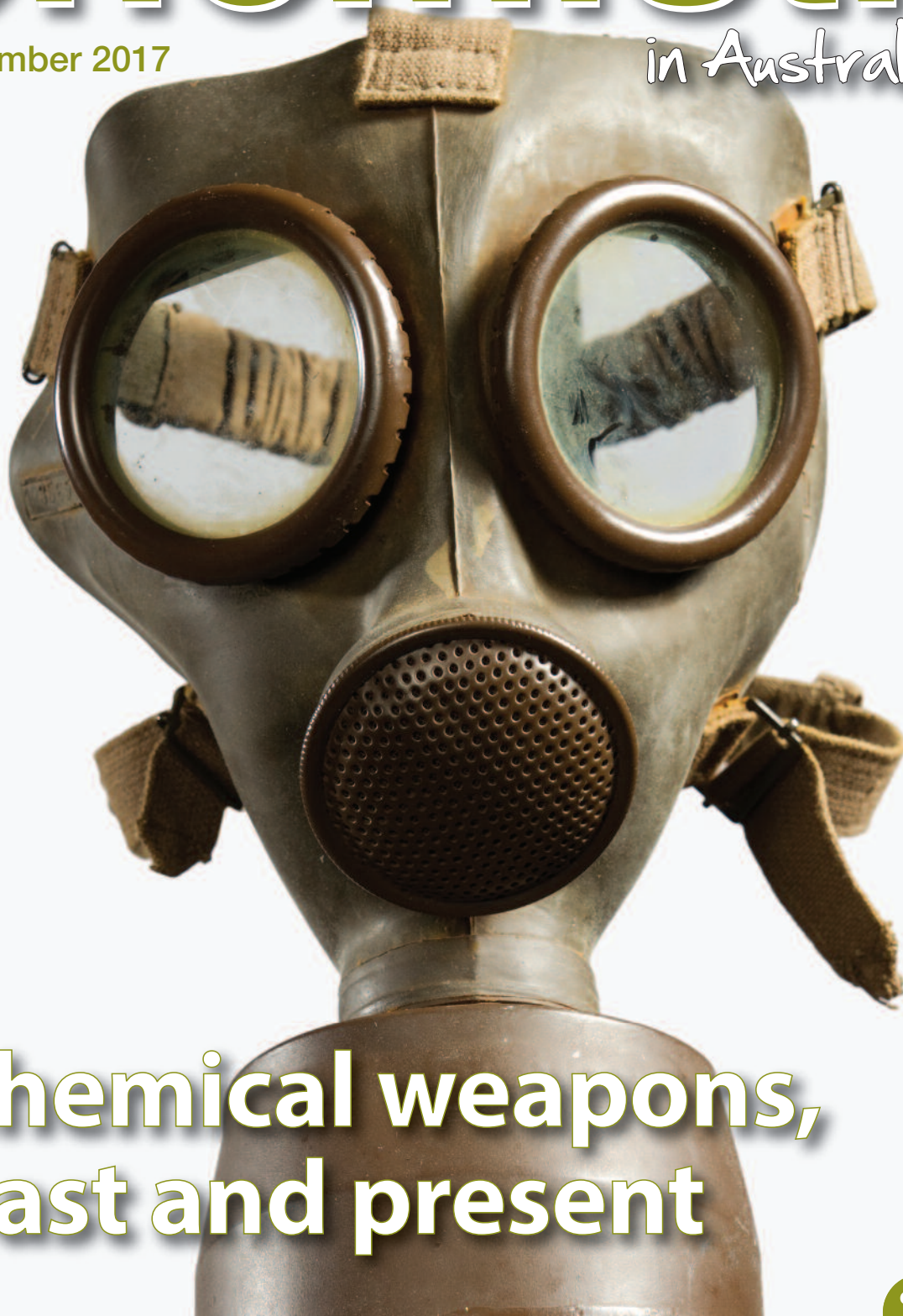


chemistry

September 2017

in Australia



Chemical weapons, past and present

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- Free software for chemists
- Rapid phenotyping in the field
- Diversity in the journal jungle

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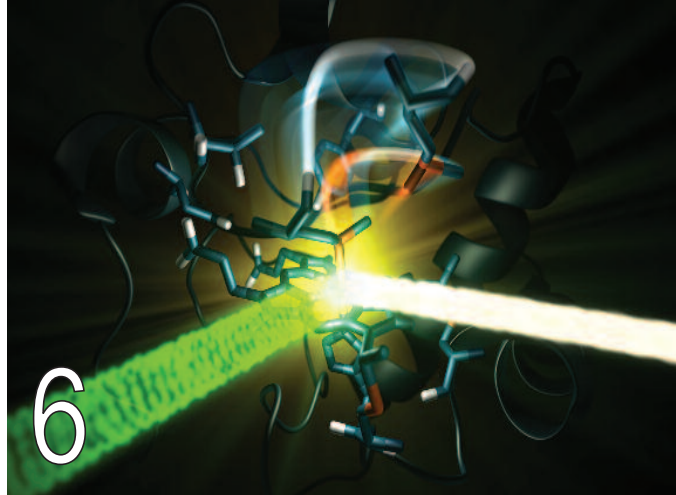
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cover story

From chlorine to sarin: chemical weapons, past and present

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Diversity in the journal jungle

As an editor, I consider reference lists as virtually everyday reading, and I'm fascinated by the variety and number of journals being published. The journal landscape can be a dangerous place, it seems, and George Koutsantonis's comments about 'predatory publishing', where publishers (sometimes of questionable reputation) are looking to increase their metrics and profit by signing up unsuspecting authors (July issue, p. 18), prompted me to revisit my ponderings.

Philosophical Transactions of the Royal Society, established in 1665 by the Royal Society, is the oldest scientific journal in the English-speaking world. More recently (a mere 210 years ago), it split into journals A and B, to accommodate physical and life sciences separately.

The Wiki list of journals – populated, at least partly, using the Chemical Abstracts Service tool – contains about 150 journals whose content is primarily regarded as being chemistry. I'm sure that most if not all of the predatory publishers don't make the cut, and some reputable chemistry journals are probably missing.

Clicking on a few journals at random, I learned that the mysteriously named *Talanta* is the *International Journal of Pure and Applied Analytical Chemistry* and that 'Tips on chips' is the delightfully named online resource associated with the miniaturisation journal *Lab on a Chip*.

According to a 2014 report by *Nature* ('The top 100 papers'), which used the Science Citation Index to gather its data, the most cited science research paper since 1900, with more than 305 000 citations, was published in 1951 and described a quantitative determination of protein in solution (Lowry O.H., Rosebrough N.J., Farr A.L., Randall R.J. *J. Biol. Chem.* 1951, vol. 193, pp. 265–75). *Nature* itself doesn't do too badly in the journal popularity stakes, with a gargantuan impact factor (over 40) and submissions of around 10 000 manuscripts each year (bit.ly/2tPg26W).

The diversity in medical publishing is truly extraordinary – I didn't have time to count the Wiki list. Looking at the titles, I felt that it would be quite sobering to read publications such as the *Morbidity and Mortality Weekly Report*. I know as a former proofreader of the *Australasian Journal of Dermatology* that many papers are not lunchtime reading material.

Relatively new among the medical journals is *Journal of Cachexia, Sarcopenia and Muscle*, which was established in 2010 and spawned two daughters, related to clinical reports and rapid communications, late last year. The research relates to changes in body composition, one of which is cachexia (wasting syndrome).

These journal metrics and statistics are dominated by English-language journals. Long gone are the days of Henry Oldenburg, first editor of *Phil. Trans. Roy. Soc.*, when science was spoken with colleagues in the native tongue and written in Latin. How much scientific knowledge gets lost in scholarly translation?

Ten years ago, University of Melbourne linguist Joe Lo Bianco described the danger of collapse in such discourse:

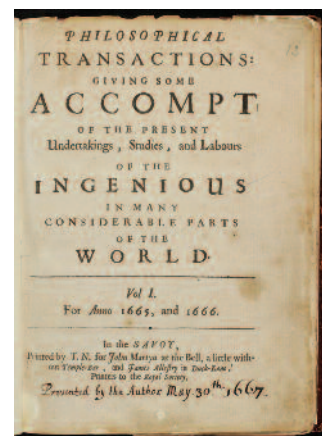
An example is Sweden's long-term acceptance of the use of English as the language of teaching in high level science and mathematics programs in its universities. However, when one of the consequences of this long-term use of English was exposed during the 1990s (the progressive deterioration of competence in Swedish in high level discourses, or domain collapse) the result was public alarm and agitation to bolster the position and security of Swedish as the national language with the full array of social and intellectual uses.

Bianco J.L. 'Language, place and learning', *Observatory Pascal*, 2007, p. 14.

Globalisation has been marvellous for science in many ways, but this 'collapse' seems to be one of its casualties. Sean Perera, currently a sessional academic at the ANU Centre for the Public Awareness of Science, has described the phenomenon, in the *International Journal of Science in Society*, as 'minimal room or no room at all ... allowed to communicators of other languages to participate in science in their own voice.' (bit.ly/2sN5aqp)



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Henry Oldenburg (Philosophical Transactions)/CC-BY4.0

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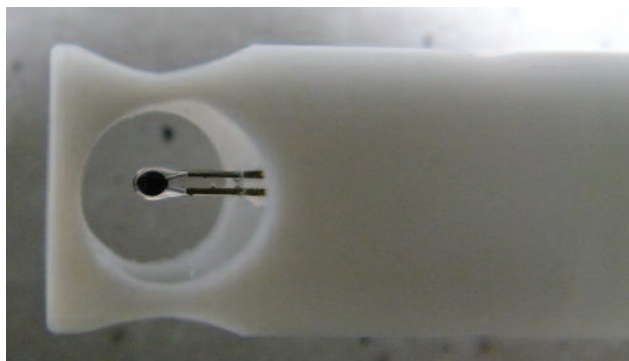
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From professional glassblowers ...



I thoroughly enjoyed Dave Sammut's engaging article 'A rare and declining craft' in the July issue (p. 26). I have always held scientific glassblowers in awe, especially as I could scarcely join two pieces of tubing together myself. My T-pieces were a source of derision.

I hold a special respect for those who work at the miniature end, especially when sealing sensors into probes. The Metroglas subsidiary of Metrohm AG solved a sealing problem with thermometric titration probes by sealing the glass-jacketed thermistor sensor into a glass-bodied probe without changing the sensing characteristics of the thermistor by excess heat. A photograph of the tip of the probe is shown here. The glass shaft encasing the leads from the thermistor is only 1 millimetre thick.

It is also worthwhile mentioning the Australian connection to glass sensor technology. The Queensland chemist and prodigious inventor John Petty, founder of electrochemical sensor company Ionode Pty Ltd, developed the first microprocessor-controlled machine to automatically produce both spherical and spear-shaped pH glass sensor membranes in the early 1980s. He also automated the production of the glass beads to make the sensor membranes, and developed his own glass formulas. This has allowed the production of high-quality pH probes at a reasonable price.

Thomas K. Smith FRACI CChem

... to amateur glassblowers

Dave Sammut continues to contribute interesting articles on a wide range of topics, and his July 2017 article (p. 26) about scientific glassblowing brought to mind a few notable memories before they disappear into the dim distant past. Professionally made soda-glass absorption tubes were chosen for reducing static gravimetric errors on microbalances and this material could be verified by rubbing on alumina with phenolphthalein, which turned pink.

For my degrees and postdoctoral work, vacuum rigs were constructed by the in-house professional glassblower. However, because thousands of sample tubes from both soda glass and double-thickness English Pyrex were needed for kinetic experiments, to save time and money, it was important to hone one's own skills and prepare these as required. Breakable soda glass components for solid catalysts were added inside the stronger Pyrex reaction tubes when needed. Another important item was a diamond-tipped pencil for numbering sample tubes, reopening samples and cutting glass as needed. Pushing hot softening glass tubing together before stretching allowed thicker walls in preconstrictions and this simplified sealing of tubes. Coordination of both hands when rotating hot glass took some time to master as did joins and T-pieces with uniform wall thickness.

Work involving liquids and gases needed freezing with liquid nitrogen before evacuating. However, for studies with methane gas, this still had a significant vapour pressure at -178°C , and required these breakseals to be made within the Pyrex glass reaction tube. More skill was needed for these because a B14 joint also had to be fused to the sample tube for later analysis.

Chemical analysis progressed from beakers and burettes in the 1960s to instrumental methods, automation and miniaturisation (e.g. flow injection analysis, capillary gas chromatography) and there have been similar developments in genetics. Nevertheless, manufacturing and preparative chemistry will always need large-scale glassware and/or appliances.

Ray Hodges FRACI CChem



My grandson's first pH experiment

Yesterday, I had my grandson of four years help with the red cabbage experiment (June issue, p. 36) and he loved the colours and their intensity as the ice blocks melted. Sadly, I did not have any lemons but they can wait for another day. Brilliant stuff, and so by the time I reach my 50 RACI years in 2019 he will, I hope, be full of exploring the chemistry and beauty of the natural world with me.

All the best to RACI and your centenary.

Ian D. MacLeod FRACI CChem

How a single chemical bond balances cells between life and death

Slight changes in the machinery of a cell determine whether it lives or begins the natural process of programmed cell death. In many forms of life – from bacteria to humans – this is determined by a single chemical bond in the protein cytochrome c. As long as the bond is intact, the protein transfers electrons needed to produce energy through respiration. When the bond breaks, the protein switches gear and triggers the breakdown of mitochondria, the structures that power the cell's activities.

For the first time, scientists have measured exactly how much energy cytochrome c puts into maintaining that bond in a state where it's strong enough to endure, but easy enough to break when the cell's life span is ending.

They used intense X-rays from two US facilities, the Linac Coherent Light Source (LCLS) X-ray free-electron laser and the Stanford Synchrotron Radiation Lightsource (SSRL) at the Department of

Energy's SLAC National Accelerator Laboratory. The collaboration, led by Edward Solomon, professor of chemistry at Stanford University and of photon science at SLAC, published their results in *Science* (<https://doi.org/10.1126/science.aam6203>).

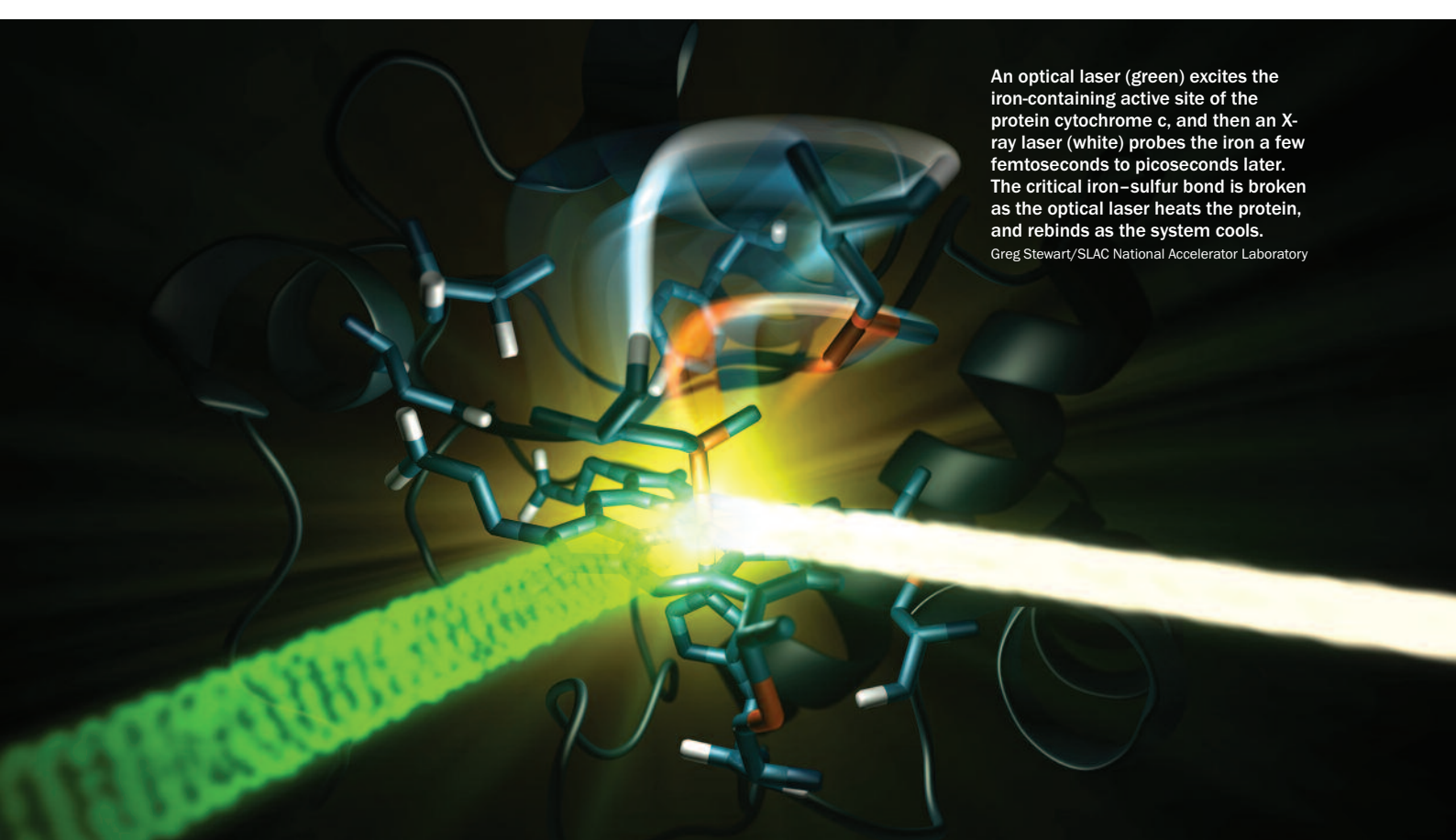
The study marks the first time that anyone has been able to experimentally quantify how the rigid structure of the cytochrome c molecule supports this crucial bond between iron and sulfur atoms in what's known as an entatic state, where the protein maintains a bond that is just strong enough to perform both of its jobs, said Michael Mara, lead author of the study and a former postdoctoral researcher at Stanford University, now at University of California, Berkeley.

'This was important because we had shown the bond is weak and shouldn't be present at room temperature in the absence of the protein constraints', said

Solomon. 'But the protein is able to contribute energy to keep this bond intact for electron transfer. In this LCLS experiment, we determined exactly how much energy the rest of the protein contributes to maintaining the bond: about 4 kcal/mol that is derived from an adjacent hydrogen bond network.'

'We were able to show how nature tunes this system to change the properties on a fundamental level and perform two very different functions', Mara said. 'The energy contribution by cytochrome c is really at a sweet spot. It makes me wonder what sort of similar effects you might see in other protein systems, and it makes us realise that there is exciting new science on the horizon.'

Cytochrome c is present in a wide range of life forms and contributes to both cellular respiration and programmed cell death, the pathway to the natural end of a cell's life cycle. How exactly the



An optical laser (green) excites the iron-containing active site of the protein cytochrome c, and then an X-ray laser (white) probes the iron a few femtoseconds to picoseconds later. The critical iron-sulfur bond is broken as the optical laser heats the protein, and rebonds as the system cools.

Greg Stewart/SLAC National Accelerator Laboratory

state of the bond relates to these two functions had not yet been demonstrated or quantified.

Scientists knew from earlier studies that a particular iron-sulfur bond is key. When iron in the protein binds to sulfur contained in one of the protein's amino acids, cytochrome c participates in electron transfer. By transferring electrons, the protein helps generate energy needed for biological processes that maintain life.

But when cytochrome c encounters cardiolipin, a lipid present in the membrane of the cell's mitochondria, the iron-sulfur bond breaks, and the protein becomes an enzyme that creates holes in the mitochondria's outer membrane – the first step in programmed cell death.

These changes occur incredibly fast, in less than 20 picoseconds, so the experiment required ultrafast pulses of X-rays generated by LCLS to take snapshots of the process.

