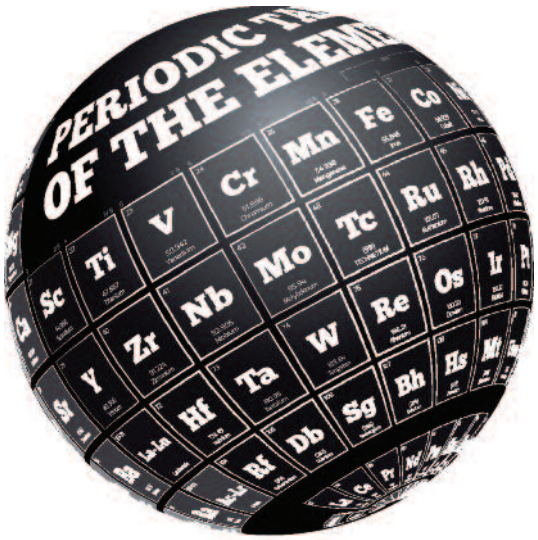
chemistry in Australia
November 2017

2019



IUPAC's centenary year is coming

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- Compliance problems with European chemical regulations
- Google's Cornforth tribute
- Eutectics in your wardrobe

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chemistry in Australia

November 2017

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cover story

IUPAC's centenary: creating the common language of chemistry

Preparations for the centenary of IUPAC in 2019 are already under way, reports Mary Garson.

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Choosing your (key)words carefully

I suspect (or at least hope) I was among the last few cohorts of students to hole-punch index cards for scientific literature searches. Computers and the internet have been a merciful release from those, and annual print indexes of key words are a thing of the past. What is the function of key words these days, and how has the internet affected their generation and use?

See and be seen

Of course, the first step on the road to being seen is to be published. Titles and abstracts have an important role here because publishers use them in deciding whether a submitted paper is worth sending for peer review. Key words can be used at this stage as an indicator of novelty and relevance. More generally, they can be signposts to peer reviewers and (in bibliometrics) to discipline trends.

A colleague employed by an online content aggregator (a business producing databases such as CAS, Web of Science and Google Scholar) eloquently explained that the purpose of key words:

> … is primarily to maximise resource discovery. … When you release content into the wild, it is wise to equip it with whatever protection possible against being instantly devoured by bigger, stronger players with insatiable appetites for attention.

Wanting to be read and cited is nothing new, but we now have access to extraordinary volumes of research, and we no longer need to find what we want by trawling through tables of contents. Readers can discover a paper via a search engine, a specialist indexed database or a link in another paper's reference list.

Authors want to be seen in different ways, and can choose their key words accordingly. If you want to reach out to colleagues in a very specific field, you might choose different key words than if you are looking for a broader audience. But how much pulling power do your key words have if the databases where your paper appears don't actually include them? (More on that later.)

Online content aggregators and SEO

The quest for high visibility has spawned countless content aggregators and, more recently, the now-burgeoning marketing discipline of SEO ('search engine optimisation'). (If you own a website, check your spam folder and you're bound to find some information about it.)

Springer Publishing refers to database indexing and search engines as a stepping stone to readers, and advises authors to choose key words with both readers and citations in mind:

> Key words are a tool to help indexers and search engines find relevant papers. If database search engines can find your journal manuscript, readers will be able to find it too. This will increase the number of people reading your manuscript, and likely lead to more citations.

However, the discovery methods I mentioned before lean more on research paper titles and abstracts than they do on key words. A colleague with experience in the journal publishing environment told me that author-chosen key words are not generally requested by online content aggregators. This suggests that titles and abstracts work harder online than key words because they are more accessible. Titles can be found as references in other people's papers, and abstracts are not hidden behind database paywalls. So would-be readers are more likely to get to the full text of a research paper based on words in its title or abstract. They won't see the key words until they arrive.

If you've used Google Analytics, you'll know that you can track data about any number of online activities. (According to their live internet statistics, Google processes more than 3.3 billion searches each day.) Search engines use robots called crawlers to collect data, for example on word occurrence. Sophisticated algorithms determine online relevance and popularity before ranking online content.

So aggregators and SEOs have a lot of power over your citations. Consider the *Wall Street Journal*, which says the publication's Google traffic dropped significantly, because of lower search rankings, after it tightened its subscriber paywall (bit.ly/2rGBjfs).

