984 obtaining a Bachelor of Science with first class honours in physical and inorganic chemistry, and completed his PhD in organometallic chemistry under the supervision of Professor Colin Raston in 1988. He currently holds a position of Professor of Chemistry and is the Head of the School of Chemistry at Monash University, Australia.

His main research interests are in rare earth and main group organometallic, organoamido and aryloxo chemistry, but has applied interests in X-ray imaging and corrosion inhibition. To date, he has published more than of 250 publications and reviews.

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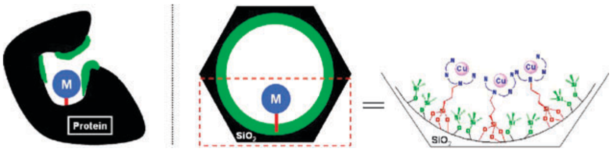
Design of grafted copper complex in mesoporous silica in defined coordination, hydrophobicity and confinement states

Sébastien Abry, Aurore Thibon, Belén Albela, Pierre Delichère, Fréderic Banse and Laurent Bonneviot*

A bio-inspired synthesis of a polydentate copper(II) complex grafted on a mesostructured porous silica is developed following the structural concept of metalloprotein where well-defined metal ion coordination state, hydrophobic environment and confined space are at stake.



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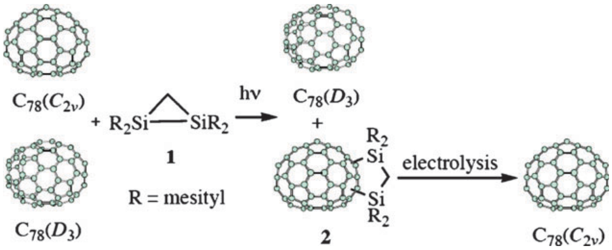
A new method for separating the D_3 and C_{2v} isomers of C_{78}

Ai Hong Han, Takatsugu Wakahara, Yutaka Maeda, Takeshi Akasaka,* Mamoru Fujitska, Osamu Ito, Kazunori Yamamoto, Masahiro Kako, Kaoru Kobayashi and Shigeru Nagase

This paper describes the efficient separation of two isomers of fullerene C_{78} (namely D_3 and C_{2v}) by using a silylation–oxidative desilylation protocol.



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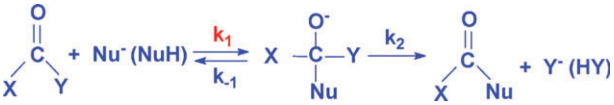
Effects of substituents on activation parameters in the reactions of carboxylic acid derivatives with anionic and neutral nucleophiles

Vladislav M. Vlasov*

$\Delta H^{\ddagger} = \delta\Delta H^{\ddagger}\sigma + \Delta H^{\ddagger}_{o}$; $\delta\Delta H^{\ddagger} = \delta\Delta H^{\ddagger}_{ext} + \delta\Delta H^{\ddagger}_{int}$; $\delta\Delta H^{\ddagger}_{int} = (-1.32 \pm 0.19) - (5.13 \pm 0.092)\rho$ ($r = 0.996$, $s = 0.75$, $n = 25$) where $\rho = \rho(k_1)$. The charge development in the transition state ($\boldsymbol{k_1}$) is mainly governed by the internal part of the activation enthalpy change, $\delta\Delta H^{\ddagger}_{int}$, which concerns to the chemical reaction.



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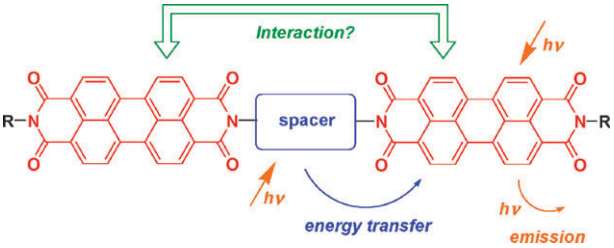
Excitation energy transfer in novel acetylenic perylene diimide scaffolds

David Shanks, Søren Preus, Katrine Qvortrup, Tue Hassenkam, Mogens Brøndsted Nielsen* and Kristine Kilså*

Dimeric perylene diimide scaffolds incorporating acetylenic bridges were prepared and excitation energy transfer in these molecules was investigated in solution and at a mica surface.



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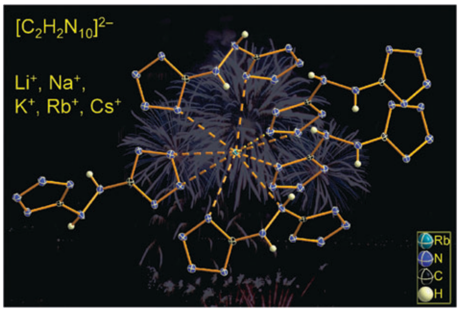

Nitrogen-rich alkali metal 5,5′-hydrazinebistetrazolate salts: environmentally friendly compounds in pyrotechnic mixtures

Moritz Ebespächer, Thomas M. Klapötke* and Carles Miró Sabaté

Energetic compounds based on the nitrogen-rich 5,5′-hydrazinebistetrazolate anion ($[C_2H_2N_{10}]^{2-}$) and alkali metals (Li^+, **2**, Na^+, **3**, K^+, **4**, Rb^+, **5** and Cs^+, **6**) are reported.