'We photoexcited the iron atoms in the protein's active site – which contains an iron-rich compound known as haem – with an ultrafast laser before probing it with the LCLS X-ray pulses at different time delays', said Roberto Alonso-Mori, LCLS staff scientist and a co-author of the study.

Each 50-femtosecond laser pulse heated the haem by a couple of hundred degrees. X-ray pulses from LCLS took images of what happened as the heat travelled from the iron to other parts of the protein. After 100 femtoseconds, the iron-sulfur bond would break, only to form again once the sample cooled. Watching this process allowed the scientists to measure energy fluctuations in real time and better understand how this critical bond forms and breaks.

Knowledge of cytochrome c's function is also valuable to the fields of bioenergy and environmental science, since it is a critically important protein in bacteria and plants.

SLAC National Accelerator Laboratory

Virtual reality chemistry lessons

MEL Science has launched its first virtual reality (VR) chemistry lessons. The MEL Chemistry VR app, which features a virtual chemistry lab, is now available for Google Daydream. The free version containing the first six lessons is available at <https://melscience.com/vr>.

VR provides new science education opportunities that teachers could previously only dream about. Chemistry is filled with abstract concepts that can be difficult for young students to grasp. The best way for kids to learn is through interaction, so MEL Science developed these chemistry lessons to bring molecular level science to life – and students could be seeing them in their classrooms soon. The lessons follow K-12 curricula, and they are designed to be used at home or in the classroom. A special version for educators will be released soon.

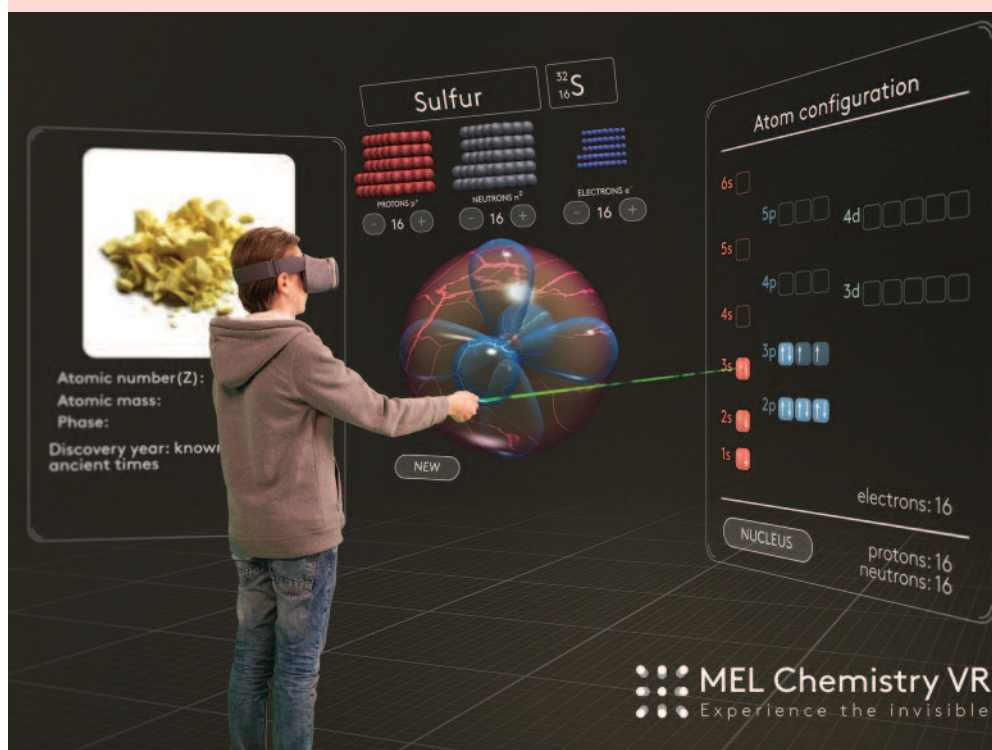
With these first lessons, students will see what it's like to dive into a pencil or a diamond and discover what it looks like at an atomic level. They'll learn about basic chemistry concepts in an interactive, friendly way, including topics such as:

- the difference between solids and gases
- the structure of an atom
- what an electron orbital is
- what an isotope is.

Students will also get the chance to build an atom of any known element with their own hands!

MEL Science plans to release over 150 lessons covering all the main topics included in schools' chemistry curricula. MEL Science also plans to add support for other VR platforms, including Google Cardboard and Samsung GearVR, later this year.

MEL Science is known for its subscription service providing science sets. With this service, parent subscribers get two new chemistry sets every month, enabling them to perform cool educational experiments at home with their kids. This fast-growing business has experienced a more than 500% year-over-year growth rate.



MEL Chemistry VR
Experience the invisible

ACS awards highest honour to Geraldine Richmond

Geraldine Richmond
Charlie Litchfield



The American Chemical Society (ACS) has chosen Dr Geraldine (Geri) Richmond, presidential chair in science and professor of chemistry at the University of Oregon, to receive its highest award, the 2017 Priestley Medal. The world's largest scientific society is recognising Richmond for her 'pioneering contributions to our understanding of the molecular properties of liquid surfaces and her extraordinary service to chemistry on the global level'.

'As a leader in and out of the lab, Geri Richmond is an outstanding choice to receive the Priestley Medal', said ACS Executive Director and CEO Dr Thomas Connelly Jr. 'Her pioneering research to understand the characteristics of surfaces in chemical processes has advanced studies related to energy, the environment and biological applications. Beyond the lab, she has been a devoted advocate for women in science and a true trailblazer in assuring a diverse workforce.'

Richmond's research examines the chemistry and physics that occur at complex surfaces that have relevance to important problems in energy production, environmental remediation and

atmospheric chemistry. In particular, her landmark experimental and computational studies of the molecular structure of organic-water interfaces have answered long-standing questions about how water molecules behave near fluid hydrophobic surfaces.

She is founder and current director of the Committee on the Advancement of Women Chemists. Since 1998, this grassroots organisation, known as COACH, has helped promote the careers of more than 15 000 women scientists and engineers in the US. In addition, Richmond has taught career-building workshops to 3000 women in more than 20 countries.

'Richmond's scientific discoveries that underlie some of the most important chemical processes on our planet, her leadership on multiple national boards that oversee scientific policy and education issues in this country and her tireless efforts to increase the diversity of our chemistry workforce make her an ideal choice for this prestigious honour', said Northwestern University chemistry professor Richard P. Van Duyne, who nominated Richmond for the award.

She is currently serving on the National Science Board and as the US science envoy to the Southeast Asian Lower Mekong River countries. Richmond is also a past president and former board chair of the American Association for the Advancement of Science.

In 2016, Richmond was awarded the National Medal of Science. Other awards for her scientific accomplishments include the ACS Olin-Garvan Medal, the ACS Joel H. Hildebrand Award and the American Physical Society Davisson-Germer Prize.

Richmond received her BSc in chemistry from Kansas State University in 1975 and her PhD in physical chemistry from the University of California, Berkeley in 1980.

Since 1923, ACS has recognised groundbreaking chemists with the Priestley Medal. The annual award includes a gold medallion designed to commemorate the work of Joseph Priestley, who lived from 1733 to 1804, and is best remembered for his discovery of the gas that would later be named 'oxygen'.

American Chemical Society

Left to right: Deakin's Carbon Nexus Director Derek Buckmaster, Chair of Deakin's Advanced Manufacturing Advisory Group Simon Crean, LeMond Composites Chief Operating Officer Nicolas Wegener, Deakin Chancellor John Stanhope AO, Deakin PhD student Maxime Maghe, LeMond Composites Founder and CEO Greg LeMond and Deakin University Vice-Chancellor Professor Jane den Hollander AO.



Deakin and Lemond Composites join forces on carbon fibre

Deakin University has paved the way to dramatically cut the cost of carbon fibre manufacturing, joining forces with LeMond Composites in a \$US44 million deal to revolutionise its use across the world.

The partnership allows LeMond Composites to license technology developed by Carbon Nexus Deakin's carbon fibre research centre.

LeMond Composites will also consider the development of a carbon fibre manufacturing plant in Geelong, which would invest more than \$30 million in construction and equipment, and create dozens of jobs for Geelong manufacturers to take the carbon fibre of the future to the global market.

The specialised carbon fibre production machinery for the plant will be manufactured by Furnace Engineering in Clayton, Victoria.

Deakin University Vice-Chancellor Professor Jane den Hollander said the new technology, developed by Carbon Nexus PhD Student Maxime Maghe and Carbon Nexus General Manager Steve Atkiss, was a game-changer for the future of manufacturing.

'We know carbon fibre has been in use in aircraft, high-end cars and bikes, among other applications for a long time now, but it remains a niche product that costs a significant amount to produce', Professor den Hollander said.

'This new technology could revolutionise the advanced manufacturing sector locally, across Australia and around the globe, because it will make carbon fibre more affordable to produce, which will make it more accessible for consumers.'

LeMond Composites Founder and CEO Greg LeMond in 1986 became the first cyclist to win the Tour de France on a carbon fibre bike. He has been a household name among cyclists for three decades, selling carbon fibre bikes under his own brand around the globe, before last year setting up LeMond Composites to realise his vision of affordable carbon fibre cycles for everyday riders.

LeMond said the ability to scale low-cost carbon fibre production had been the biggest hurdle to bring the material to the masses.

den Hollander said the scope for future growth of Deakin and LeMond's partnership had potential to help transform a new future for Geelong.

'We all know that Geelong's reliance on manufacturing has changed and the future will be driven by high-value advanced manufacturing', den Hollander said.

'Just three months ago, Deakin joined with the City of Greater Geelong and G21 to launch Geelong Economic Futures – a blueprint for a number of projects that included scope for development to help lead this city's future and carbon fibre development was a key project highlighted, so it is pleasing to see a key in this vision come to fruition.'

The Carbon Nexus centre was established in 2014 as a research facility to conduct basic and industrial-scale research into carbon fibre production methods and composite manufacturing techniques.

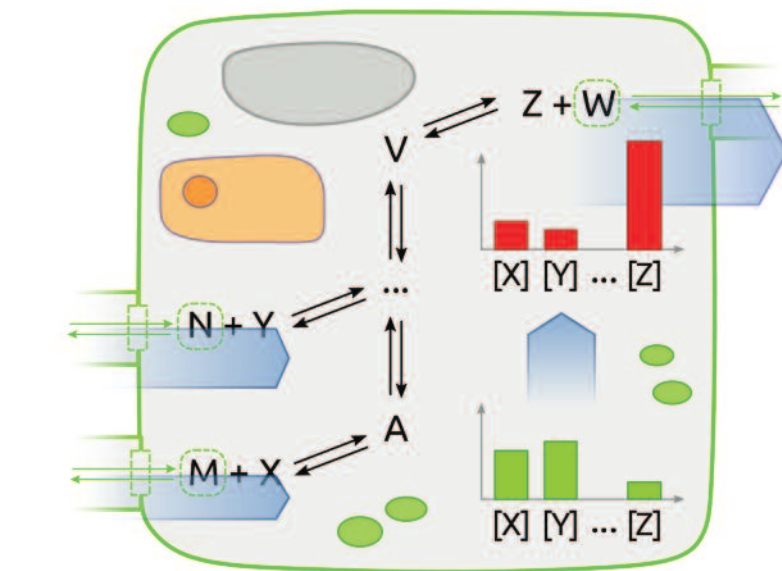
Deakin University

Using mathematical methods to study complex biological networks

Complex biological processes, such as metabolism, often involve thousands of different compounds coupled by chemical reactions. These process chains are described by researchers as chemical reaction networks. Researchers from the University of Luxembourg have developed new mathematical methods to study the energetic properties of these networks. The scientists published their findings in *Physical Review X* (<https://doi.org/10.1103/PhysRevX.6.041064>).

The paper was prepared by the research group led by Professor Massimiliano Esposito that investigates how very small biological systems work at the molecular level. These systems are subject to large fluctuations in mass which make their behaviour difficult to predict. In order to be able to describe them, the researchers use a probabilistic approach that calculates the dynamics of these systems based on the statistical likelihood that changes occur. Using these probabilistic descriptions, the group studies how these systems exchange energy and matter with their environment and how much energy they dissipate during these processes – a discipline known as stochastic thermodynamics. However, in the realm of complex chemical reaction networks, probabilistic descriptions become unfeasible because thousands of molecules are involved. The authors showed how the mathematical methods developed for small systems can be used to investigate these networks.

‘Currently, rigorous thermodynamic models for this kind of networks are lacking. Our work paves the way for thermodynamic characterisations of real chemical networks, such as metabolism’, explained Riccardo Rao, the main author of the paper. ‘We think of these networks as machines transforming some



Understanding the dynamics and thermodynamics of the chemical reaction networks of cells is the researchers' long-term goal.

compounds into others. Some compounds are consumed as they 'fuel' the processes. Our description allows us to answer questions such as: Is this process efficient? How much energy does it dissipate? If we slightly tweak the system, how will it react?

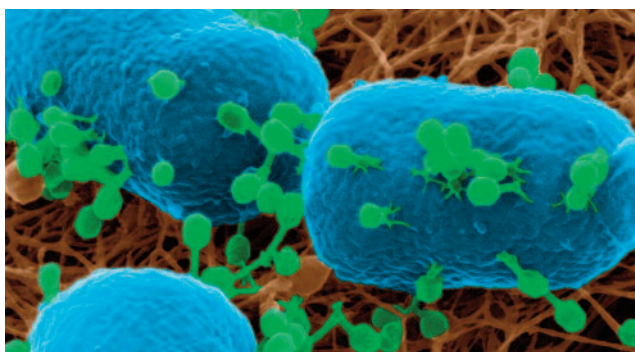
At the moment, their research focuses on models of metabolic networks, for which some simplifying approximations are required. 'We are now using this framework to investigate specific classes of chemical reaction networks, such as metabolic networks', Rao said. Also, the research team will work with biologists and chemists to test and apply the results to concrete biological systems. Research in this direction with groups from the Luxembourg Center for Systems Biomedicine is already ongoing.

University of Luxembourg

... the researchers use a probabilistic approach that calculates the dynamics of these systems based on the statistical likelihood that changes occur.

Helium ions reveal how viruses attack bacteria

An interdisciplinary research consortium from the Nanoscience Center at University of Jyväskylä in Finland (group leaders Dr Lotta-Riina Sundberg and Professor Ilari Maasilta) has found that bacteria and viruses can be imaged with helium ions in contrast to electrons, which are the standard workhorse in nanoscale microscopy. Helium ions, being more massive than electrons, can be focused to a much tighter spot down to the atomic length scales. By measuring the electrons generated by the ion bombardment, an image can be formed from the sample with biological features visible below the nanometre length.



Bacteriophages (green) attached to *E. coli* (blue) on an agar substrate (brown), imaged with a helium ion microscope.

University of Jyväskylä

The novel technique, called helium ion microscopy (HIM), was used to image hard-to-see interactions between bacteria and bacteriophages – viruses infecting bacteria. These phages are currently actively considered as a novel ‘smart weapon’ against bacterial infections, which are becoming more and more difficult to treat with traditional antibiotics. The images demonstrated clearly the different stages of how the phages in question attacked the bacteria (*E. coli*), for example showing the process where the virus has latched onto the bacterial surface, grabbing it with a tentacle-like structure, and in the process of injecting its genome into the bacterial cell.

The researchers also demonstrated that the ions can be used as a nanoscale scalpel, to cut portions off individual bacterial cells, or to reveal bacterial colonies under the surfaces of samples. They feel confident that HIM offers many more possibilities to help to study microbes and viruses in their natural state, interacting with each other and other cells.

The research was published in *Advanced Biosystems* (<https://doi.org/10.1002/adbi.201700070>).

University of Jyväskylä

Antioxidants against sepsis

During sepsis, cells are swamped with reactive oxygen species generated in an aberrant response of the immune system to a local infection. If this fatal inflammatory path could be interfered with, new treatment schemes could be developed. Now, Korean scientists report in *Angewandte Chemie* (<https://doi.org/10.1002/anie.201704904>) that zirconia-doped ceria nanoparticles act as effective scavengers of these oxygen radicals, promoting a greatly enhanced surviving rate in sepsis model organisms.

Sepsis proceeds as a vicious cycle of inflammatory reactions of the immune system to a local infection. Fatal consequences can be falling blood pressure and the collapse of organ function. As resistance against antibiotics is growing, scientists turn to the inflammatory pathway as an alternative target for new treatment strategies. Taeghwan Heyon, Director of the Center for Nanoparticle Research of Institute for Basic Science and Professor of Chemical and Biological Engineering at Seoul National University, Seung-Hoon Lee at Seoul National University Hospital, South Korea, and collaborators explore ceria nanoparticles for their ability to scavenge reactive oxygen species, which play a key role in the inflammatory process. By quickly converting between two oxidation states, the cerium ion can quench typical oxygen radical species like the superoxide anion, the hydroxyl radical anion, or even hydrogen peroxide. But in the living cell, this can only happen if two conditions are met.

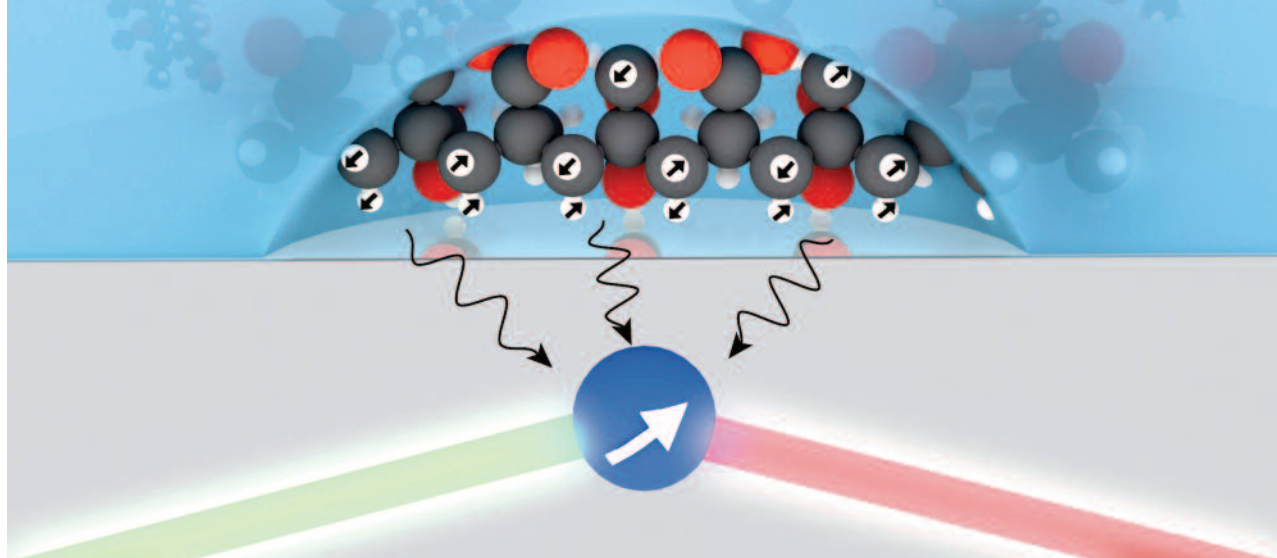
The first condition is the size and nature of the particles. Small, two-nanometre-sized particles were coated by a hydrophilic shell of poly(ethylene glycol)-connected phospholipids to make them soluble so that they can enter the cell and remain there. Second, the cerium ion responsible for the quenching (Ce^{3+}) should be accessible on the surface of the nanoparticles, and it must be regenerated after the reactions. Here, the scientists found out that a certain amount of zirconium ions in the structure helped, because ‘the Zr^{4+} ions control the Ce^{3+} -to- Ce^{4+} ratio as well as the rate of conversion between the two oxidation states’, they argued.