Vocab-controlled key words and indexed key words

I said earlier that online content aggregators don't usually include author-chosen key words. What they do publish are vocabulary-controlled key words, from extensive and hierarchical thesauruses. These nested lists of words are available as machine-readable data from, for example, the US Library of Medicine, the provider that revises and updates Medical Subject Headings (MeSH; bit.ly/1QznhVX). This control achieves consistency because it helps readers to find what they're looking for, even if they search using a non-preferred variant of a term. By contrast, author-chosen key words offer flexibility, particularly in instances where terms are very new or specific. The trade-off is relevance of results and thus online rankings.

My content aggregator colleague explained that 'Key words enable application of natural-language terms; controlled vocabs are more highly refined and predefined'. However, neither an aggregator nor a search engine index will know that a certain esoteric concept in your paper, which is discussed but not named, is important. The only way to draw it out is to give it key word status. The uniqueness of author-chosen key words is in the name: they are still the most meaningful indicator of what an author most wants to say.

So key words still have unique uses, but knowing which ones appear where will give your choices more mileage.

Sally Woollett (editor@raci.org.au) With thanks to the journal editors and online content professionals who have discussed this fascinating topic with me.

Historical clarity

The obituary for Dr Peter Wilkinson (September, p. 32) shone light on earlier truncated communications and why I missed seeing Peter at the spectacular RACI Centenary Congress in Melbourne. The obituary reporting Peter's time as National RACI President, identical to mine (1987–88), activated my pedant gene to revisit the name change for the University of New South Wales (UNSW). UNSW was incorporated in 1949 and initially named the NSW University of Technology. The timing (1958) of the UNSW name change was referenced in an 'official' UNSW history and repeated in an issue of *Chemistry in Australia* (June 2016, p. 5). In reality, students studying at UNSW in 1960 were enrolled with the NSW University of Technology.

It is remarkable that Sydney Technical College spawned two universities: UNSW (1949) and University of Technology, Sydney (UTS; 1964). It is noteworthy that UNSW set up another two universities: Newcastle University (1951) and University of Wollongong (1961).

All of the above institutions evolved from the Sydney Mechanics' School of Arts (SMDA), a precursor for Sydney Technical College (now TAFE). The SMDA (1833) is still a very active institution, and I recently attended a joint lecture shared between SMDA and the Royal Society of NSW (1821). The current Chairman of the Royal Society of NSW is the well-known Emeritus Professor Brynn Hibbert FRACI CChem.

So for the record, the name change from 'NSW University of Technology' to 'University of New South Wales' happened around the time the last tram passed by UNSW, 1961 (the near completion of the new light rail construction along Anzac Parade, Kensington, is surely another case of 'back to the future').

Robert F. Ryan FRACI CChem

More science for fun

Ian MacLeod (September, p. 5) was not the only granddad to try out Jeremy Just's red cabbage juice pH experiment (June, p. 36) with grandchildren. My eight- and five-year-old granddaughters were similarly fascinated by colourful kitchen chemistry's pH indicator.

Ian Southwell FRACI CChem

'Your say' guidelines

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

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ISSN 0314-4240 e-ISSN 1839-2539