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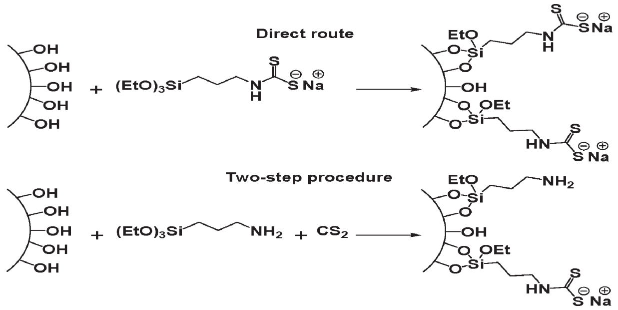

Synthesis of dithiocarbamate-functionalized mesoporous silica-based materials: interest of one-step grafting

Stéphanie Goubert-Renaudin, Fabrice Gaslain, Claire Marichal, Bénédicte Lebeau, Raphaël Schneider and Alain Walcarius*

Direct grafting of siloxydithiocarbamate provides is a more efficient way to prepare dithiocarbamate-functionalized silica than the classical two-step procedure involving the reaction of CS_2 on preformed amine-grafted silica, which leads to residual amine groups.

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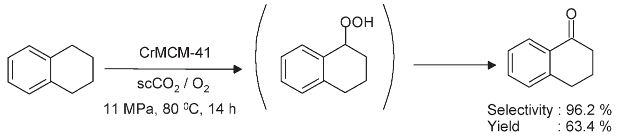

Highly selective oxidation of tetralin to 1-tetralone over mesoporous CrMCM-41 molecular sieve catalyst using supercritical carbon dioxide

Sudhir E. Dapurkar,* Hajime Kawanami,* Toshirou Yokoyama and Yutaka Ikushima

A high selectivity and a good yield of 1-tetralone was obtained *via* oxidation of tetralin with molecular oxygen over chromium containing mesoporous molecular sieve (CrMCM-41) catalyst using $scCO_2$ solvent.

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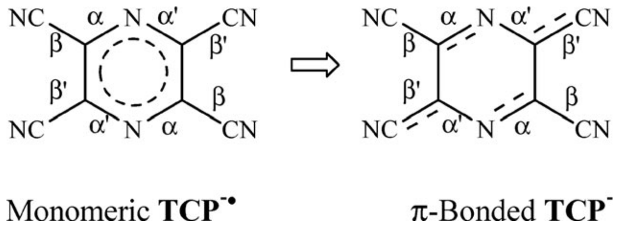

Unusual structural effects of intermolecular π-bonding in the tetracyanopyrazine (ion-radical) dimer

Sergiy V. Rosokha,* Jianjiang Lu, Bing Han and Jay K. Kochi

The long-distance π-bonding of tetracyanopyrazine anion-radicals results in formation of unusual dianionic π-dimers which show ~30° rotation and "quasi-quinonoidal" distortion of monomers arranged co-facially near the limit of their van der Waals separations.


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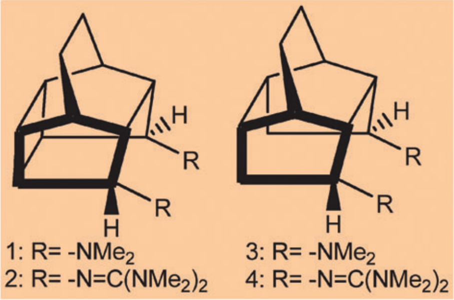
DFT studies on a new class of cage functionalized organic superbases

Ajeet Singh and Bishwajit Ganguly*

According to DFT calculations, pentacyclo[6.4.0.0^{2,7}.0^{3,11}.0^{6,10}]dodecane (PCD) derivatives have been predicted as organic super bases. The new molecular framework (PCD) is versatile in terms of anchoring different functional groups to achieve high basicities in both gas and solvent phase.



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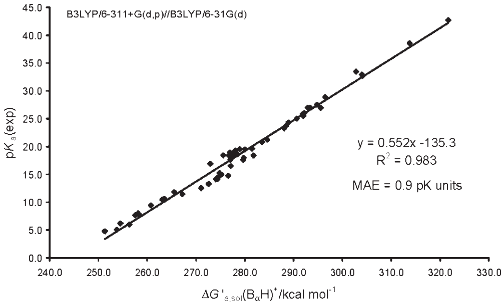
Basicity of organic bases and superbases in acetonitrile by the polarized continuum model and DFT calculations

Zoran Glasovac,* Mirjana Eckert-Maksić and Zvonimir B. Maksić

We report the accurate prediction of pK_a in acetonitrile for nitrogen bases possessing multiple intramolecular hydrogen bonds, employing linear correlation between experimental pK_a and $\Delta G'_{a,sol}$ for a set of known nitrogen bases.



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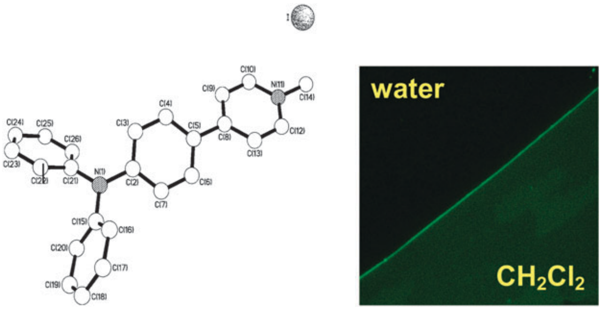
Synthesis and characterisation of substituted diphenylamines—charge-transfer, donor–acceptor systems localised at water–oil interfaces

K. Kowalski, N. J. Long,* M. K. Kuimova, A. A. Kornyshev, A. G. Taylor and A. J. P. White

A range of charge-transfer dyes have been synthesised and subjected to crystallographic and spectroscopic studies. Two of the compounds localise selectively on the water/oil interface, illustrating their potential as light-driven optical machines.



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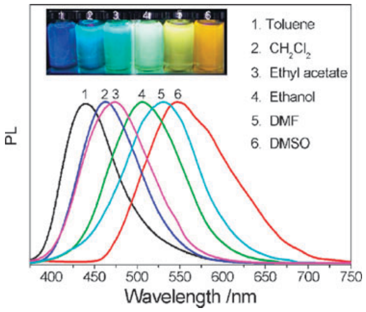
Solvent-resolved fluorescent Ag nanocrystals capped with a novel terpyridine-based dye

Yuanhao Gao, Jieying Wu, Qiong Zhao, Lingxia Zheng, Hongping Zhou, Shengyi Zhang, Jiaxiang Yang and Yupeng Tian*

A stable, fluorescent Ag system has been set up by capping a novel terpyridine-based dye onto the surface of Ag nanocrystals (NCs). The capping dye renders the Ag NCs soluble, with solvent-resolved fluorescence taking place in organic solvents.



