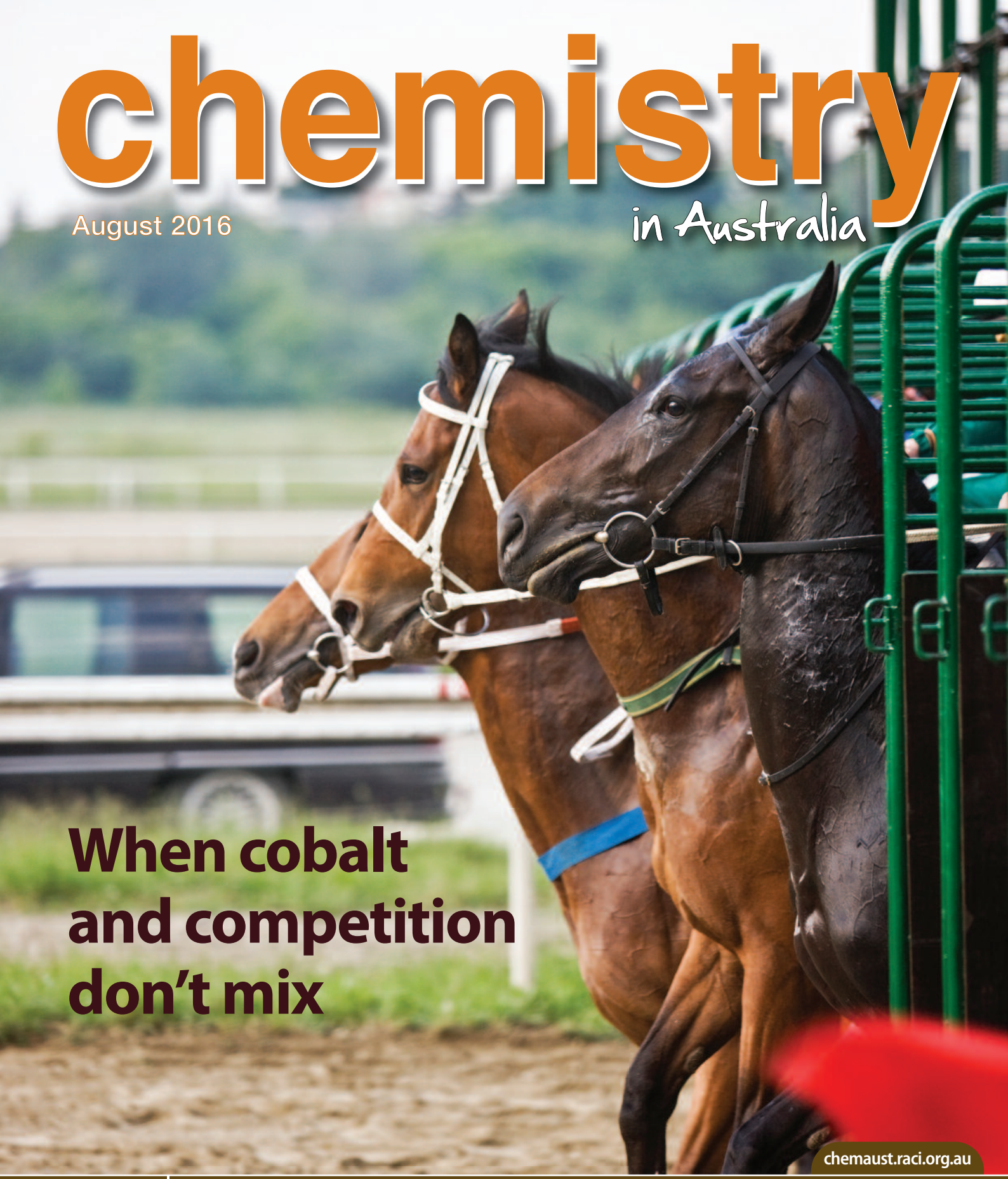
chemistry in Australia

August 2016



When cobalt and competition don't mix

chemaust.raci.org.au

raci
Royal Australian Chemical Institute

- A passion for chemistry and crystals
- What makes a great chemistry teacher?
- National Science Week: STEM for schools

23-28 July 2017 | Melbourne

www.racicongress.com

#RACI100

Centenary Congress

The Organising Committee would like to invite you to the 2017 RACI Centenary Congress.

The RACI is the oldest scientific or technical professional society in Australia. The Centenary Congress is an opportunity to celebrate the contributions that chemistry has made to Australia's (and the world's) social, economic and intellectual advancement over the past century.

17 ACC
17th Asian Chemical Congress and 19th General Assembly of FACS

ACCC6
6th Asian Conference on Coordination Chemistry

AIMECS 2017
11th AFMC International Medicinal Chemistry

Registration opens

July 2016

Call for abstracts closes

November 2016

For all enquiries, please email
info@racicongress.com

Carbon 2017
World Conference on Carbon

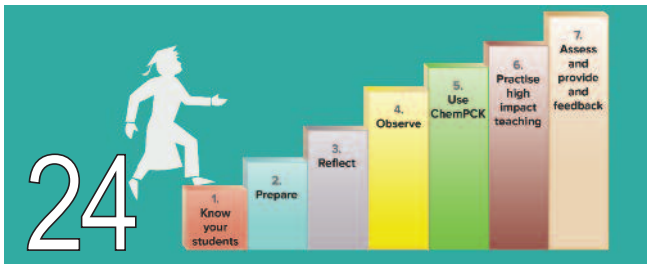
Chemeca 2017
Australian and New Zealand Federation of Chemical Engineers Annual Conference

GSC8
8th International Conference on Green and Sustainable Chemistry

Tetrahedron
18th Asian Edition Tetrahedron Symposium

chemistry in Australia

August 2016




iStockphoto/webphotographeer

chemaust.raci.org.au

Centenary Congress: conferences and celebration in 2017

23-28 July 2017 | Melbourne

Centenary Congress

#RACI100 www.racicongress.com

On behalf of the Organising Committee, it is with great pleasure that I invite you to the 2017 RACI Centenary Congress. That's right; the RACI will soon be 100 years old! We're the oldest scientific or technical professional society in Australia. The Centenary Congress is an opportunity to celebrate the contributions that chemistry has made to Australia's (and the world's) social, economic and intellectual advancement over the past century as well as to look forward to the challenges and opportunities in the century ahead.

The Centenary Congress will bring together several thousand delegates from across the breadth of the chemical sciences and technologies. The Congress will encompass the RACI's Centenary Conference, based on the traditional national scientific gathering of chemists from across the breadth of our discipline, both technical and geographic. However, the Congress will be so much more as it is being held in collaboration with several partner conferences, including the 17th Asian Chemical Congress (17ACC), which is the biennial gathering of the Federation of Asian Chemical Societies, Carbon 2017 (The World Carbon Conference), Chemeca (Australian and New Zealand Federation of Chemical Engineers Conference), AIMECS17 (The Asian Federation of Medicinal Chemists' Conference), ACCC6 (The Asian Conference on Coordination Chemistry), GSC8 (8th International Conference on Green and Sustainable Chemistry), Elsevier's Tetrahedron – an Asian seminar, and the Asian Hub for e-Drug Discovery (AHeDD) conference.

Centenary Congress delegates will be freely able to contribute to and enjoy the scientific and technical programs of all of these partner meetings at no extra cost. The Congress will celebrate Australian chemistry's place in the Asia Pacific region and the world. It will incorporate the energetic and enthusiastic contributions of many student and early-career scientists and engineers from academia and industry as well as industrial leaders, world-renowned researchers and leaders in chemistry education. Congress Plenary speakers include several Nobel laureates, and several other outstanding chemists who may well be future laureates.

The Congress is being held in Melbourne at the Melbourne Convention and Exhibition Centre, which is located in the heart of the city, with easy access to a wide range of accommodation within walking distance or via an excellent public transport network. Melbourne hosts a vibrant social life with excellent restaurants, bars and performing arts venues. Moreover, for those addicted to sport, Melbourne is Australia's 'sporting capital' with options to watch top-tier professional sporting events including Australian Football and Rugby League matches only a short stroll from the Congress venue. Melbourne is an international city, easily accessible from any part of the world. It's a fantastic base to explore south-east Australia and enjoy some of the best food, wine and unique flora and fauna that Australia has to offer.

A key element of the centenary Congress will be the comprehensive exhibition program showcasing the latest innovations in chemistry, and we encourage interested organisations to make contact.

I am very pleased to welcome you to attend the RACI Centenary Congress in Melbourne in July 2017. I'm sure you'll enjoy an intellectually stimulating and socially enjoyable event. Details can be found at www.racicongress.com. Please check the website regularly for up-to-date information.

Mark Buntine FRACI CChem, Centenary Congress Chair

chemistry in Australia
chemaust.raci.org.au

EDITOR
Sally Woollett
Ph (03) 5623 3971
editor@raci.org.au

PRODUCTION EDITOR
Catherine Greenwood
catherine.greenwood@bigpond.com

ADVERTISING SALES
Gypsy Media & Marketing Services
Marc Wilson, ph 0419 107 143
marc@gypsymedia.com.au

PRODUCTION
Control Publications Pty Ltd
science@control.com.au
www.control.com.au

BOOK REVIEWS
Damien Blackwell
damo34@internode.on.net

RESEARCH HIGHLIGHTS
David Huang
david.huang@adelaide.edu.au

GENERAL ENQUIRIES
Robyn Taylor
Ph/fax (03) 9328 2033/2670
chemaust@raci.org.au

PRESIDENT
Paul Bernhardt FRACI CChem

ISSN 0314-4240 e-ISSN 1839-2539

Randwick recollections

I was interested to read in the June issue (p. 5) Robert Ryan's recollections and musings, and took particular note of his statement that trams to the University of New South Wales stopped in 1961.

In the early 1960s, the University of NSW acquired the site of the tramway workshops in adjacent Randwick, which became the Randwick subcampus of the university.

During my time at the University of NSW (1987–95), I was frequently at the Randwick subcampus where, among other buildings, there was (is?) a fuel technology laboratory. It was designed by Dr Ken Basden MRACI CChem, whose obituary I wrote for the July 2011 issue of *Chemistry of Australia*. Ken's first tertiary qualification was an ASTC (Associate of the Sydney Technical College), which provides a further link with the theme of Robert Ryan's article.

I did a little research on the history of the area once, and saw photographic evidence that trams would be out in force on a day when there was a major event at Randwick racecourse!

Clifford Jones FRACI CChem

'Your say' guidelines

We will consider letters of up to 400 words in response to material published in *Chemistry in Australia* or about novel or topical issues relevant to chemistry. Letters accepted for publication will be edited (no proof supplied) for clarity, space or legal reasons and published in print and online. Full name and RACI membership type will be published. Please supply a daytime contact telephone number (not for publication).

Publication does not constitute an endorsement of any opinions expressed by contributors. All letters become copyright of the Royal Australian Chemical Institute and must not be reproduced without written permission.

Send letters to editor@raci.org.au.

Apology

RACI does not endorse the comment related to Dolly Parton in the book review of *Rare: the high stakes race to satisfy our need for the scarcest metals on Earth*, published in the June issue of *Chemistry in Australia* (p. 34). The comment has been removed from the online issue. We apologise for any offence caused.

Laboratory safety taskforce calls for renewed research safety commitment

University-wide efforts to renew and strengthen a culture of research safety are necessary to avoid tragic accidents, according to a guide released by the Association of Public and Land-grant Universities' (APLU) Task Force on Laboratory Safety. In the document and on a companion website (bit.ly/1WRJnWV), the taskforce provides US university presidents and chancellors with 20 recommendations to strengthen the culture of safety.

The task force was created by APLU in coordination with the American Chemical Society (ACS), the Association of American Universities and the Council on Government Relations. It was composed of senior research officers, environmental and health safety experts, and representatives from industry and national labs.

American Chemical Society

Given the recent number of serious academic lab accidents, APLU's report should serve as a critical clarion call to improve lab safety

Thomas Connelly, ACS Executive Director and CEO

Cancer technology could help cure crop disease problems

Researchers at the Centre for Crop and Disease Management (CCDM), co-supported by Curtin University and the Grains Research and Development Corporation (GRDC), are using digital polymerase chain reaction (dPCR) cancer detection technology to discover fungicide resistance mutations in crop disease.

dPCR works by allowing researchers to collect multiple samples from one crop, pool them, and extract fungal DNA to look for resistance mutations. dPCR is also capable of quantifying the amount of DNA that contains the resistance mutations.

Curtin University

... it is now clearer than ever before that fungicide resistance is widespread ... requiring integrated disease management options ...

Dr Fran Lopez-Ruiz, leader of Fungicide Resistance Group, Centre for Crop and Disease Management

Funding for commercial waste-to-biofuel plants

Technology of Australian renewable energy start-up Licella, co-founded by Professor Thomas Maschmeyer FRACI CChem and developed in partnership with the University of Sydney, is the subject of a new contract with global investors that allows the re-imagining of the huge pulp and paper industry as biorefineries – turning waste into renewable or recycled fuel blend-stocks. The Catalytic Hydrothermal Reactor (Cat-HTR™) technology converts low-cost, non-edible, waste biomass into a stable biocrude oil.

Canadian pulp and paper producer CanFor has announced it will invest funds sufficient for a full-scale commercial operation that will transform the resource-intensive pulp and paper industry by turning biomass waste into a petroleum substitute, biocrude. Also known as bio-oil, it will be ready to go into existing petrochemical refinery streams to generate renewable fuels and/or chemicals.

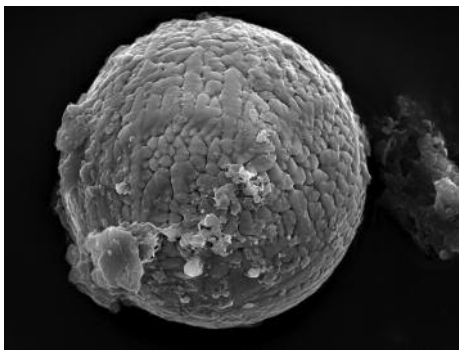
University of Sydney

Using the whole tree and not just a minor part will move the industry towards biorefining.

Dr Len Humphreys, Licello CEO

Cosmic dust reveals Earth's ancient atmosphere

Using the oldest fossil micrometeorites (space dust) ever found, Monash University-led research has made a surprising discovery about the chemistry of Earth's atmosphere 2.7 billion years ago.



This is one of 60 micrometeorites extracted from 2.7-billion-year-old limestone, from the Pilbara region in Western Australia. These micrometeorites consist of iron oxide minerals that formed when dust particles of meteoritic iron metal were oxidised as they entered Earth's atmosphere, indicating that the ancient upper atmosphere was surprisingly oxygen-rich. Andrew Tomkins

The findings of a new study published in *Nature* (doi: 10.1038/nature17678) – led by Dr Andrew Tomkins and a team from the School of Earth, Atmosphere and Environment at Monash, along with scientists from the Australian Synchrotron and Imperial College, London – challenge the accepted view that Earth's ancient atmosphere was oxygen-poor. The findings indicate instead that the ancient Earth's upper atmosphere contained about the same amount of oxygen as today, and that a methane haze layer separated this oxygen-rich upper layer from the oxygen-starved lower atmosphere.

Tomkins explained how the team extracted micrometeorites from samples of ancient limestone collected in the Pilbara region in Western Australia and examined them at the Monash Centre for Electron Microscopy (MCEM) and the Australian Synchrotron.

'Using cutting-edge microscopes, we found that most of the micrometeorites had once been particles of metallic iron – common in meteorites – that had been turned into iron oxide minerals in the upper atmosphere, indicating higher concentrations of oxygen than expected,' Tomkins said.

'This was an exciting result because it is the first time anyone has found a way to sample the chemistry of the ancient Earth's upper atmosphere,' Tomkins said.

Imperial College researcher Dr Matthew Genge – an expert in modern cosmic dust – performed calculations that showed oxygen concentrations in the upper atmosphere would need to be close to modern-day levels to explain the observations.

'This was a surprise because it has been firmly established that the Earth's lower atmosphere was very poor in oxygen 2.7 billion years ago; how the upper atmosphere could contain so much oxygen before the appearance of photosynthetic organisms was a real puzzle,' Genge said.

Tomkins explained that the new results suggest Earth at this time may have had a layered atmosphere with little vertical mixing, and higher levels of oxygen in the upper atmosphere produced by the breakdown of CO_2 by ultraviolet light.

'A possible explanation for this layered atmosphere might have involved a methane haze layer at middle levels of the atmosphere. The methane in such a layer would absorb UV light, releasing heat and creating a warm zone in the atmosphere that would inhibit vertical mixing,' Tomkins said.

Tomkins outlined the next steps in the research.

'The next stage of our research will be to extract micrometeorites from a series of rocks covering over a billion years of Earth's history in order to learn more about changes in atmospheric chemistry and structure across geological time. We will focus particularly on the great oxidation event, which happened 2.4 billion years ago when there was a sudden jump in oxygen concentration in the lower atmosphere.'

Monash University

New IChemE president

Professor Jonathan Seville, Executive Dean of the Faculty of Engineering and Physical Sciences at the University of Surrey, UK, is the new President of the Institution of Chemical Engineers (IChemE).

Seville studied chemical engineering at Cambridge, and joined the research division of Courtaulds Ltd before returning to academia to complete a PhD at Surrey under the supervision of Professor Roland Clift. He then embarked on a successful academic career, which took him to the University of Birmingham, UK, as the head of chemical engineering where he established the UK's first research centre in formulation engineering. He then moved to the University of Warwick, UK, where he served three years as dean of engineering, before returning to Surrey in 2011.