The prepared nanoparticles were then tested for their ability to detoxify reactive oxygen species, not only in the test tube, but also in live animal models. The results were clear, as the authors stated: ‘A single dose of ceria–zirconia nanoparticles successfully attenuated the vicious cycle of inflammatory responses in two sepsis models.’ The nanoparticles accumulated in organs where severe immune responses occurred, and they were successful in the eradication of reactive oxygen species, as evidenced with fluorescence microscopy and several other techniques. And importantly, the treated mice and rats had a far higher survival rate.

This work demonstrates that approaches in sepsis treatment other than killing bacteria with antibiotics are possible. Targeting the inflammatory signal pathways in macrophages is a very promising option, and the authors have shown that effective scavenging of reactive oxygen species and stopping inflammation is possible with a suitably designed chemical system like this cerium ion redox system provided by nanoparticles.

Angewandte Chemie International Edition

Quantum probes dramatically improve detection of nuclear spins



A nitrogen-vacancy (dark blue) quantum probe in diamond (light grey) performing nanoscale NMR spectroscopy on molecular hydrogen sitting on the diamond's surface. A green laser controls the quantum state of the probe, which is tuned to the resonant frequency of target nuclear spins. The probe responds to the nuclear spins of the hydrogen atoms and provides a direct measurement via the red light emitted.

David Broadway/cqc2t.org

Researchers at the University of Melbourne have demonstrated a way to detect nuclear spins in molecules non-invasively, providing a new tool for biotechnology and materials science.

Important research in medicine and biology relies on NMR spectroscopy, but until now, it has been limited in spatial resolution and typically requires powerful microwave fields. A team led by Professor Lloyd Hollenberg at the University of Melbourne has used a quantum probe to perform microwave-free NMR at the nanoscale. The results were published in *Nature Communications* (<https://doi.org/10.1038/NCOMMS15950>).

'This quantum probe delivers a dramatic improvement in NMR technology. In addition to being able to detect NMR in far smaller samples than conventional machines, our technique does not require the application of microwave fields that might disrupt biological samples', said Hollenberg, who is Deputy Director of the Centre for Quantum Computation and Communication Technology (CQC2T) and

Thomas Baker Chair at the University of Melbourne.

'In NMR the goal is to detect the magnetic signal from the nuclei of the atoms comprising molecules. But the signal from the nuclear "spin" is very weak and conventional NMR machines require many millions of nuclear spins to detect anything. However, using the quantum properties of a "defect" in diamond, our technique can detect much smaller volumes down to only thousands of spins.'

The discovery may overcome significant limitations with conventional NMR methods, which depend on machines that can exceed 10 tonnes.

'The problem with the large NMR machines in widespread use today is that the signals we're trying to detect are extremely small, and the distance from the measurement device to the object being measured is very large', said Dr Alastair Stacey, a postdoctoral researcher in CQC2T.

'This creates two problems: the machine can only see a larger collection

of molecules, reducing the accuracy of the measurement. It also has to use very strong microwaves and magnetic fields to reach the sample, but these processes are invasive and can affect delicate bio-samples, particularly when trying to see the molecular structure of liquids.'

Lead author James Wood describes the technique as 'a dramatic simplification of the nuclear detection process, where we essentially shine light on an atomic-sized defect in diamond and observe its natural response, at a fundamentally quantum level, to the target nuclear spins nearby.'

'A great benefit of our approach is that we don't interfere with the sample when imaging it.'

'With these advances in quantum sensing technology, we are opening the door to a new world of scientific investigation that could lead us to gain a better understanding of the smallest building blocks of life', said Hollenberg.

ARC Centre of Excellence for Quantum Computation and Communication Technology (CQC2T), University of Melbourne

Earth's magnetic field 'simpler than we thought'

Scientists have identified patterns in Earth's magnetic field that evolve on the order of 1000 years, providing new insight into how the field works and adding a measure of predictability to changes in the field not previously known.

The discovery will also allow researchers to study the planet's past with finer resolution by using this geomagnetic 'fingerprint' to compare sediment cores taken from the Atlantic and Pacific oceans. Results of the research were recently published in *Earth and Planetary Science Letters* (<https://doi.org/10.1016/j.epsl.2017.05.022>).

The geomagnetic field is critical to life on Earth. Without it, charged particles from the sun (the 'solar wind') would blow away the atmosphere, scientists say. The field also aids in human navigation and animal migrations in ways scientists are only beginning to understand. Centuries of human observation, as well as the geologic record, have shown dramatic changes in the field's strength and structure over time.

Yet in spite of this importance, many questions remain unanswered about why and how these changes occur.

'We've known for some time that the Earth is not a perfect dipole, and we can see these imperfections in the historical record', said lead author Maureen Walczak. 'We are finding that non-dipolar structures are not evanescent, unpredictable things. They are very long-lived, recurring over 10 000 years – persistent in their location throughout the Holocene.'

Some 800 000 years ago, a magnetic compass needle would have pointed south because Earth's magnetic field was reversed. These reversals typically happen every several hundred thousand years.

A secondary pattern of geomagnetic 'wobble' within periods of stable polarity, known as paleomagnetic secular variation (PSV), may be a key to understanding why some geomagnetic changes occur.

Earth's magnetic field does not align perfectly with the axis of rotation, which is why true north differs from magnetic north. In the northern hemisphere this disparity in the modern field is apparently driven by regions of high geomagnetic intensity that are centred beneath North America and Asia.

When the magnetic field is stronger beneath North America, or in the 'North American Mode', it drives steep inclinations and high intensities in the North Pacific, and low intensities in Europe with westward declinations in the North Atlantic. This is more consistent with the historical record.

Around Earth's equator, bright swaths of colour ('airglow') can appear hovering at about 80–500 kilometres above the surface of Earth. These are the result of a complex interaction between Earth's magnetic field lines and terrestrial weather.

NASA's Goddard Space Flight Center/Duberstein

The alternative 'European mode' is in some ways the opposite, with shallow inclination and low intensity in the North Pacific and eastward declinations in the North Atlantic and high intensities in Europe.

'The magnetic field is somewhat less complicated than we thought', said co-author Joseph Stoner. 'It is a fairly simple oscillation that appears to result from geomagnetic intensity variations at just a few recurrent locations with large spatial impacts. We're not yet sure what drives this variation, though it is likely a combination of factors including convection of the outer core that may be biased in configuration by the lowermost mantle.'

The researchers were able to identify the pattern by studying two high-resolution sediment cores from the Gulf of Alaska that allowed them to develop a 17 400-year reconstruction of the PSV in that region. They then compared those records with sediment cores from other sites in the Pacific Ocean to capture a magnetic fingerprint, which is based on the orientation of the magnetite in the sediment, which acts as a magnetic recorder of the past.

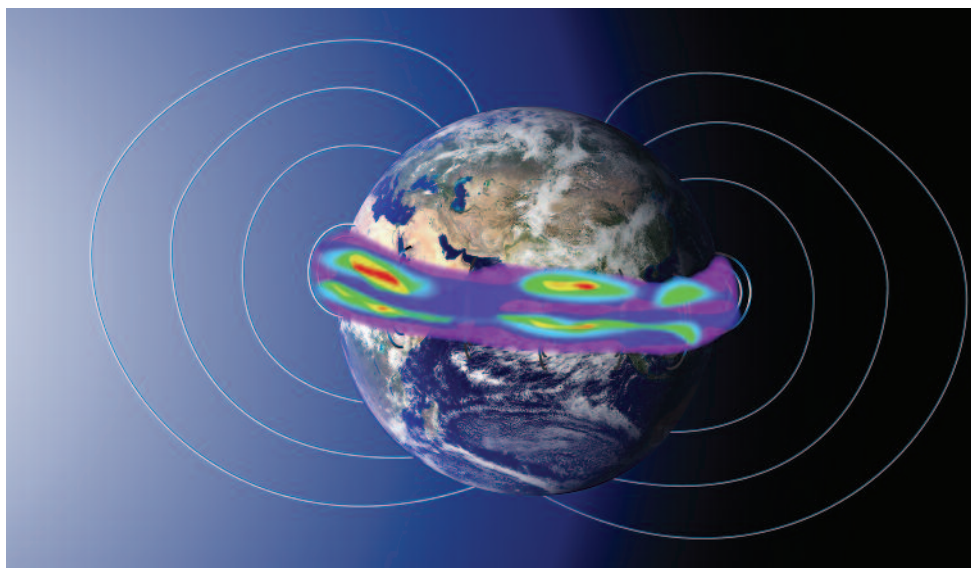
The common magnetic signal found in the cores now covers an area spanning from Alaska to Oregon, and over to Hawaii.

'Magnetic alignment of distant environmental reconstructions using reversals in the paleomagnetic record provides insights into the past on a scale of hundreds of thousands of years', Walczak said. 'Development of the coherent PSV stratigraphy will let us look at the record on a scale possibly as short as a few centuries, compare events between ocean basins, and really get down to the nitty-gritty of how climate anomalies are propagated around the planet on a scale relevant to human society.'

The magnetic field is generated within Earth by a fluid outer core of iron, nickel and other metals that creates electric currents, which in turn produce magnetic fields. The magnetic field is strong enough to shield Earth from solar winds and cosmic radiation. The fact that it changes is well known; the reasons why have remained a mystery.

Now this mystery may be a little closer to being solved.

Mark Floyd, Oregon State University



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New measurement will help redefine international unit of mass

Using a state-of-the-art device for measuring mass, researchers at the US National Institute of Standards and Technology (NIST) have made their most precise determination yet of Planck's constant, an important value in science that will help to redefine the kilogram, the official unit of mass in the SI, or international system of units. Accepted for publication in the journal *Metrologia* (<https://doi.org/10.1088/1681-7575/aa7bf2>), these new results came ahead of a 1 July international deadline for measurements that aim to redefine the entire SI in terms of fundamental constants of nature.

The new NIST measurement of Planck's constant is $6.626\,069\,934 \times 10^{-34} \text{ kg} \cdot \text{m}^2/\text{s}$, with an uncertainty of only 13 parts per billion. NIST's previous measurement, published in 2016, had an uncertainty of 34 parts per billion.

The kilogram is currently defined in terms of the mass of a platinum-iridium artifact stored in France. Scientists want to replace this physical artifact with a more reproducible definition for the kilogram that is based on fundamental constants of nature.

Planck's constant enables researchers to relate mass to electromagnetic energy. To measure Planck's constant, NIST uses the Kibble balance, originally called the watt balance. Physicists widely adopted the new name last year to honour the late British physicist Bryan Kibble, who invented the technique more than 40 years ago.

NIST's Kibble balance uses electromagnetic forces to balance a kilogram mass. The electromagnetic forces are provided by a coil of wire sandwiched between two permanent magnets. The Kibble balance has two modes of operation. In one mode, an electrical current goes through the coil, generating a magnetic field that interacts with the permanent magnetic field and creates an upward force to balance the kilogram mass. In the other mode, the coil is lifted at a constant velocity. This upward motion induces a voltage in the coil that is proportional to the strength of the magnetic field. By measuring the current, the voltage and the coil's velocity, researchers can calculate the Planck constant, which is proportional to the amount of electromagnetic energy needed to balance a mass.

There are three major reasons for the improvement in the new measurements, said physicist Stephan Schlamminger, leader of the NIST effort.

First, the researchers have much more data. The new result uses 16 months' worth of measurements, from December 2015 to April 2017. The increase in experimental statistics greatly reduced the uncertainty in their Planck value.

Second, the researchers tested for variations in the magnetic field during both modes of operation and discovered they had been overestimating the impact the coil's magnetic field was having on the permanent magnetic field. Their subsequent

adjustment in their new measurements both increased their value of Planck's constant and reduced the uncertainty in their measurement.

Finally, the researchers studied in great detail how the velocity of the moving coil affected the voltage. 'We varied the speed that we moved the coil through the magnetic field, from 0.5 to 2 millimetres per second', explained Darine Haddad, lead author of the NIST results.

In a magnetic field, the coil acts like an electric circuit consisting of a capacitor, a resistor and an inductor. In a moving coil, these circuit-like elements generate an electrical voltage that changes over time, said Schlamminger. The researchers measured this time-dependent voltage change to account for this effect and reduced the uncertainty in their value.

This new NIST measurement joins a group of other new Planck's constant measurements from around the world. Another Kibble balance measurement, from the National Research Council of Canada, has an uncertainty of just 9.1 parts per billion. Two other new measurements use the alternative Avogadro technique, which involves counting the number of atoms in a pure silicon sphere.

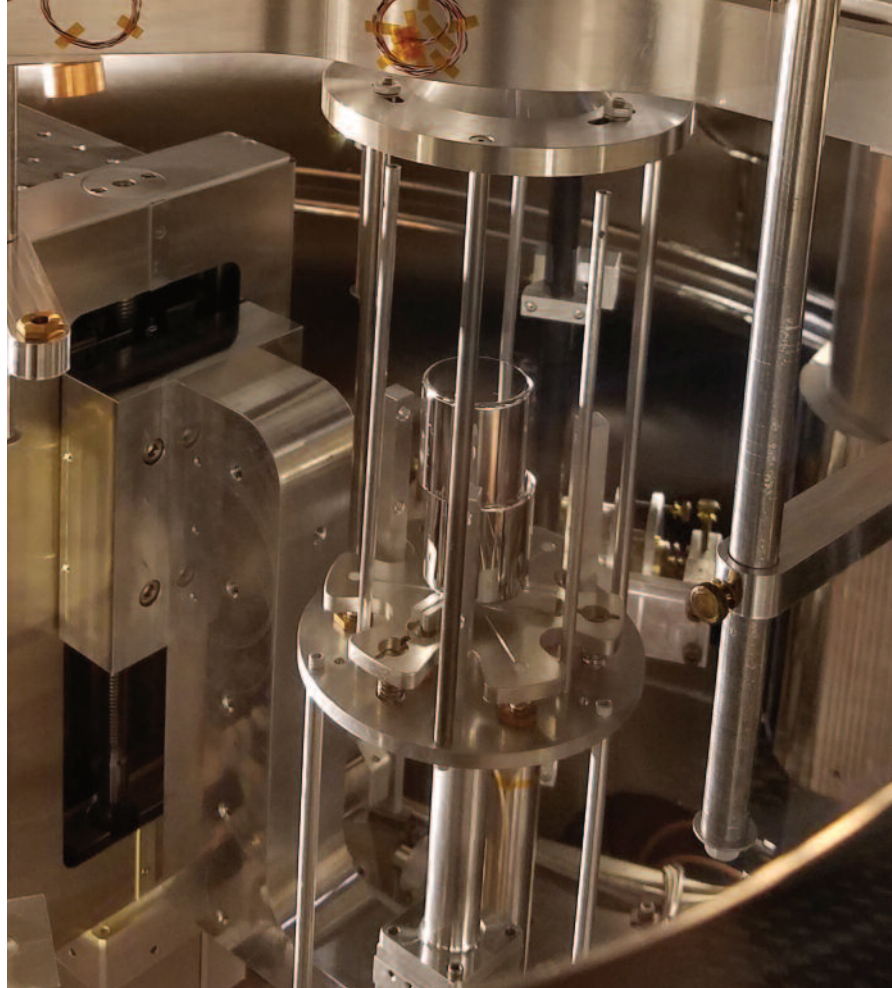
The new measurements have such low uncertainty that they exceed the international requirements for redefining the kilogram in terms of Planck's constant.

'There needed to be three experiments with uncertainties below 50 parts per billion, and one below 20 parts per billion', Schlamminger said. 'But we have three below 20 parts per billion.'

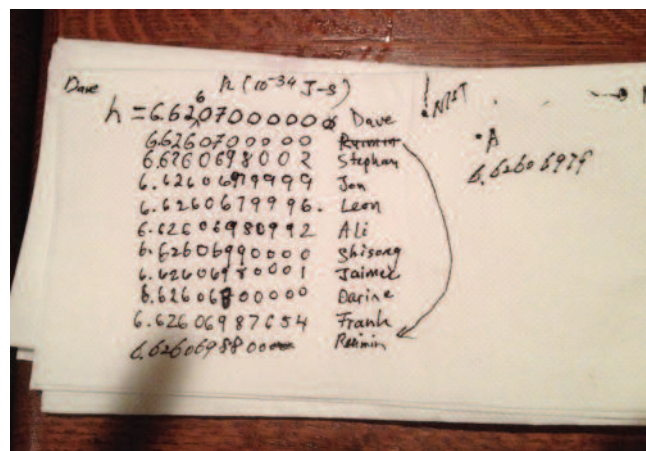
All of these new values of the Planck's constant do not overlap, 'but overall they're in amazingly good agreement', Schlamminger said, 'especially considering that researchers are measuring it with two completely different methods'. These values will be submitted to a group known as CODATA ahead of a 1 July deadline. CODATA will consider all of these measurements in setting a new value for Planck's constant. The kilogram is slated for redefinition in November 2018, along with other units in the SI.

Before they started these experiments, Schlamminger and his group went to lunch in December 2013. On a lunch napkin, each group member wrote his or her prediction of the value of Planck's constant that the group would determine through their measurements. They tucked away this napkin under their Kibble balance nearly four years ago, and they have now compared the predictions. Shisong Li, a guest researcher from Tsinghua University in China, came closest. His prediction differed by only about 5 parts per billion from the measured result. There is no word yet on how the team plans to celebrate the winner's guess.

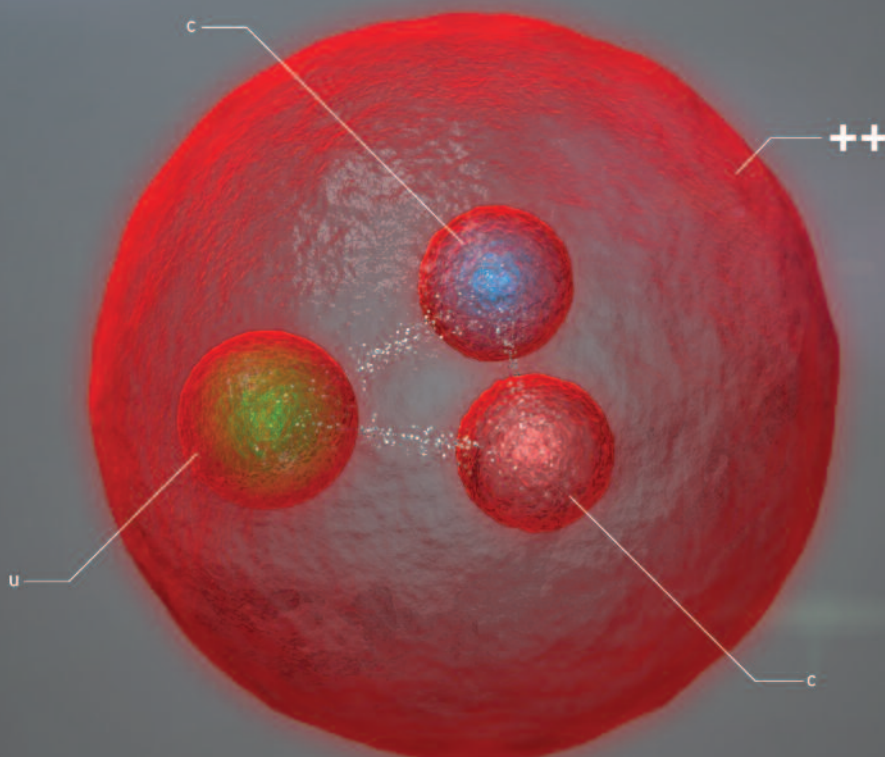
National Institute of Standards and Technology



In measuring Planck's constant with the NIST Kibble balance, researchers carefully measured the effects of the magnetic field that is generated to counteract the weight of masses. In their experiments, they varied the mass from half a kilogram to two kilograms. In this image, NIST kilogram K85 lies on top of NIST K104 for the two-kilogram measurement. NIST



In December 2013, before NIST began its experiments on its newest Kibble balance, group members wrote their predictions on the value of Planck's constant they would measure. Shisong Li, a guest researcher from Tsinghua University in China, came closest. His prediction differed by only about 5 parts per billion from the measured result. NIST



Large Hadron Collider detects new particle

The Large Hadron Collider has once again done what it does best – smash bits of matter together and find new particles in the carnage.