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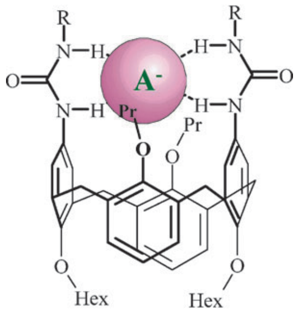

Anion recognition by diureido-calix[4]arenes in the 1,3-*alternate* conformation

Petra Cuřínová, Ivan Stibor,* Jan Budka, Jan Sýkora, Kamil Lang and Pavel Lhoták*

A series of diureido-calix[4]arenes immobilised in the *1,3-alternate* conformation was synthesised and systematically studied for their complexation ability. As revealed by ^{1}H NMR and UV/vis titrations, this structural motif leads to efficient ligands for anion recognition in nonpolar solvents.

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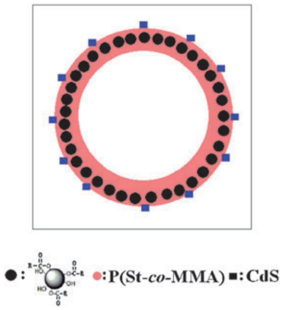

Design and fabrication of hollow, magnetic and fluorescent CdS–magnetite–poly(styrene-*co*-methyl methacrylate) microspheres

Song Yang, Huarong Liu* and Zhicheng Zhang

A facile and mild approach to multifunctional nanocomposite microspheres which possesses simultaneously magnetic, fluorescent, hollow properties under room temperature and at ambient pressure is reported. It should have great potential in biological applications.

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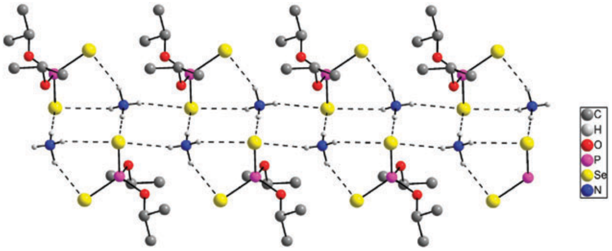
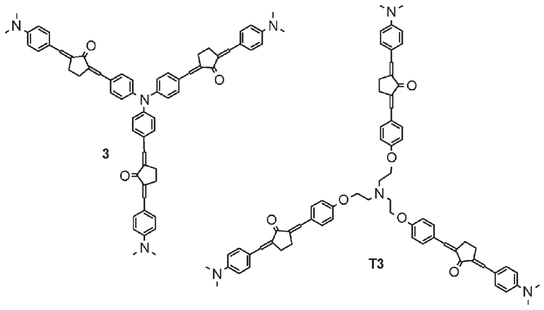


The chemistry of phosphorodiselenoates: structure, catalysis and formation of Se-esters

Bijay Sarkar, Chiang-Shiang Fang, Lee-Yan You, Ju-Chun Wang and C. W. Liu*

The ammonium salt of phosphorodiselenoic acid is structurally characterized. $NH_4Se_2P(OR)_2$ salts mediate Fe catalyzed condensation of acetone–ammonia to form an 4-oxopiperidine ring and act as a nucleophile to form Se-esters of the phosphorodiselenoic acid.

634



Study of electronic and vibronic contributions to cooperative enhancement of two-photon absorption in multibranched structures

Jianqiang Xue, Yuxia Zhao,* Jie Wu, Feipeng Wu* and Xiangyun Fang

Electronic coupling and vibronic coupling contributions to cooperative enhancement of two-photon absorption in multibranched structures were revealed. The crucial contribution for this enhancement was confirmed to be an electronic coupling effect. In addition, no contribution of vibronic coupling was observed.

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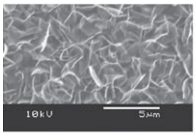
Vanadium selenoether and selenolate complexes, potential single-source precursors for CVD of VSe_2 thin films

Andrew L. Hector,* Marek Jura, William Levason,
Stuart D. Reid and Gillian Reid

V^{III} and V^{IV} selenoether and selenolate complexes have been prepared and investigated as reagents for deposition of vanadium selenide; $[(Cp)_2V(Se^tBu)_2]$ functions as a precursor to VSe_2 thin films *via* low pressure CVD.



$$[(Cp)_2V(Se^tBu)_2] \xrightarrow{LPCVD} VSe_2$$

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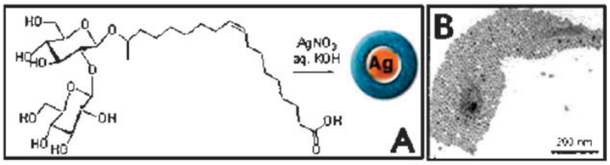
A direct method for the preparation of glycolipid–metal nanoparticle conjugates: sophorolipids as reducing and capping agents for the synthesis of water re-dispersible silver nanoparticles and their antibacterial activity

Sanjay Singh, Pitamber Patel, Swarna Jaiswal,
A. A. Prabhune,* C. V. Ramana* and B. L. V. Prasad*

The production of a new class of glycolipid–metal nanoparticle conjugates, namely, sophorolipid reduced/capped silver nanoparticles is demonstrated.