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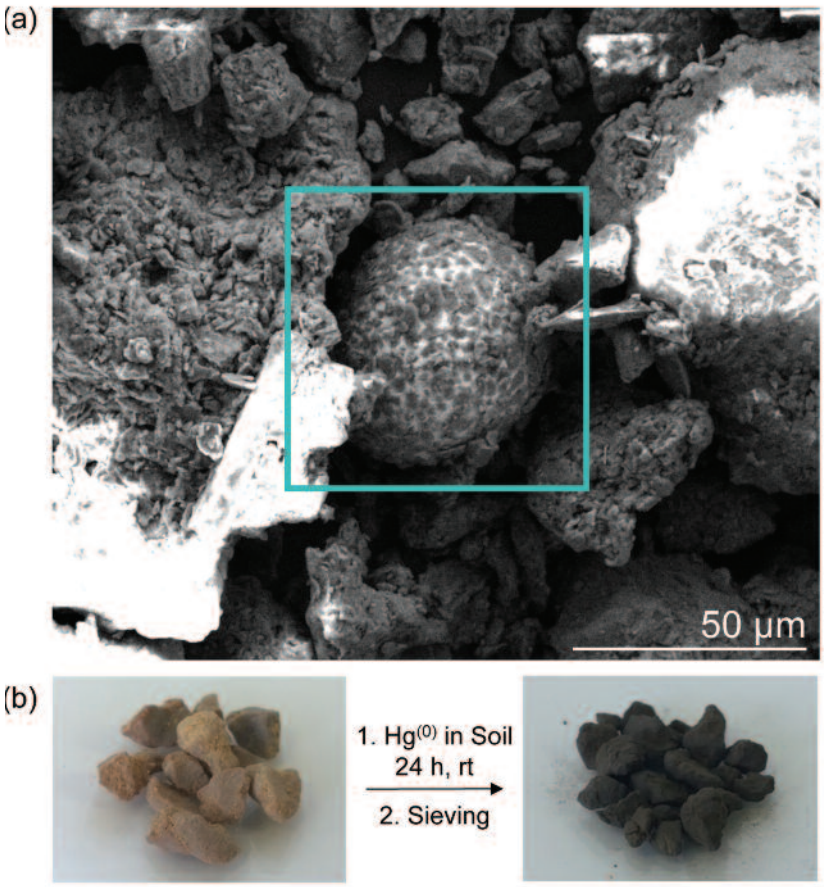
New way to clean up mercury pollution

The porous polymer cubes (the high surface area version of the polymer) are very effective at capturing inorganic mercury in water, organomercury compounds and mercury vapour.
Max Worthington



(a) Mercury bead (in green box) contaminating soil and (b) the polymer before (left) and after (right) capturing the mercury so it can be removed from soil.

Scientists have devised a way to use waste cooking oil and sulfur to extract the neurotoxin mercury from the environment.

For the first time, researchers have demonstrated that the dynamic new canola oil polymer can trap the most dangerous and common types of mercury pollution – mercury metal, mercury vapour and highly toxic organo-mercury compounds – which harm both aquatic and terrestrial systems.

'Our previous research studied a single type of inorganic mercury, so this is a significant advance', said Dr Justin Chalker, senior lecturer in synthetic chemistry at Flinders University.

'With the Minamata Convention on Mercury coming into force around the world this year, this discovery is an important advance in protecting the environment and human health.

'We can use this material to protect the environment by capturing toxic mercury pollution – a pernicious problem around the world, causing brain damage and loss of IQ points in unborn children.

'At the same time, every atom of the mercury-binding material can be derived from industrial by-products, so this is also an exciting advance in recycling and re-purposing waste.'

Chalker and fellow researchers from around the world have combined second-hand cooking oil and sulfur – a common, low-cost by-product from petroleum production – to produce a new kind of polymer to use in remediation of soil, water and even the air.

After absorbing mercury pollution, the novel rubber-like polymer changes colour to indicate the job is done. More of the affordable polymer mixture can then be placed in the area to continue to process.

The material is being tested in field trials at mining sites and areas where mercury-based fungicides are used.

Flinders University

Why whisky tastes better with water

There is a reason why whisky is diluted with water before being bottled. The same reason also makes many whisky enthusiasts add a few drops of water in their glasses – it makes the whisky taste better. But why is this so?

Whisky is a chemically complicated beverage. After malting, mashing, fermentation, distillation and maturing, for at least three years in oak barrels, the whisky is bottled. However, first it is usually diluted to around 40% of alcohol by volume by the addition of water, which changes the taste significantly. For that same reason, whisky enthusiasts often add a little water in their glasses.

But why and how does water enhance the taste of whisky? Up until recently, no one had been able to answer this question, but now Björn Karlsson and Ran Friedman, researchers in chemistry at Linnaeus University, have solved a piece of the puzzle that will help us better understand the chemical qualities of whisky (http://doi.org/10.1038/s41598-017-06423-5).

'The taste of whisky is primarily linked to so-called amphipathic molecules, which are made up of hydrophobic and hydrophilic parts. One such molecule is guaiacol, a substance that develops when the grain is dried over peat smoke when making malt whisky, providing the smoky flavour to the whisky', Karlsson explained.