This time, physicists have come across a real charmer. It's four times heavier than a proton and could help challenge some ideas about how this kind of matter sticks together.

We've seen a lot of interesting new particles from CERN's Large Hadron Collider 'beauty' (LHCb) collaboration, which is a little sister to the ATLAS and CMS experiments that brought us the famous Higgs boson a few years back.

The experiments run in CERN's colliders all involve accelerating matter and then bringing it to a quick stop. The resulting burst of energy results in a shower of particles with different properties, most of which we're pretty familiar with.

Running these experiments over and over again and doing the maths on the sizes and behaviours of the particles as they form and interact with one another can occasionally provide something different.

We can now officially add a new kind of baryon to the zoo of particles, one that was already predicted to exist but never before seen.

Baryons are effectively triplets of quarks, which are elementary particles. Quarks come in a variety of flavours, called up, down, top, bottom, charm and strange. It's combinations of these that give us different bosons. Current models predict there are a bunch of ways quarks can make baryons, with some more common than others.

Protons consist of two ups and a down quark, while neutrons are two downs and an up. These quarks stick together under what's called the strong nuclear force, which is caused by the swapping of particles called gluons. Never let it be said that physicists lack a sense of humour.

This new baryon – made when two charm quarks and a single up are bound together – was given the less whimsical name $\Xi_{cc^{++}}$, so they can't all be winners.

Quarks have different masses, and charm is a beefy one. That makes this baryon a touch on the heavy side, which is good news for particle physicists.

'Finding a doubly heavy-quark baryon is of great interest as it will provide a unique tool to further probe quantum chromodynamics, the theory that describes the strong interaction, one of the four fundamental forces', said Giovanni Passaleva, the spokesperson for the LHCb collaboration.

Seeing how this particle keeps itself together compared to the predictions made by current models will help give the going theories a good shake.

Being made of two heavy quarks should give $\Xi_{cc^{++}}$ a slightly different structure from protons and neutrons.

'In contrast to other baryons, in which the three quarks perform an elaborate dance around each other, a doubly heavy baryon is expected to act like a planetary system, where the two heavy quarks play the role of heavy stars orbiting one around the other, with the lighter quark orbiting around this binary system', said former collaboration spokesperson Guy Wilkinson.

If you're wondering where this baryon has been hiding all this time, like many particles it doesn't hang around very long. It wasn't seen directly, but was recognised by the particles it broke into.

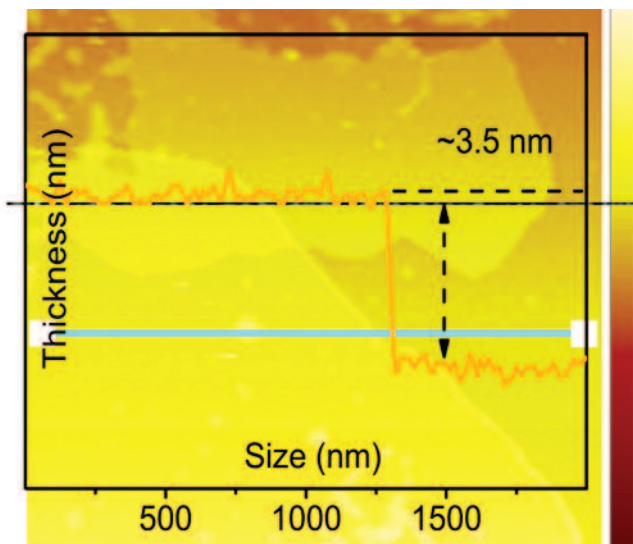
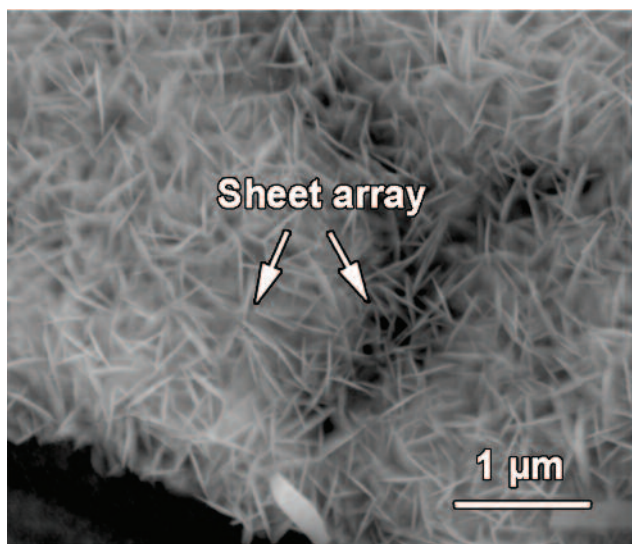
The LHCb experiment is a champion at spotting these kinds of decay products, as well as making heavy quarks.

The discovery has a high statistical significance at seven sigma. Physicists break out the champagne at five sigma, so we can be pretty confident $\Xi_{cc^{++}}$ was produced.

This research has been submitted to *Physical Review Letters*.

Mike McRae, ScienceAlert

New ultrathin MOF material for efficient water splitting



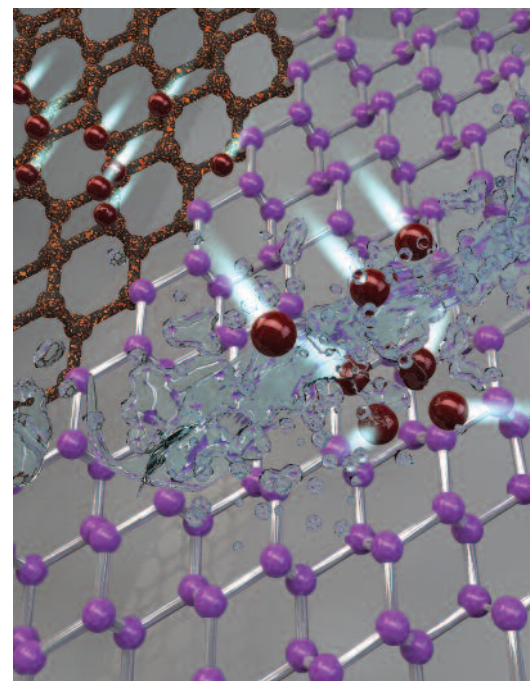
Metal–organic frameworks (MOFs) are a family of versatile porous materials with a wide variety of potential applications, including fuel storage, drug delivery and carbon capture. But conventional MOFs have poor electrical conductivity and low macroporosity, which limit charge transfer, mass transport and applications in electrochemical processes. To address these problems, researchers at the University of New South Wales have developed a ‘bottom-up’ strategy to fabricate an ultrathin 2D MOF architecture on various substrates (Duan J.J., Chen S., Zhao C. *Nat. Commun.* 2017, **8**, 15 341). The synthesised nanosheet arrays of MOFs

possess remarkable structural properties, including highly exposed metal sites, improved electrical conductivity by 2D nanostructurisation, and a combination of micro-, open and macro-pores for facile electrolyte ion diffusion and fast gas dissipation. The researchers report a nickel–iron-based MOF array, which demonstrates spectacular electrocatalytic performance towards oxygen evolution reaction and hydrogen evolution reaction. The finding challenges a common concept that MOFs are inert electrocatalysts, and can potentially expand MOF applications beyond electrochemistry.

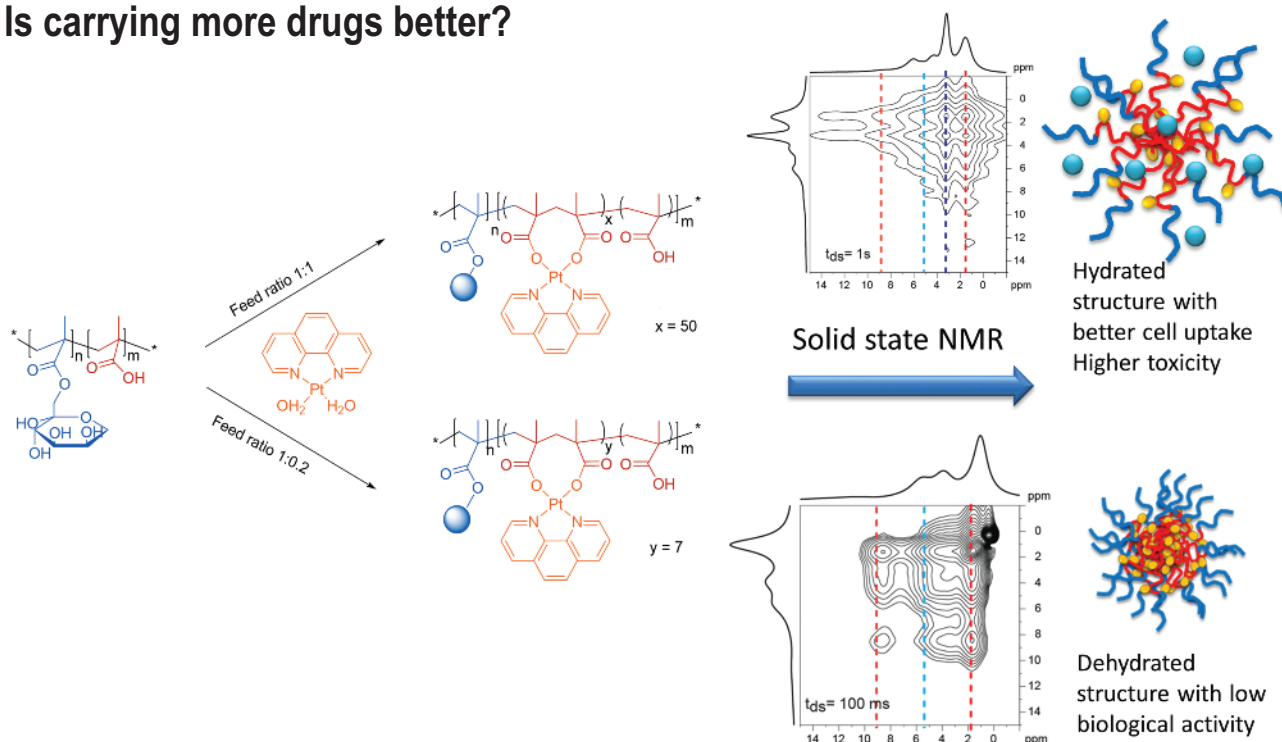
Ionic liquid traps stop black phosphorus degradation

Black phosphorus and its atomically thin form (phosphorene) are potential materials for a variety of applications in sensing, electronics, catalysis and energy storage. A fundamental challenge limiting use of black phosphorus in practical devices is its varied stability under ambient conditions, which results in the loss of its ultra-high semiconducting properties. Recently, a multidisciplinary team led by researchers at RMIT and including scientists from the University of Technology, Sydney, CSIRO Manufacturing, Monash University and the University of Granada, Spain, has used ionic liquids to trap damaging reactive oxygen species that are responsible for degrading of black phosphorus (Walia S., Balendhran S., Ahmed T., Singh M., El-Badawi C., Brennan M.D., Weerathunge P., Karim M.N., Rahman F., Russell A.,

Duckworth J., Ramanathan R., Collis G.E., Lobo C.J., Toth M., Kotsakidis J.C., Weber B., Furher M., Dominguez-Vera J.M., Spencer M.J.S., Aharonovich I., Sriram S., Bhaskaran M., Bansal V. *Adv. Mater.* 2017, **29**, article 1700152. The strategy draws inspiration from the unique ability of biological systems to avoid photo-oxidative damage caused by reactive oxygen species. The ionic liquid acts as a functional chemical barrier, rapidly capturing reactive oxygen species generated on the black phosphorus surface without interfering with the material’s semiconducting properties. This approach led to a significant enhancement in device lifetime. Future work is directed towards improving device scalability, durability and functionality for specific end-use applications.




Is carrying more drugs better?



It is strongly believed that it is best to pack as many drugs as possible into a drug-delivery carrier. This makes sense as the empty drug carrier can be considered waste that needs to be cleared from the body after use. So maximising drug loading should minimise the waste produced for a given drug dosage. But increasing the amount of a drug inside a nano-sized drug carrier may affect the way in which the carrier interacts with the environment and thus its cellular uptake. Professor Martina Stenzel and Dr Aditya Rawal from the University of New South Wales and their co-workers have shed light on this matter by preparing micelles based on glycopolymers made from fructose and a block copolymer with pendant platinum drugs, in which

the amount of the drug was varied (Callari M., De L., Rawal A., Stenzel M.H. *Angew. Chem. Int. Ed.* 2017, **56**, 8441–5). Interestingly, the micelles with low drug loading displayed higher cell uptake and higher toxicity. Solid-state NMR spectroscopy was subsequently employed to unveil the internal structure of the micelles, which showed that a high drug loading had a tendency to dehydrate the glycopolymers layer. On the other hand, a low drug loading resulted in micelles with high water content, which most likely allowed better display of the bioactive fructose and thus better cellular uptake.

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.*, *Chem. Sci.*) are encouraged to contribute general summaries, of no more than 200 words, and an image to David.



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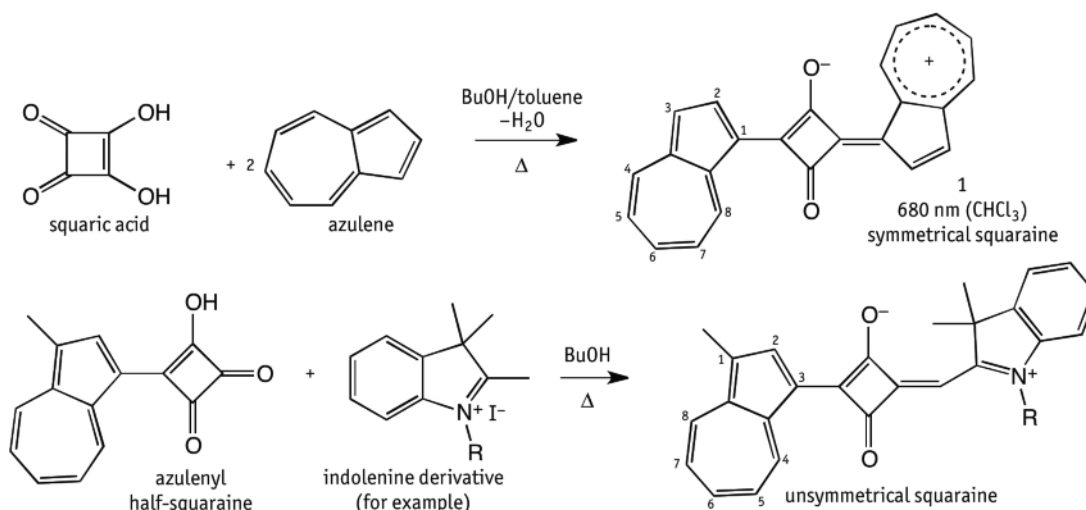
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Highlights from the August issue



Highlights of the August 2017 issue of *Australian Journal of Chemistry* include two reviews, one each from the UK and India, and a research article from Northern Ireland.

Daniel Lynch of Exilica Ltd (UK) and Darren Hamilton of the Department of Chemistry, Mount Holyoke College, USA, provide a historical overview of azulenyl squaraines, a class of organic dye that possesses properties that make the dyes highly attractive for optical data storage. These organic molecules are defined as either symmetrical or unsymmetrical squaraine compounds prepared through the 1:2 condensation reaction of 3,4-dihydroxycyclobut-3-ene-1,2-dione (squaric acid) and azulene (or an associated derivative such as an aza-azulene), or condensation of an azulenyl half-squaraine with a suitable electron-donating aromatic system such as an N-substituted 2,3,3-trimethylindolenine (see scheme). From the first reported synthesis of an azulenyl squaraine in 1966, these compounds have been intensely investigated because they absorb within the wavelength range of a semiconductor laser beam, i.e. within an approximate range of 700–900 nm. The authors report on the fascinating synthesis chemistry and on potential novel applications such as in biomedicine as photosensitisers in photodynamic therapy.

Bubum Banerjee of the Department of Chemistry at Indus International University, India, provides a comprehensive review on ultrasound-assisted synthesis of *N*-heterocycles at ambient temperature. Heterocycles, which make up more than half of all organic compounds, are widely distributed privileged structural subunits that possess a range of key biological activities. *N*-Heterocycles have been reported to have, among other actions, antimicrobial, antihistamine, antimalarial and anti-inflammatory action. Although a large number of methods are available for their syntheses, they commonly suffer from harsh reaction conditions that can significantly impact upon overall yields. In the past decade, considerable efforts have led to the development of methods for the synthesis of *N*-heterocycles under mild conditions at ambient temperature with ultrasonic irradiation in organic synthesis proving to be particularly beneficial. The review describes the successful application of such methods to a variety of complex *N*-heterocycles, leading to their detailed biological study.

A notable contribution by Kenneth Seddon and his team at The Queen's University of Belfast, Northern Ireland, and his collaborators, reports on the development of ionic liquid countercurrent chromatography (ILCCC) as a viable means for the separation of organic, inorganic or

bio-based materials. Countercurrent chromatography (CCC) is a liquid chromatography process based on the partition of solutes between two immiscible liquid phases as they interact in a thin tube under a centrifugal force field. The mobile and stationary phases are both liquids and form a biphasic liquid system. Centrifugal fields are needed to hold the liquid stationary phase when the mobile phase is pushed through it. Ionic liquids possess properties that have been shown to be beneficial as additives in chromatography. However, their high viscosity has prevented their routine use in CCC as instrumentation is unable to cope with the high back pressure generated by these liquids. The use of dilute solutions of ionic liquids in CCC has been sporadically reported. The Northern Ireland team report on the custom design of a CCC instrument that enables the use of ionic liquids in which their viscosity, density and interfacial tension can be manipulated to allow the separation of virtually any soluble mixture. The effectiveness of such ILCCC was demonstrated in the separation of transition metal salts, arenes, alkenes and sugars on the 0.1–10-gram scale. It promises to be a valuable addition to the armoury of chromatographic methods available to the chemist today.

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



From chlorine to sarin

Chemical weapons, past and present

BY **COLIN A. SCHOLES**

Ongoing conflict in Syria has returned the weaponisation of chemicals to maim and kill military combatants and civilians to the public consciousness.

The incidents of chemical weapons use in Syria, as part of the ongoing civil war, have globally demonstrated the tragedy these weapons can inflict. Conversely, the award of the 2013 Nobel Peace Prize to the Organisation for the Prohibition of Chemical Weapons (OPCW) has demonstrated efforts and success in reducing and in some cases eliminating weapons stockpiles.

The origins of chemical weapons go back 160 years to the British forces in the Crimean War and the Union forces in the American Civil War. Artillery shells were filled with chlorine gas (a pulmonary agent) and fired into the opposition lines, though in only limited instances. The full weaponisation of chemicals occurred

during World War I, where all sides used a range of agents to inflict heavy casualties. Chlorine gas was used throughout the conflict. In the beginning, chlorine gas attacks had devastating consequences, most notable in the second battle of Ypres, because gas masks and protective equipment had yet to be widely distributed. However, its effectiveness over the period of the war became limited because of its visibility to soldiers as a pale green mist, which provided time for soldiers to take countermeasures.

The declining effectiveness of chlorine gas led to the use of phosgene (COCl_2) as a weapon, given it is colourless. Exposure to phosgene causes severe chemical burns to the skin and eyes, and impedes a soldier's

ability to breathe. Death is caused by suffocation due to a build-up of fluid in the lungs. Phosgene was so effective that it has been attributed to 85% of deaths due to chemical weapons during World War I, and the eerie outcome of an attack has been brilliantly captured in Erich Maria Remarque's 1929 novel, *All quiet on the Western Front*.

The tragedy of both of these chemicals is that neither was developed for military purposes – chlorine gas has been known to chemists since Sir Humphry Davy reported it in 1810, while phosgene was developed as a precursor for a range of chemical syntheses.