Throughout his career, Seville has championed the application of chemical engineering to the design and manufacture of products for the pharmaceutical, home care and fast-moving consumer goods industries. He is also active in energy-related projects, including biomass conversion and solar power, and is co-founder of the successful spin-out company Recycling Technologies.

John McGagh, Chief Digital Officer at renewable energy supplier, Snowy Hydro, was confirmed as IChemE's Deputy President. He will succeed to the presidency at the end of Seville's 12-month term, in May 2017. Allyson Black, Corporate Development Manager at Caltex Australia, will replace McGagh as Australian Board representative.

Institution of Chemical Engineers

Successful pilot method for chemical risk data

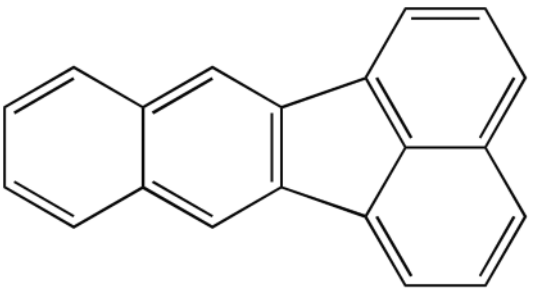
US federal government researchers have successfully pilot tested a new method to more quickly and cheaply collect data that can help define the potential cancer and other human health risks for more than 80 000 chemicals now in commerce and the environment. The research lays the groundwork for far-reaching advances in managing chemical risks.

The new approach will help government regulatory agencies, such as the US Environmental Protection Agency, decide which among the thousands of chemicals should receive greater scrutiny first. Priorities would be set on the basis of chemicals' potential hazardous effects on humans and on their potential to get into human lungs and other organs. Using rapidly evolving computer-based methods to integrate data and information from many sources, the researchers say, will make it possible to start defining levels at which chemicals might cause harm and then select those chemicals in the environment that should be more fully assessed. That ability has long been recognised as a critical unmet need.

'In my opinion, this work is starting to lay the foundation that will allow risk assessors and risk managers around the world to couple high-throughput screening tests and adverse outcome pathways for risk assessment,' said Dr Lyle D. Burgoon of the US Army Engineer Research and Development Center. Quantitative high-throughput screening (qHTS) uses robotics and other technological devices. These technologies allow researchers to quickly conduct millions of chemical tests. Adverse outcome pathways, or AOPs, trace changes in biological systems that lead to harmful effects.

To assess the usefulness of the qHTS-AOP approach, Burgoon worked with colleagues from the Oak Ridge Institute for Science and Education. Their research used the cancer-causing chemical benzo[*k*]fluoranthene to pilot test the promising chemical risk assessment method and was published in the online version of *Risk Analysis* (doi: 10.1111/risa.12613). The research focused on benzo[*k*]fluoranthene's putative ability to cause steatosis, a cell disease in which excess fatty molecules build up in cells. It also focused on the chemical's potential to damage DNA as a result of oxidation, which can cause electron losses associated with some diseases and cancers.

Burgoon says the qHTS-AOP approach is especially critical for the chemicals currently in the environment for which data are lacking. 'High-throughput screening provides an avenue to get more data on these chemicals in a shorter amount of time, at an overall lower cost. As scientists generate more data from these high-throughput tests, our approach will allow these data to be integrated together, to create a better sense of what a safe exposure may be.'



Benzo[*k*]fluoranthene

Ideally, risk assessors would use qHTS data in combination with reverse dosimetry data and models. Such data are based on levels of chemicals found in biological samples (from human hair, blood etc.). The samples are used to define chemical levels in the environment that caused the exposures, but data derived from reverse dosimetry are currently insufficient. Until the gap in reverse dosimetry data can be filled, the qHTS method will allow chemicals to be ranked for regulatory attention. Priorities will depend on which chemicals the qHTS tests find are potentially more harmful relative to other chemicals. Those findings will be paired with real-world data on how much of the chemical is found in air, water or other places.

'Overall, we feel confident that as more qHTS data become available we will be able to translate these into risk assessment research needs and risk screening assessments,' the authors wrote. 'We are equally confident that transparency can be enhanced over time, as we continue to migrate towards more computationally efficient, semi-automated methods.'

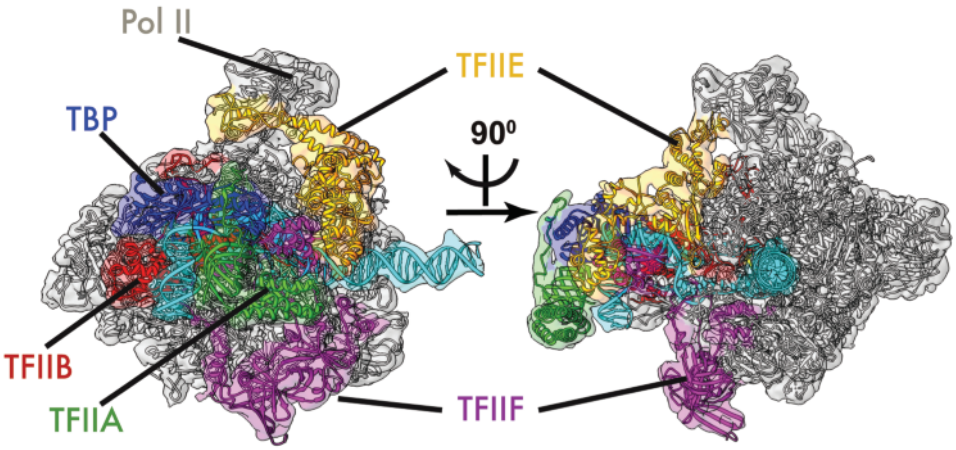
Society for Risk Analysis

New, detailed images of DNA transcription

An unprecedented molecular view of the critical early events in gene expression, a process essential for all life, has been provided by researchers at Georgia State University, the University of California at Berkeley and Northwestern University.

Cryo-electron microscopy (cryo-EM), a technique that studies samples at cryogenic temperatures, combined with state-of-the-art computational modelling, allowed researchers to visualise large transcription pre-initiation complexes (PIC) at near-atomic resolution. The PIC is a protein assembly that positions the enzyme RNA polymerase so it can start transcription.

The new structures shed light on the sequential conformational changes in the PIC throughout the transcription initiation process, including recognising the promoter region of DNA where transcription of a gene starts, opening this promoter region and initiating transcription. The study was published in *Nature* (doi: 10.1038/nature17970).



Architecture of the human transcription pre-initiation complex (PIC). A critical step in transcription is the process of promoter opening, resulting in a nascent transcription bubble. This is accomplished by RNA polymerase (Pol II) in association with general transcription factors that assemble to form the PIC. The structure of the core PIC is fitted into the cryo-EM density map and shown in two orientations.

Genes are made up of DNA, which serves as a repository of all our genetic information. To use the information encoded in a gene, RNA polymerase must make a copy in the form of messenger RNA. The copying process – transcription – is one of the central activities necessary for life.

At the beginning of this tightly controlled process, RNA polymerase and general transcription factor proteins assemble at a specific site along the DNA to form a PIC. The PIC assembly is required for opening the double-stranded DNA helix of the promoter, positioning the DNA in the active site of RNA polymerase and starting the transcription process. The messenger RNA transcripts are then used to produce proteins, the building blocks of human bodies.

'This paper provides detailed structural information on the complexes that participate in the early stages of the transcription process,' said Ivaylo Ivanov, associate professor of chemistry at Georgia State University. 'We explore the steps that RNA polymerase and general transcription factors take in order to open the transcription bubble and begin the process of transcription. This is a very important system that wasn't accessible by either crystallography or any other structural method before. This is the very first near-atomic cryo-EM reconstruction of the human PIC assembly.'

Chemical cross-linking and crystallography had provided glimpses of partial RNA polymerase complexes from eukaryotic organisms such as yeast, but these techniques could not solve the structure of the entire PIC complex. The events and processes leading to DNA unwinding by the PIC and the formation of a transcription bubble, a molecular structure that occurs during transcription when a portion of the DNA double strand is unwound, were insufficiently understood.

To build detailed atomic models of the PIC complex, Ivanov and his team applied integrative molecular modelling techniques. The calculations relied on modern supercomputing technology available though the National Science Foundation Extreme Science and Engineering Discovery Environment program and the National Energy Research Scientific Computing Center. The researchers showed that judicious combination of complementary techniques – molecular dynamics flexible fitting and refinement of atomic coordinates with the Phenix crystallography software package – led to models comparable in quality to crystal structures in the same resolution range.

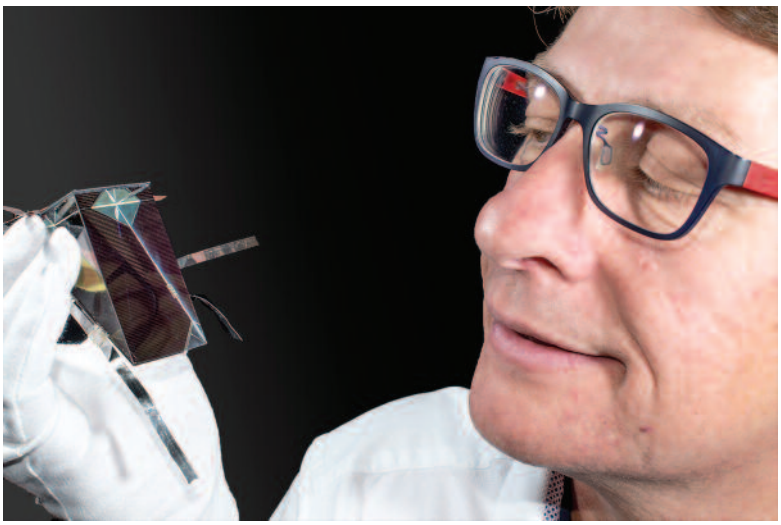
The researchers captured the human PIC in three different functional states: a closed state engaged with the DNA double helix of the promoter region; an open state engaged with the transcription bubble; and an initial transcribing complex poised to carry out the chemistry of messenger RNA synthesis. They were also able to visualise numerous previously undetermined components of the human PIC assembly. The findings revealed the complete subunit organisation of a transcription factor called TFIIH, which has a critical role in opening the promoter region. TFIIH proved one of the most difficult pieces of the PIC assembly to resolve.

Comparisons between the closed, open and initial transcribing states of the PIC provide new mechanistic insights into the processes of DNA engagement, promoter melting and transcription bubble stabilisation.

Georgia State University

Milestone in solar cell efficiency

By Wilson da Silva



Dr Mark Keevers with one of the spectrum-splitting, four-junction mini-modules developed at the University of New South Wales.

A new solar cell configuration developed by engineers at the University of New South Wales has pushed sunlight-to-electricity conversion efficiency to 34.5% – establishing a new world record for unfocused sunlight and nudging closer to the theoretical limits for such a device.

The record was set by Dr Mark Keevers and Professor Martin Green, Senior Research Fellow and Director, respectively, of the University of New South Wales's Australian Centre for Advanced Photovoltaics, using a 28 cm^2 four-junction mini-module – embedded in a prism – that extracts the maximum energy from sunlight. It does this by splitting the incoming rays into four bands, using a hybrid four-junction receiver to squeeze even more electricity from each beam of sunlight.

The new result, confirmed by the US National Renewable Energy Laboratory, is almost 44% better than the previous record – made by Alta Devices of the US, which reached 24% efficiency, but over a larger surface area of 800 cm^2.

'This encouraging result shows that there are still advances to come in photovoltaics research to make solar cells even more efficient,' said Keevers. 'Extracting more energy from every beam of sunlight is critical to reducing the cost of electricity generated by solar cells as it lowers the investment needed, and delivering payback faster.'

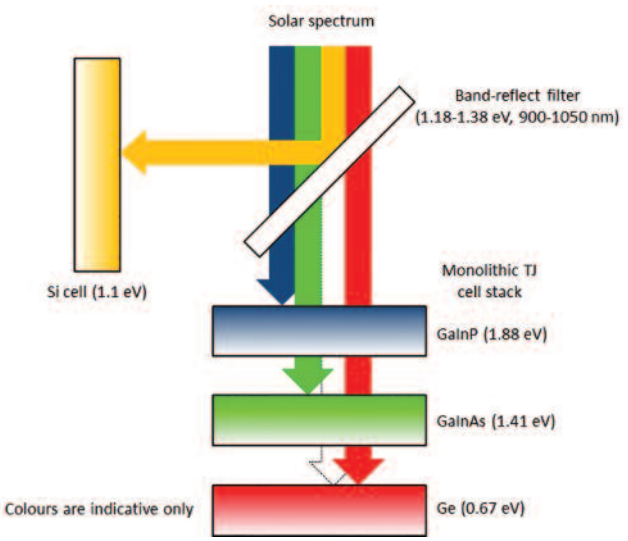
The result was obtained by the same team that set a world record in 2014, achieving an electricity conversion rate of over 40% by using mirrors to concentrate the light – a technique known as CPV (concentrator photovoltaics) – and then similarly splitting out various wavelengths. The new result, however, was achieved with normal sunlight with no concentrators.

'What's remarkable is that this level of efficiency had not been expected for many years,' said Green, a pioneer who has led the field for much of his 40 years at the University of New South Wales. 'A recent study by Germany's Agora Energiewende think tank set an aggressive target of 35% efficiency by 2050 for a module that uses unconcentrated sunlight, such as the standard ones on family homes.'

Australia's research in photovoltaics has already generated flow-on benefits of more than $8 billion to the country, Green said. Gains in efficiency alone, made possible by PERC cells, are forecast to save $750 million in domestic electricity generation in the next decade. PERC cells were invented at the University of New South Wales and are now becoming the commercial standard globally.

The record-setting mini-module combines a silicon cell on one face of a glass prism, with a triple-junction solar cell on the other.

The triple-junction cell targets discrete bands of the incoming sunlight, using a combination of three layers: indium–gallium–phosphide, indium–gallium–arsenide, and germanium. As sunlight passes through each layer, energy is extracted by each junction at its most efficient wavelength, while the unused part of the light passes through to the next layer, and so on.



A diagram of the spectrum-splitting, four-junction mini-module.

Some of the infrared band of incoming sunlight, unused by the triple-junction cell, is filtered out and bounced onto the silicon cell, thereby extracting just about all of the energy from each beam of sunlight hitting the mini-module.

The 34.5% result with the 28 cm^2 mini-module is already a world record, but scaling it up to a larger 800 cm^2 – thereby leaping beyond Alta Devices' 24% – is well within reach. 'There'll be some marginal loss from interconnection in the scale-up, but we are so far ahead that it's entirely feasible,' Keevers said. The theoretical limit for such a four-junction device is thought to be 53%, which puts this result two-thirds of the way there.

Multi-junction solar cells of this type are unlikely to find their way onto the rooftops of homes and offices soon, as they require more effort to manufacture and therefore cost more than standard crystalline silicon cells with a single junction. But the team is working on new techniques to reduce the manufacturing complexity, and create cheaper multi-junction cells.

However, the spectrum-splitting approach is perfect for solar towers, like those being developed by Australia's RayGen Resources, which use mirrors to concentrate sunlight, which is then converted directly into electricity.

The research is supported by a $1.4 million grant from the Australian Renewable Energy Agency (ARENA). The University of New South Wales team is working with another ARENA-supported company, RayGen, to explore how the advanced receiver could be rolled out at concentrated solar PV power plants. Other research partners are Trina Solar, a PV module manufacturer and the US National Renewable Energy Laboratory.

Thermal analysis webinars

Thermal analysis plays an important role in the development and production of many products, including food, polymers and metal, but reliable results are sometimes difficult to obtain. Attend Mettler Toledo's free thermal analysis webinars to learn more about principles that enhance accuracy and get answers to your application questions.

Mettler TOLEDO's year-long calendar of live webinars will cover a full range of thermal analysis methods, giving lab assistants, engineers and other interested professionals an opportunity to explore how these robust analyses can be used to gain materials insight, investigate product failure, and improve product quality. Attendees will also learn tips for obtaining reliable, reproducible results using enabling technology.

Webinars will address thermal analysis themes from various standpoints, including:

- specific techniques, such as differential scanning calorimetry (DSC)
- different methods, such as kinetics studies
- application fields, such as thermoplastics.

Each webinar will also offer a Q&A session where attendees can have their most pressing thermal analysis application questions answered by METTLER TOLEDO experts without leaving the comfort of their office chairs.

For the complete calendar, or to register for one or more of these interactive sessions, please visit our thermal analysis webinars webpage (bit.ly/1TiHaNG).

Register now to access our free Mettler Toledo on-demand thermal analysis webinars (bit.ly/1TGMb29). To register for an e-training course, please visit our Thermal Analysis e-training course webpage (bit.ly/1TmqeYX).

Additional information about Mettler Toledo can be found at www.mt.com.

Member ADVANTAGE®

raci
Royal Australian Chemical Institute

Planning a holiday?