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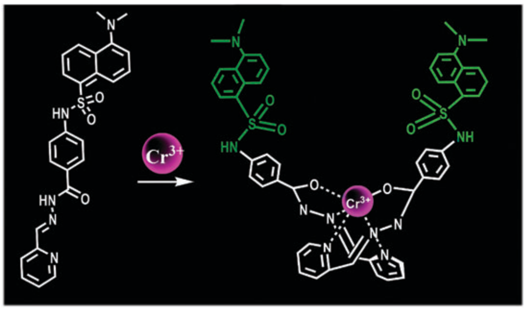
Dansyl-based fluorescent chemosensors for selective responses of Cr(III)

Hongmei Wu, Peng Zhou,* Jian Wang, Liang Zhao and
Chunying Duan*

Selective fluorescent chemosensors for Cr^{3+} are reported that incorporate carboxhydrazones as the ionophores and a dansyl dye as a fluorophore.



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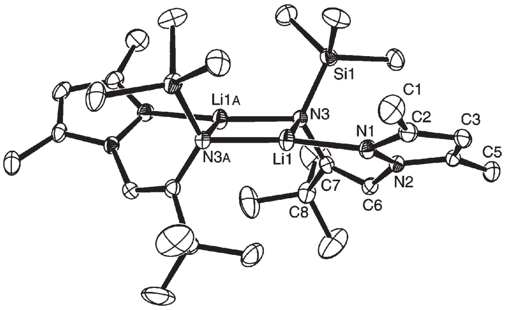
Synthesis and characterization of lithium, aluminium and zinc complexes supported by pyrazolyl-based N,N′-chelate ligands

Can Jin and Zhong-Xia Wang*

Novel pyrazole-based N,N′-chelate ligands and their lithium, aluminium and zinc complexes were synthesized and characterized.



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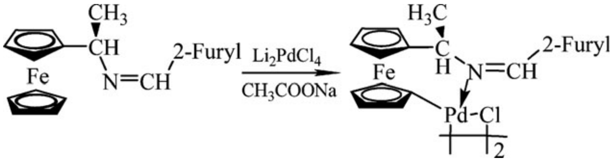
Synthesis and structure of heteroannular cyclopalladated chiral ferrocenylimines: theoretical interpretation of the cyclopalladated complexes based on density functional calculations

Hengyu Qian, Xiuling Cui,* Mingsheng Tang, Chunhui Liu, Cheng Liu and Yangjie Wu*

Reaction of novel chiral ferrocenylimines **3** and **6** with Li_2PdCl_4 produced heteroannular palladacycles and Pd(N^N) complexes, respectively. Quantum calculations based on (DFT) were carried out to explain the experimental results.



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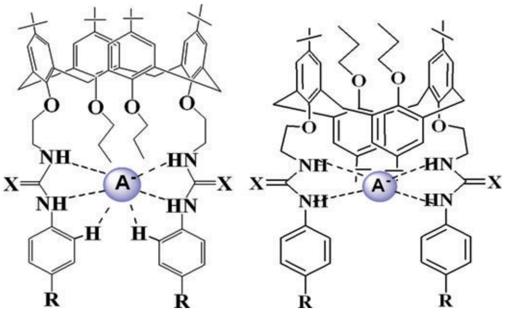
Chloride ion recognition using thiourea/urea based receptors incorporated into 1,3-disubstituted calix[4]arenes

J. Nagendra Babu, Vandana Bhalla, Manoj Kumar,* Rajiv Kumar Puri and Rakesh K. Mahajan

New calix[4]arene derivatives with thioureido/ureido moieties have been synthesized in *cone* and 1,3-*alternate* conformations which exhibit strong binding affinity for chloride ions.



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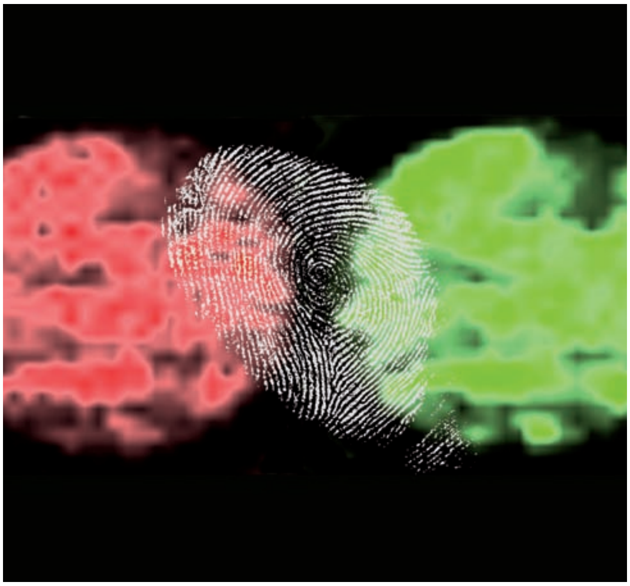
March 2009 / Volume 6 / Issue 3 / ISSN 1478-6524 / CSHCBM / www.rsc.org/chemicalscience

Chemical Science

Silica dusting agent allows drug detection in fingerprints

When the dust settles



The silica dust can give additional chemical information from fingerprints

UK scientists have devised a simple route to detecting illicit drugs and their metabolites in dusted fingerprints.

Frederick Rowell and colleagues of ROAR Particles Ltd in Durham, have developed a silica dusting agent that not only develops fingerprints, but also allows for the direct detection of drugs in the fingerprints by mass spectrometry. Rowell says that there is considerable interest in being able to obtain additional information from developed fingerprints, especially since a considerable fraction are smudged and therefore do not provide a clear image for routine identification purposes.

A hydrophobic silica dusting agent was used to develop fingerprints, which were then lifted using commercial tape. The lifted fingerprints subsequently underwent direct analysis by mass spectrometry, analysing for various chemical residues within the print. The procedure successfully confirmed the presence of parent drug compounds and their metabolites, providing unique fragmentation patterns for each chemical.

Graham Cooks of Purdue University in West Lafayette, US, says that the significance of this work lies in the fact that this technique 'can be used to record chemical fingerprints' and 'show the distribution of chemicals associated with latent fingerprints'. Cooks adds that the advantage of this method over existing ones is the 'dual use of powder as a latent print dust and as a mass spectroscopy matrix'.