World War I is often associated with mustard gas, also known as sulfur mustard and by its proper name 1-chloro-2-((2-chloroethyl)sulfanyl)-ethane. It was named because in its impure weaponised form the gas is yellow-brown with an odour resembling mustard and garlic. Mustard gas is a blistering agent because its absorption into the body through the lungs, eyes and skin causes severe chemical burns and thus large blisters form across the body. The macabre purpose of sulfur mustard was to incapacitate soldiers, as well as overload an opponent's medical facilities in treating both military and civilian casualties.

Sulfur mustard was first synthesised almost a century before World War I, but its hazardous nature was only established in 1913, when English biochemist Hans Clarke, while working with German chemist Emil Fischer, was hospitalised after being exposed to a concentrated form in the laboratory in Berlin.

The use of mustard gas in warfare represented a change in weaponisation of chemicals compared to chlorine and phosgene. Sulfur mustard as a vapour cannot be readily dispersed, and hence to increase the effectiveness it was delivered as an aerosol, in which the sulfur mustard is contained within a fine solvent drop.



Pallets of 155-millimetre artillery shells containing mustard gas at Pueblo chemical weapons storage facility in Colorado, USA. The USA has been steadily destroying its entire stockpile of chemical weapons and will continue to do so until none remain.

US Government via Wikimedia Commons

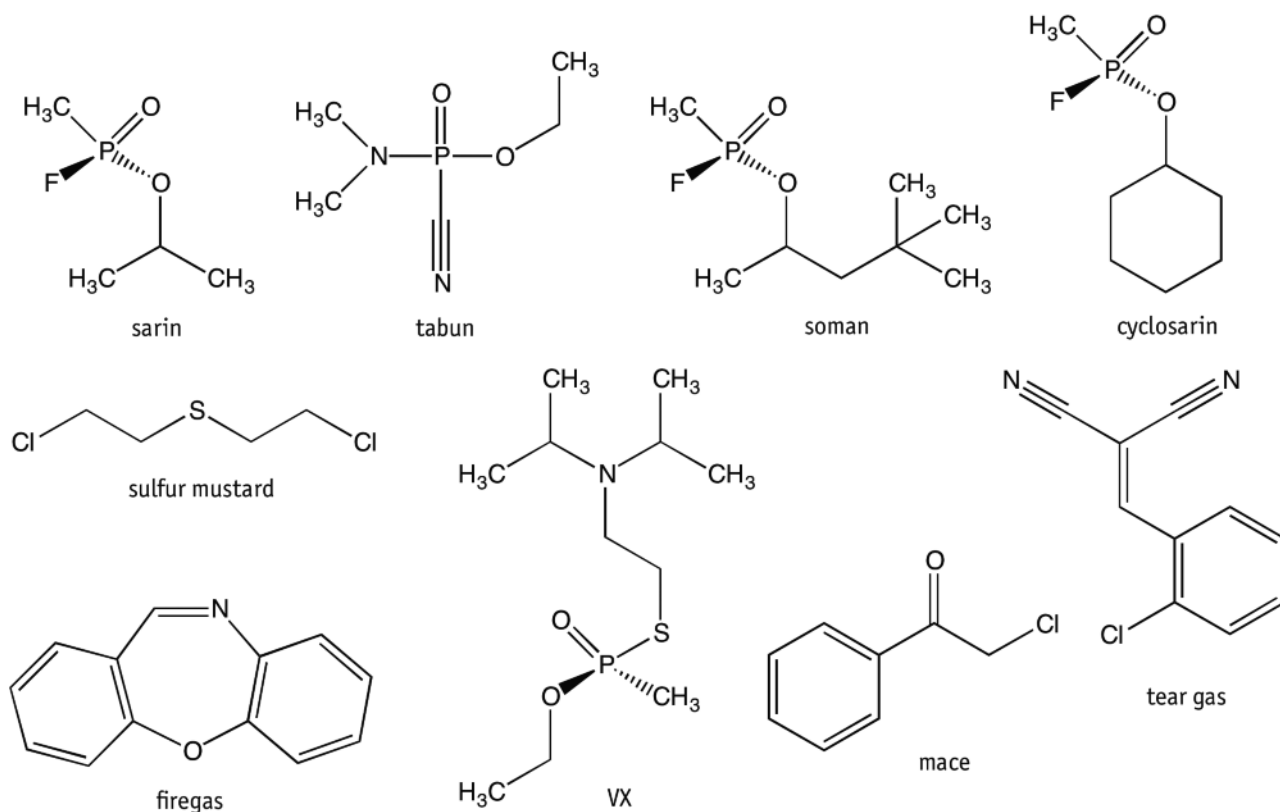
This dramatically increased the distribution area of an attack and led the way for other non-gaseous chemical agents to become weaponised. The stability of sulfur mustard also meant the active agent could persist in the soil and water of contested areas for extended periods of time, and hence have continual impact on soldiers and military personnel long after the initial attack had ceased.

Aerosol distribution has been used to deliver other chemical weapons, for example those classed as blood agents. These are based on cyanogen chloride and arsine (AsH_3) derivatives. On their own, these chemicals are too volatile to be weaponised in a gaseous form, and hence are delivered in an aerosol to ensure dispersion over a wide area and increased the probability of contact with enemy personnel. Blood agents enter the blood through contact within the lungs, where they react with haemoglobin, destroying red blood cells.

Again, both cyanate- and arsine-based chemicals were not originally developed for warfare; rather they

were the product of inquisitive chemists in the preceding century, with arsine known since the late 18th century. Similarly, aerosols and the wide-scale land distribution of chemicals in aerosol form had initial application in the agricultural industry (September 2014 issue, p. 20). This highlights the insidious nature of chemical warfare – so much of the technology has been derived from the advancements chemists have made in other, more beneficial, fields of endeavour.

The macabre purpose of sulfur mustard was to incapacitate soldiers, as well as overload an opponent's medical facilities ...



The Syria incidents have been attributed to sarin, a nerve agent. Nerve agents were specifically developed for warfare. Sarin (also given the code GB) was originally developed by Germany before and during World War II, and is classed in the G-series of nerve agent along with tabun (code GA), soman (GD) and cyclosarin (GF). These are so named because German scientists were the first to synthesise them. Other chemical weapons that Syria has stockpiled in preceding decades have been sulfur mustard and VX (another nerve agent). Stockpiles of these chemicals, including sarin, are currently being destroyed under a UN-sponsored agreement.

Sarin is based on (*RS*)-propan-2-yl methylphosphonofluoride, which inhibits the acetylcholinesterase enzyme in nerve cells, causing them to fire continually. This causes convulsions as well as involuntary urination and defecation because a person loses all muscle control. Death is almost always due to asphyxiation



Sarin (red) inhibits the enzyme acetylcholinesterase (yellow), which degrades the neurotransmitter acetylcholine (blue). Acetylcholine builds up in the synaptic cleft and nerve impulses are effectively continuously transmitted.

RichHard-59/CC BY-SA 3.0

because of loss of respiratory muscle control – victims can no longer breathe. Nerve agents' primary method of delivery is through the respiratory tract in the form of aerosols, but they can be absorbed through the skin, which means soldiers must don full chemical protective suits when under nerve agent attack. Sarin and other G-series agents have immediate effect on those exposed, as evident by the events in Syria; however, they do not persist in the environment.

The other nerve agents, V-series, do persist in the environment because they do not degrade or wash away easily, meaning they will remain on clothes and exposed surfaces for long periods of time. This enables a military to essentially poison terrain and disrupt the movement of enemy forces. Such chemical weapons are known as area denial weapons. The most dangerous of the V-series is VX, short for 'venomous agent' and known to chemists as ethyl ((2-(bis(propan-2-yl)amino)ethyl)sulfanyl)(methyl)-

phosphinate. VX is 10 times more toxic than sarin, and is odourless and tasteless, with exposure possible through skin and eyes and by inhaling. The only military use of VX has been alleged in the Halabja chemical attack by Iraq against Kurds in 1988, with traces of VX found on armaments. However, recently VX has been attributed to the alleged assassination of Kim Jong-nam (brother of North Korean leader Kim Jong-un), in Malaysia in February 2017.

All of the previously mentioned chemical agents are considered weapons of mass destruction, and their use, production and stockpiling is outlawed under the Chemical Weapons Convention. However, some chemical agents are used legally to inflict injury on people. These are incapacitating agents (identified as Schedule 2 substances under the Convention). The most common is tear gas, used by police and military forces worldwide to control riots and disperse crowds. The official name is CS gas, and it is a controlled substance under the Chemical Weapons Convention, meaning it can be produced, stockpiled and used by government agencies in a controlled manner. The active ingredient is 2-chlorobenzalmalononitrile, which causes strong irritation to the nose, mouth and throat as well as tearing in the eyes, hence its name. The victim's response is dependent on the amount of exposure, but it is generally severe

The Syria incidents have been attributed to sarin, a nerve agent. Nerve agents were specifically developed for warfare.



US soldiers wearing full chemical protection. US Government via Wikimedia Commons

enough to result in the victim needing to keep their eyes closed and hence become disoriented.

Pepper spray, another incapacitating agent, is based on capsaicin, which causes irritation to the eyes, leading to pain, tears and temporary blindness. Not considered a controlled substance, it is found in a range of personal protective sprays and animal repellants. Pepper spray is often called Mace; however, Chemical Mace, also known as CN gas, is based on an aerosol of phenacyl chloride. This is a much stronger incapacitating agent than capsaicin and tear gas, though with increased toxicity.

An older incapacitating agent that has gone out of favour was known as firegas, also called CR gas, which is based on dibenzoxazepine, and which is 10 times more powerful than tear gas. Exposure leads to immediate incapacitation because of intense irritation to the eyes, throat and skin; but it can be lethal in enclosed spaces because of its increased toxicity.

A more devious incapacitating agent is known by the stylised name of Agent 15, BZ, Buzz, or in Russia as Substance 78. This is an aerosol of 3-quinuclidinyl benzilate, which results

in confusion and stupor response, rather than an irritation response. The chemical agent can also result in hallucinations in victims, sometimes causing them to disrobe because of the confusion. It was originally developed for treating gastrointestinal ailments but was found more suitable by the US military as a chemical warfare agent through their research into psychoactive incapacitating agents. This is another example of fundamental chemistry research being appropriated for military purposes.

The development of chemical agents for warfare represents a horrendous pursuit of the chemistry field and the appropriation of discoveries made for more benign applications a travesty of chemistry research. The activities of the Organisation for the Prohibition of Chemical Weapons must be continually supported and strong international responses must be made to investigate alleged and proven chemical weapons incidents.

Colin Scholes FRACI CChem is a lecturer in the Department of Chemical Engineering at the University of Melbourne. A partner article about protection in and prevention of chemical warfare will be published in a forthcoming issue of *Chemistry in Australia*.



Free software for chemistry

BY **DAVID WINKLER**

The main tools of scientific enquiry are increasingly being enriched by computational modelling and simulation.

Working together, the three complementary research methodologies of theory, experimentation and computational modelling and simulation are accelerating the rate of scientific discovery, providing otherwise intractable access to mechanistic details of many physical and biological processes.

While there is much useful software available for chemistry, the cost of commercial packages can be a deterrent to wider application. Fortunately, several open-access movements make high-quality software available for little or no cost.

The following examples of free software of potential interest to chemists are not exhaustive – many thousands of packages are available for chemical applications. Virtually every area of chemistry has relevant free packages available.

These include, but are not limited to:

- simulation of chemical reactions
- software for chemical inventories
- simulation of physical properties
- simulation of NMR, IR, Raman, and UV/visible spectra
- analysis of mass spectrometry data for small molecules and peptides
- chemical database and property filtering
- molecular modelling using quantum chemical, molecular dynamics and molecular graphics
- electronic laboratory notebooks
- cheminformatics and bioinformatics
- molecular structure–property relationships modelling
- machine learning and statistical analysis
- kinetics and thermodynamics
- chemical structure drawing, editing and display
- docking of ligands to proteins
- toxicity prediction
- teaching demonstrations.

The number of open-access and free chemistry software packages is dynamic and constantly growing, making a printed list or website unrealistic. These packages can save considerable time compared to carrying out the same operations by hand. A large commercial project in which I was involved used AutoDock to conduct 300 000 docking calculations for all unique proteins in the Protein Data Bank. Most software packages are available for Windows operating systems, and a large majority run on multiple operating systems.

Artificial intelligence, machine learning, statistical modelling, QSAR

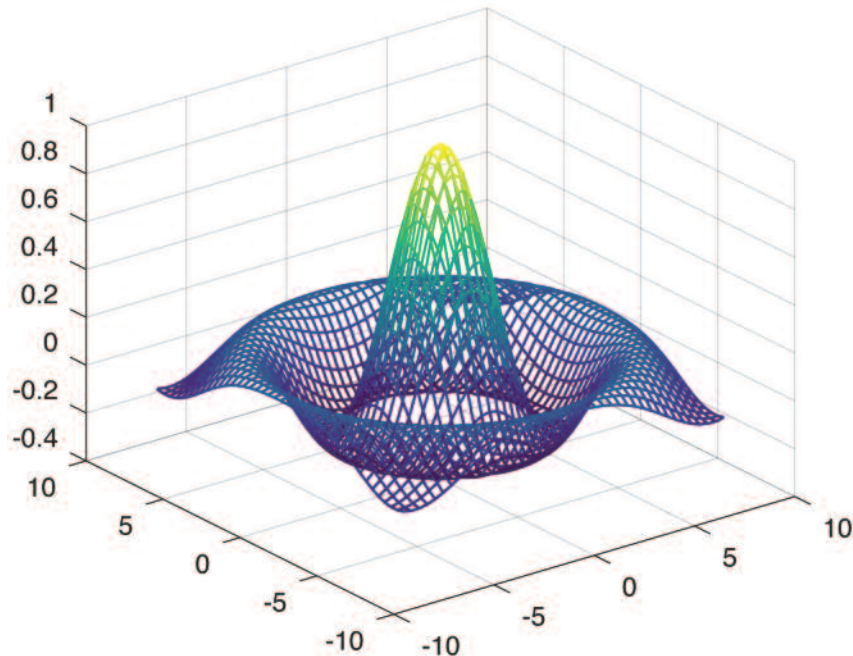
Octave A high-level programming language for numerical computations using a language that is mostly compatible with the commercial package MATLAB. Supports the Shogun machine learning package (<http://shogun.ml>), amongst others. (www.gnu.org/software/octave)

TensorFlow Developed by the Google Brain Team within Google's Machine Intelligence research organisation for machine learning and deep neural networks research. (www.tensorflow.org)

Weka A collection of machine learning algorithms for data mining tasks written in Java, developed at the University of Waikato. (www.cs.waikato.ac.nz/~ml/weka)

Chemical reaction prediction

AutoClickChem A computer algorithm that performs myriad click-chemistry reactions in silico. (<https://sourceforge.net/projects/autoclickchem>)



An example of the 3D graphing capabilities of Octave. Octave

Cheminformatics

Chemistry Development Kit (CDK) A collection of modular Java libraries for processing chemical information that are free and open source. (<https://cdk.github.io>)

OpenBabel A chemical toolbox mainly used to interconvert chemical file formats. (http://openbabel.org/wiki/Main_Page)

Knime An open-source data analytics, reporting and integration platform whose components include machine learning and data mining. KNIME allows users to visually create data flows (or pipelines). (www.knime.org)

Drawing and visualisation

XDrawChem A package for chemical structure drawing and editing. It can simulate NMR spectra and predict pK_a and octanol water partition coefficients. (www.woodsidelabs.com/chemistry/xdrawchem.php)

Molsketch A 2D molecular editing tool for drawing molecules for publication. (<https://sourceforge.net/projects/molsketch/?source=directory>)

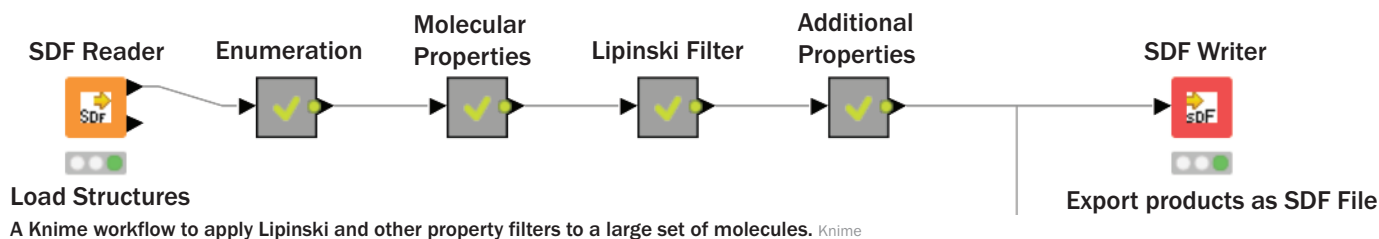
WebChemViewer A simple, open-source program that generates output suitable for viewing on a web browser without needing additional software. (<https://sourceforge.net/projects/webchemviewer>)

Molecular docking

AutoDock and Vina A suite of automated docking tools that predicts how small molecules (peptides or drug candidates) bind to a target protein. Vina is a fast, well-validated package that automates and combines the grid calculations and docking required to locate favourable binding sites in proteins. (<http://autodock.scripps.edu>)

rDock A versatile package for docking small molecules against proteins and nucleic acids in high throughput virtual screening and binding mode prediction studies. (<http://rdock.sourceforge.net>)

DOCK A comprehensive protein docking software package from the University of California, San Francisco. (<http://dock.compbio.ucsf.edu>)



NASA software catalogue: free access to technologies for earthly applications



The new NASA software catalogue includes the code LEWICE, developed to help study the effects of ice on an aircraft in flight and to help create ice detection systems. NASA

NASA's 2017–18 software catalogue offers an extensive portfolio of software products for a wide variety of technical applications, all free to the public, without any royalty or copyright fees.

Available in both hard copy and online, this third edition of the publication has contributions from all the agency's centres on data processing/storage, business systems, operations, propulsion and aeronautics. It includes many of the tools NASA uses to explore space and broaden our understanding of the universe. A number of software packages are being presented for release for the first time. Each catalogue entry is accompanied by a plain language description of what it does.

'The software catalogue is our way of supporting the innovation economy by granting access to tools used by today's top aerospace professionals to entrepreneurs, small businesses, academia and industry', said Steve Jurczyk, associate administrator for NASA's Space Technology Mission Directorate (STMD) in Washington.

NASA published the first edition of its software catalogue in April 2014, becoming the first comprehensive listing of publicly available software to be compiled by a federal government agency – the largest creator of custom code. Since then, NASA has shared thousands of its software programs with students, industry, individuals and other government agencies.

Some of the software available include codes for more advanced drones, and quieter aircraft. While access restrictions apply to some codes, NASA has automated and updated its software release process over the last two years to ensure that it is as quick, easy and straightforward as possible.

The software catalogue is a product of NASA's Technology Transfer program, managed for the agency by STMD. The program ensures technologies developed for missions in exploration and discovery are broadly available to the public.