It's just a click away with thousands of competitive rates at more than 700,000 hotels worldwide!

www.memberadvantage.com.au/raci/hotels

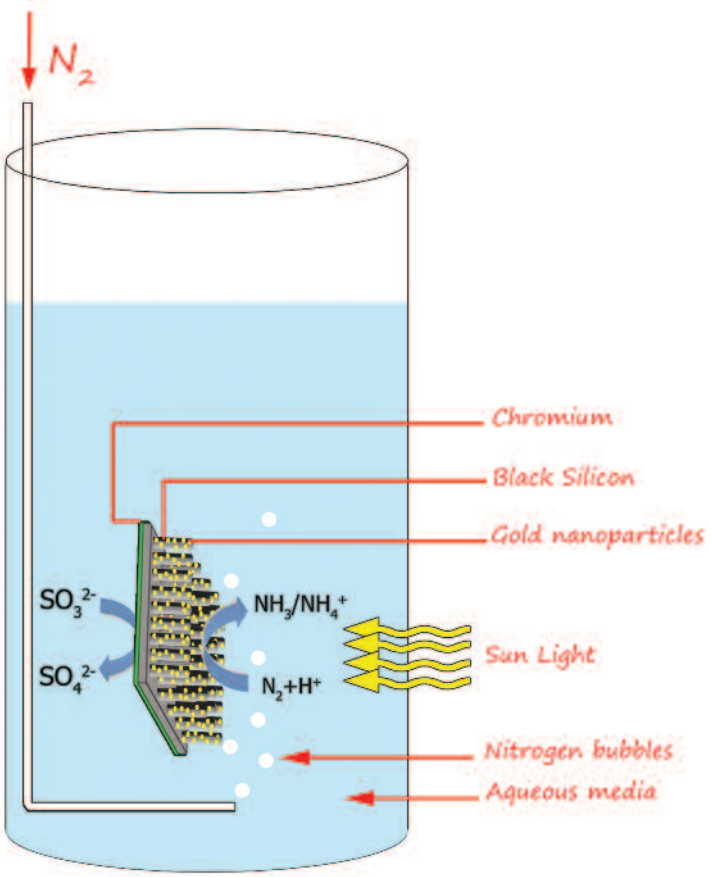
Your RACI Member Advantage program recently launched its new hotel booking service with one of the world's largest online travel agencies, allowing you to enjoy thousands of promotional deals and great competitive rates when booking your next holiday.

The choices are endless, with an extensive range of properties, from resorts, villas and motels, to executive apartments and five-star luxury suites, in more than 71,000 destinations worldwide.

Contact RACI Member Advantage at info@memberadvantage.com.au or call 1300 853 352

Fixing nitrogen with light

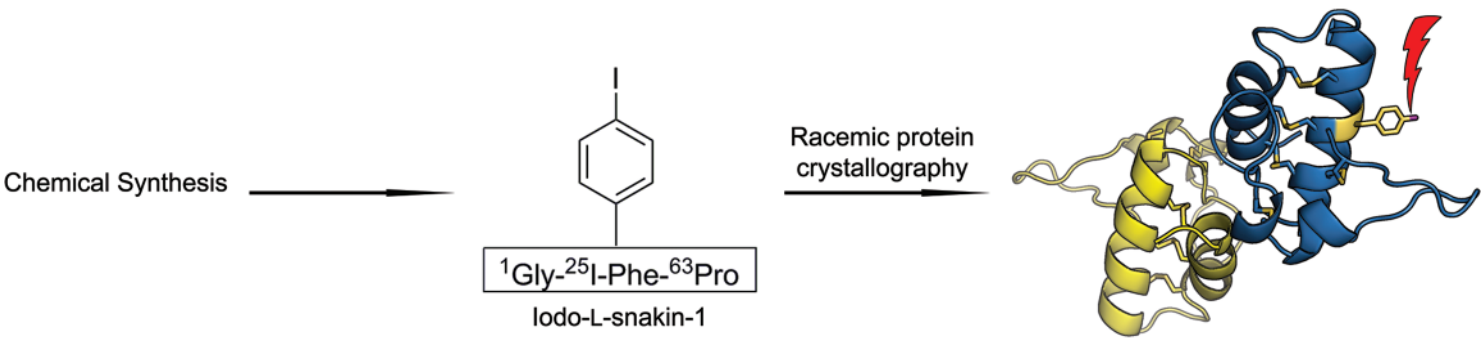
Ammonia has played a pivotal role in the expansion of society over the past century, as the basis for chemical fertilisers that have improved crop yields and fed a growing world population. However, the industrial production of ammonia (roughly 200 million tonnes/year) is an energy-intensive process that consumes approximately 3% of world energy supplies. Finding new and sustainable methods to generate ammonia without carbon-based energy is therefore a strategic goal to combat global warming. Besides its use in fertilisers, ammonia also has a bright future as a fuel. Fuel cells that provide power to vehicles and devices can be designed to use ammonia, making it a carbon-free fuel source. In recent work published by Professor Douglas MacFarlane and co-workers at Monash University, a new method to reduce nitrogen to ammonia using light has been discovered (Ali M., Zhou F., Chen K., Kotzur C., Xiao C., Bourgeois L., Zhang X., MacFarlane D.R. *Nat. Commun.* 2016, **7**, 11 335). The method relies on a nanostructured silicon wafer with gold nanoparticles deposited on its surface to absorb light and use the absorbed energy to reduce molecular nitrogen to ammonia in an aqueous electrolyte. Electrons generated in the nanostructured silicon semiconductor under illumination are sufficiently energetic to accomplish the six-electron reduction reaction. The ammonia yields are currently not sufficient for large-scale application, but there is much scope to improve this process in the future.



Structure determination using radiation-damaged quasi-racemic crystals

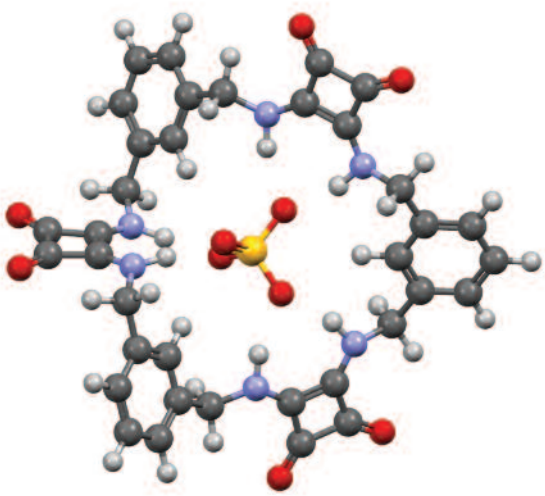
In recent years, advances in chemical protein synthesis have enabled racemic protein crystallography, a method by which both L- and D-amino-acid-containing proteins are mixed together to promote crystal growth and to remove a major bottleneck in structure determination. The research groups of Distinguished Professor Margaret Brimble and Dr Christopher Squire at the University of Auckland have solved the structure of the snakin-1 protein through a novel combination of racemic protein crystallography and radiation damage-induced phasing (Yeung H., Squire C.J., Yosaatmadja Y., Panjikar S., López G., Molina A., Baker E.N., Harris P.W.R., Brimble M.A. *Angew. Chem. Int. Ed.* 2016, doi: 10.1002/anie.201602719).

The incorporation of an unnatural 4-iodophenylalanine residue inside a quasi-racemic crystal of the protein and the subsequent breakage of the exogenous C–I bond by X-irradiation were critical factors in the successful structure determination. The structure of this protein is the first from the GASA/snakin superfamily, whose members are involved in development, hormonal cross-talk and antimicrobial defence in many plant species. The structure provides a starting point for rational antimicrobial peptide design, and also suggests the general applicability of the 4-iodophenylalanine residue in radiation-mediated phasing of crystals prepared from chemically synthesised proteins.

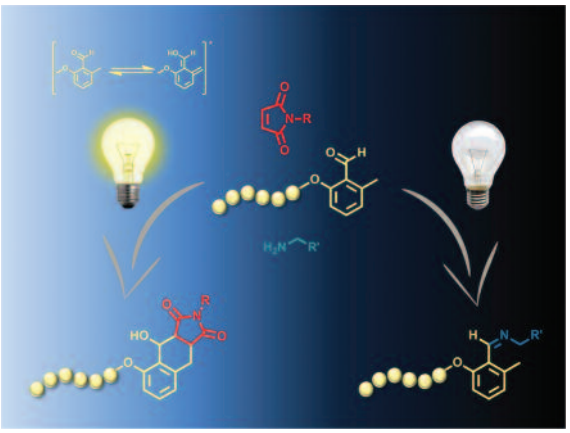


Selectively sensing sulfate

Anions play essential roles in biology, medicine, catalysis and the environment. So the ability to selectively detect anions has numerous real-world applications. Most of these applications require anion recognition to occur in water. However, selective anion receptors that operate in water are exceptionally rare, particularly when the target anion is inorganic sulfate, which is heavily hydrated in aqueous solution. Nature has overcome this challenge by employing an idealised arrangement of hydrogen-bonding interactions in the sulfate-binding protein. This has served as the inspiration for a series of macrocyclic sulfate receptors synthesised in the Jolliffe research group at the University of Sydney (Qin L., Hartley A., Turner P., Elme R.B.P., Jolliffe K.A., *Chem. Sci.* 2016, doi: 10.1039/C6SC01011C.) These macrocyclic structures are simple to prepare and their structures can be readily tuned to provide solubility in different solvents, including aqueous mixtures. They were found to be extremely potent and selective ligands for inorganic sulfate, with one of the receptors better able to discriminate between sulfate and chromate than the sulfate-binding protein.

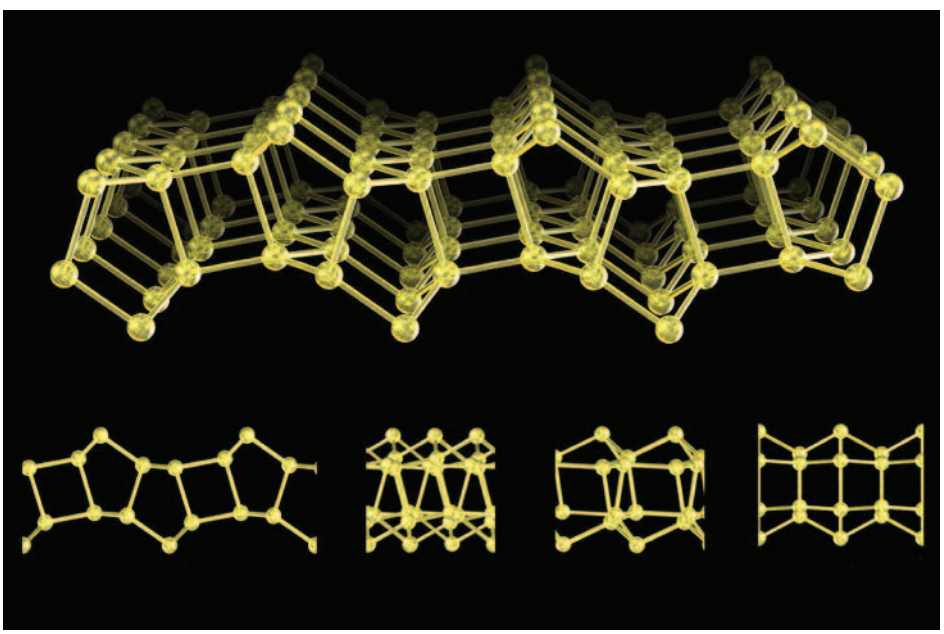


Light switch for polymerisation products



The concept of orthogonality in macromolecular synthesis – the ability to create a series of polymers with varied architecture or sequence from a single reaction mixture through independent chemical reactivity – has wide-reaching applications. The team of Dr James Blinco at the Queensland University of Technology and Professor Christopher Barner-Kowollik at the Queensland University of Technology and the Karlsruhe Institute of Technology in Germany have done just this and it is as easy as switching a light on and off (Hiltebrandt K., Eiles K., D'hooge D.R., Blinco J.P., Barner-Kowollik C. *J. Am. Chem. Soc.* 2016, **138**, 7048–54). The researchers introduced a reaction manifold for a polymer with an *o*-methylbenazaldehyde end group. When mixed in a solution containing a primary amine and a maleimide, different ligation products were achieved depending on the presence or absence of a light stimulus. When irradiated, the end group underwent photo-enolisation, activating it for Diels–Alder cycloaddition. If left in the dark, the imine reaction preferentially occurred. Through controlled irradiation, the composition of the final product formed could be adjusted from 100% imine (0% photo product) to less than 5% imine (95% photo product). The team also demonstrated that the methodology is not only amenable for polymer end-group modification but also for the linking of two polymer chains to form block copolymers.

Stabilising silicenes



Silicene is a two-dimensional nanomaterial that is the silicon analogue of graphene. It holds great potential for next-generation electronics, batteries and gas sensors (see September 2014 issue, pp. 24–7). But the full application of silicene is hindered by its instability under ambient conditions and high reactivity with oxygen (Spencer M.J.S., Morishita T. *Sci. Rep.* 2015, **5**, 17570). Dr Michelle Spencer (RMIT University) and Dr Tetsuya Morishita (National Institute of Advanced Industrial Science and Technology, Japan) have recently edited the first book on silicene (*Silicene: structure, properties and applications*, Springer, 2016). The groups of Dr Spencer, Dr Morishita and Dr Hideyuki Nakano (Toyota Central R&D Labs, Japan) have also recently discovered a new allotrope of silicon containing four-, five- and six-membered sp^3-hybridised silicon rings (Yaokawa R., Ohsuna T., Morishita T., Hayasaka Y., Spencer M.J.S., Nakano H. *Nat. Commun.* 2016, **7**, 10 657). In total, three types of bilayer silicenes were obtained after treating calcium-intercalated monolayer silicene ($CaSi_2$) with a BF_4^--based ionic liquid. The bilayer silicenes were sandwiched between planar crystals of CaF_2 and/or $CaSi_2$, making them highly resistant to oxidation and thus providing scope for new applications of bilayer silicene that require greater stability under atmospheric conditions.

Compiled by **David Huang** MRACI CChem (david.huang@adelaide.edu.au). This section showcases the very best research carried out primarily in Australia. RACI members whose recent work has been published in high impact journals (e.g. *Nature*, *J. Am. Chem. Soc.*, *Angew. Chem. Int. Ed.*) are encouraged to contribute general summaries, of no more than 200 words, and an image to David.

Communications: do we need them?

It is fair to say that the process of publishing a manuscript has changed remarkably over the course of our academic careers. While, unlike our older colleagues, we were spared the tedium of typewritten manuscripts with carbon paper providing the copies, we still had to endure the tyranny of distance, served by the postal service. We must remember that the whole process of academic publishing was considerably slower, the copies of the manuscript had to be posted to the editor and from there to the referees. All deliberations were by post and it could take up to six months to publish a paper. In fact, in our own journal, which went fully electronic in 1997 and was the first of the CSIRO journals to do so, the average time from submission to online publication was six months. Gradually, authors started to provide their manuscripts on electronic media, which shortened typesetting times as prior to that the text was re-keyed in by our in-house typesetters.

It was in this environment that the Communication was created to serve the community. Communications were used to provide our peers with the quickest possible dissemination of important results. Our own journal suggests that a Communication should be for 'short reports of urgent research findings, and should not exceed 2000 words and three graphics.' However, some Communications could still take up to a year from submission to publication. Once we went to conferences to hear the most important new results, but now they are really opportunities to network because no one likes to report their unpublished results given the possibilities afforded by the accelerated publishing process.

The current publishing paradigm sees us with drastically shorter submission to publication times with articles appearing online sometimes within a month of submission depending on the rate-determining step of the reviewing process. So the question is, do we need the Communication as an article type in any journal? Perhaps not! People will point to impact factor as a reason to publish in these journals but these are often inflated by the incorporation of review articles, perhaps the very opposite of 'short reports of urgent research findings'.

Our view is that the chemical community would be better served by the publication of full papers in which all the details and full scope of the work are provided. There is still a place for a shorter full paper telling a complete story but in our minds there is no need for 'urgent' publication because if you want you can tweet it! It just won't be peer reviewed.

What do our readers think?

George Koutsantonis FRSC, FRACI CChem and **John D. Wade** FRSC, FRACI CChem, Co-Editors-in-Chief, *Australian Journal of Chemistry*

iStockphoto/olgalT

Cobalt blues

BY **DAVE SAMMUT**

Alongside inspiring stories in elite sport are those centred on the use of banned substances such as cobalt.

Public scandals of doping in sport have become legendary. A tiny minority of competitors seek unfair advantage through the misuse of therapeutic and other drugs, and this creates problems for all. The fall of Western greats such as Ben Johnson and Lance Armstrong and the 2015 suspension of the entire Russian athletics federation from international competition show that this is a global sporting issue.

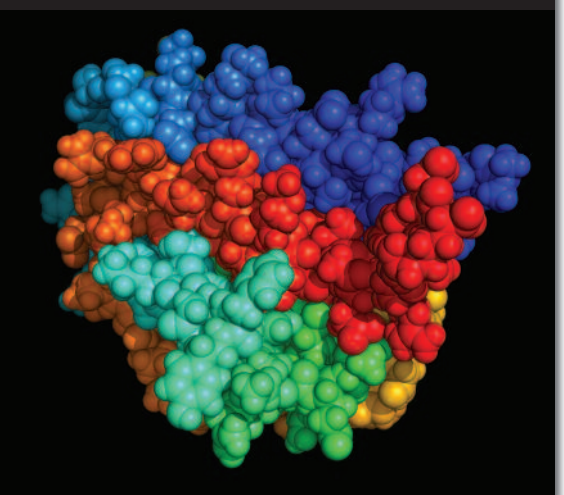
The problem is much wider than just the issue of cheating. Many of the drugs and techniques used in doping have serious and long-term health consequences. Danish cyclist Knud Jensen died suddenly during competition in the 1960 Olympics, with one autopsy finding amphetamines and the drug pyridin-3-ylmethanol (a vasodilator) in his system. The causes of Jensen's death are debated even today, but this tragic event prompted the International Olympic Committee to establish its first medical committee, the start of ongoing efforts to protect the health of athletes and the fairness of competition.

A fundamental aspect of performance in elite sport – human or animal – is the oxygenation of the muscles. So there are many routes by

How cobalt(II) activates EPO production

The erythropoietin (EPO) gene and other oxygen-regulated genes are controlled by the transcription factor hypoxia inducible factor 1a (HIF-1α). This is a specific protein required for the initiation of the synthesis of RNA, using a DNA template catalysed by an RNA polymerase enzyme.