'We need to undertake trials for these contact residues and for biomarkers with large numbers of individuals before our methods can be considered for routine forensic analysis,' says Rowell. 'In order to achieve maximum sensitivity for detecting chemicals present in trace amounts, it is necessary to reduce interference in the analysis step from the major components. This is proving a challenge but we think we have found a simple but effective solution.'

Mary Badcock

Reference

F Rowell, K Hudson and J Seviour, *Analyst*, 2009, DOI: 10.1039/b813957c

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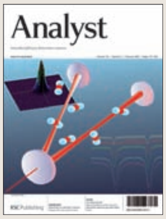
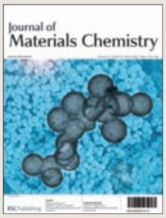
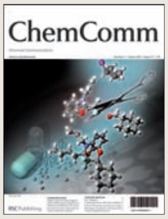


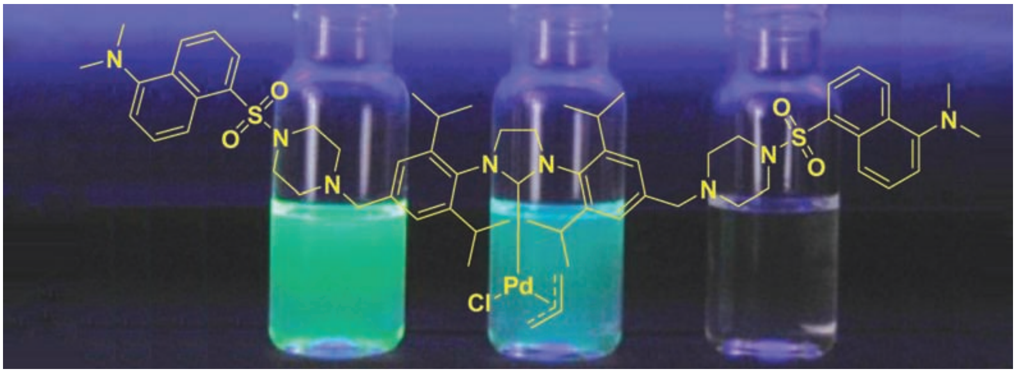




A snapshot of the latest developments from across the chemical sciences

Tagging a catalyst allows its progress through a reaction to be monitored

Fluorescent dyes to see catalysts in action



The fluorescence signal changes at each stage of the reaction

German researchers have used a fluorescent tag to monitor the state of a catalyst during a chemical reaction.

Herbert Plenio and colleagues from the Darmstadt University of Technology tagged an *N*-heterocyclic carbene ligand in a palladium catalyst with a fluorescent dye. They followed the catalyst's progress in a Suzuki cross-coupling reaction using fluorescence spectroscopy. The team found that the fluorescence signal changed at each stage of the reaction. When the catalyst was activated by a base, the signal decreased within a few seconds. It then remained stable until the substrate was added, then decreased gradually until the end of the reaction. The tag also allowed Plenio to see any catalyst impurities left in the product.

'Our work provides a highly sensitive tool to monitor catalysts in action in low concentrations,' says Plenio. 'Little is known about the nature of catalyst complexes involved in catalytic transformations. By definition, the amount of a catalyst is small compared to the substrates and, to make things worse, this often acts as only a reservoir for the even smaller amount of active species that is actually doing the work.'

Fluorescence has the high sensitivity required to detect these very small quantities, even with just a few nanograms of palladium. 'This is a nice application of fluorescence that allows a deeper insight into catalytic processes,' says Jay Winkler, an expert in the photochemistry of transition metal complexes at the California Institute of Technology, Pasadena, US.

Plenio says he hopes that in the future, he will have tags that are sensitive enough to reveal the concentration of the active species in the catalytic cycle and the nature of the metal complexes involved. 'We still need to understand so much more about fluorescence dyes and the photophysics behind them,' he says, 'but I am optimistic – Shimomura, Chalfie and Tsien's 2008 Nobel Prize award for the discovery and development of the green fluorescent protein is providing a strong stimulus.'

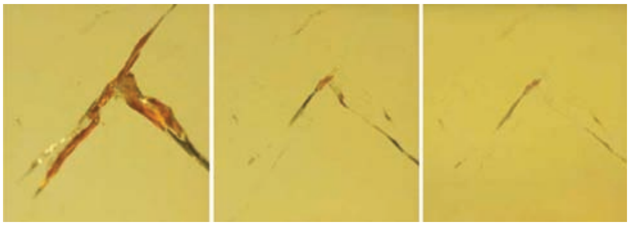
Michael Spencelayh

Reference

V Sashuk, D Schoeps and H Plenio, *Chem. Commun.*, 2009, 770 (DOI: 10.1039/b820633c)

Chinese scientists find the key to self-healing polymer

Smoothing the cracks in epoxy resin



Heating mends the cracks in damaged epoxy resin

Researchers in China have developed a self-healing epoxy resin which can be repaired by heating when cracks form.

Epoxy resin is a tough polymer with many uses from glues to circuit boards, aerospace engineering to art restoration. Epoxy materials are often used under harsh conditions where long-term service and durability are needed. So, it would be ideal if damaged epoxy resin could self-heal, a property recently developed for other polymers.

Conventional epoxy resin is based on epoxides to which an additive (or curing agent) is added to form cross-linking between the chains strengthening the polymer. However, these cross-linked bonds are usually irreversible meaning that if cracks form, the bonds cannot be remade to repair the material.

Min Zhi Rong and co-workers from Zhongshan University, Guangzhou, China, have solved this problem by making a new epoxy material which contains both epoxide and furan groups in the same molecule. To this they add a maleimide-based curing agent, as well as the conventional anhydride curing agent.