NASA

Rosetta A suite of software for modelling protein structures, structure prediction, protein design, and remodelling of proteins and nucleic acids. (www.rosettacommons.org/software)

Molecular dynamics

GROMACS A molecular dynamics package mainly designed for simulations of proteins, lipids and nucleic acids. (www.gromacs.org)

LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) A classical molecular dynamics code for simulating solid-state materials (metals, semiconductors), soft matter (biomolecules, polymers) and coarse-grained or mesoscopic systems. (<http://lammps.sandia.gov>)

NAMD (Not Another Molecular Dynamics Program) An efficient molecular dynamics simulation package. (www.ks.uiuc.edu/Research/namd)

Molecular visualisation

Avogadro A cross-platform use in, for example, computational chemistry, molecular modelling, bioinformatics and materials science. (<https://sourceforge.net/projects/avogadro>)

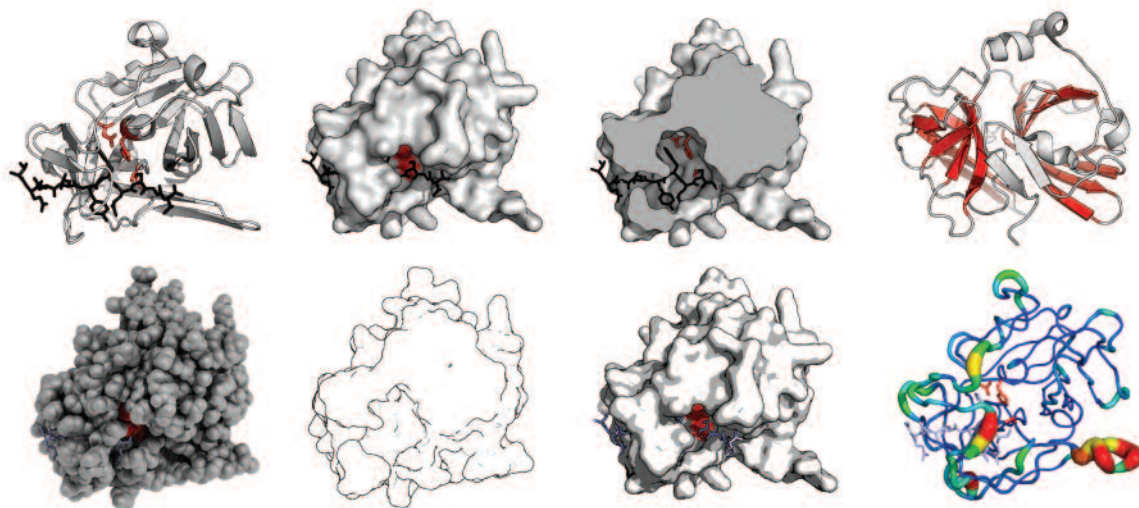
JMol A molecular viewer for chemical structures that can read many file types, including PDB, SDF, MOL, and those generated by Spartan Gaussian, GAMESS, MOPAC, VASP, CRYSTAL, QuantumEspresso, VMD and many other quantum chemistry packages. (<https://sourceforge.net/projects/jmol>)

PyMOL A user-sponsored, open-source molecular visualisation system released under the Python Licence. It generates publication-quality 3D images of small molecules and proteins. (www.pymol.org)

RasMol A molecular graphics program intended for the visualisation of proteins, nucleic acids and small molecules. (<http://rasmol.org>)

Quantum chemistry

MOPAC7 A semi-empirical molecular orbital software package with a long



PyMOL representations of tobacco etch virus protease rendered in different modes. Standard cartoon, surface, cut-through of surface, highlighted barrels, 'QuteMol'-like, 'Goodsell'-like, glossy-surface, and b-factor putty. Thomas Shafee/CC BY 4.0

and distinguished development history. (<https://sourceforge.net/projects/mopac7>)

NWChem A versatile, high performance quantum chemistry suite capable of running Hartree–Fock, density functional theory (DFT), MP2 and CASSCF calculations on biomolecules, nanomaterials, and small molecules. (www.nwchem-sw.org/index.php/Main_Page)

QuantumEspresso An integrated suite of codes for electronic-structure calculations and materials modelling based on density-functional theory, plane waves and pseudopotentials. (www.quantum-espresso.org)

GAMESS GAMESS can perform Hartree–Fock (DFT), generalised valence bond (GVB), and multi-configurational self-consistent field (MCSCF) calculations and includes solvent and relativistic effects. (www.msg.ameslab.gov/gamess/download.html)

Spectroscopy and mass spectrometry

Mass-Up A MALDI-TOF data analysis software package for proteomics. (<https://sourceforge.net/projects/mass-up/?source=directory>)

Raman Tool Set Software for processing and analysis of Raman spectra and spectroscopy data. (<https://sourceforge.net/projects/raman-toolset/?source=directory>)

MatNMR A collection of MATLAB/Octave scripts to analyse and display NMR and EPR data. Unlike other packages, MatNMR provides direct access to the data matrices. It can also create publication-quality 1D, 2D and 3D plots. (<http://matnmr.sourceforge.net>)

Toxicity prediction

ToxTree An application that estimates toxic hazard of chemical compounds. (<https://sourceforge.net/projects/toxtree/?source=directory>)

TEST Toxicity Estimation Software Tool from the US EPA that uses QSAR (quantitative structure–activity relationship) to estimate chemical toxicity to aquatic species and rats, and predicts water solubility, melting point and bioconcentration factors. (www.epa.gov/chemical-research/toxicity-estimation-software-tool-test)

Hopefully, this article will stimulate chemists to explore the internet more widely for useful tools. Visit the Wikipedia page for free and open-access software (https://en.wikipedia.org/wiki/List_of_free_and_open_source_software_packages) and the chemistry sections of open access sites, such as Sourceforge (sourceforge.net), GNU (www.gnu.net) and GitHub (www.github.com). NASA recently opened their extensive software repository for public download (<https://software.nasa.gov>; see box p. 26). This contains useful software for materials, propulsion and environmental science, and image processing.

It is worth the effort implementing an automated search for new software in your research area of interest, or performing regular searches online to benefit from updates and new software offerings.

Professor David Winkler FRACI CChem is a computational chemist and molecular designer who recently left CSIRO for academic positions at Monash and La Trobe universities. He has published extensively on the design, modelling and simulation of bioactive molecules and materials for therapeutic and regenerative medicine, and was the recent recipient of the Adrien Albert award from the RACI and the Herman Skolnik award from the American Chemical Society.

Rapid progress

Phenotyping in the field

BY **DAVE SAMMUT**

A recently fledged business is about to take its new phenotyping technique to market.

Australia hasn't always had the best track record in commercialising the ideas coming out of its universities. There are plenty of barriers and hurdles in the way of success. Happily, there are some instances where academia, government and entrepreneurship have come together to great effect.

The team at Rapid Phenotyping (www.rapidphenotyping.com) first came together while studying for their respective PhDs at the University of Newcastle. After forming their company just a year ago, they are now poised to launch their product to market.

The starting point for Rapid Phenotyping's journey was Dr Antony Martin's and William Palmer's academic study of high-yield sorghum grass varieties for both first- and second-generation biofuel production. Total sugar yields are important for first-generation biofuel production, while the biomass component and the 'digestibility' of that biomass is also considered for high-yielding second-generation biofuel crops. Breeding for these traits required high-throughput measures of the chemistry of both the sugar component in the juice and the cell wall components of the biomass.


The existing phenotyping techniques were laboratory-based wet chemical assays. These techniques were laborious and time consuming, involving considerable sample preparation, and results would take days or weeks to obtain. Put simply, they were unsuitable for high-throughput analyses, for mobile devices or for real-time decision-making *literally* in the field(s).

Martin and Palmer's work came together with that of neuroscientist Dr Jamie Flynn. Coming from their various studies, the team have brought together a novel product for the agricultural industry – with visions for much wider application.

'We started working with technologies like near-IR and FTIR spectroscopy', says Martin, 'and applying some fairly common techniques to build predictive models of certain components of plants. We developed some novel components and built some novel models, but we saw restrictions on getting this technology out to consumers and farmers who might want to apply this technology in a much more usable way.'

'We started on a journey that involved firstly improving the technology, including building new





The work started from a breeding program for new, high-sugar sorghum varieties optimised for biofuel production.

devices. We're pushing the boundaries of the techniques in the device. We've done a lot of innovative optical work, incorporating a number of spectroscopic techniques into one device, then improving the designs of the devices to manufacture them much more cheaply, making them smaller and portable for people in the field to take these sort of measurements. We've done a lot of work on the hardware, and that's where we're filing patents at the moment.

We're expanding the capabilities of technologies like near-IR to be able to measure pretty much any solid or liquid material, and measure components that are present in much smaller quantities.'

The other aspect of the technology is the software. The team started out using standard regression-based modelling techniques like PLS (partial least squares). That works quite well, but they were struggling to detect certain molecules using near-IR and PLS. So the team ventured into the world of AI, using PLS alongside more

sophisticated mathematical modelling techniques and intelligent data transformations. Applying new machine learning techniques to a combination of processes, Rapid Phenotyping's system automates the process of building and optimising very accurate predictive models. 'We're seeing something like a 50% improvement in error rates,' says Martin.

'We've packaged it together in an easy-to-use platform for people who want to use this without the need for specialists in the area.'

The work started from a breeding program for new, high-sugar sorghum varieties optimised for biofuel production. Sorghum is a type of grass, often grown for cattle feed. With a variety that looked more like sugar cane – tall, with a thick stem – the breeding was generating thousands of samples, and a new analytical technique was required to make the characterisation of the sugar components practicable.

The particular advantage of field analysis for phenotyping is timing. For

example, in the application of fertiliser, there is a lot of benefit to being able to know the nitrogen and phosphorus requirements in real time. Most particularly, there are real advantages to being able to analyse the grain at harvest time.

Knowing when the sugars, proteins or oils have peaked will allow the optimisation of quality and yields, which isn't possible if the farmer is waiting one or two weeks for analytical data. So while a winemaker might use a Brix meter to analyse sugars in the grapes at harvest time, Rapid Phenotyping claims that its device can yield simultaneous data about the acid content, another key variable in the grape, and most other components that would be tested in a wet laboratory.

Rapid Phenotyping is focusing on agricultural products in the near term. Progressing through an 'early adopter' trial program, it is building towards the launch of its product in early 2018.

Asked about the challenges of getting this far, Martin said 'We've all

come from a research science background. We're not trained in commercialisation or business, but as we're working with customers and developing the business model and manufacturing processes, we've really had to call on others with varying expertise.'

'One of our early successes, right at the beginning, was to approach the business community in the Hunter region. We found a bunch of

experienced advisers who've built businesses in the region. We have set up a support network who have been able to guide us through the processes – that has been absolutely invaluable to the project. Then more recently, we've brought on board new team members who have that experience in business and commercialisation.'

So what's Martin's advice to other PhD students? 'Give it a shot. Don't be

scared. But seek advice from people who know how to do this stuff. When you go out and ask people for help, they're generally more than willing to offer their time when you value their expertise.'

Importantly, government support has proved similarly useful to Rapid Phenotyping's early progress. Some early cash from the NSW Tech Voucher program allowed the company to build its first prototype. The company has

Dual-purpose biofuel crops could extend production, increase profits



Haibo Huang, an assistant professor at the Virginia Polytechnic Institute and State University, squeezes bio-oil out of PETROSS sugarcane to process into biodiesel. Haley Ahlers/PETROSS

Today, many biofuel refineries operate for only seven months each year, turning freshly harvested crops into ethanol and biodiesel. When supplies run out, biorefineries shut down for the other five months. However, according to recent research, dual-purpose biofuel crops could produce both ethanol and biodiesel for nine months of the year –increasing profits by as much as 30%.

'Currently, sugarcane and sweet sorghum produce sugar that may be converted to ethanol,' said co-lead author Stephen Long, Gutsell Endowed Professor of Plant Biology and Crop Sciences at the Carl R. Woese Institute for Genomic Biology at the University of Illinois. 'Our goal is to alter the plants' metabolism so that it converts this sugar in the stem to oil – raising the levels in current cultivars from 0.05% oil, not enough to convert to biodiesel, to the theoretical maximum of 20% oil. With 20% oil, the plant's sugar stores used for ethanol production would be replaced with more valuable and energy dense oil used to produce biodiesel or jet fuel.'

A paper published in *Industrial Biotechnology* simulated the profitability of Plants Engineered to Replace Oil in Sugarcane and Sweet Sorghum (PETROSS) with 0%, 5%, 10% and 20% oil. They found that growing sorghum in addition to sugarcane could keep biorefineries running for an additional two months, increasing production and revenue by 20-30%.

Today, PETROSS sugarcane produces 13% oil by dry weight, 8% of which is the kind of oil used to make biodiesel. At 20% oil, sugarcane would produce 13 times more oil – and six times more profit – per acre than soybeans.

A biorefinery plant processing PETROSS sugarcane with 20% oil would have a 24% international rate of return – a metric used to measure the profitability of potential investments – which increases to 29% when PETROSS sorghum with 20% oil is processed for an additional two months during the sugarcane off-season.

'When a sugarcane plant has to shut down, the company is still paying for capital utilisation; they have spent millions of dollars on equipment that isn't used for five months,' said co-lead author Vijay Singh, Director of the Integrated Bioprocessing Research Laboratory at Illinois. 'We propose bringing in another crop, sweet sorghum, to put that equipment to use and decrease capital utilisation costs.'

By decreasing capital utilisation costs, the cost to produce ethanol and biodiesel drops by several cents per litre. Processing lipid-sorghum during the lipid-cane off-season increased annual biofuel production by 20 to 30%, thereby increasing total revenue without any additional investment in equipment.

The simulations in this paper accounted for the equipment required to retrofit ethanol plants to produce biodiesel. In the US, about 90% of ethanol plants are already retrofitted to produce biodiesel. According to Singh, in places like Brazil where they produce a large amount of sugarcane, it makes sense to retrofit ethanol plants. 'Our study shows that it is cost effective to do it.'

Carl R. Woese Institute for Genomic Biology, University of Illinois at Urbana-Champaign

‘We’re expanding the capabilities of technologies like near-IR to be able to measure pretty much any solid or liquid material, and measure components that are present in much smaller quantities.’

also received \$360 000 through the Accelerating Commercialisation program. ‘This has been hugely beneficial,’ says Martin, ‘You’re assigned a business adviser with that – someone to ask all the questions that we lacked experience in.’

More than just monetary help, AusIndustry, Jobs 4 NSW and the NSW Department of State and Regional Development have all been extremely supportive. ‘Just by approaching the government’, says Martin, ‘we’ve been inserted into networks that have been invaluable in getting us this far.’

‘I met with Antony, Wil and Jamie over 18 months ago to talk about a project they were developing at the University of Newcastle and was impressed with their technology and ideas, which had the potential to make a significant impact on global food production’, says Nicolas Van der Voort, of the Hunter Office of Regional Development. ‘As a business development manager for NSW Trade and Investment (now Premier and Cabinet) I connected the guys with a number of NSW state and federal agencies, including the NSW Tech Voucher program for engineering design of tumblers, leveraging support for commercialisation (AusIndustry), and export/trade commission support



The Rapid Phenotyping team (L-R): Jamie Flynn, William Palmer, Antony Martin, Peter Tyler and Jacob Lorber. They are eagerly anticipating the imminent launch of their innovative device.

(NSW TradeStart), plus local business contacts with potential synergies.’

With good ideas and great support, Rapid Phenotyping has been fortunate in the early success of the company. This has been supported by good attention to cash flow. Founding the company in March 2016, the entrepreneurs initially supported themselves by seeking funding for the design and implementation of an associated 3D microscope project for the Hunter Medical Research Institute, and in their spare time brought in consulting revenues to build

spectroscopic models for early clients. That work proved the concept, paving the way for the new product.

‘We’re doing something different in Australia by trying to build new hardware. There are a whole lot of challenges that go along with that, but we’re overcoming them. We’re very excited about our new product.’

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.

Peter Roy Wilkinson

A learned, engaging and compassionate man

The *West Australian* of 13 November 1941 reported the names of the 50 children who had won secondary school scholarships to commence in 1942. The list included Robert J.L. Hawke (future PM), John O. Stone (future Secretary to the Treasury), John M. Wheeldon (future Senator for Western Australia), Peter R. Wilkinson and Lloyd S. Zampatti (future head of Swan Breweries and Castlemaine Tooheys).

Peter Wilkinson was the only winner who had been educated by correspondence classes. Peter lived on his family's farm in Aldersyde in the Western Australian wheat belt, 165 kilometres south-east of Perth. The scholarship was worth £50 a year, including the cost of living away from home. The family chose to send him to Albany High School. He lived, as he described it, 'at an establishment catering for about eight boys'. His letters to home came back corrected in red ink by his mother, still being the correspondence teacher! At Albany High School, he claimed to be 'good at classwork, but a dud at metalwork, woodwork and sport'. When the family moved from Aldersyde to Perth, Peter transferred to Perth Modern School. He described his new classmates Hawke, Stone, Wheeldon and Zampatti as having 'incisive minds, rapid repartee and withering wit'. As indeed, did Peter!

Peter did well in his final year at Perth Modern School, including passing a subject called 'Industrial History and Economics', possibly useful background for his later career. His results earned him a scholarship for children of ex-servicemen and he commenced a science degree at the University of Western Australia. He obtained first class honours in physical



chemistry in 1950 and completed a Master's degree in mid-1952. Both of the theses were on the photoconductivity of aromatic hydrocarbons. His supervisor was Professor N.S. Bayliss, RACI President 1955–6.

In February 1952, Peter applied for both an Australian Canteen Trust Fund scholarship to go to the University of Bristol for his PhD studies and a research officer position at the CSIRO Division of Forest Products in Melbourne. He was informed of his success in the CSIRO application in March of 1952 and of the scholarship application in 1953. He worked for CSIRO from June 1952 until July 1953.

He married Violet (Vi) Garvey in 1953 and they went almost immediately to the University of Bristol. Peter studied for a PhD with the distinguished surface chemist D.D. Eley. His 1960 *Proceedings of the Royal Society* paper with Eley on this work has 124 citations, including two in 2017.

In 1957, ICIANZ was recruiting for its new Central Research Laboratories at Ascot Vale, a suburb of Melbourne, and Peter secured a position. He worked there until 1964 doing research on catalysts in hydrocarbon processing plants before transferring to head office as a planning officer in the Development Department. He became the leader of the New Development Section in 1965 and was the company's chief economist when he retired in 1991. His main task was to

Peter retired from ICI Australia in 1991 but continued to be very intellectually active. His paper 'Professionalism and economic advantage in the chemistry profession in Australia, 1914–1932' ... is a great insight into Peter's way of thinking.

interact with the main economic forecasters, senior public servants and politicians and report to the ICIANZ senior management and directors. This job 'suited my talents'.

He was an active member of the Australian Labor Party from 1963 until 1987 when Paul Keating allowed Rupert Murdoch to own The Herald and Weekly Times. His aim was to be the Minister for Science or Minister for the Environment by entering Parliament as the Member for Maribyrnong. He tried out as a candidate for the then safe Liberal seat of Isaacs in the 1966 election. Internal factional politics within the Victorian Branch saw Dr Moss Cass endorsed for the seat of Maribyrnong in the 1969 election. Dr Moss Cass did become the Minister for the Environment and Conservation in the Whitlam government. I first met Peter in the early 80s when we both were members of the Victorian Branch Energy and Resources Policy Committee. Once again, he lost his position on this committee because he lacked factional backing.

Peter was always interested in the industrial and professional interests of chemists. In 1961, he was approached to be the President of the Association of Professional Scientists of Australia and stayed in that position until 1972 when the organisation had been registered as a union and the first awards were secured.

The RACI was his next interest. Two of his friends from school and university days, Athel Beckwith and Jim O'Donnell, were Vice-President or President from 1983 to 1986 and I, a fellow graduate of the University of Western Australia, was in those positions from 1985 to 1987. Peter was the Honorary General Secretary during all these years and became the Vice-President himself in 1987 and President in 1988. The WA connection was a happy coincidence! His period of office was quite an eventful time for the RACI and the country. Within the RACI, he oversaw the change of Executive Secretary from Peter Woodhouse to Noel Hart (temporarily) and then Fred Bryant, and within the country, the floating of the Australian dollar and the general lowering of tariffs. A busy time for the ICI Chief Economic Advisor! As President, I certainly valued his advice.

Peter retired from ICI Australia in 1991 but continued to be very intellectually active. His paper 'Professionalism and economic advantage in the chemistry profession in Australia, 1914–1932' (*Historical Records of Australian Science*, 1997, vol. 11, pp. 481–499) is a great insight into Peter's way of thinking.

His wife, Vi, became ill in the early part of the century and Peter became her carer until her death in August 2008.

Many of Peter's friends enjoyed his company at the Victorian Branch's Retired Chemists Lunches until late in 2016.