Under normoxic conditions, HIF-1α is rapidly degraded by a proteasome, an intracellular enzyme that degrades misfolded or damaged proteins and modulates the quantity of regulatory proteins (like HIF-1α) in the cell. Co^{2+} induces a form of hypoxia, and thereby markedly inhibits the degradation of HIF-1α. The HIF-1α then binds to HIF-1β, crosses the nuclear membrane and powerfully activates erythropoietin gene transcription.



The glycoprotein erythropoietin includes four alpha helices stabilised by disulfide links. Wikimedia/CC-BY-SA-3.0

which athletes and their trainers seek to enhance the capacity of the body to carry oxygen.

Arguably at its most benign, anaerobic training at high altitude creates hypoxic conditions in the system, which stimulates a natural increase in production of haemoglobin, which in turn enhances performance on return to the oxygen partial pressures at sea level. Within the body, sea level oxygen partial pressures are medically termed 'normoxia' (see box).

The same principle applies to the technique of drawing the athlete's blood over time and then re-injecting it just before race day. However, whether natural or forced, higher red-blood cell levels pose a risk to the system by increasing the viscosity of the blood, placing a greater strain on the heart to pump the blood around the body.

The recent AFL supplements scandal embodies a key problem with doping. The athletes were found to have been doped, allegedly without their knowledge or consent, with the prohibited substance thymosin beta-4. These players have incurred substantive sporting sanctions, and now face unknown long-term health effects.

Take this one more step to the issue of doping in horse racing, where the animals can in no way give consent to their treatment, therapeutic or otherwise. According to Racing NSW: 'United States racing officials became concerned with the use of cobalt in January 2013 when officials detected its presence in a large number of samples that were taken at The Meadowlands in New Jersey'.

Why cobalt? Since the 1980s, a key challenge for antidoping authorities has been the detection and control of the use of erythropoietin (EPO). EPO is the hormone responsible for controlling the generation of red blood cells ('erythropoiesis') in bone marrow. So the use of EPO represents another method of boosting haemoglobin levels in the blood. However, as the analytical techniques to detect EPO in both blood and urine, particularly recombinant human EPO (rhEPO) and its analogues, have improved, and because EPO is expensive, unscrupulous athletes and trainers are increasingly seeking alternatives. Cobalt(II) is known to activate EPO production in the body (see box).

Cobalt is found in trace levels in a wide range of foodstuffs, including nuts, green leafy vegetables, fish and cereals. In both humans and animals, it is active in various coenzymes such as cobalamins, the best known of which is vitamin B12. It is therefore a critical micronutrient. However, there are no published reports of cobalt dietary deficiency in humans, nor in horses. Indeed, there are reports of healthy horses grazing in cobalt-deficient grasses that are unable to support sheep or cattle.

The US National Research Council recommends a minimum daily cobalt intake of 0.5 milligrams of cobalt per day for a 500-kilogram horse. This should be readily achievable from dietary sources for a healthy adult horse, but supplementation might be legitimately used for the treatment of diseases that interfere with the take-up of vitamins and minerals.

In a 1958 human study (doi: 10.3181/00379727-99-24395), the administration of 120–150 mg/day of cobalt chloride induced additional haemoglobin production up to 20% above pre-treatment levels in six subjects within 7–22 days, returning to normal levels within 9–15 days after cessation of cobalt administration.

From the 1940s to the 1970s, cobalt was used therapeutically to treat various types of anaemia in humans (septic infection, myeloid hypoplasia, sickle-cell disease), as well as rheumatoid arthritis and chronic kidney disease. However, these treatments were associated with significant harmful side-effects: organ damage, gastrointestinal illness, neurological dysfunction, impaired thyroid activity and myocardial function, reversible hearing loss and long-term loss of visual acuity. Given these serious side-effects, cobalt treatments for anaemia were abandoned in the 1970s in favour of androgens, until rhEPO became available in the 1980s.

Although cobalt is known to have therapeutic benefits in humans, there

is little or no evidence that cobalt supplements enhance racing performance for healthy horses. The first direct study of single-dose intravenous cobalt administration in 18 horses (Knych et al., 2014, doi: 10.1002/dta.1737) did not find any change in blood EPO concentrations, red blood cell parameters or heart rate within the period studied. Instead, its use in horses appears to be based on anecdotal evidence and extrapolation from its former use in human therapeutics.

Various sources of cobalt are readily accessible and cheap. It is also found in various veterinary therapeutics, and commercially available supplements.

The unregulated abuse of cobalt in horse racing has yielded some major consequences. Given in excessive doses, it has caused side effects such as 'shaking, trembling and sweating up'. According to news reports, there has been a number of unexplained deaths of US racehorses, later found with high levels of cobalt in their system.

In a scathing article in the September 2015 *Veterinary Journal* (doi: 10.1016/j.tvjl.2015.04.005), authors Mobasheri and Proudman stated '… the lay public does not have access to detailed information about the potential risks and many trainers do not have the scientific knowledge to assess the risk : benefit ratio for the use of cobalt salts.'

Harness Racing NSW took the lead in regulating cobalt in Australian horse racing. In December 2013, it introduced a threshold limit of 200 μg/L of cobalt in race-day urine samples. Dr Terence Wan, considered a world leading racing analyst, advised the authority that 'no untreated horse should have a level greater than 60 μg/L but, to be safe, a level of 100 μg/L would clearly represent a treated horse on raceday'. Racing Victoria and South Australia followed suit in 2014. A national threshold of 200 μg/L was subsequently implemented by Racing Australia in 2015.

Emeritus Professor Brynn Hibbert FRACI CChem, newly inducted President of the Royal Society of New South Wales, conducted statistical analyses for the racing industry, concluding that: 'it was reasonable to infer that those [horses] below 50 μg/L had not been treated'. Hibbert advised that if 50 μg/L can be taken as an upper level of a 'normal' population, then an action level (level at which regulatory action would be taken) of 100 μg/L gives odds of 1 : 116 000 against such a concentration in a normal population.

Speaking to the author, Hibbert emphasised that up to 50 μg/L was the range used to establish the typical population, but that higher levels don't automatically imply doping. However, above 200 μg/L 'the chances are essentially zero that a typical horse would have these levels'.

Using the threshold of 200 μg/L, the Victorian Civil and Administrative Tribunal handed leading horse trainers Mark Kavanagh and Danny O'Brien multi-year suspensions in January 2016 after they were convicted for administering cobalt to horses in their charge. Two other trainers, Lee and Shannon Hope, were found guilty of administering cobalt to their horses the previous November. Some cobalt values in these prosecution were in considerable excess of the 200 μg/L limit.

The unregulated abuse of cobalt in horse racing has yielded some major consequences. Given in excessive doses, it has caused side effects such as 'shaking, trembling and sweating up'.

NSW Racing currently uses the National Measurement Institute for its cobalt analysis, pending the procurement, development and validation process of its own ICP-MS analysis technique. This is the 'gold standard' method, and works well for these types of samples. Hibbert advises that a limit of detection of 1 μg/L is practical, with a median level for a typical population of several thousand horses of approximately 3 μg/L cobalt.

The good news is that, based on further studies, Hibbert reports that cobalt levels in horse racing are falling appreciably. The trainers are taking note, and the goal of protecting the welfare of the horses in the industry is being achieved in this respect.

Dave Sammut FRACI CChem is principal of DCS Technical, a boutique scientific consultancy, providing services to the Australian and international minerals, waste recycling and general scientific industries.

Expressing a passion for chemistry and crystals

The Crystal Crew (Left to right: Harriet, Faduma, Maria and Emma), University of Warwick Chemistry Department.

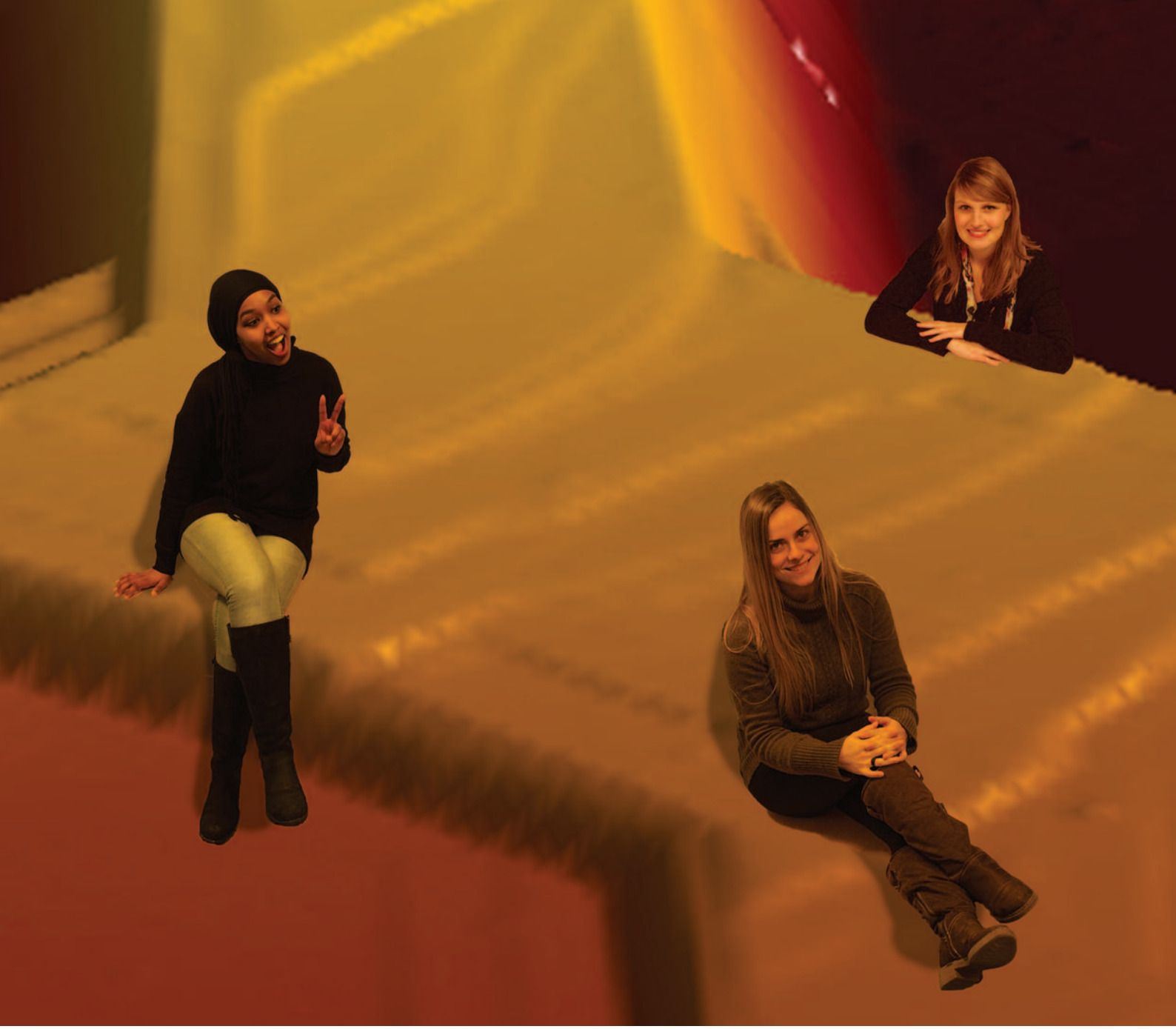
BY **UNIVERSITY OF WARWICK**

An optical microscope image of a partially dissolved crystal of an API becomes a very curious character in Mary Courtney's piece entitled 'The idea was crystallising himself'.

Four PhD students at the University of Warwick are exploring the creative side of crystal research.

Emma Ravenhill, Faduma Maddar, Harriet Pearce and Maria Adobes-Vidal have a passion for chemistry and crystals. They want to share and celebrate the contributions women make to chemistry in today's world. They are part of the Electrochemistry Group at Warwick University, which is composed of 45% women. The Head of the Department of Chemistry, Professor Alison Rodger, is also a woman.

Emma, Faduma, Harriet and Maria are PhD students in the Electrochemistry and Interfaces



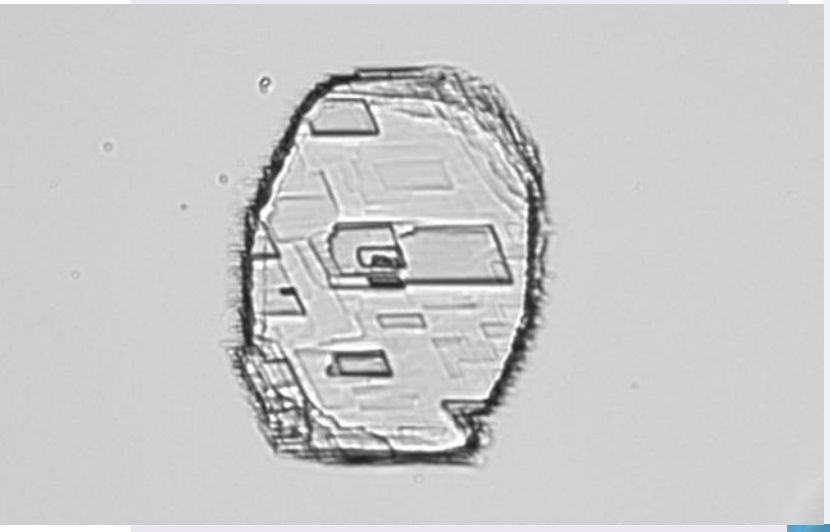
Group at Warwick University. They use state-of-the-art microscopes and instruments in new ways to reveal the properties of crystalline materials with applications from engine deposits to kidney stones. Their work helps to improve the composition of drugs, improve fungicides, enhance drug development and benefit industry.

Faduma, Harriet and Maria all study the growth and dissolution kinetics and mechanism of organic crystals. They monitor in situ topography changes of single crystals at the micro and nano scale by using Raman spectroscopy, X-ray diffraction, vertical scanning interferometry, optical microscopy, scanning ion-conductance microscopy and atomic force microscopy to provide a holistic view of the processes involved. The data inform mathematical modelling to obtain quantitative information of the driving force and the rate-limiting step of the growth/dissolution processes.

Known on campus as the Crystal Crew, the chemists produce images that not only assist their research into crystals but also reveal a strange and beautiful micro-world. Because their work provides lots of interesting new images, the Crystal Crew is involved in a Chem-Art project led by Professor Patrick R. Unwin and Mary Courtney, an artist in residence at the University of Warwick's Chemistry Department supported by the Leverhulme Trust. The project, 'Drawing on the nanoscale', uses high-resolution probe microscopes to allow the chemists to express a different side to their creativity. These images serve as inspiration for some of Mary's creations.

Maria Adobes Vidal

I am particularly interested in active pharmaceutical ingredients (the active component in drugs) and pathological crystals (for example kidney stones) due to their importance for human health. Understanding the process of dissolution or growth of these crystals makes it possible to improve the composition of drugs for a better performance or develop new strategies or treatments to cure certain illnesses.



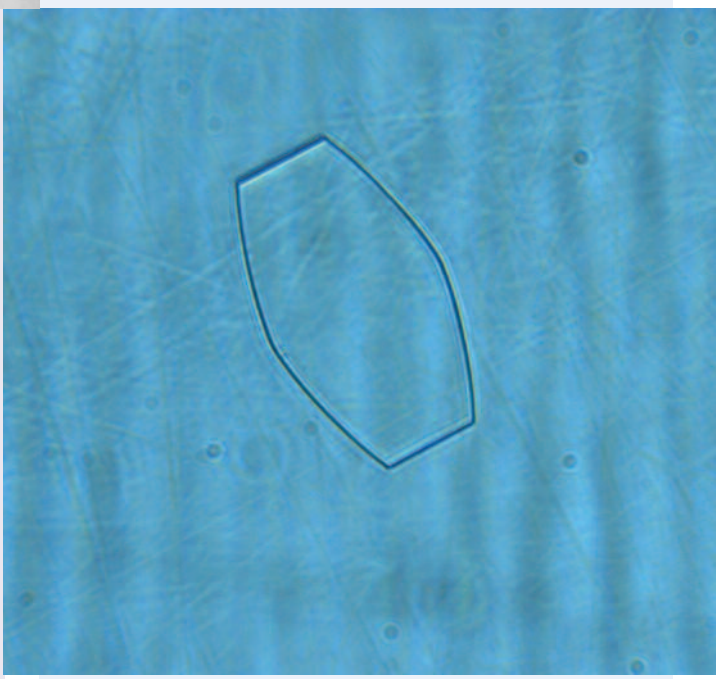
Optical image of a partially dissolved crystal of an active pharmaceutical ingredient.

Maria concentrates on organic crystals with a great impact on human health, such as active pharmaceutical ingredients or pathological crystals, for example kidney stones. L-Cystine crystals are the cause of kidney stones associated with the genetic disorder cystinuria and the available treatments for this condition are not totally effective in the removal (dissolution) or prevention (growth) of new stones. As a consequence, there is considerable interest in understanding the growth/dissolution kinetics of these crystals in order to improve the treatment of cystinuria. Maria has worked with Professor Michael D. Ward at New York University imaging the dissolution of L-cystine crystals by in situ atomic force microscopy. They were able to record movies of the surface process that occurred by the formation of hexagonal spirals formed from screw dislocations.

Harriet Pearce

The use of fungicides is vital for farmers to avoid crop losses. I want to understand the dissolution and growth processes of the fungicide crystals to make them more efficient to use.