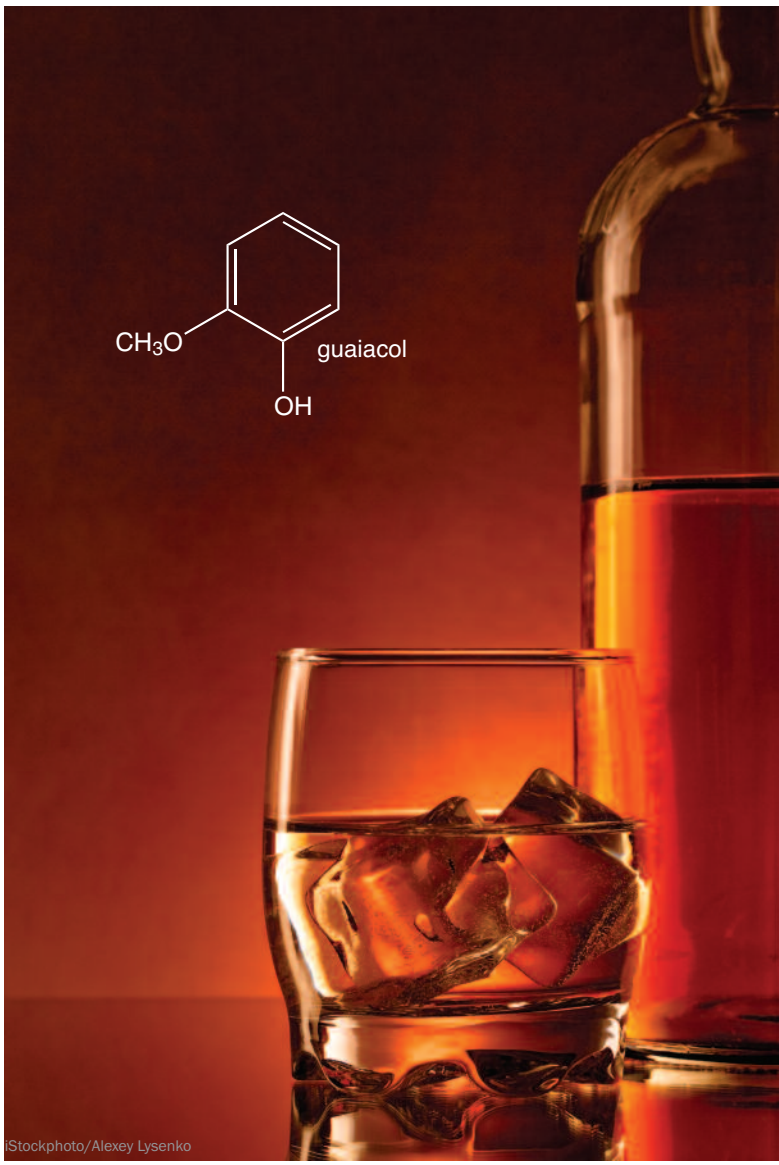
Karlsson and Friedman carried out computer simulations of water–ethanol mixtures in the presence of guaiacol to study its interactions. They found that guaiacol was preferentially associated with ethanol molecules and that in mixtures with concentrations of ethanol up to 45% guaiacol was more likely to be present at the liquid–air interface than in the bulk of the liquid.

'This suggests that, in a glass of whisky, guaiacol will therefore be found near the surface of the liquid, where it contributes to both the smell and taste of the spirit. Interestingly, a continued dilution down to 27% resulted in an increase of guaiacol at the liquid–air interface. An increased percentage, over 59%, had the opposite effect, that is to say, the ethanol interacted more strongly with the guaiacol, driving the molecule into the solution away from the surface', Friedman continued.

Combined, these findings suggest that the taste and aroma of guaiacol, and similar compounds in whisky, are enhanced when the spirit is diluted prior to bottling and this taste may be more pronounced on further dilution in the glass. So what is the optimal number of water drops to put in your whisky?

'How we experience taste and aroma is highly individual. Some people choose to add ice cubes to their whisky, to cool it down and give it a milder taste. Thus, there is no general answer to how much water you should add to your whisky to get the best taste experience', Karlsson concluded.