Peter was born in Perth on 12 December 1929 and died in Melbourne on 27 April 2017. He is survived by his younger brother Fred, his children Meredith, Roy and Luke and four grandchildren.

Tom Spurling FRACI CChem was assisted by family members and an autobiography written by Peter for his family. Quotes from this are in quote marks.

New Fellow

Ajayan Vinu has been working as a Professor of Nanomaterials at the University of South Australia since October 2015. Before moving to the University of SA, he was working as a full professor at the University of Queensland from September 2011 to September 2015.

Professor Vinu is recognised as a world leader in the field of nanoporous materials, with specific interest in the material's application in carbon capture, energy storage, adsorption and separation, and catalysis. He has introduced a new field of research on nanoporous nitrides and developed novel methods for making new highly ordered nanoporous materials with improved textural parameters and multiple functions. His significant contributions to the field include the discovery of the first nanoporous carbon nitride materials with tunable pore structures and textural parameters; the discovery of the first nanoporous boron nitride and boron carbon nitride materials; and the development of a new class of carbon nanoporous materials with novel architectures, including carbon nanocage, and nanocoops, hexagonal and cubic nanoporous carbons. These nanostructures aim to enhance mechanical, conducting, field emission and energy storage properties for use in advanced materials for supercapacitors, catalysis, fuel cells and the photo-electrochemical conversion of greenhouse gas.

The quality of his research has been recognised with several international awards including Scopus Young Researcher Award (2014), Friedrich Wilhelm Bessel award by the Humboldt Society (2010), JSPS Senior Invitational Fellow (2014), Australian Future Fellowship (Professorial Level) (2010), Indian Society for Chemists and Biologists award for excellence (2010), Catalysis Society of India Young Scientist award (2010), Chemical Society of Japan Award for the Young Scientist (2008), Laureate of Khwarizmi International Award (2008), Asian Excellent Lectureship Award, and ICYS fellowship. Vinu is a Fellow of the Royal Society of Chemistry, an elected Fellow of the World Academy of Ceramics and Foreign Fellow of Maharashtra Academy of Sciences. His contribution in the field of nanoporous materials led to more than 300 papers in high-impact-factor journals with about 14 000 citations and an H-index of 61 (Google Scholar).

Vinu is married to Siji Dhasan and blessed with two smart boys (STEVIN – NIVETS; enantiomers!). He loves to spend time with his family and play cricket and tennis with his boys.



ChemCentre appoints RACI Fellow as new CEO

ChemCentre, a provider of chemical and forensic science services in Western Australia, has announced the appointment of its new CEO, Peter McCafferty FRACI CChem.

McCafferty's scientific expertise spans 35 years, including almost 25 years at ChemCentre and the past 15 years as the Director of ChemCentre's Scientific Services Division (SSD).

Outgoing ChemCentre CEO Peter Millington said an extensive international search was undertaken to find his replacement and he was thrilled that the best candidate for the job was one of ChemCentre's own.

'As Director of SSD, Peter currently supervises more than sixty staff in areas including Emergency Response, Environmental Chemistry, Food and Agricultural Chemistry, Water Chemistry, Petroleum Chemistry, and Occupational Hygiene,' Millington said.

'Peter has directed this diverse group through significant periods of change including transition to a statutory authority, increased financial accountability, absorbing the National Measurement Institute's (NMI) former analytical services in WA, and establishing a strategically focused Research and Development portfolio.

'Mr McCafferty has been an essential member of ChemCentre's Executive team since its creation as a statutory authority in 2007, and has acted as CEO of ChemCentre on many occasions.'

Among his professional achievements, McCafferty is ChemCentre's principal scientific consultant to the WA Government on the Perth Children's Hospital lead issue. He headed the ChemCentre team which was awarded the 2013 Australian Water Association WA Water Award for Water Recycling, and was a key participant in the interagency team that received the 2013-14 Premiers Award for 'Managing the Environment'. Mr McCafferty was also awarded the 2004 RACI Wilf Ewers Citation for 'services to the Profession of Chemistry'.

ChemCentre

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2017 ARC Laureate Fellowships announced

Professor Michelle Coote FRACI CChem (pictured) from the ANU Research School of Chemistry has received the Georgina Sweet Australian Laureate Fellowship for science and technology for a project to establish a new approach to chemical catalysis.

Coote's \$2.3 million fellowship will help establish a new approach to chemical catalysis using the electrostatic effects of pH-switchable charged functional groups.

Using a combination of theory and experiment, she hopes to establish a game-changing approach to controlling chemical reactions, while training the next generation of chemists in the principles of computer-aided chemical design.

'I am particularly pleased to receive the Georgina Sweet Fellowship and see this as an outstanding opportunity help address long-standing gender inequities in chemistry and STEM disciplines generally,' Coote said. 'It will also bring modern cutting-edge solid-state NMR techniques developed overseas to Australia and provide advanced training for Australian NMR researchers.'

Professor Christopher Barner-Kowollik MRACI CChem is a Professor of Materials Science at the Queensland University of Technology and an adjunct research group leader at the

Karlsruhe Institute of Technology. He received his \$3.3 million fellowship award for a project entitled 'Light-induced chemical modularity: a new frontier in macromolecular design'.

Professor Shizhang Qiao FRACI CChem is Chair of Nanotechnology within the School of Chemical Engineering at the University of Adelaide. He received \$2.7 million in funding as a 2017 Laureate Fellow. His research expertise is in nanomaterials and nanoporous materials for new energy technologies, such as electrocatalysis, photocatalysis, batteries, fuel cells and supercapacitors.

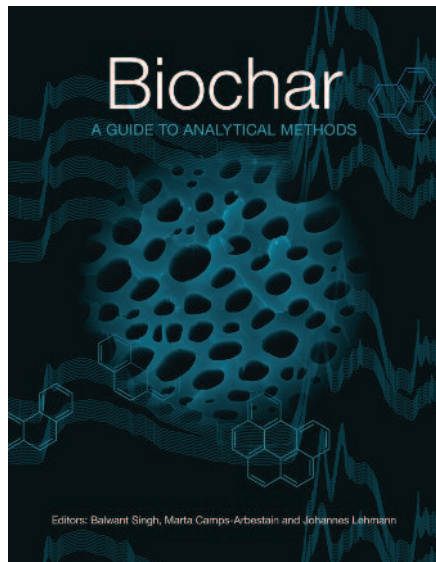
Other chemistry-related recipients included:

- Professor George Zhao, a professor within the School of Chemical Engineering at the University of Queensland, and currently a Vice-Chancellor's Research and Teaching Fellow there. His research focus is nanoporous materials for energy and environmental applications
- Professor Gottfried Otting, head of biomolecular NMR spectroscopy at the ANU Research School of Chemistry, for a project designed to have immediate benefits in the design of lead compounds in drug development.

Australian National University

Biochar: a guide to analytical methods

Singh B., Camps-Arbestain M., Lehmann J. (Eds), CSIRO Publishing and CRC Press, 2017, paperback, ISBN 9781498765534, 310 pp., \$99.95 (Amazon.com price US\$51.36. Online access options available at www.publish.csiro.au/books/ebooks)



Biochar seems to be a bit of a buzzword in soil chemistry and environmental science at present. If you have not heard of the term before, biochar is a type of *charcoal* produced by the conversion of *biomass* (hence the name) via pyrolysis. Different forms can be produced for different applications and soils by varying the type of the initial material used as feedstock and/or the pyrolysis conditions (e.g. temperature, rate of heating and oxygen delivery).

What differentiates biochar from charcoal is its purpose; it is usually produced as an additive to soils, mainly to improve nutrient retention and carbon storage. Advocates also claim it could have applications in everything from climate change mitigation and waste management, through soil fertility and microbiology to biofuel production and pollution remediation. There is certainly a lot of interest in the topic.

The central premise of *Biochar: a guide to analytical methods* is that in order to see if biochar lives up to its hype, it is necessary to be aware of, and be able to accurately measure and assess, its properties. Proper analysis of biochar is therefore very important; and if you want to analyse biochar, then this is definitely the book for you. There are 24 chapters each of which are very comprehensive and provide procedures and guidelines for both routine and advanced characterisation methods. Between them they cover pretty much every type of analysis you could wish to perform on charcoal – everything from absorbance to X-ray analysis is included, and while I suspect the target audience is students and researchers in biochar science, the content is well written and detailed enough that it would also be useful for industry and policymakers in the area.

The book is laid out logically with Chapter 1 discussing recommendations on sampling, storage and preparation of specimens for analysis. Further chapters then detail testing methods to assess physical properties (such as porosity and sorption) and many forms of chemical testing, including (but certainly not limited to) proximate and elemental analysis, binding capacity, elemental analysis, as well as tests for pH, electrical conductivity, liming potential and cation exchange capacity. Each chapter is written by active researchers in the field, from all over the world. A good range of examples and illustrations for all the important points is included, and the advantages and disadvantages of each technique are discussed in depth. I was quite pleased to see that each chapter includes data for the methods presented, from a range of biochar samples. Indeed, the editors seem to have made it a requirement that chapter authors practise what they preach so to speak.

The presentation of the book is also really nice, with consistent formatting and clear and well-defined figures, in high resolution throughout. The latter point may sound trivial, but in this reviewer's humble opinion at least, there are many technically sound science books let down by poor-quality images and figures. Thankfully, this is certainly not the case here. Overall, the editors have done a great job bringing together material from a range of authors into a cohesive whole and for this they should be applauded.

A minor negative is that, as the name suggests, the book focuses entirely on analytical methods, which is fair enough. However, I think it would have been helpful to include an introductory chapter with a discussion of what biochar is and how it is formed, a comparison with similar materials (such as hydrochar), plus some of the historical context such as the *terra preta* soils found in the Amazon Basin. This is, however, a very small gripe on what is overall a very well written, interesting and, above all, useful tome.

Oliver Jones FRACI CChem

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Why is my patent specification so repetitive?

Dr Jacqueline Warner, Associate and Registered Patent Attorney, FB Rice



Have you ever wondered why your patent specification is so repetitive and difficult to read in sections? Patent attorneys draft specifications in this way to ensure it is in the best form possible for prosecuting before the European Patent Office (EPO) and other jurisdictions that have strict amendment laws.

Ideally, a patent specification is drafted so that it can be prosecuted in any jurisdiction. It is almost inevitable that the claims of a specification will need to be amended in each jurisdiction, to some degree, to address any number of objections ranging from novelty to clarity objections. To give the patent applicant the freedom to amend the claims in any jurisdiction, in a manner that will address objections raised by an examiner and still provide a claim scope that is meaningful, the patent attorney aims to draft the specification to a standard that will withstand the toughest examining jurisdiction.

The EPO has a strict assessment on claim amendments and a problem facing many applicants is how to introduce claim amendments without facing the dreaded 'added subject matter' objection under Article 123(2) EPC. Added subject matter objections typically arise when the applicant attempts to amend the scope of a claim to distinguish it from a cited prior art document, and where support for the amendment is not present in the specification as filed.

Types of amendments that are likely to attract an added subject matter objection by the EPO include:

- a) removing features from an independent claim where the feature is arguably essential;
- b) combining features from different embodiments when the resulting combination is not disclosed in the application as filed; and
- c) making intermediate generalisations where a specific feature is isolated from an originally disclosed combination of features, including the examples, to de-limit the claimed subject matter.

In order to avoid an added subject matter objection, the specification is drafted to include as many perceivably different fall-back embodiments as possible. If a fall-back embodiment is not available, then the applicant may need to resort to unnecessarily narrow claims. The skill of the Patent Attorney in interacting with inventors to elucidate all combinations of features is therefore very important.

Accordingly, patent specifications often include:

- separate descriptions for each feature and possible combinations of those features to describe increasingly narrower embodiments;
- a broad range of values followed by a number of progressively narrow ranges which lead to a preferred value;
- a number of intermediate embodiments disposed between the broadest embodiments and the preferred embodiment;
- multiple dependent clauses which provide basis for a variety of different combinations;
- repetition of parts of an embodiment, which may mirror an independent claim, with a different limiting feature to ensure there is support for any one of the limiting features that the claim may need to be limited to at some stage during prosecution; and
- claims (or equivalent text) in multiple-dependent format.

This understandably results in sentences and paragraphs being repeated with only slight variations in language and context.

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

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The IP Navigators

Balance, buffers and bubbles

These experiments involve only kitchen chemicals and so avoid issues of OH&S (if not ethics).

The equilibria explored in these experiments are important in the buffering (resistance to pH change) of our blood. They are important in understanding some of the consequences of increased carbon dioxide in the atmosphere and thus the oceans. They are terribly important in producing a good sparkling wine or beer as well as for common fizzy drinks. So we ask a question, do some simple kitchen experiments, and suggest an answer.

Part 1: Why does adding soda to soda water get rid of bubbles?

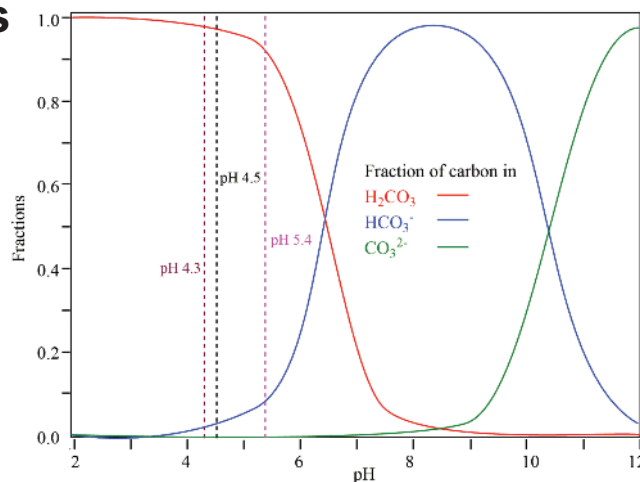
This experiment illustrates the carbon dioxide (carbonic acid)–bicarbonate (carbonate) equilibrium as seen from the side of aqueous carbon dioxide (see diagram below).

What you'll need

- Six pack of small soda water bottles
- Small amount of washing soda
- Spatula or teaspoon
- Lemon
- Drip tray to collect spray from shaken soda bottles

What to do

- 1 Half empty three soda water bottles (labelled 1, 2 and 3) carefully to minimise the loss of gas bubbles. Place them on the drip tray.
- 2 Dissolve a pinch* of washing soda (sodium carbonate) in a teaspoon of water. As a control, dissolve some sugar or salt in another teaspoon of water.
- 3 With gentle stirring, to bottle 1 add the soda solution, and to bottle 2 add the sugar or salt solution. Keep bottle 3 as a second control.
- 4 In bottles 1 and 2, the disturbance will release a small amount of gas. Let it settle.
- 5 Shake or stir the bottles to release bubbles. Bottle 1 will not show any bubble release while bottles 2 and 3 will, and will behave roughly the same.



For optimum carbonation, pH is between 4.3 and 4.5. A.J. deLange

In spite of adding more potential carbon dioxide by adding soda, the soda's strong alkaline nature increases the pH of the solution and this shifts the equilibria so that dissolved carbon dioxide (aka carbonic acid) is changed into (non-gassing) sodium bicarbonate (see graph).

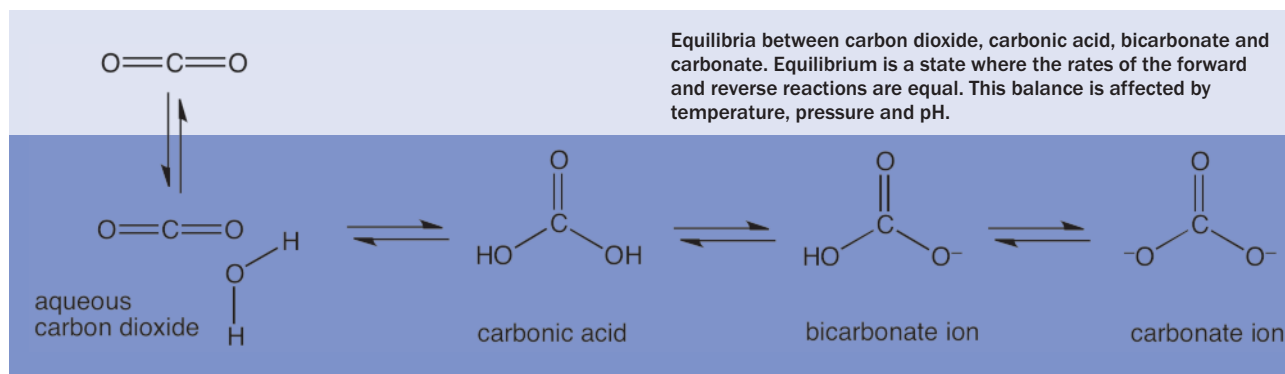
Some *soda* waters say they contain *potassium* bicarbonate and theoretically should more correctly be called 'potash water'. As they're more expensive, maybe they really are 'posher water'. Can you taste the difference?

Because of the extra equilibria, Henry's law does *not* apply to this gas–liquid interface. More on that in part 2.

Want to get your bubbles back in bottle 1? Just lower the pH again by squeezing in some lemon juice and reverse the direction of the equilibrium.

Part 2: Equilibrium from the bicarbonate side

The traditional experiment illustrates the bicarbonate–carbonate equilibrium from the carbonate side. For this, carbon dioxide is blown (from breath or other source) into limewater (calcium hydroxide) to initially precipitate calcium carbonate, and then more carbon dioxide is added, dissolving the



*The amounts need experimentation. Some soda waters might be buffered, possibly with bicarbonate or, less likely, citric acid (sometimes declared as acidity modifier) and will thus need more soda to raise the pH.

carbonate to produce the (more) soluble calcium bicarbonate. For this experiment, let's step to the left and take a look.

What you'll need

- Large (2 L) beaker or kitchen pot
- Eno antacid powder or equivalent (but not tablets, which are just bicarbonate/carbonate and binder, and rely on stomach acid for effervescence)
- Teaspoon

What to do

- 1 Carefully sprinkle a quarter of a teaspoon of antacid powder over the surface of a largish volume (e.g. two litres or more) of water and watch it dissolve.
- 2 Sprinkle another quarter of a teaspoon and another ... until effervescence occurs to the same extent as when adding the powder to a small volume (say a glass) of water. Why this difference?

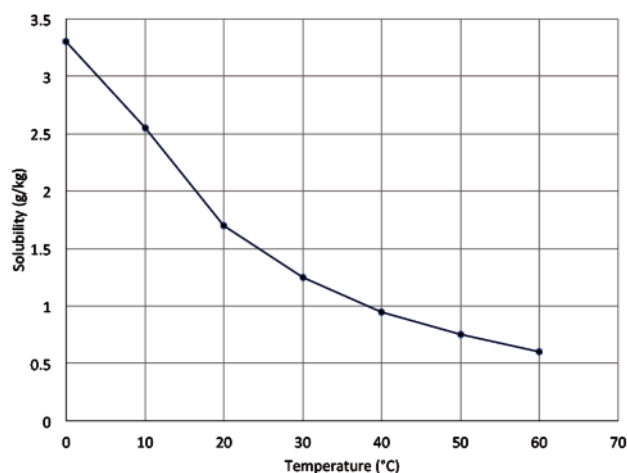
Appropriate antacids are a mixture of (at least) bicarbonate and citric acid. The acid and base react in water to form carbon dioxide, which relieves gastric distress.

The first dose of powder does release carbon dioxide, but it all dissolves. With more added powder, the solubility of carbon dioxide (2.5 g/L at 10°C, 1.5 g/L at 20°C) is exceeded and bubbles are released in quantities similar to those formed when adding the powder to a small amount of water.