Harriet focuses on agricultural fungicide formulations in aqueous media with surfactants. The active ingredient (AI) is an organic crystalline molecule with poor aqueous solubility and the surfactant aids its uptake into the plant from the leaves. Fungicides are normally delivered by a spray-dry process where the formulation exhibits a variety of liquid-crystalline phases as water (anti-solvent) evaporates from the surface of the leaf. Evaporation of water increases the organic content of a droplet on the leaf and thus the solubility of the AI. The crystalline AI can then dissolve, becoming available for uptake. Furthermore, if it rains, the spray deposit will pick up water, causing the AI to become insoluble and crystallise on the leaf surface. Hence, dissolution and crystallisation cycling of organic crystals is important in determining the efficacy of AIs with a view to improving the delivery process.

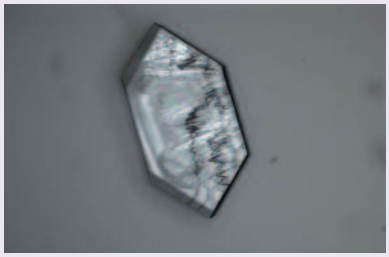


A bicalutamide crystal.

Faduma Maddar

I am looking into new approaches, combining optical imaging, microscopy and spectroscopy techniques to provide further in depth understanding and in turn assist in enhancement of drug development and formulation.

Faduma works in collaboration with pharmaceutical company AstraZeneca, developing new approaches to understand the dissolution of active pharmaceutical ingredients. In pharmaceutical science, dissolution testing is a key step to determine the rate at which an active pharmaceutical ingredient is released and is made available for absorption in the gastro-intestinal tract. Despite this importance, the general processes governing dissolution and crystallisation of crystals are poorly understood. As a case study, Faduma has focused on bicalutamide, the active pharmaceutical ingredient in AstraZeneca's product CASODEX. Bicalutamide belongs to class II of the biopharmaceutics classification system (low solubility, high permeability). The low solubility/dissolution rate of bicalutamide is a key factor limiting its oral bioavailability and clinical application. In fact, nearly 40% of newly developed compounds face the same problem and so in-depth understanding of dissolution of such compounds is fundamental as it is the rate-limiting step for in vivo absorption.

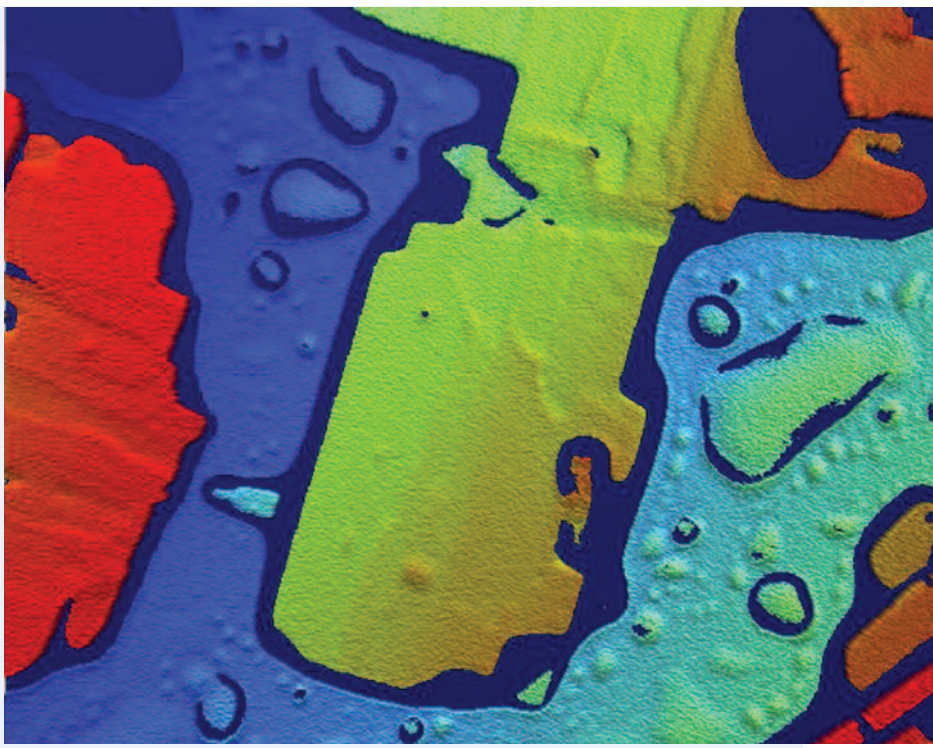


Optical image of a bicalutamide single crystal.

Emma Ravenhill

All gasoline and diesel car engines contain a range of essential additive chemistries. These are required, for example, to inhibit corrosion, enhance lubrication, and keep the engine clean. My project involves using microscopy and analytical techniques to study the crystal growth processes behind this deposit formation, allowing us to tailor future additives to prevent these unfavourable reactions from taking place.

Emma's project is focused on the study of engine additives. Although each additive plays a key role in protecting the engine, unfavourable side reactions take place between them, resulting in the formation of crystalline deposits. She uses in situ optical microscopy and analytical techniques such as Raman spectroscopy and X-ray diffraction to study the crystal growth processes, crystal morphology and polymorphism behind this deposit formation, obtaining information to tailor future additive chemistries that will prevent these unfavourable reactions and improve engine performance.



Calcium sulfate crystal interferometry.

Not all is science for Emma, Faduma, Harriet and Maria. Emma plays the guitar, paints in her spare time and bakes fantastic cakes. Harriet has been part of the Croydon Youth Theatre Organisation and loves going to the theatre. She also plays canoe polo and enjoys climbing and going hiking with her dog. Faduma is an amazing photographer, enjoys sketching and loves running. Maria was a ballet dancer before becoming a chemist and now she enjoys the adrenaline rush of skiing, kayaking and climbing. They also do other activities like fundraising for charity. Faduma and Maria are taking part in an upcoming UWCB (Ultra White Collar Boxing) event organised together with Cancer Research UK, and will have a proper boxing match (but not against each other).

First published by University of Warwick and adapted with permission.

What makes a great chemistry teacher?

Findings of the ChemPCK project

BY **MADELEINE SCHULTZ**

Pedagogical content knowledge from teachers and academics has been captured and coded to create a new resource for chemistry education.

It is surprising that science academics who place high levels of importance upon evidence-based practice for research do not consider the same evidence-base as being important in their teaching.

da Silva K.B. (2008). *Raising the profile of teaching and learning: scientists leading scientists*. ALTC. p. 25

Classroom teaching practice is a personal skill that develops with experience and through reflection. Teacher behaviour involves responding to a specific group of students in a particular class and so is impossible to completely plan in advance. However, steps towards the development of more effective teaching methods are possible even with limited time and resources.

Associate Professor Gwen Lawrie from the University of Queensland and I, together with research assistants Bronwin Dargaville and Chantal Bailey, have spent the past two years investigating teaching strategies within the framework of pedagogical content knowledge (PCK) as described in the September 2014 issue. PCK can be loosely defined as ways of teaching specific content, including the choice of representations, examples and analogies along with an understanding of typical student difficulties. While there is a vast body of research into PCK at the secondary level and it is explicitly taught and practised, PCK has been investigated less at the tertiary level.

The motivation for this project came from the recognition that in general, novice teachers in universities rarely


iStockphoto/ViktorCap

receive professional development in discipline-specific teaching practices. Instead they rely on a mixture of their own learning experiences, advice or mentoring provided by their colleagues and learning from their own mistakes as they gain experience. This process is in stark contrast to the culture in secondary school teacher training in which awareness of how students learn is linked to a disciplinary context to help teachers develop their PCK, and PCK is often taught explicitly.

A decade prior to this project, internationally renowned chemical educator Professor Bob Bucat from the University of Western Australia wrote in *Chemistry Education Research and Practice*, 2004, vol. 5(3), pp. 215–28):

> *The chemical education enterprise is crying out for 'applied research' that probes and documents the topic-specific PCK of respected teachers.*

> *Currently in the teaching profession the accumulated PCK of each of its participants grows with experience, peaks at retirement, and then disappears - often with hardly a contribution to the collective wisdom of the profession. (p. 225)*

To try to capture some of the wisdom to which Bucat refers, this project has collected topic-specific PCK from more than 50 chemistry academics from around Australia within workshops. In addition, we conducted interviews with ten recognised exceptional tertiary teachers about their personal teaching strategies. The interviewees were chosen on the basis of institutional or national awards for teaching excellence and were a mix of teaching and research-intensive academics representing different subdisciplines of chemistry. The resulting data from workshops and interviews were coded and a website was built (chemnet.edu.au/chem-pck), which distils the specific teaching strategies that are used for particular topics in chemistry. The site can be searched by chemistry topic or type of teaching strategy. Teaching strategies have been collated for a range of topics and subtopics (see table).

The website has been live since April this year and has attracted national and international attention. Feedback from users has been very positive, showing that it is a useful resource, particularly for those new to teaching a particular topic. Further teaching strategies will be added and readers are invited to contribute their own favourite strategies to the website.

We collected many insightful quotes from the expert teachers. Combining these with the current educational literature led to the development of a series of seven steps (see box) to

ChemPCK website topics and subtopics

Topic	Subtopics
General chemistry	Chemical bonding Electronic structure/electronegativity/shape Foundations of chemistry Nature of matter Practical chemistry Stoichiometry/equations/formulae
Organic chemistry	Functional groups Mechanisms Organic structure and bonding Stereochemistry Structure determination/NMR
Inorganic chemistry	Acid–base chemistry Electrochemistry Aqueous solutions
Physical chemistry	Chemical and physical properties Equilibrium Intermolecular forces Kinetics Phase transitions Quantum mechanics Thermodynamics
Analytical chemistry	Spectroscopy Other analytical techniques

enhance teaching that are applicable in any discipline. The website and the steps are recommended to any academics in the early stages of their teaching careers.

We found that the most favoured teaching strategies evolve with increasing numbers of years of teaching experience. In the first two years of teaching, most academics' teaching strategies rely on demonstration and explanation. Participants with three to seven years of teaching experience were more likely to use examples and real-world applications as their most favoured teaching strategies. After eight years of teaching, the most common strategies involve student participation, and this persists through to the most experienced and expert academics. Thus, these strategies are likely to be most effective and novice teachers could attempt to move towards expert behaviour.

Tertiary chemistry teachers typically have a focused research background within a specific chemistry subdiscipline other than chemical education. This background influences their epistemological perspectives and can inform their understanding and explanations of basic chemical concepts. This project aimed to capture the PCK of chemistry teachers with a variety of backgrounds to compare their teaching strategies for the same topics and to seek common threads that tie together chemistry PCK.

Some quotes illustrate the depth of interviewees' affiliation to their subdiscipline. For example, an organic chemist, describing the use of curly arrows to understand reaction mechanisms, said

> *... it takes organic chemistry from a rote learning discipline ... to an understanding and an intuitive discipline ... for students that can make that transition and can fully understand that concept, then they have a much deeper and more profound understanding of and relationship with the whole discipline ...*

A bioinorganic chemist had a different perspective on what is most important:

> *It is imperative for all future understanding of chemistry that they understand that molecules are 3D things, they have a spatial requirement and a 3D shape that may change when the molecule reacts with something.*

Perhaps the strongest statement about what is fundamental to understanding chemistry came from an inorganic chemist:

> *... that's the underpinning of all chemistry. If you don't understand how atoms bond together, you can't do chemistry, or you can't understand chemistry ... chemistry is all about electrons and electron configuration, and you can forget everything else, it's just what's your electron configuration? How does that atom attain more stable electron configuration? And that's chemistry.*

The expert teachers gave examples of advice they wished they had received when starting out. For example, in terms of preparation: 'it's very important to be able to know what's coming, know what's gone behind and know what you're doing at the moment fits both ways'. During class time, perceptive comments were 'focus on what they're doing rather than what you're doing' and 'teaching through intuition is not good enough, and teaching the way you were taught is not good enough'. The value of experience is shown by the quote: 'it's taken me a little while to realise is that the students weren't understanding what the question was'.

Finally, to help combat what Bucat has called 'professional amnesia', a metareview of all outcomes of federally funded chemistry education projects in Australia over the past 20 years was completed. The outcomes from the 22 grants for which information was available form a major source of PCK and TSPK (topic specific professional knowledge), and

Steps to transform your teaching

1 **Know your students**
Find out who they are and be willing to adjust to their needs: students in tertiary classes are usually more diverse than you assume. Question the students – a show of hands gives you quick feedback.

2 **Prepare**
Quarantine 20–30 minutes before you teach to think about what you are aiming for students to learn in your class that day and how you will know whether they have understood you. Plan the strategies that you will use to address important concepts.

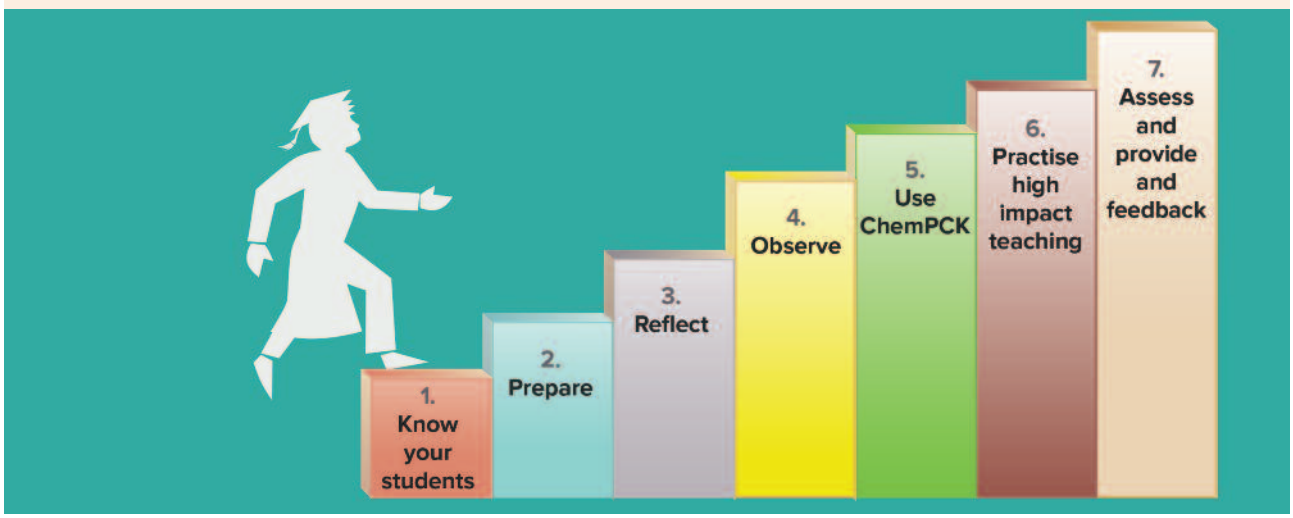
3 **Reflect**
Reflect on what you did after each teaching experience and make a note of what you could adjust. Did you feel that you communicated the essential concepts effectively? Did students engage with the material and the teaching strategies that you used? How many students grasped the concepts?

4 **Observe your peers teaching and invite them to observe you**
Invite colleagues to observe you and to give you feedback on your teaching, and also ask whether you can observe their teaching.

5 **Use ChemPCK**
The website chemnet.edu.au/chem-pck contains teaching strategies and insights from a large number of tertiary chemistry teachers. You can search by topic that you are teaching to find specific strategies that have been successfully used by others.

6 **Practise high-impact teaching**
- Flipping: move the bulk of the new content into resources that students access before class time, such as readings, videos or screen casts.
- Peer teaching (with or without flipping): during class, have the students work in small groups to discuss stimulus material or problem solve.

7 **Assess student learning and provide feedback**
Assessment informs teachers of what their students know and can do, and this information is important when choosing teaching strategies.



the outputs provide additional resources relevant to this project's community. The review will be published in the *Australian Journal of Education in Chemistry* in 2016 and the collected resources are available on the website.

If you are interested in more detail on the project or would like to contribute a teaching strategy to the PCK website please email madeleine.schultz@qut.edu.au.

Madeleine Schultz MRACI CChem was a senior lecturer in chemistry at Queensland University of Technology until recently and is currently working at the European Molecular Biology Laboratory in Heidelberg, Germany, synthesising fluorescent dyes for live cell microscopy. Support for this project has been provided by the Australian Government Office for Learning and Teaching (SD14-3737). The views expressed in this project do not necessarily reflect the views of the Australian Government Office for Learning and Teaching.

New Fellows

Ian Eckhard graduated from Loughborough University with a BTech (1966) and a PhD (1969). After postdoctoral fellowships in Palo Alto, California (1970), University of Newcastle, Australia (1972), and University of Warwick, Coventry (1973), he returned to Australia and worked in the biochemistry department of Royal Prince Alfred Hospital for 10 years. While there, he set up the first benchtop gas chromatograph–mass spectrometer imported into Australia, where it was used for drug screening and quantitative drug analyses.

In 1985, Eckhard joined Australian Analytical Laboratories as chief chemist and operated a variety of analytical equipment used in environmental, pharmaceutical, food and trade waste industries. In 1995, soon after the company was taken over by Amdel, he left to join Australian Environmental Laboratories to advise management on strategies and equipment requirements to keep the company at the forefront on environmental analysis.

In 1998, Eckhard joined the Australian Government Analytical Laboratories as Manager and Principal Residue Chemist in Organic Residues with responsibility for managing various major environmental projects. There he assisted in setting up the dioxin analysis facility since at that time there were no facilities for measuring dioxin levels in the environment in Australia. For this he was awarded an Australia Day Medallion in 2003.

In 2003, together with three other ex-AGAL employees, Eckhard started Advanced Analytical Australia P/L and took the role of technical director. It was intended to set up the business for the analyses of organic and inorganic compounds that no other company were prepared to accomplish, rather than analyse routine environmental and food contaminants. The company grew successfully over the next 10 years and continues to occupy a niche market in the analytical industry.

Eckhard has been a NATA assessor for 15 years and a member of the New South Wales RACI Analytical and Environmental Group for 20 years.