Linnaeus University



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... in mixtures with concentrations of ethanol up to 45% guaiacol was more likely to be present at the liquid–air interface than in the bulk of the liquid.

Tiger snake toxin overturns venom evolution paradigm


Ian W. Fieggen/CC BY-SA 3.0

Australian tiger snakes have 'hit the jackpot' because prey cannot evolve resistance to their venom.

While that may sound foreboding, University of Queensland School of Biological Sciences expert Associate Professor Bryan Fry said this discovery had medical benefit for humans.

That's because tiger snake antivenom has an extraordinary level of cross-reactivity against other snake species, and can therefore neutralise the lethal effects on humans in snakebite cases.

'The level of conservation in the toxin sequences is not only really unusual, but this is why the corresponding tiger snake antivenom is so useful in treatments against bites from many Australian snakes that affect the blood in the same way', Fry said.

'No other antivenom in the world is so spectacularly effective against such a wide range of snakes this way and now we know why.'

Fry said the research had overturned a central paradigm of venom evolution.

'A long-held belief is that snake venom varies with diet – that is, as the snakes evolve into new species and specialise on new prey, the venom changes along with it', he said.

'Our research has shown that tiger snakes and their close relatives have toxins that are almost identical, despite this group of snakes being almost 10 million years old.

'We worked out the reason was that the toxins target a part of the blood-clotting cascade that is almost identical across all animals.

'So we have a new addition to the theory of venom evolution: that when the target itself is under extreme negative selection pressure against change, then the toxins themselves are under similar such pressure.

'This is a novel twist to the chemical arms race which most snake venoms evolve under. But it is one with direct human benefit since this is why tiger snake antivenom is so effective against treating the effects on the blood by quite a few other Australian snakes. No other antivenom is so widely useful.'

Fry said normally, snake venom placed pressure on the target so that animals with some variance were more resistant to the poison, which in turn put pressure back onto the venom for change.

'In this case, if the animals had variation in their blood-clotting proteins, they would die because they would not be able to stop bleeding', he said.

Fry's team studied the venom of 16 tiger snake populations from across Australia, including five island populations in the Bass Strait, and venoms from 11 other snakes in related genera.

'This is the most comprehensive examination of this clade of medically important snakes ever undertaken, including the first examination of the venom of the enigmatic Lake Cronin snake from Western Australia', he said.

'This study is a great example of the human medical benefits that can come from studying evolution.'

The study involving researchers from the University of Queensland's Venom Evolution Lab, Swansea University, UK, University of Melbourne, Venom Supplies South Australia, Snakes Harmful & Harmless, Western Australia, and the Fauna Vet Wildlife Veterinary Consultancy, Beerwah, is published in *Comparative Biochemistry and Physiology, Part C* (doi: 10.1016/j.cbpc.2017.07.005).

University of Queensland

Students building a prosthetic limb. Left to right: Roshan Doherty (St Hilda's), Kate Kang (Methodist Ladies' College), Amy Boyd (St Hilda's) and Jaime Dunn (Methodist Ladies' College).

Girls encouraged to follow careers in STEM

More than 100 Year 9 and 10 female students recently learnt about some of the exciting career opportunities available to them in science, technology, engineering and mathematics (STEM) subjects at an event held at the University of Western Australia.

Girls in Engineering Discovery Day is part of the Girls in Engineering program at the University of WA, which is supported by foundational partner Rio Tinto. The event aimed to inspire young women interested in a STEM career by breaking gender stereotypes and encouraging them to pursue a career that they are most passionate about.

A report issued by the Office of the Chief Scientist in 2016 estimated that only around 16% of Australia's qualified STEM workers were female.

The students got involved in activities ranging from working in robotics and programming miniature robots, to developing prosthetic limbs, using virtual reality systems to create experiences that help those with physical and mental impairments and completing activities to understand how algorithms, patterns and maths can be used to help solve some of the world's most complex problems.

A keynote speech by world leader in cancer research Professor Christobel Saunders from the University of WA Medical School's surgery division, who was also a recent recipient of a Premier's Science Award, was a highlight of the day, with Saunders imparting her knowledge and advice to the students.

Saunders said engineering was a wonderful career for women, with incredibly broad options and the opportunity to make a big difference.