The anhydride forms irreversible strong bonds with the epoxide groups but the maleimide makes bonds with the furan groups which are reversible at 110°C. So when cracks form in the cured polymer, it is heated to 120°C to break the reversible bonds and then cooled to 80°C so the broken bonds could reform.

Fred Wudl, a polymer expert from University of California, Los Angeles, US, says Rong's work 'is an interesting step towards creating remendable epoxy resins, following on from previous work in the field.'

Rong says that his group is currently working to make an epoxy resin which will be able to self-heal at lower temperatures.

Ruth Doherty

Reference

Q Tian *et al*, *J. Mater. Chem.*, 2009, 1289 (DOI: 10.1039/b811938d)

Scientists turn waste plastic into useful ultra-strong carbon spheres

New lease of life for used cola bottles

Discarded plastic bottles can be broken down to make ultra-strong carbon spheres that could be used in lubricants.

Vilas Pol from Bar-Ilan University, Ramat-Gan, Israel, and colleagues produced strong carbon microspheres from waste polyethylene terephthalate (PET). They heated used cola bottles at 700 °C for three hours in a closed reactor. The plastic then decomposed under self-generated pressure to form the hard carbon spheres with diameters between two and ten micrometres. 'We broke one diamond knife and damaged a second while cutting a cross-section of the spheres,' says Pol.

'The strength of these materials is interesting,' says Neil Coville, coordinator of the Carbon Nanotubes and Strong Composites group at the University of the Witwatersrand, Johannesburg, South Africa. 'The results are impressive and suggest others should be measuring this property in the future.'

JUPITER IMAGES

Carbon spheres from decomposed plastic could be used in lubricants

Reference
S V Pol *et al*, *Green Chem.*, 2009, DOI: 10.1039/b819494g

'The process is particularly interesting,' says Philippe Serp, an expert in carbon nanostructures at the National Center for Scientific Research, Toulouse, France, 'as it does not use any catalyst.' Pol's scalable process also does not require solvents and improves on existing methods that can be limited by low yields and poor separation of the spheres from carbon soot.

Carbon spheres are used in energy storage and nanodevices. Pol's microspheres can withstand significant pressure, so they could be used in lubricants. Lowering the reaction temperature to below 700 °C gives larger carbon particles that could be used in printers, toners and filtration technology.

'The challenge facing today's scientific community to find an innovative solution to the degradation of waste polymers motivated us,' explains Pol's colleague Aharon Gedanken. 'Our process demonstrates a way to remediate waste PET polymer to fabricate value-added products.'

Kathryn Wills

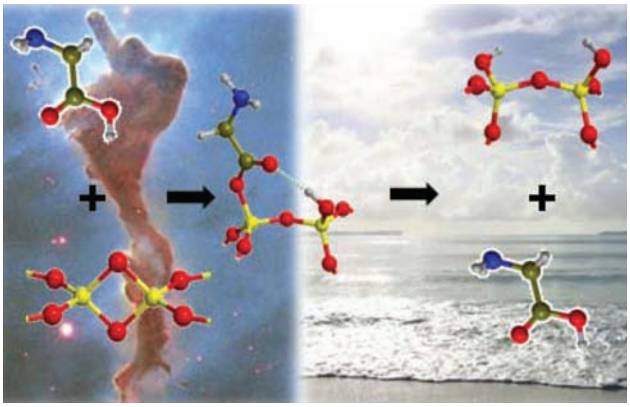
Life's building blocks may have travelled to Earth on interstellar silica dust

Did space dust start life on Earth?

Amino acids could have found their way from deep space to start life on Earth, say scientists in Italy.

Piero Ugliengo and Albert Rimola from the University of Turin used quantum mechanics to show that amino acids synthesised in deep space molecular clouds can be captured by interstellar dust particles. Ugliengo says that the particles could have travelled to Earth, where the amino acids were released into the 'primordial soup' ready for the synthesis of early proteins.

Ugliengo and Rimola simulated the reaction between the amino acid glycine and interstellar silica dust. Their calculations show that glycine can bond to defects on the silica particles' surface – defects that could have been caused by extreme heat given off by young stars. They tested the particles' stability by simulating conditions in space, such as cosmic rays and UV radiation. They also showed that hydrolysis of the particles, which would have happened when the dust landed in the ocean, released the glycine to become part of the primordial soup.



Amino acids may have been captured by silica particles in deep space and released in the primordial ocean

Ugliengo says that he hopes that experimental evidence will match their findings. 'The key role of the mineral surfaces as a catalyst in the prebiotic era is a very broad and promising one,' he says. 'We need to merge accurate quantum-mechanical modelling studies with carefully designed experimental measurements if any real progress in this exciting field is to be seen.'

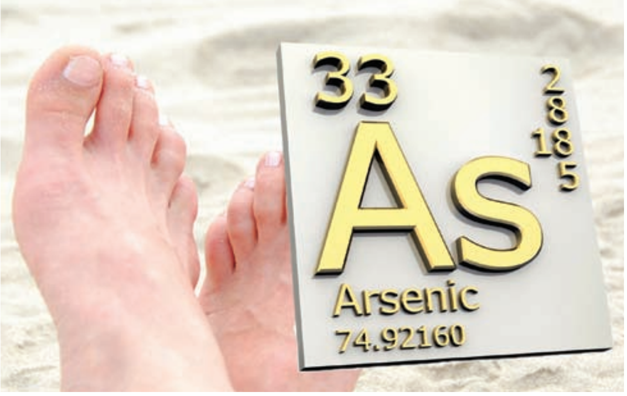
'This work not only helps us understand the survival of amino acids formed in the harsh conditions of the interstellar medium, but it also suggests that some of these compounds may have arrived intact to the primitive Earth,' says Antonio Lazcano, a leading scientist in the origin of life and prebiotic chemistry fields, National Autonomous University of Mexico, Mexico City. 'The primitive soup was likely formed by chemical reactions that took place on the Earth but it was clearly spiced by extraterrestrial compounds arriving on board micrometeorites. The richer the broth, the tastier it becomes!'