Eckhard is married with two children and five grandchildren. He retired in February and was presented with his RACI Fellowship at his retirement dinner by Professor Roger Reid. He intends to travel both in Australia and overseas for long periods over the next few years.

Jonathan Morris is an organic/medicinal chemist based at the University of New South Wales, where he currently is an Associate Professor and the Deputy Dean of Graduate Research.

He was born in Perth but grew up in the Pilbara region of Western Australia. He received his BSc(Hons) (first class) from the University of Western Australia in 1990, then moved to the labs of Lew Mander at the RSC at the Australian National University. His PhD research focused on the total synthesis of rare gibberellins and he completed his PhD in 1994. From 1994 to 1996, he carried out postdoctoral research with Phil Magnus at the University of Texas at Austin. On the flight back to Australia, he interviewed for a lectureship at the University of Canterbury in New Zealand, which he was successful in securing. He worked at the University of Canterbury from 1997 to 2004, then moved to the University of Adelaide. In late 2009, he was recruited to the University of NSW as an Associate Professor to direct the new Bachelor of Medicinal Chemistry degree that had just been set up.

Morris has supervised 13 PhD students, three Masters students and numerous Honours students, with many of these now working in biomedical research and pharmaceutical companies. He was awarded the 2014 Vice Chancellors Award for Teaching Excellence.

Morris' research interests are in the broad areas of organic and medicinal chemistry. He is interested in utilising the power of synthetic organic chemistry to investigate biological problems. Much of his work is centred on the synthesis of biologically active natural products, with the goal of restoring access to these valuable materials so that further biological investigations can be initiated. In recent years, his group has focused on the development of inhibitors of the kinases that control alternative splicing as these kinases are implicated in many diseases. In 2013, his work on SRPK1 inhibitors led to the establishment of Exonate Ltd, which is a start-up company focused on the discovery and development of small molecule drugs that modulate alternative mRNA splicing to address diseases of high unmet medical need.

Morris has been very active in the RACI, especially since his return to Australia. He was Vice-President of the South Australian Branch of the RACI in 2004 and is currently the treasurer for two different Divisions: Organic Chemistry (since 2012) and Medicinal Chemistry and Chemical Biology (since 2013).

He is married to Joanna Drimatis, who is a musician. They have two daughters, Zoe (14) and Eva (7).

2015 Archibald D. Ollé Prize

The Archibald D. Ollé Prize is an annual national RACI award for a published treatise, paper or journal article on any topic of interest to the Institute. The award is administered by the New South Wales Branch. The 2015 Prize was awarded to Professor Stephen Pyne FRACI CChem, University of Wollongong, by Dr Joseph Bevitt (ANSTO), RACI NSW President, at the NSW Branch Presidents' Dinner and Awards Night on 7 April 2016. The award was for the book chapter 'The boronic acid Mannich reaction' (S.G. Pyne, M. Tang, *Organic reactions*, 2014, Wiley, vol. 83, Ch. 2, pp. 211–498).

The boronic acid Mannich reaction (or Petasis reaction) is a three-component coupling reaction involving boronic acids or boronate esters, carbonyl compounds and amines. This reaction is extremely versatile for preparing important chiral starting materials for the synthesis of molecules of biological interest, including chiral α-amino acids, 1,2-amino alcohols, 2-aminoalkyl phenols, heterocycles and alkaloids. This chapter addresses the mechanism, stereochemistry and scope and limitations of each of the three components of this reaction. Some typical experimental conditions are provided along with a comprehensive tabular survey.

RACI Board elections

Nominations are open for the following positions on the RACI Board.

- President elect
- Treasurer
- Ordinary board member

Forms are available at www.raci.org.au/theraci/corporate-governance/board-elections-2016

Nominations close 20 August and elections will be held the first week in October.

Successful women ceramic and glass scientists and engineers: 100 inspirational profiles

Madsen L.D., Wiley, 2016, hardback, ISBN 9781118733608, 640 pp., $92.95

Successful women ceramic and glass scientists and engineers presents the profiles of 100 female professionals, some of whom were pioneers in the ceramics industry. These profiles feature current and retired university researchers, professors and industry contributors to the glass and ceramics community. The author, Dr Lynnette Madsen, is herself an industry professional working as a consultant and for the US National Science Foundation. She describes her intentions of compiling the book as multifaceted – 'for the reader to find someone in this book who reflects who they are and where they want to go' – and to recognise the contribution of women to the industry as a whole. The book is also designed as a resource for future collaboration and networking by listing personal contact details for each profile.

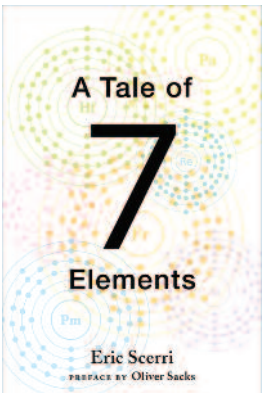
The individual profile format (while relatively simple) provides the best of both worlds with a detailed professional biography and a selection of personal remarks. Each professional biography provides details such as education and career history, awards received and details of publications. Many of the profiled women were awarded multiple degrees in their field, and held positions in some of the most recognised scientific organisations in the world (including NASA, MIT, Cambridge University and UNESCO). Nonetheless, the book's highlights are the personal reflections of the women featured. Their responses to 'Challenges', 'On being a woman in this field', 'Words of wisdom' and 'Proudest career moment' are each incredibly honest, unique and inspirational. Thus from Lisa Klein: 'What has helped me over the years is the idea that we are all in it together. And if we stick together, everyone will move forward ...'

One of the drawbacks of the book is its limited indexing, and while there is a 'quick guide', it does not provide a clear way to navigate the entire group of profiles. Most of the women featured are from Europe and the US, although there are a number of Australian-born women featured including Sylvia Marian Johnson (NASA), Rachel Caruso (University of Melbourne) and Cathy Patricia Foley (CSIRO, NSW). A number of other women feature who participate in Australian research and industry, but they are from home countries other than Australia.

There are a number of applications for the enormous amount of information contained in this book – among them taking inspiration from the personal remarks. The women featured in the book provide an opportunity to see a modelled career path, to select contributors to professional events and to make personal contact if preferred. *Successful women ceramic and glass scientists and engineers* provides an opportunity to recognise the contributions of female scientists and engineers. It also provides an avenue to ensure that the contributions of women continue to be recognised in scientific research and in the ceramics and glass industry.

Samantha Profke MRACI

A tale of seven elements



Scerri E., OUP, 2013, hardback, ISBN 9780195391312, 270 pp., $20.95

Chemistry is about understanding our physical world, how and why things are as they are and why they behave as they do. However, it is also very much a science of prediction, of anticipation of what is likely, or unlikely, to occur in any set of defined, sometimes imagined, circumstances. Assuredly, one of the most significant milestones in the long history of chemistry was the invention of that great unifying and classifying tool, now something of a scientific icon, the periodic table.

The periodic table emerged as a somewhat rough draft, which has undergone a lot of amendment and adapting on the way to becoming the form now familiar to us. For sure, there is plenty of argy-bargy and numerous tales of jealousy, nationalism, racism, bitter disputes, obfuscation, chicanery and downright dishonesty to be found in the story of the modern periodic table's emergence. In my view, we try too hard to hide the essential humanity of our great chemistry forbears behind the gloss of their glorious achievement. They were real people, with all the same strengths, weaknesses and foibles as the rest of us. Surely, this has to be inspirational! For my money, 'warts and all' is best.

Eric Scerri, probably the best historical analyst of the periodic table, wrote *The periodic table: its story and its significance* (OUP, 2007). Everybody ought to read it. Plenty of 'warts and all' and jolly interesting too. *A tale of seven elements* is, if you like, a worthy appendix to his earlier work, insofar as it is a detailed exploration of the discovery of the last seven elements, which existed as gaps in the 92-element periodic table about the beginning of the 20th century. These seven elements, in order of their discovery, were 91-protactinium, 72-hafnium, 75-rhenium, 43-technetium, 87-francium, 85-astatine and 61-promethium. The time span covered is 1917 (^{91}Pa) to 1947 (^{61}Pm), part way through World War I until after World War II. Unless you have a photographic memory, at this stage you might find it helpful to grab a copy of the periodic table and see just where these elements fit in.

Bear in mind that Mendeleev published his version of the periodic table in 1869, although his underlying premise was not quite right (by a long shot). However, it was a pretty

groundbreaking effort, and, equally, the credit might well have gone to a German (Meyer). There are tinges of nationalism here in ascribing credit. All of this was accompanied by a huge explosion of knowledge about atomic and subatomic structures from about 1900. You can see how geopolitics and science get entangled. Scerri devotes several chapters to elaborating on these themes, in addition to his seven elements.

The chemical research leading to the discovery of the seven 'unknowns' makes great reading and highlights some of the serendipity of chemistry. Things don't always go to plan and there are many instances of lucky discoveries on record. I guess the real skill is to recognise your discovery, before you say 'Oh! @@##!!!' There are also wrong turns and missed opportunities in every chemist's career. This happened along the way to discovery of these seven elements: sometimes people got lucky; sometimes they just got it wrong; sometimes the cards just didn't fall right. Science at its best is altruistic and everything noble and exalted, but it is not always like that. There are bitter disputes, disputed and spurious claims, and plenty of rancour, hatred, detestation and nationalism littering the glorious history of chemistry. If you don't believe me, then read this book to find some excellent examples.

I really enjoyed reading this book. It is a well written, interesting, informative and thoroughly fascinating account of how our central guiding tenet, the periodic table, came to its full fruition. It taught me a lot in a painless way. You can read it on the bus; you can read it on the train; or, like me, you can read it in bed at night. The chapters are short and more-or-less self-contained. Read it! You'll love it.

The chemical research leading to the discovery of the seven 'unknowns' makes great reading and highlights some of the serendipity of chemistry.

R. John Casey FRACI CChem


iStockphoto/Jirkab

Drones, droids and robots

The Australian Government's 'National Innovation and Science Agenda' is hosting the schools theme of 'Drones, Droids and Robots' as part of National Science Week this month. The aim of this theme is to 'embrace [in schools] … real-world application of autonomous technologies in areas including agriculture, mining, manufacturing, medicine and space and deep ocean exploration'.

A robot is pretty much any device that automatically performs physical tasks, sometime repetitively. The border between machines and robots can be quite fuzzy, but we can say this: all robots are machines but not all machines are robots. Generally speaking, robots include very high levels of computer control and many sensors, and, in some form or another, they often replicate one or more human functions.

Consider a welding robot in an automotive manufacturing facility. It looks very much like a large and quite intimidating human arm, performing similar functions to a human arm but with much greater speed, higher accuracy and precision, lower overall costs and virtually no occupational health and safety risks.

Droids are a subset of robots – those that are mobile and that often have a humanoid form. Until recently, droids only existed in science fiction books and movies, but they have now become a reality as technology has allowed the production of autonomous droids for all sorts of functions. These include soccer-playing droids created for the Robocup competition and household 'butler' droids that have popped up on crowd-sourcing funding sites.

At a tradeshow in China, I noticed a little droid running around one of the neighbouring booths. It combined the functions of vacuuming and drink delivery. The novelty value of such an oddity probably outweighed the risks of people tripping over it.

The autonomy of real-life droids sometimes requires a form of 'artificial intelligence' to provide functionality. Today this artificial intelligence is usually developed within extremely limited physical environments (such as a soccer pitch) and is really just binary software code that is able to make 'decisions' in most possible scenarios within such a closed physical environment.

Certainly no machine, droid or otherwise, has completely passed the Turing test in an *open environment*. The Turing test requires that a machine can fool a human into 'perceiving' that the machine is a human. Indeed, in order to pass this test in an open environment a machine would probably require, in addition to artificial intelligence, both artificial sentience and artificial consciousness; we are a long way off developing such a machine.

A drone is very different from a robot or droid. It is a vessel guided by humans using remote control. The ready availability of cheap technologies for wireless communications and high-density electric battery storage, usually containing lithium, has allowed for the introduction of low-cost flying drones (unmanned aerial vehicles or UAVs), which have captured the imagination of many large businesses, hobbyists and small business entrepreneurs. In addition to UAVs, there are many ground vehicles and water-borne vehicles that are also drones.


iStockphoto/Marco Maccolini

Lithium polymer batteries use lithium ion chemistries but have polymer separators that effectively reduce energy capacities compared to lithium ion batteries but permit higher discharge rates. Lithium polymer batteries can have a flat pack configuration as compared to the cylindrical shape of lithium ion batteries. This ease of packaging combined with higher discharge rates has resulted in a situation where most UAVs are powered by lithium polymer batteries.

The future for robots is a given. They have been with us for decades and will continue to get more sophisticated, especially in the manufacturing sector where ever-increasing productivity requires the removal of labour from factories. A similar trend is also occurring in the agricultural and mining sectors, where labour is seen as an inhibitor to cost reductions and productivity gains. This trend is underpinned by the fact that robot technology is steadily becoming cheaper and more sophisticated.

Of more interest in the near term is how the specific categories of drones and droids will evolve. Drones and droids, in their modern context, have only just emerged from high-tech laboratories as cost-effective technologies that are available for real-world applications. Previously, costs were so high that

In some cases, UAVs (unmanned aerial vehicles) are replacing what was formerly ground-based commerce, such as high-value cargo transport. In other cases, such as cinematography, drones are allowing video filming of what was previously not possible to capture.

these technologies were limited to very high-value niche applications.

In terms of commercial deployment, drones have gone through a massive non-linear uptake in consumption primarily driven by UAV applications. Droids, although threatening such a leap, have yet to take off in quite the same way.

For UAVs there are five interesting trends.

- The maximum flight time and distance of UAVs is slowly increasing as battery technologies improve.
- The payload of UAVs is slowly increasing with improved motors, better batteries and higher strength but still light chassis.
- Authorities are limiting the application of UAVs, for safety and privacy reasons, while at the same time exploring policies that will allow widespread commercial applications of UAVs.
- The cost of UAVs (per kilometre of flight or per kilogram of payload per kilometre of flight) is rapidly decreasing.
- Technology groups are developing autonomous flight systems, i.e. fly-by-GPS systems. Strictly speaking, when a UAV flies according to GPS settings, it is no longer a drone but more of a flying robot.

All of these trends are pointing towards multiple commercial applications of UAVs. In some cases, UAVs are replacing what was formerly ground-based commerce, such as high-value cargo transport. In other cases, such as cinematography, drones are allowing video filming of what was previously not possible to capture. Indeed, every time I talk to an entrepreneur working with UAVs, I discover a new and unexpected use of the technology.

Dow Chemical has recently used UAVs to inspect its chemical plants for issues such as cracks in pipes and tanks. Before it could do so, however, Dow had to apply to the US Federal Aviation Administration for approval to fly the UAVs over Dow's own property.

This is an area where government regulations can accelerate or hinder technology deployment. For large-scale commercial deployment of UAVs, it is critical that standards for flight path systems and guidance systems are developed. What is most needed is international standards in the area so that the same technology can be deployed globally and thus benefit from the greatest economies of scale. In English, this means that costs will come down quicker.

Standing in the way of such efforts is the fact that it may take years for different nations to collaborate on what is currently seen by many as just a nuisance to aviation. In the meantime, many technology groups are busily filing patents in the area, and these will further confound future efforts to standardise technologies in the UAV market.

Ian A. Maxwell (maxwell.comms@gmail.com) is a serial (and sometimes parallel) entrepreneur, venture capitalist and Adjunct Professor in Electrical and Computer Engineering at RMIT University and Visiting Professor in the Faculty of Engineering and Information Technology, UTS, who started out his career as a physical polymer chemist.

Patent strategy essentials

Dr John Landells, Partner and Registered Patent Attorney, FB Rice

The chemical sciences provide a competitive and commercially innovative technology area where, in many cases, patenting is critically important for commercialisation. The chemical sciences, in particular the chemical life sciences, is an area that often presents significant barriers to commercialisation, for example where there are high costs in developing an invention into a marketable product, or where chemical products can be easily and cost-effectively copied by competitors. Maintaining an invention as a confidential trade secret is a sensible option in some situations, such as for some industrial chemical processes. However, relying on confidentiality also carries risk, particularly with many organisations having a large number of transiting employees working in collaborating teams. Patenting can provide protection for an invention for up to 21 years in most countries, with confidentiality being maintained for the first 18 months.

Without patent protection for a chemical invention, it may be very difficult to attract investment necessary for commercial development. Seeking patent protection is often essential to establishing and building value in an organisation's research and development efforts.

A successful approach around patent protection involves more than simply the preparation, filing and grant of patent applications. Some patent strategy essentials are as follows.

- PATENT LANDSCAPE AND PRIOR ART REVIEW – maintain a regular understanding of the patent landscape and prior art in your technology area, particularly by identifying the closest documents from the point of view of identifying opportunities for patenting new inventions, and in understanding the extent of your freedom to commercialise your invention without infringing other patents.
- INVENTORSHIP/OWNERSHIP – carefully document all contributions from each individual involved in development of the invention and ensure ownership has been assigned in a written agreement by each of the individuals, preferably before they contribute.
- CONFIDENTIALITY – control disclosures to ensure confidentiality is maintained at least until a first (provisional) patent application is filed, and preferably until all applications (e.g. an international application) have been filed.
- WHEN TO FILE – filing your patent application early reduces the risk that another party researching in the same area will publish or file its own patent application before you do. However, this needs to be weighed against how far developed your own invention is (see below).
- WHAT TO FILE ON – the breadth of protection that a patent will provide depends on factors including the nature of the prior art and the data/research results provided to support the patent. In many cases, a patent application that contains more supporting data will allow for broader protection to be obtained. Broad patent filings based on little supporting data may have the undesired result of allowing only narrow protection to be obtained while at the same time creating prior art that is detrimental to possible future patent applications in the same research area. The right decision on how broadly to file will depend on the circumstances, but it should form part of your discussions with your patent attorney.
- PATENT PORTFOLIO REVIEW – carry out a regular review of your patent portfolio in view of changing commercial circumstances, including considering whether existing patents still cover the proposed commercial product and if so whether there are new opportunities for patent filings, balancing commercial importance against projected patent costs, particularly prior to time points where significant patent costs are incurred such as at national phase entry (30 months after first filing) and validation of a European patent.