'It's not just about building roads or machines that go "bang"; engineering is a hugely diverse career that encompasses a lot of other things within science', Saunders said.

'I think inspiring young women is really important and it's also important to help them realise that there is a spark there and you really can make a difference in the world through what you choose to study.

'This is an incredibly bright bunch of motivated girls and I'd love to see them enjoy a rewarding career in STEM.'

St Hilda's Anglican School for Girls student Amy Boyd, 14, of Bicton said the event was a rewarding experience and opened up many possibilities of what she might like to study after school.

'I really enjoyed the work we did using virtual reality, the possible uses of this technology to improve areas such as medicine and how it can be used to carry out different surgeries without needing to hurt anyone or be invasive', Miss Boyd said.

'I'm interested in pursuing a career in chemical and biomedical engineering, which looks pretty fun and it was great to see some of the options in practice at the Girls in Engineering Discovery Day.'

Participating schools at the Girls in Engineering Discovery Day included St Hilda's Anglican School for Girls, Methodist Ladies' College, St Mary's Anglican Girls College, Belmont City College and Governor Stirling Senior High School.

University of Western Australia

Ancient pottery tests positive for wine

The storage jar was discovered in a cave in the province of Agrigento, Sicily. Alun Salt/CC BY-SA 2.0

Chemical analysis conducted on ancient pottery could dramatically predate the commencement of winemaking in Italy. A large storage jar from the Copper Age (early fourth millennium BCE) tested positive for wine.

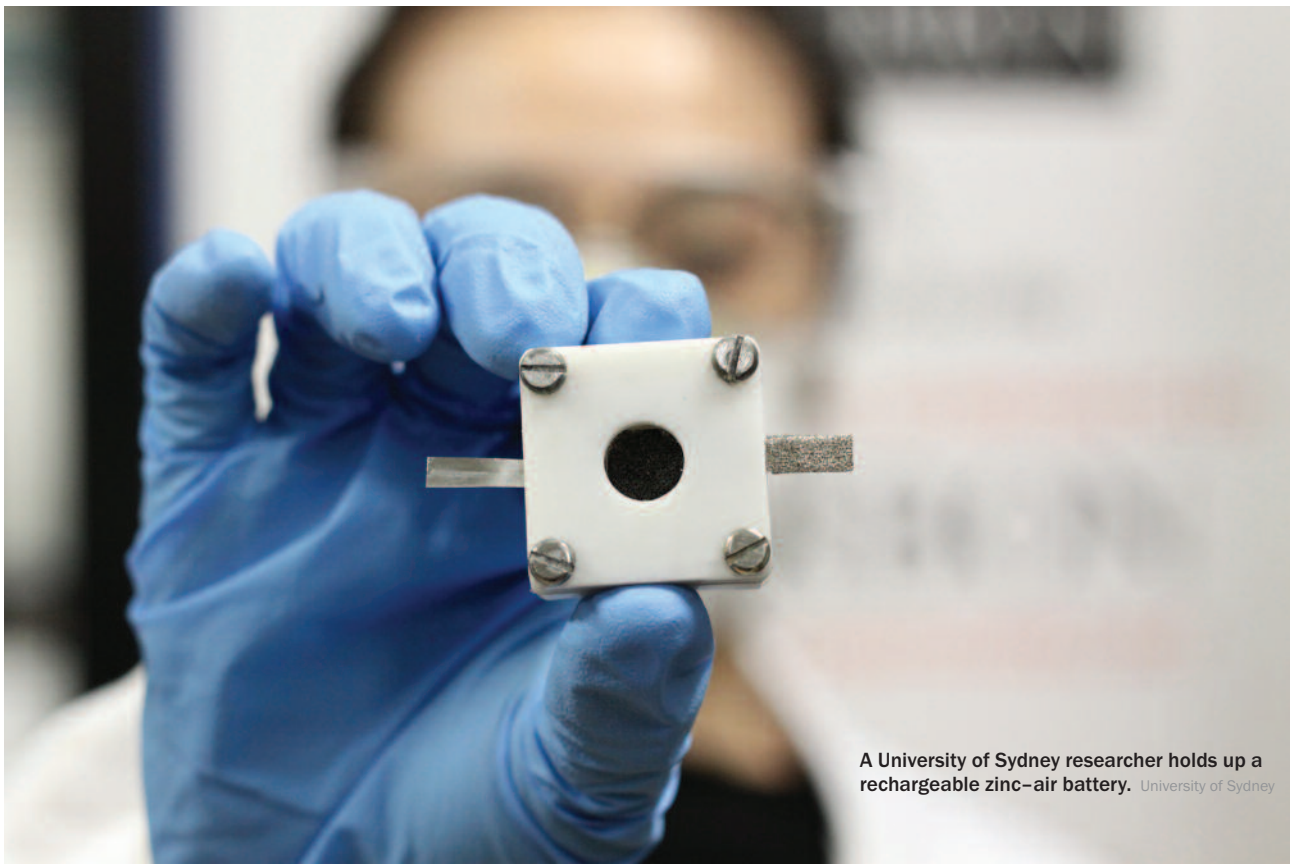
This finding published in *Microchemical Journal* (http://doi.org/10.1016/j.microc.2017.08.010) is significant as it's the earliest discovery of wine residue in the entire prehistory of the Italian peninsula. Traditionally, it's been believed wine growing and wine production developed in Italy in the Middle Bronze Age (1300–1100 BCE) as attested just by the retrieval of seeds, providing a new perspective on the economy of that ancient society.