Sarah Dixon

Reference
A Rimola and P Ugliengo, *Phys. Chem. Chem. Phys.*, 2009, DOI: 10.1039/b820577a

Poisonous element detected in toenail exam

Toenails reveal arsenic exposure



UK scientists have finally found a use for toenail cuttings. Mark Button at the British Geological Survey in Nottingham, UK, and colleagues are using the clippings to detect human exposure to elevated environmental levels of arsenic.

Button's group collected toenails from residents living near a former arsenic mine in Devon, UK. They washed and acid digested the samples under microwave irradiation. They then analysed the samples using inductively coupled plasma mass spectrometry. The toenails showed significantly elevated arsenic levels compared to those seen in samples taken from people that had no contact with the element.

Arsenic occurs naturally in the environment and people can be exposed to it in several ways, for example through contaminated water, food or soil. Chronic exposure is associated with increases in lung, liver, bladder and kidney cancers.

Once ingested, arsenic is absorbed into the bloodstream and then accumulates in several body parts. Evidence disappears from blood and urine after a few days but arsenic accumulates long term in keratin rich materials such as hair and nails. This makes them potentially more useful as biomarkers of chronic arsenic exposure. Toenail samples in particular are an attractive possibility as they are easy to collect, store and transport and are less liable to contamination than hair samples.

'This research', says Button, 'highlights the suitability of toenails as a biomarker of exposure to potentially harmful elements in areas such as the south-west of the UK where more extensive biomonitoring studies are long overdue.'

Richard Kelly

Reference

M Button *et al*, *J. Environ. Monit.*, 2009, DOI: 10.1039/b817097e

Chemical Science

Instant insight

Metal detectors for clean fuel

Guilhem Caumette, University of Pau - IFP, France, outlines the techniques used to find metal contaminants in petroleum and how they will lead to superior fuels

Petroleum is, and always has been, the primary source of energy on our planet. The shortage of oil reserves, combined with increasing energy demands has brought a surge of interest in revisiting petroleum processing technology in the quest for better performing and cheaper fuels. Oil companies are searching for alternative sources of carbonaceous fuels, such as biofuels and gas condensates, or are trying to improve the efficiency of heavy crude oil (and heavy distillation fractions') conversion to transportation fuels.

Metals and sulfur found in these heavy petroleum fractions can poison the catalysts used during refining processes. They also corrode equipment and contaminate the environment. So investigations focus on detecting metal content in petroleum and petroleum products. The metals' behaviour during the refining processes depends on their speciation – their chemical form. Knowing the size and structure of metal complexes is crucial in choosing catalysts suitable for removing them. Their identity can also give information about the geological origin and migration of oils, and can be used to find new oil fields.

Yet, despite progress in analytical methodology, relatively little is known about the metal species in crude oils. Metalloporphyrin complexes with nickel and vanadium are often cited, but non-porphyrin complexes with molecular weights reaching several thousand Daltons should also be present. More information is available about the forms of sulfur in petroleum or mercury and arsenic in gas condensates but there is no definite agreement on their exact nature.

Analysing the elements in petroleum is a nightmare for analysts as the fuel contains thousands of molecules of different sizes and polarities, which interact with different forces. Direct analysis is barely possible and multistep analytical techniques are required to separate and properly identify target metallomolecules. The interest in speciation of metals and other heteroelements in petroleum-related products has led analysts to develop dedicated analytical techniques and methods. They include direct analytical techniques such as x-ray absorption spectroscopy, electron paramagnetic resonance and molecular mass spectrometry (using laser desorption, electrospray and chemical ionisation) as well as hyphenated techniques that combine chromatography's high separation potential (for example, high performance liquid chromatography or gas chromatography) with an element specific detector's sensitivity (for example, atomic absorption spectrometry).

As these dedicated techniques become more widely available, identifying metal species in complex organic mixtures such as petroleum becomes easier and meeting the challenge of removing them for cleaner fuels becomes a step away.

Reference

G Caumette *et al*, *J. Anal. At. Spectrom.*, 2009, DOI: 10.1039/b817888g

Relatively little is known about the metal species in crude oils

Read more in 'Element speciation analysis of petroleum and related materials' in issue 3, 2009 of Journal of Analytical Atomic Spectrometry.

Would anyone really put a Formula One engine in a family saloon?
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Chemistry, life and longevity

Jyoti Chattopadhyaya talks to Marie Cote about chemistry's role in our lives, the secrets of a successful business and delivers his message to younger scientists

Jyoti Chattopadhyaya

Jyoti Chattopadhyaya is Professor of Bioorganic Chemistry at the University of Uppsala, Sweden. His research focuses on a biophysical/bioorganic approach towards understanding the structure–function of nucleic acids, encompassing the design of biological mimics with synthetic chemistry and their structural studies *via* NMR and computation, and kinetics, for a better understanding of the chemistry–biology interface.

What inspired you to be a scientist?

Curiosity inspired me. I am driven by curiosity and the unknown. I also wanted to pass on my knowledge, to let people know what I know. Science is for society, and we, as scientists, have a duty to keep the public informed.

What motivated you to study chemistry?

Once I realised the bountiful gifts of nature as an undergraduate, I understood how chemistry has made our lives so successful. From drugs to clothes to hygiene, chemistry plays a fundamental role. Look at the longevity of the human race today: in Sweden, where I live, you can hope to reach 85–86 years old. Can such longevity be possible without chemistry?

With this in mind, we need to work towards a cleaner environment so that toxicity levels are lowered and controlled. In this way, the positive effects of chemistry will come into focus. If chemistry can find its way into the containment of carbon monoxide and carbon dioxide emissions, then let's hope it won't be unusual to live to 150! We want to live long and productive years, and not perish like the dinosaurs. To reduce carbon dioxide pollution, we need help from all corners of research, for example, to develop hybrid cars for the next generation. Politicians also need to take responsibility. More money should be invested in these research fields and chemistry and politics must work together.