For more information, email jlandells@fbrice.com.au.

Directly reduced iron technology: steel-making using gas

The production of steel from coal and iron ore by the blast-furnace route accounts for the major portion of the world's steel production of 1650 Mt/year. This route has good economies of scale and is now practised in facilities producing volumes of about 1 million tonnes of iron per year or more. Steel production is seen by many countries as a strategic necessity and for many countries (such as New Zealand) production of steel on this scale is not warranted. This develops the opportunity for smaller scale technologies, many of which are grouped as directly reduced iron (DRI).

DRI technology has been commercialised for over 100 years. In essence, there are two approaches, one uses coal and the other uses natural gas. Of the approximately 75 Mt/year of DRI produced, about 80% is produced from gas. The coal-based DRI technologies are generally all different, being developed to process particular ores and coals. In recent times new facilities have been built that use coal as coke oven gas or coal gasification to provide the reducing gas.

For gas-based technologies, a shaft-based system developed and promoted by the Midrex Corporation (www.midrex.com) has achieved a high level of take-up. In this process, iron ore lumps (>6.3 millimetres) are loaded into the top of the shaft-furnace and are reduced by an upward flowing stream of reducing gas, a mixture of hydrogen and carbon monoxide.

The reducing gas is produced in a steam reforming unit from the natural gas. Relative to other steam reformers that produce synthesis gas for ammonia or methanol production, reducing gas reformers operate at high temperatures and low pressures, which maximises hydrogen and carbon monoxide concentrations.

As the iron ore is reduced, water and carbon dioxide are produced, which could reverse the reaction if the concentration becomes too high. To prevent this, excess reducing gas is fed to the furnace and recycled after water and carbon dioxide have been removed. Reduced iron is separated from the ash. As produced, DRI is pyrophoric and is passivated by a briquetting process prior to shipment.

Because of the demand for lump ore for this technology (and its benefits to blast furnace operations), there is a significant price premium for lump ore over fines, typically 20%. Fines can be used but require pelletising at additional cost prior to use. Because of this price differential, there have been attempts to use iron ore fines in the direct reduction process.

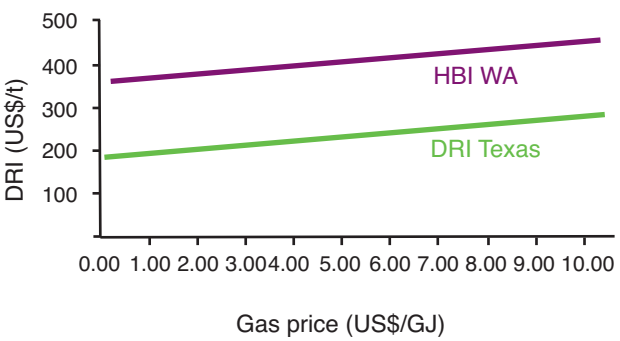
In the 1970s, Esso succeeded in the fine iron ore reduction (FIOR) process on a semicommercial plant in Texas. The technology required the fines to be fluidised in an ascending stream of reducing gas. Four sequential reactors were required with fresh ore charge to the first reactor and passing progressively to other reactors, which completed the reduction process. However, attempts to transfer the technology at full scale to ore reduction in the Orinoco region of Venezuela failed because the ore used, on partial reduction, became sticky and aggregated and clogged the reactors.

The technology was improved by Voestalpine (an Austrian steel conglomerate), who managed to get the technology to work and marketed this as the FINMET process.

In the late 1980s, BHP decided to use the FINMET process rather than the more proven Midrex process for a very large-scale DRI operation at Boodarie in Western Australia. This was known as the BHP HBI (hot briquetted iron) plant. It ran intermittently for several years but seems to have suffered from the same problems as the original Esso FIOR plant: sticky, partly reduced ore, which adversely impacted on production rates. A fatal accident at the site persuaded the company not to persevere with the process and the facility was closed in 2005.

Prior to steel making, the DRI is melted in an electric arc furnace, which separates impurities from the iron as a slag. Unlike the blast furnace, an electric arc furnace has limited ability to handle slag and this limits the level of impurities in the feed. The main feed competitor to DRI for electric arc

Rio Tinto HIsmelt facility. This high-intensity smelting facility was deconstructed in 2013. Liberty Industrial



Comparison of DRI production costs in Western Australia and Texas.

BHP's hot-briquetted iron facility. The facility was demolished in 2011.

Liberty Industrial

furnace operations is scrap steel for which there is a large and extensive international market – especially good-quality scrap containing few tramp metals produced by the scrapping of ships, particularly the oil tanker fleet, which has a high turnover rate.

Despite BHP's experience, the large reserves of natural gas and iron ore in Western Australia will always attract DRI type operations. The graph illustrates some of the key economic issues for the cost of DRI production. The graph plots the production costs for an HBI operation in Western Australia and a conventional DRI facility in Texas against the prevailing gas price. The salient data are given in the table for the two facilities of similar scale. The HBI data have been escalated from published BHP SEC filings (capital cost $A2.6 billion in 1999) and the Texas DRI from Midrex/Voestalpine publications for an export DRI operation based near Corpus Christie. This has just been completed. For comparison the cost of good quality scrap (US market, May 2016) is $250/t.

Data for DRI operations

	DRI Texas	HBI WA
Capacity (kt/year)	2000	2000
Capital (late 2015) (US$ million)	770	2875
Iron ore (type)	Lump	Fines
Iron ore pricing basis*	FOB fines + 20%	Run on mine cost
Iron ore price (US$/t)	66	35
Gas usage (PJ/year)	19.7	19.7

FOB, free on board. (FOB fines = US$55/t)

The main difference clearly evident is that despite low gas prices (<US$5/GJ) and lower iron ore cost (run of the mine cost), the very high capital cost for operations in Australia makes DRI production in Australia non-viable. This is in contrast to the US Gulf area where both low capital costs and low gas costs (typically $3/GJ) can deliver DRI well below the cost of scrap. This makes export of DRI from the US to Europe viable.

DRI operations are of interest because of their relatively lower emissions of carbon dioxide. Other methods that have been tried include the CSIRO/Rio Tinto HIsmelt process, which reduced ore with powdered coal in a molten metal bath. This project has now been abandoned in Australia and the technology transferred to India for further development.

A fully 'renewable' route would be to use wood charcoal for the reduction. This has been practised in the past (prior to the coal age) and is still found in some countries, such as India. The problem is that blast furnaces are restricted in size and require enormous quantities of biomass (wood) for the operation.

Duncan Seddon FRACI CChem is a consultant to coal, oil, gas and chemicals industries specialising in adding value to natural resources.

National Science Week: taking STEM education out of the classroom

National Science Week is an annual celebration of science and technology at all levels and in all areas of education, but especially through non-formal and informal education as outreach events by the CSIRO, the RACI, museums, Scouts, Guides and other community groups. This year, National Science Week will be held during 13–21 August. Its popularity has increased over the years – it has increased from seven days to nine, including two weekends, with some events being held in the weeks before and after the formal National Science Week.

One highlight of National Science Week 2016 will be a live stage show, *A Journey into Deep Space*, by English physicist and BBC presenter Professor Brian Cox. There will be approximately 1000 other events, all aiming to encourage an interest in scientific pursuits among the general public, and to encourage younger people to be fascinated by the world we live in. A few other examples will illustrate the scope of the events.

The ScienceWorks Museum in Melbourne is presenting *STEMania*. This is a series of theatrical sketches to create hilarious and fact-filled scenes that are based on STEM (science, technology, engineering and maths) themes. The scientific method will be applied to a cricket game, showing how science is all about asking and answering questions. An engineer, trying to design a new car, will solve complex problems through artistry, testing and the implementation of trial and error. There will also be sketches about technology and maths.

The Chemistry of Scouting is a collaboration between Scouts ACT and the Australian National University's Research School of Chemistry. Each participant will attend a talk by a scientist, have two hands-on laboratory sessions, watch a fire safety demonstration, make ice cream using liquid nitrogen and take part in water-testing, as well as seeing various hands-on displays.

Last year, more than 700 workplaces around the country registered to celebrate National Science Week by organising a Brain Break Morning Tea. There are no hard-and-fast rules for the Brain Break: there can be science-related quizzes, group activities or a few quick science demonstrations. Other ideas include science-themed foods such as molecular models made from lollies and toothpicks, cakes decorated with dinosaurs and biscuits in the shape of lab equipment.

The 2009 report *Learning Science in Informal Environments: People, Places, and Pursuits* by the National Research Council (USA), found that, by some estimates, individuals spend as little as 9% of their lives in schools, and that many often overlook or underestimate the potential for science learning in non-school settings, where people actually spend most of their time:

> Contrary to the pervasive idea that schools are responsible for addressing the scientific knowledge needs of society, the reality is that schools cannot act alone, and society must better understand and draw on the full range of science learning experiences to improve science education broadly.

Scouts Science Night, National Science Week 2015.

I have previously discussed the differences between formal, non-formal and informal education (see October 2014 issue, p. 33; December 2014 issue, p. 38). Learning science in non-formal and informal environments both complements and supplements formal science education, and education generally. In recent years, the *Journal of Chemical Education* has been publishing about one article per month on science outreach, science camps and public engagement.

One important aspect of National Science Week is that it takes STEM education out of the school classroom, where STEM experiences often seem divorced from the daily lives of young people. National Science Week and other out-of-school STEM activities can help young learners enhance and support their learning in other contexts.

See the National Science Week website (www.scienceweek.net.au) to find an event near you. Better still, why not run your own Brain Break Morning Tea or other event?

Kieran F. Lim (林百君) FRACI CChem (kieran.lim@deakin.edu.au) is an associate professor in the School of Life and Environmental Sciences at Deakin University.

Chardonnay or anything but

Chardonnay is an amazing grape cultivar that seems to thrive in most wine-growing regions throughout the world. In Australia, the success of Chardonnay was the driving force for our export markets to the UK and Europe. Our ability in Australia to blend across regions and to use oak and especially oak chips when they were not approved for use in Europe gave rise to wines that were seen by consumers as consistent in style and full of flavour. Jacob's Creek Chardonnay is a classic example.

One consequence of the Chardonnay success ('Chardonnay mania' it was sometimes called) was that many consumers had difficulty in differentiating between a wine made from the Chardonnay grape and wine in general. In a winery where I worked on occasions, a group of customers came to the cellar door, asking to try the white Chardonnay. When advised that this wine was not made at the winery, they then asked to try the red Chardonnay. In a survey of UK consumers, Chardonnay was listed as a wine region in Australia, along with the Barossa Valley and Hunter Valley.

The success of Chardonnay led to a surge in plantings in Australia and other new world wine countries, especially New Zealand and the US (California). In Australia, there are more than 25 000 hectares planted to Chardonnay or 17% of total plantings; in California, plantings are more than 38 000 hectares or 20% of total vines; whereas Argentina has under 7000 hectares (3%). Plantings in France are more than 47 000 hectares, which is only 6% of total grapevine plantings.

It is perhaps in the Burgundian region of France that the expression of the Chardonnay character reaches its peak. This region is often regarded as the homeland of Chardonnay. There is even the village of Chardonnay and the local tourism industry can effectively piggy-back on the name. However, it is the region around Montrachet in Burgundy that produces some of the spectacular and certainly the most expensive wines from this cultivar. For example, in a list of the five most expensive white wines, four of the five came from Burgundy (see bit.ly/1TDxaig).

The craze in purchasing high-priced Montrachet led *Forbes Magazine* in 1996 to run a divorce settlement carton (see image) with the caption 'She gets to keep the chalet and the Rolls, I want the Montrachet'. Montrachet even rates a mention in the movie *Hopscotch*, in which Glenda Jackson responds to

It is perhaps in the Burgundian region of France that the expression of the Chardonnay character reaches its peak. This region is often regarded as the homeland of Chardonnay.

winefolly.com/update/24-funny-wine-quotes/CC BY-NC-SA 3.0

Walter Matthau's suggestion of gin and ginger ale for her by saying 'Mine was *never* gin and ginger ale. Montrachet '69, right next to the beer'.

The other region of France where Chardonnay comes to the fore is Chablis. This cool climate region produces wines of marked acidity that allows good fruit expression and a steely or gunflint character on the palate. The use of new oak tends to be minimal, which allows better expression of fruit characters.

Chardonnay is grown in most regions in Australia. During my time at Charles Sturt University, I had the opportunity to explore Chardonnay wines made from grapes grown on irrigated vines in warm to hot conditions. While acid adjustment was always necessary, careful vineyard management and winemaking produced wines of character at a price that suited many consumers. The cooler climate regions such as Margaret River, Adelaide Hills, Tasmania and the Yarra Valley produce Chardonnay wines of distinctive character. Acid adjustment is still required because we do not seem to be able to reach the acidity levels that are common in Chablis, for example.

The success of Chardonnay, especially the big, fruity, over-oaked styles, led some wine consumers to seek ABC wines (Anything but Chardonnay; bit.ly/1WQ1hsn). But these ABC days would seem to be well and truly over, as discussed by Michael Austin recently in the *Chicago Tribune* (http://trib.in/1sdUIn4). Perhaps part of the reason for the swing back to Chardonnay is better knowledge of the impact of grape-growing and winemaking on the characters of the wine. This is where chemistry comes to the forefront! Joanna Gambetta and co-authors from the University of Adelaide have reviewed the science behind the aroma composition as influenced by production techniques (*J. Agric. Food Chem.* 2014, vol. 62, pp. 6512–34). I shall look at these findings in my next column.

Geoffrey R. Scollary FRACI CChem (scollary@unimelb.edu.au) was the foundation professor of oenology at Charles Sturt University and foundation director of the National Wine and Grape Industry Centre. He continues his wine research at the University of Melbourne and Charles Sturt University.

The gentle art of quitting

I have come to realise that I am good at something that may not at first appear to be a particularly desirable talent: I'm a good quitter. It's a weird thing to be proud of, I know, especially in a society that seems to emphasise 'sticking with it' and 'being in it for the long haul'. But I've actually found quitting isn't necessarily a bad thing and sticking with it isn't necessarily a good one.

How often have you found yourself with a job, responsibility, relationship or living situation that isn't working out for you? And how often have you stuck it out out of a sense of obligation, duty or fear of being in a worse situation than if you quit? I'm sure each of us could think of at least one job, apartment lease or relationship that has gone on too long. Wouldn't we have been better off if we just quit?

So if quitting is often a necessity of life, doesn't it make sense to be good at it? The thing is, most people have so little experience with quitting that they have little opportunity to perfect this (in my opinion) essential skill.

I am not advocating wanton abandonment of all responsibility. No, there are some things that are worth resisting the urge to head out the door when the going gets tough. But some just aren't.

Let me give you an example. I recently quit a job. This was particularly difficult to do because it was my first job in a new country and marked the culmination of a long and painful job search (six months). But it was clear to me, from the first day, that I was going to be unhappy in the job. The work culture wasn't one that resonated with my values and I found the tasks to be far less demanding than I was anticipating. So on day 5, I walked up to my boss and let her know that I was quitting.

This was pretty brave, given that I was staring down the barrel of further unemployment with no end in sight, but I decided that the opportunity cost of sticking it out was too high. Every minute I spent at this job was one I didn't spend looking for another. And so I quit and I was unemployed again. And two weeks later I was interviewing for a job with tremendous potential and one I was really excited about. It was a great interview and I made it to the final round of selection and only missed out because there was an excellent internal candidate.

So did I do the right thing by quitting? Especially given that I sit here typing this as an unemployed scientist? Absolutely! I had a shot at a perfect job, which I would not have got if I was in the other job. I had a great interview experience and impressed a potential employer who I am still in contact with. None of this would have happened if I hadn't quit and released the bird in my hand to chase the nicer one in the bush.

Since I consider myself so good at quitting, here are three small bits of advice to all the bashful quitters.

- Be honest. I told my employer exactly why the job wasn't working out. I explained that I didn't want to be anything less than an excellent employee and I would prefer they had a candidate in the role who truly appreciated it.

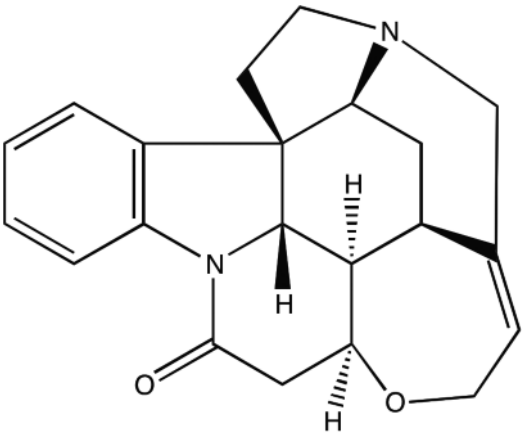
iStockphoto/Ximagination

- Be professional. I let my boss know that I would stick around as long as possible to ease the transition for the new person. She actually asked me to stay a couple of weeks longer, which I thought was worth it to not sour a relationship. I've heard of people giving two weeks notice and then taking two weeks of personal leave – not really all that classy.
- Be diligent. I worked just as hard on my last day as on my first. I was fast friends with all my co-workers and they were sad to see me leave even though we'd only known each other for a short time. This is really important to me since the last thing I want is to give people a bad impression as I walk out the door.