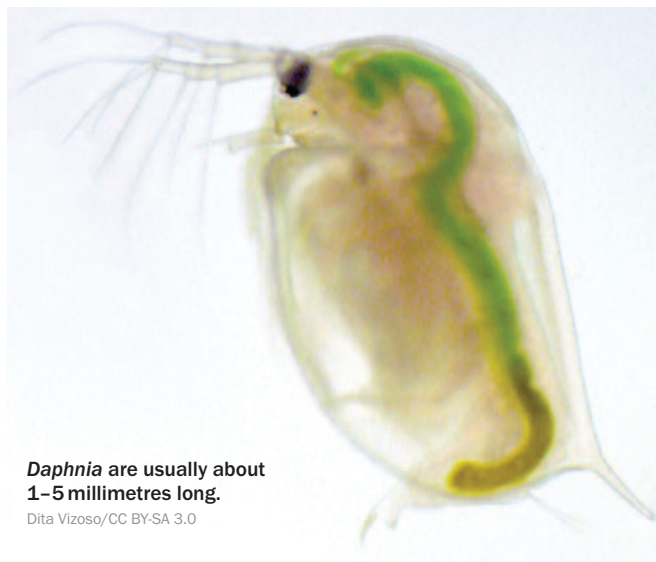
The equilibrium amount of carbonic acid (H_2CO_3) is only about one-thousandth of that of $\text{CO}_2(\text{aq})$, but it is important in being depleted by the next equilibrium, bicarbonate. That's why Henry's law does not apply.

Part 3: *Daphnia* and toxicology testing

Eutrophication (change caused by excessive nutrients) is a serious problem in waterways where carbon dioxide is produced and oxygen is consumed. *Daphnia* are used for toxicology testing of water.



Water solubility of carbon dioxide gas with temperature.



Daphnia are usually about 1–5 millimetres long.

Dita Vizoso/CC BY-SA 3.0

What you'll need

- *Daphnia* (water fleas; see picture) from a pond, dam or lake where there is organic decomposition

What to do

- Drop the *Daphnia* into soda water. Carbon dioxide dissolves at 2.5 g/L (at 10°C) and there is probably not much oxygen left in a bottle of soda water. The water fleas should pass out peacefully in a few minutes.

I have this great idea of running the equivalent of a series of garden sprinkler hoses in parallel across our beaches, bubbling excess carbon dioxide from our coal-burning power stations through the sea. Any tempted crossing shark will cough and splutter while cetaceans such as dolphins as well as turtles would be safe. As an added bonus, surfers could scoop up plenty of floating fish to slip onto the beach barbie. Tongue in cheek.

Ben Selinger FRACI CChem is Emeritus Professor of Chemistry at ANU and, along with ANU colleague Associate Professor Russell Barrow, released the sixth edition of *Chemistry in the marketplace* (CSIRO Publishing) in June 2017. For more information, visit www.publish.csiro.au/book/7366. The author thanks Kerrie Mullins-Gunst for helpful advice.

Solubility by the sea

Have you ever noticed the white crystals formed by the evaporation at the edge of pools of sea water left high and becoming dry by the retreating tide? These crystals are not NaCl. NaCl only appears when the water has been reduced to around 15% of its initial volume.

The first salt to crystallise out, but only in tiny amounts, is calcium carbonate because it is the only species near saturation. Just as well it is, or sea organisms that make shells (such as corals, oysters, mussels and periwinkles) would have difficulty extracting it. And with *rising* carbon dioxide levels in sea water, they do have more difficulty. Now that is counter-intuitive!



Cork closures strike back

A recent article in Reuters (<http://reut.rs/2rMRyXD>), 'Once tainted, Portugal's cork industry fights back', outlines the strategies being undertaken to improve the quality of cork closures for wine bottles to win back cork's market share. 'Tainted' refers to the release of chemicals from the cork into the wine with consequent negative impact on the wine's sensory characters. About 15 years ago, producers of screw cap seals and plastic stoppers, so-called non-cork closures, entered some markets in a big way, drastically reducing the market success of the traditional cork closure. Acceptance of non-cork closures was not uniform across all markets, especially those where there is a strong preference by consumers for cork.

Cork taint is commonly related to the presence of 2,4,6-trichloroanisole (TCA is the common acronym), which is released from the cork when in contact with wine. Common descriptors for TCA in wine include wet dog, mouldy newspaper and damp cellar. The taint can be so strong that it reduces the impact of the wine's own aromas. On several wine evaluation sessions, we have argued about whether a wine was 'corked' or not and it was the overall reduction in wine aroma that was the giveaway. On one memorable occasion in a restaurant where the waiter disputed our claim of 'corked', one group member said 'I made this wine and I know it is corked!'. That brought out the replacement bottle.

The Australian Wine Research Institute (AWRI) comments in its advisory note on cork-type taints (bit.ly/2t1yB6S) that there are several compounds, including guaiacol, geosmin, 2-methylisoborneol, 1-octen-3-ol, 1-octen-3-one and 2-methoxy-3,5-dimethylpyrazine, that contribute a musty aroma similar to TCA taint. Of these compounds, TCA has the lowest aroma threshold, ranging from 1.4 ng/L to 4 ng/L depending on wine style and taster's sensitivity. Some AWRI tasters were able to detect TCA at less than 1 ng/L. Just to add to the complexity, occasionally 2,3,4,6-tetrachloroanisole and 2,4,6-tribromoanisole have been found.

While there is considerable evidence that TCA in wine originates from the cork closure, some oak-related products used in winemaking, including barrels, staves and chips, can also be a source of TCA (*J. Agric. Food Chem.* 2010, vol. 58,

pp. 10 528–38). Routine quality control of both corks and oak products is thus highly recommended. For example, the AWRI offers a service for corks, oak chips and shavings from barrels or staves (bit.ly/2tZpvVA). Corks are soaked in model wine overnight or seven days for oak chips and shavings before TCA determination by GC-MS. The GC-MS procedure is described in the *Australian Journal of Grape and Wine Research* (1996, vol. 2, pp. 184–90). A considerable amount of pre-planning is required for this check to be performed before use of the material.

About 10–15 years ago, the cork industry decided to address the taint issue through significant investment in quality control of the corks themselves before release to the market. Cork exports from Portugal have risen dramatically and company share prices have increased. All this is good news for wine traditionalists, of which I am unashamedly one.

As chemistry was used to identify the compounds contributing to cause taint, so chemistry has been used, in combination with engineering, to address the issue and significantly improve the quality of cork closures. Amorim from Portugal has invested €10 million over a five-year period with the outcome being a cork closure with a non-detectable level of TCA. The NDtech cork, as it is known, assesses a non-detectable TCA concentration down to a quantifiable limit of 0.5 ng/L (bit.ly/2tFhN3y). Establishing an independently validated sampling protocol, the use of robotics for sample processing and significant reduction in the time required for the chromatographic procedure has enhanced the sample throughput. The chromatography is very smart: the analysis time has been reduced from 14 minutes to a few seconds. This allows for corks that exceed the 0.5 ng/L limit to be removed before entering the packaging process. A rather smart development overall.

For those who like to twist when opening a wine bottle, Helix is now available in some countries (bit.ly/2u2jveM). The release of Helix is a great example of consumer research and cork and bottle engineering. A partnership between Amorim and O-I, an international bottle manufacturer, resulted in a grooved cork closure that matches the threads on the inside neck of the bottle. Just hold the bottle and twist the cork and 'pop' comes the wine. No waiter's friend or other type of corkscrew is needed. If one wishes, the cork can be re-inserted to seal the remaining wine. More detail on these corks and the market success they are achieving can be found in Amorim's *Bark to bottle* publication (bit.ly/2t1VkQf).



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.

Seeing red about strontium

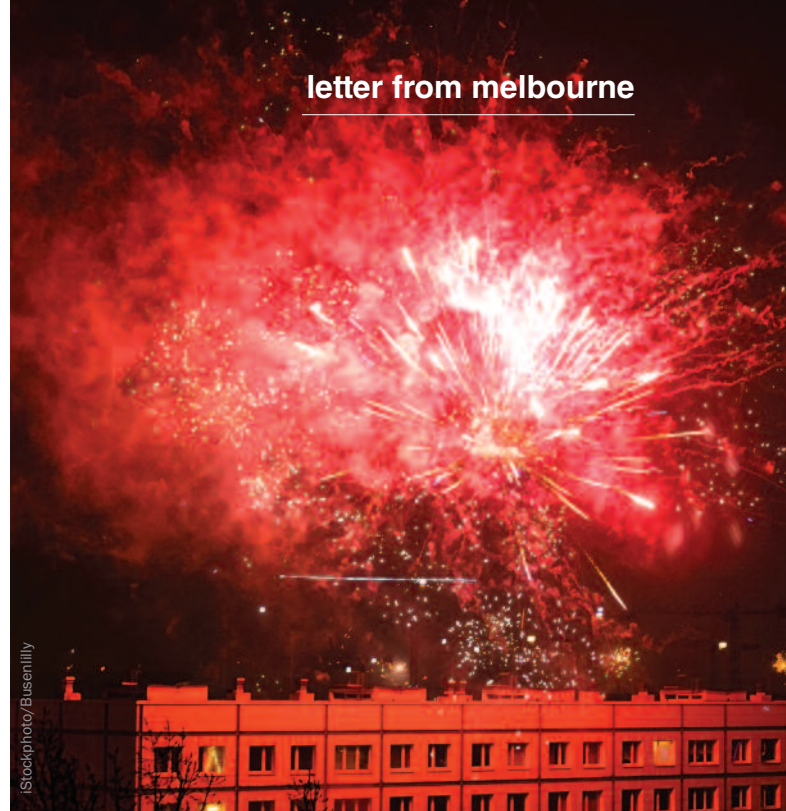
Some years ago, I was driving around a lonely peninsular in western Scotland when I came to the town of Strontian. The name seemed familiar but it still took a few minutes for the alkaline-earth metal to drop. In the late 18th century, it was recognised that a mineral found in a nearby mine was the carbonate of a new element. The mineral was named strontianite and the metal, strontites. Early in the next century, Davy prepared the element by electrolysis of the molten chloride, and renamed it strontium.

Most of us are familiar with the brilliant red colour that strontium atoms impart to a flame, and its use in pyrotechnics, but that's about it for personal experience. There is another story attached to strontium, too, but it's quite a different one. Strontium makes up 0.02–0.03% of the Earth's crust. We ingest 4 mg/day, and a typical human body burden is 0.3–0.4 g, mostly in our bones where it is found with its periodic table mate, calcium.

There are four stable isotopes of strontium, in order of natural abundance ^{84}Sr (0.56%), ^{87}Sr (7.00%), ^{86}Sr (9.86%) and ^{88}Sr (82.58%), but for a few decades in the second half of the 20th century there was a lot of interest in a radioactive strontium isotope, ^{90}Sr , that does not occur naturally but is produced in nuclear fission reactions. It is a β^- emitter with a half-life of 28.79 years, and its release into the environment by nuclear test explosions led to its status as a marker of radioactive contamination.

As the bomb testing ramped up, Australia was among countries to initiate a monitoring program in the late 1950s, sampling soil, air, wheat, milk, cabbages and bone from humans and sheep. In his 2014 book *Maralinga* (subtitled *The chilling exposé of our secret nuclear shame and betrayal of our troops and country*), Frank Walker made much of the fact that the human bone samples had been taken without permission and he cited the case of a woman who had been surprised to learn that samples had been taken from the body of her stillborn baby without her knowledge or consent. Hospitals were actually paid for providing the bone samples.

The bones were ashed and, as were samples from other materials, their radioactivity levels were measured in Britain or the US. I was interested to see that one of the co-authors, the officer in charge of the measuring facility at the Woolwich Outstation of the UK Atomic Energy Research Establishment, was Fred Bryant, who was later (1987–93) RACI Executive Director. Although the broad outline of the program was published annually in the *Australian Journal of Science* under the heading 'Strontium-90 in the Australian Environment', it did not attract much attention in the scientific community and members of the public were probably unaware of its findings. E.W. Titterton, Professor of Nuclear Physics at the Australian National University, who headed the project and was co-author of the scientific papers, came in for a good deal of criticism from Walker. Although the radioactive results were given in



some detail, the sources of the bones were never explicit although Titterton said that pathologists who supplied the bones had discussed what was involved with next-of-kin.

In 2001, the then Minister for Health, Dr Michael Wooldridge, convened a small group to give him advice on 'ethical and practical issues concerning ashed bones from the Commonwealth of Australia's strontium 90 program 1957–1978'. The group recommended (to his successor, Minister for Health and Ageing Senator Kay Patterson) that the Australian Radiation Protection and Nuclear Safety Agency (ARPANSA) should provide information to the institutions that had provided the bone samples so that they could reply to inquiries from next-of-kin. Institutions were not to initiate contact, but the Commonwealth should issue an invitation to next-of-kin. This would mirror the practice followed with organs retained after autopsy. As we might expect, specific disclosures like this flushed out some very unhappy people.

The data for 1958–60 showed that values in Australia were one-half to one-third of those in the northern hemisphere. The authors quoted the National Radiation Advisory Committee to the effect that 'even on the most pessimistic assumptions, the risks to the Australian population are insignificant when compared to the normal hazards of everyday life'.

For those with a taste for numbers and units, the results were first expressed in ' $\mu\text{mC/gm}$ ' which I took to mean $10^{-6} \times 10^{-6}$ curies per gram and found this confirmed in later papers when it became ' pCi/g '. Typical results were 0.5–1.0 for infants and 0.1–0.3 for adults. There was a good deal of scatter, and some variations as tests came and went, there was no substantial change over the years.



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.

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Current Trends in Mass Spectrometry and Chromatography

25–27 September 2017, Atlanta, Georgia, USA

<http://massspectra.com>

2nd International Conference on Pharmaceutical Chemistry

2–4 October 2017, Barcelona, Spain

<http://pharmaceuticalchemistry.conferenceseries.com>

ChemComm Symposia on Energy Science and Materials – Beijing

9 October 2017, Beijing, China

www.rsc.org/events/detail/26254/chemcomm-symposia-on-energy-science-and-materials-beijing

6th Modern Solid Phase Peptide Synthesis and its Applications Symposium

12–14 October 2017, Fraser Island, Qld

www.solidphase.org

International Conference and Exhibition on Pharmaceutical Nanotechnology

27–29 October 2017, Rome, Italy

<http://nanotechnology.pharmaceuticalconferences.com>

2nd International Conference on Applied Chemistry

30 October – 1 November 2017, Chicago, Illinois, USA

<http://appliedchemistry.conferenceseries.com>

Emerging Polymer Technologies Summit

22–24 November 2017, RMIT University, Melbourne, Vic.

<http://epts17.org/index.html>

QACS 2017 – Qld Annual Chemistry Symposium

27 November 2017, Queensland University of Technology, Brisbane, Qld

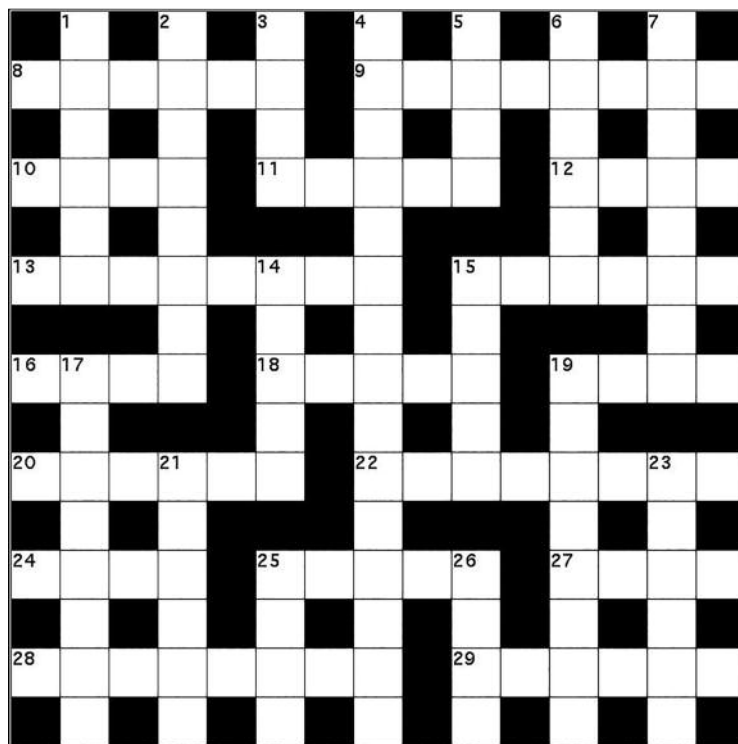
WattsFest2017

27–29 November 2017, Hydro Majestic Hotel, Blue Mountains, NSW

Email Jeffrey.Reimers@uts.edu.au or fs@unimelb.edu.au for more information.

Corrigendum

In the July issue (p. 18), Sir David Orme Masson was referred to as the first professor of chemistry at the University of Melbourne. This was incorrect because he was the second professor of chemistry at the University of Melbourne. He was preceded by J.D. Kirkland (1882–5).



Across

- 8 & 9 Across** Pretty much laid back Friday revelers get smashed. (6,8)
- 9** See 8 Across.
- 10** Notice about melting point is a bit wet. (4)
- 11** Trims advantages. (5)
- 12** Solid lipids made fast. (4)
- 13** A gas mine producing pericase. (8)
- 15** Pertaining to shape of Spooner derived from HCOOH. (6)
- 16** Employs operations. (4)
- 18** Summer reptile. (5)
- 19 & 29 Across** Seek hotter reaction for R-CO-R'-O-R'' examples, perhaps. (4-6)
- 20** Red over iodine for a different colour. (6)
- 22** New device missing tungsten reaction data. (8)
- 24** 8973 proceedings. (4)
- 25** Called for marked sheets of document. (5)
- 27** Bird went deep. (4)
- 28** Union chose altered charged species. (8)
- 29** See 19 Across.

Down

- 1** Is able to notice a state. (6)
- 2** Derivatives of cycloheptatrienone put stop on 75th rearrangement. (8)
- 3** Kind class. (4)
- 4** Regarding garnet rock and RMgX. (8,7)
- 5** See 7 Down.
- 6** Like better PUMPER. (6)
- 7 & 5 Down** Treatment of rust is secret: give limited access! (8,4)
- 14** Sweeping cut to sulfur fulminate. (5)
- 15** Irishman said Spooner asked: 'Where is everybody?' (5)
- 17** Switch second voter. (8)
- 19** Potassium set holding back had a method for determination of organic nitrogen. (8)
- 21** Is game changer making representations? (6)
- 23** Caesium binds more than screens. (6)
- 25** Particular phosphorus edge. (4)
- 26** Papers recording inclusion of halide education. (4)

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



IUPAC Distinguished Women in Chemistry awards

To celebrate International Women's Day on 8 March, IUPAC announced the awardees of the IUPAC 2017 Distinguished Women in Chemistry or Chemical Engineering. Frances Separovic, RACI Fellow and professor at the Bio21 Institute, was among them (see May issue, p. 32).

The awards ceremony took place during the IUPAC World Chemistry Congress in São Paulo, Brazil, in July.

Details of forthcoming deadlines for

2018 awards will be published at <https://iupac.org/category/deadline>. IUPAC says that 'Awardees will be selected based on excellence in basic or applied research, distinguished accomplishments in teaching or education, or demonstrated leadership or managerial excellence in the chemical sciences. The Awards Committee is particularly interested in nominees with a history of leadership and/or community service during their careers.'

IUPAC 2017 Distinguished Women in Chemistry or Chemical Engineering at the award ceremony (left to right, holding awards): Professor Ingrid Montes-González, University of Puerto Rico; Professor Misako Aida, Hiroshima University; Dr Veronika Ruth Meyer, Swiss Federal Laboratories for Materials Science and Technology; Professor Yvonne Mascarenhas, University of São Paulo; Professor Zafra Lerman, Malta Conferences Foundation; Frances Separovic FRACI CChem, Bio 21 Institute, University of Melbourne; Professor M. Concepción Gimeno, CSIC-University of Zaragoza; Professor Thisbe K. Lindhorst, Universität Kiel; Professor Lifeng Chi, Soochow University. Absent award recipients were Professor Jihong Yu, Jilin University; Dr Jaqueline Kiplinger, Los Alamos National Laboratory; and Professor Ekaterina Lokteva, M.V. Lomonosov Moscow State University.

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