What led you to specialise in the biophysical aspects of nucleic acids?

If you wish to carry out synthetic organic chemistry, you need to understand the physical chemistry behind it. In order to understand biological functions, there must be interplay between physical and synthetic chemistry. Chemistry cannot be distinguished into separate branches as it used to be 30–40 years ago.

How do you see nucleic acid chemistry progressing over the next 10 years?

There is a metamorphosis going on in this field, but nucleic acids do not stand alone – they have a role to play with other biopolymers and ligands. Nucleic acids alone cannot achieve the whole process from transcription and translation to glycosylation of proteins. This can only take place through the interaction of different ligands and biopolymers.

You have initiated many start-up companies. What is the secret to setting up a successful business?

The secret is to understand that we cannot have companies without patents, we cannot have patents without fundamental discoveries, and we cannot have fundamental discoveries without solid support behind us – it's a continuum. The dynamic of the process is very important and the market force alone cannot dictate what will actually make it to the market. I would like to see more commitment from the representatives of our democratic society; I would be happy to see some of the profits from the start-up companies go back to the tax payers.

What would your message for younger scientists be?

Have trust in yourself, and be ready to put your heart and soul into the game. We as teachers have a responsibility to communicate to the younger generation about the science of today and how it has developed. However, I can only paint my own picture: the students have to decide for themselves. Science pays off, but it demands a full commitment. The younger generation takes it for granted, because they have not seen days without antibiotics or a flushing toilet. We would not be what we are today without science and many people tend to forget this. That is the message I want to give to them.

What would you be if you were not a scientist?

I wasn't very good at sports. I played some chess, but I was not alpha plus in that either. But I am good at what I do, and that is what I want to be. I want to keep sharpening my mind and look forward: there is still much to learn.

Essential elements

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2009 spring conferences

With the 2009 spring conference season about to begin, RSC Publishing staff will be spread around the globe at a number of major conferences over the forthcoming weeks.

Meet RSC staff at Pittcon in Chicago, US, from 8–12 March. This comprehensive annual meeting on laboratory science this year celebrates 60 years of service to the scientific community. Visit the RSC at booth #3410 and meet Niamh O'Connor, the editor of *Analyst* and *JAAS*, the market leader in spectrometric techniques. Pick up free copies of RSC journals and enter our competition to win an iPod touch when you sign up to journal e-alerts. Keep up-to-date with forthcoming RSC Pittcon announcements at www.rsc.org/publishing

The RSC will also be at the American Physical Society (APS) meeting in Pittsburg, PA, US, from 16–20 March, where around 7000 scientists gather to share research on a wide range of physics and physics-related topics. Visit us at booth #117.

Salt Lake City, US, hosts the 237th ACS National Meeting & Exposition, from 22–26 March. Enjoy the rich programme of scientific papers on a variety of multidisciplinary topics, including thematic programming around nanoscience. Meet Geoff Ozin (a speaker in the Naturally Nano session on Tuesday 24 March) who will be at RSC booth #1525 signing copies of his best selling book, *Nanochemistry*. The 2nd edition highlights the latest breakthroughs using more than eighty new case histories, problem sets and teaching principles.

If you're travelling to these or other conferences, look out for RSC Publishing staff – they will be happy to meet you. Visit our stand and pick up sample copies of journals, look out for special offers on the RSC book collection and keep up-to-date with the latest developments and exciting new announcements from RSC Publishing.

Faraday Discussions grow in popularity

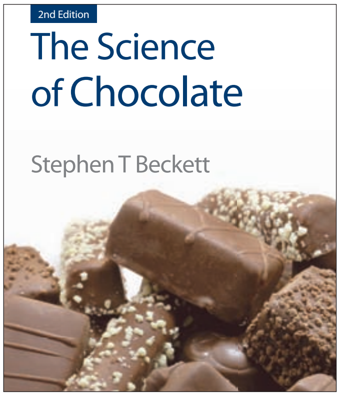
Faraday Discussions, the long-established series of meetings providing unique international views on newly acquired physical chemistry, chemical physics and biophysical chemistry results, has increased its frequency this year from three to four meetings. These meetings take a special format, in which papers are distributed to all participants in advance of the conference and almost all of the meeting is devoted to discussion of the papers. Previous *Faraday Discussions* volumes are available to buy online at www.rsc.org/books.

Faraday Discussions' latest impact factor is 5.0, emphasising its highly cited and well respected accounts by world-class experts in physical chemistry. Philip Earis, editor for *Faraday Discussions* comments: 'The unique format of *Faraday Discussions*, and the world-class speakers that discussions attract, lead to outstanding and stimulating debate in topical areas of physical chemistry.'

2009 sees the discussion of Cold and ultracold molecules; Soft nanotechnology; Multi-scale modelling of polymers, colloids, mesophases and membranes; and Frontiers in physical organic chemistry. Registration is now open for the first meeting in April which will be held at Durham University, UK. Visit www.rsc.org/faraday for further information on past and future *Faraday Discussions*.

And finally...

As part of this year's food theme, the RSC's book programme will showcase titles focused on, or related, to the food sciences. The RSC already has an extensive food science list catering for scientists at all levels from schools and universities through to industry. *The Science of Chocolate*, *Chemistry and Biology of Winemaking* and *Food: The Chemistry of its Components* (5th edition) are already established as best selling titles, used by the scientific community and professionals globally.



2009 begins with the publication of the *Microbiology Handbook (Diary)*, shortly followed by other exciting new food titles including *Nanotechnologies in Food* (from the RSC's landmark *Nanoscience and Nanotechnology* series) and *Handbook of Culture Media for Food and Water Microbiology*. These titles will be complemented further by other exciting projects to be published throughout the year.

For more information please visit www.rsc.org/books

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