So there you have it. My three little steps to being a better quitter. I encourage you to try it with something small first and see if you like it. If you don't, well … you can always quit quitting.

The author is trying to break into the corporate world in Portland, Oregon. It is a long-term goal and he isn't about to quit. Yet.

Chakravarti and the strychnine story



Strychnine

R.N. (Ram Narayan) Chakravarti (1916–2007) was an Indian chemist who spent two years in the late 1940s working on the structure of the alkaloid strychnine at Oxford with Sir Robert Robinson. Chakravarti returned to India and worked at the Calcutta School of Tropical Medicine before becoming Director of the Indian Institute of Experimental Medicine. Robinson visited him when he was at the Indian Science Congress in 1950 but they failed to meet up when Robinson spent a few days in Delhi in 1960 on his way to the IUPAC Natural Products Congress in Australia. However, both were great letter writers and they exchanged more than 200 letters over three decades.

In 1986, on the centenary of Robinson's birth, Chakravarti published a long article about his work at Oxford, concentrating on unpublished results and the discussions he had with Robinson. In those days before the widespread adoption of spectroscopic methods, structure determination of natural products proceeded by stepwise degradation. A key step, in this case, was the conversion of strychnine into *neo*strychine. There were several known methods for effecting this change but none gave a good yield, the best, 15%, being achieved by boiling a solution of strychnine with selenium. In Chakravarti's hands the yield was improved to 50% but the smell of hydrogen selenide militated against widespread adoption of the method. Driven to discover a new procedure, Chakravarti found that a quantitative yield could be obtained by boiling a solution of strychnine in xylene with finely divided Raney nickel. Others in the lab were unable to reproduce his success.

*Neo*strychine is an isomer of strychnine, and is formed by the shift of a double bond in the bridged ring structure, something that would have been hard to characterise by the methods then available to organic chemists. Chakravarti described the change as 'hydrogenation *cum* dehydrogenation' and I suppose that's a good summary of the change that has taken place, essentially a 1,3-shift of a hydrogen atom. Elemental selenium had long been used, just as elemental sulfur was, to effect dehydrogenations and it was probably used with strychnine in an attempt to reveal (as an aromatic ring system) the carbon skeleton of the alkaloid. It's hard to see how selenium could have produced the observed isomerisation, but since the yield was so low, and other products were not identified, I should put the reaction in the anything-can-happen basket. On the other hand, Raney nickel is a hydrogenation catalyst and since the finely divided metal is a hydrogen-carrier, it's a bit easier to see how it might produce the change.

The failures in the hands of other competent chemists were due, according to Chakravarti, to their not exactly following the method he had devised and communicated to them. First, the Raney nickel had to be freshly prepared and well washed with alcohol, and the last traces of alcohol and water had to be removed by azeotropic distillation of a small portion of the xylene. Second, the Raney nickel had to be kept in suspension and this was achieved by allowing the solution to 'bump' as the mixture at the bottom of the flask became superheated during the boiling process. Bumping was normally avoided, but it was a good way to stir up the heavy metal powder. The flask, condenser, sand-bath and support stand needed to be robust and well supported to avoid accidents.

Three of the failures were explained in detail. K.H. Pausacker, an Australian postgraduate student, 'had a fire, due to which a fume-chamber was burnt, because he did not fix the sand-bath with the tripod stand he used. He went out with his wife for dinner and on coming back at night he saw the fire'. Professor D.S. Tarbell, a visitor from the University of Rochester, New York, 'for avoiding the bumping … heated the flask immersed in an electrically heated oil-bath. There was, no doubt, very smooth boiling and no bumping, but the catalyst remained practically as a hard cement-like sediment at the bottom of the flask'. Conversion was poor and although there were no by-products, the difficulty of separating strychnine and *neo*strychine was a complicating factor. Third, South African A.M. Stephen failed because his Raney nickel catalyst was no good. Following a published method that began with 300 grams of the Raney Ni–Al alloy, Stephen reduced everything by a factor of 30 and set off with 10 grams. While proportionate reduction was appropriate for quantities such as solvent volume and amount of alkali, he was wrong to reduce the reaction time by a factor of 30 and to use three washings with distilled water instead of the recommended 30. 'I saw the white particles of scum actually floating on the catalyst prepared by him', wrote Chakrvarti, and 'his catalyst was not only coated with aluminium hydroxide but there was also presence of the hindering agent, sodium hydroxide, as a consequence of grossly incomplete washing'.

Needless to say, Robinson was delighted by all this but Chakravarti didn't make many friends.

Ian D. Rae FRACI CChem (idrae@unimelb.edu.au) is a veteran columnist, having begun his Letters in 1984. When he is not compiling columns, he writes on the history of chemistry and provides advice on chemical hazards and pollution.

events

NZIC-16
21–24 August 2016, Millennium Hotel, Queenstown, New Zealand
www.nzic16.org

Southern Highlands Conference on Heterocyclic Chemistry
28–30 August 2016, Peppers Manor House, Moss Vale, NSW
www.chemistry.unsw.edu.au/SHC16

6th International Meeting on Antimicrobial Peptides
1–3 September 2016
Leipzig, Germany
http://peptideconferences.org/imap-2016

European Symposium of Biochemical Engineering Sciences (ESBES)
11–14 September 2016, Dublin, Ireland
www.esbes2016.org

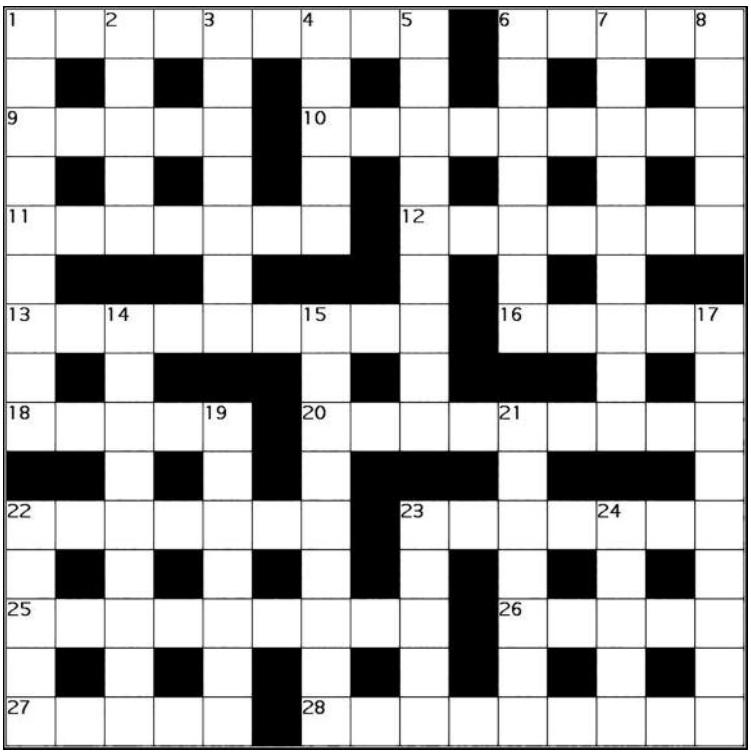
Chemeca 2016
25–28 September 2016, Adelaide Convention Centre, Adelaide, SA
www.chemeca2016.org

6th International Conference and Exhibition on Pharmaceutical Regulatory Affairs and IPR
29 September – 1 October 2016, Orlando, Florida, US
http://regulatoryaffairs.pharmaceuticalconferences.com

AusBiotech 2016
24–26 October 2016, Melbourne Convention Centre, Vic.
www.ausbiotechnc.org

RACI events are shown in blue.

cryptic chemistry



Across

1 Changes answers. (9)
6 Burn boron and not lift a finger. (5)
9 Test court case. (5)
10 Vein sites become painful. (9)
11 1 Down is one place where one feels comfortable. (7)
12 Dry house wrecked when final bottle lost but holds water. (7)
13 Hikes in wrinkles. (9)
16 Program is Par Matches. (5)
18 Digger sounds small. (5)
20 Chemistry phenomena adversely centred on naming errors. (9)
22 Relation 3719A32. (7)
23 Does NaI need to change nucleobase? (7)
25 Can Chairs work out $C_7H_5NO_3S$? (9)
26 Figured on making further comment. (5)
27 Controlled with lines. (5)
28 Expel cobalt and mendelevium making bound ligand and metal. (9)

Down

1 In honour of the Russian empire hum tune 77 badly. (9)
2 Bearing $-N_3$ and making a comeback in the work of Reed Izatt. (5)
3 Lone ute crashed compound. (7)
4 Beginning attack. (5)
5 Combination shy, sets in chaos. (9)
6 Accumulation of publicity. (5-2)
7 R_2NO^- ion a mixed bag. (9)
8 Neon in 4 Down and argon in 16 Across. (5)
14 A form contributing to the structure of six elements. (9)
15 In proportion to my crimes undermining loss of oxygen. (9)
17 Interrupted hanging. (9)
19 About painful hit. (7)
21 Lover 13 unlucky in general. (7)
22 Shining light on Spooner's seaman. (5)
23 Year in which roman numerals were first used. (5)
24 Order ratio. (5)

Graham Mulroney FRACI CChem is Emeritus Professor of Industry Education at RMIT University.
Solution available online at Other resources.

Connection between gas flaring and Arctic pollution

Researchers have suspected for several years that the flaring of waste natural gas from industrial oil and gas fields in the Northern Hemisphere could be a significant source of nitrogen dioxide and black carbon pollution in the Arctic. Research from a NASA-sponsored study lends new weight to that hypothesis.

Nitrogen dioxide is a well-known air pollutant that is central to the production of ground-level smog and ozone. It is closely associated with black carbon (also known as soot), which is an agent of global warming, particularly in the Arctic. In addition to absorbing sunlight while aloft, black carbon darkens snow when it settles on the surface. Both processes lead to heating of the air and the land surface, accelerating the melting of snow and ice.

The amount of black carbon that reaches the Arctic is poorly estimated, but scientists know that any soot could have a significant impact. 'The Arctic starts from a very clean state, as there are no significant local sources of dust or smoke pollution,' said Nickolay Krotkov, an atmospheric scientist at NASA's Goddard Space Flight Center and a member of a team examining the origins of Arctic black carbon. 'In this kind of pristine environment, even small anthropogenic sources make a big difference.'

Previous research has suggested that gas flares from oil and natural gas extraction near the Arctic could be a key source of black carbon. But since international inventories of industrial emissions have gaps in observations and in reporting, they often over- or under-estimate the amount of pollutants.

Gas flares are an often-overlooked subset in that already messy data set. Regional estimates from Russia, for example, suggest that gas flaring may account for 30% of all black carbon emissions. But with few monitoring stations near flaring sites, the scientific community has had great difficulty getting accurate estimates of emissions.

Can Li and other researchers at NASA Goddard were recently asked by atmospheric modellers to see if they could provide flaring estimates based on satellite data. Black carbon levels in the atmosphere cannot be directly measured by satellites, but they can be derived indirectly. Black carbon is associated with nitrogen dioxide and with the total concentration of aerosol particles in the atmosphere. Nitrogen dioxide and black carbon particles are often produced at the same time when fossil fuels are burned.

The modellers were simulating the trajectories of pollution through the atmosphere based on existing, flawed emission inventories. And their results generally underestimated the amount of black carbon reaching the Arctic compared to what scientists in the field were measuring directly.

The first step for Li, Krotkov and colleagues was to find gas flares. They compiled 'night lights' data from the Visible Infrared Imaging Radiometer Suite on the Suomi NPP satellite (see back cover). They examined four known fossil fuel extraction sites: Bakken, North Dakota; Athabasca Oil Sands in Alberta, Canada; the North Sea near Great Britain and Norway; and western Siberia, Russia. The researchers pinpointed gas flares by excluding electric light from nearby towns and roads.

For each study site, Li and Krotkov analysed nitrogen dioxide data from the Ozone Monitoring Instrument aboard the Aura spacecraft. Fellow NASA researchers Andrew Sayer and Christina Hsu retrieved aerosol concentration data from the Moderate Resolution Imaging Spectroradiometer aboard NASA's Aqua satellite.

'We found a pretty good match-up between the gas flare signals from the night lights and the nitrogen dioxide retrievals for two regions – Bakken and the Canadian oil sands'

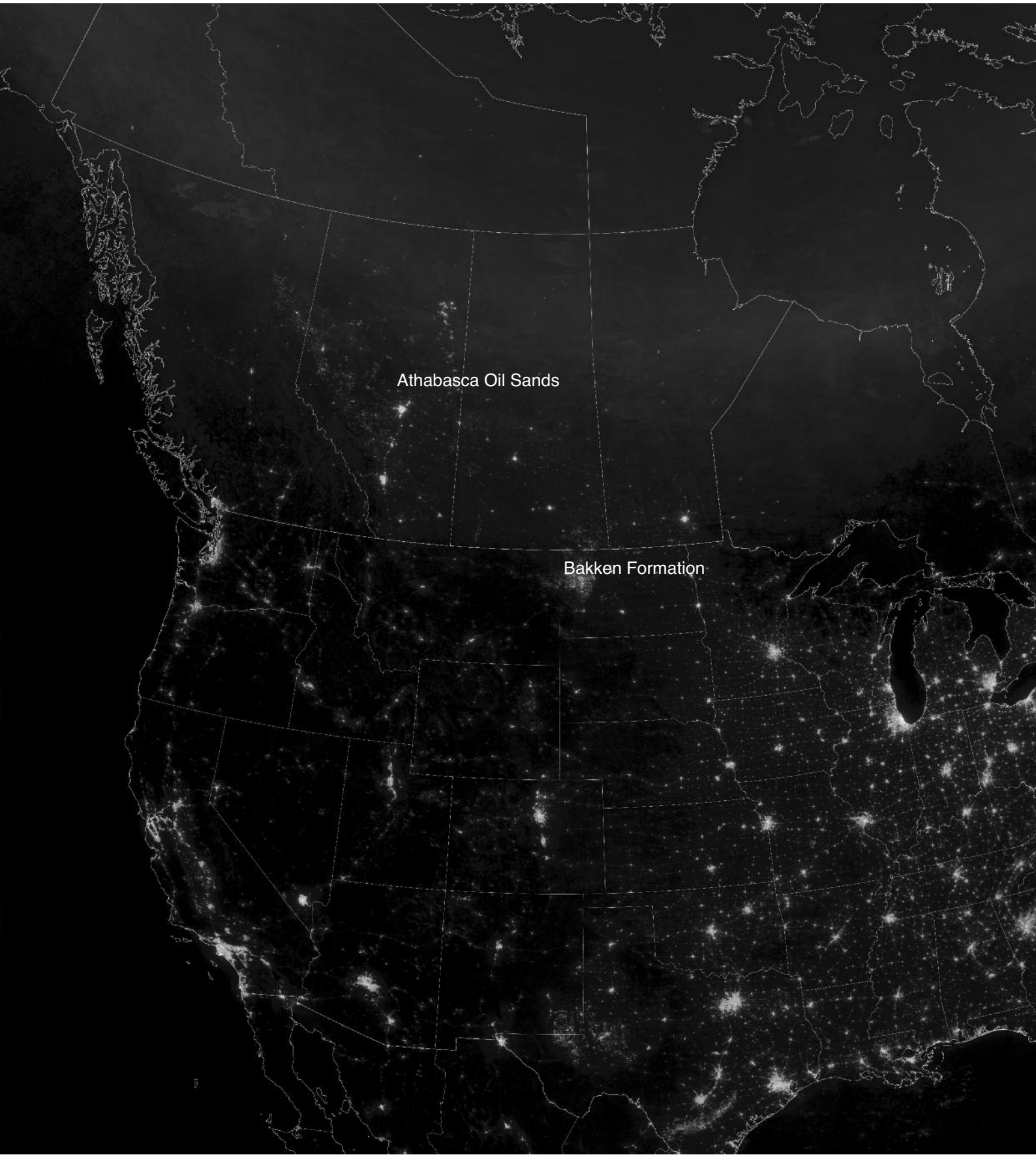
'We found a pretty good match-up between the gas flare signals from the night lights and the nitrogen dioxide retrievals for two regions – Bakken and the Canadian oil sands,' said Li. Every year from 2005 to 2015, the levels of atmospheric NO_2 rose about 1.5% per year at Bakken and about 2% per year at Athabasca. This means the concentration of black carbon produced by those flares was also likely on the rise.

The team saw a smaller rise in nitrogen dioxide in western Siberia, and no discernable flaring signal from well-established oil rigs in the North Sea. According to Li, the North Sea signal was likely obscured by the abundance of nitrogen dioxide pollution in Europe.

Aerosol data were less conclusive. Aerosols tend to linger in the atmosphere longer than nitrogen dioxide, making it more difficult to establish whether there was an increase due to oil field activities, as opposed to general background levels, Sayer said.

The new observational results fit well with modelling done by Joshua Fu, an atmospheric modeller at the University of Tennessee at Knoxville and a collaborator on the paper. When Fu and colleagues added the gas flare locations and estimated emissions into a model of chemical transport in the atmosphere, they were able to reproduce the amount of black carbon observed in the Arctic by ground stations and aircraft.

Visible Infrared Imaging Radiometer Suite day-night band (back cover) courtesy of the Suomi National Polar-orbiting Partnership (NPP) Earth Observation Group. Suomi NPP is the result of a partnership between NASA, the National Oceanic and Atmospheric Administration, and the Department of Defense. Text by Ellen Gray, NASA Earth Science News Team, with Mike Carlowicz.



'Night lights' data of fossil fuel extraction sites Athabasca Oil Sands (Canada) and Bakken Formation (US) from the Visible Infrared Imaging Radiometer Suite on the Suomi National Polar-orbiting Partnership (NPP) satellite (see page 43). Suomi NPP Earth Observation Group