Lead author Dr Davide Tanasi, University of South Florida in Tampa, conducted chemical analysis of residue on unglazed pottery found at the Copper Age site of Monte Kronio in Agrigento, located off the south-west coast of Sicily. He and his team determined that the residue contained tartaric acid and its sodium salt, which occur naturally in grapes and in the winemaking process.

It's very rare to determine the composition of such residue because it requires the ancient pottery to be excavated intact. The study's authors are now trying to determine whether the wine was red or white.

University of South Florida

Charging ahead with zinc–air batteries



A University of Sydney researcher holds up a rechargeable zinc–air battery. University of Sydney

University of Sydney researchers have found a solution for one of the biggest stumbling blocks preventing zinc–air batteries from overtaking conventional lithium–ion batteries as the power source of choice in electronic devices.

Zinc–air batteries are powered by zinc metal and oxygen from the air. The global abundance of zinc metal makes these batteries much cheaper to produce than lithium–ion batteries, and they can also store more energy (theoretically five times more than that of lithium–ion batteries), are much safer, and are more environmentally friendly.

While zinc–air batteries are currently used as an energy source in hearing aids and some film cameras and railway signal devices, their widespread use has been hindered by difficulties with recharging them. This is due to the lack of electrocatalysts that successfully reduce and generate oxygen during the discharging and charging of a battery.

Published in *Advanced Materials* (http://doi.org/10.1002/adma.201701410), a paper authored by chemical engineering researchers from the University of Sydney and Nanyang Technological University, Singapore, outlines a new three-stage method to overcome this problem.

According to lead author Professor Yuan Chen, from the University of Sydney's Faculty of Engineering and Information Technologies, the new method can be used to create bifunctional oxygen electrocatalysts for building rechargeable zinc–air batteries from scratch.

'Up until now, rechargeable zinc–air batteries have been made with expensive precious metal catalysts, such as platinum and iridium oxide. In contrast, our method produces a family of new high-performance and low-cost catalysts', he said.

These new catalysts are produced through the simultaneous control of the composition, size and crystallinity of metal oxides of earth-abundant elements such as iron, cobalt and nickel. They can then be applied to build rechargeable zinc–air batteries.

Paper co-author Dr Li Wei, also from the Faculty of Engineering and Information Technologies, said trials of zinc–air batteries developed with the new catalysts had demonstrated excellent rechargeability – including less than a 10% battery efficacy drop over 60 discharging/charging cycles of 120 hours.

'We are solving fundamental technological challenges to realise more sustainable metal–air batteries for our society', Chen added.

University of Sydney

Out, damned purple spot!

What's under that purple spot? Italian researchers working in the Secret Vatican Archive had been struggling to read a five-metre long parchment written in 1244 because it's covered in purple spots. Sparing ancient documents from the ravages of time is a difficult process, and while they are now kept in rooms with carefully controlled environmental conditions, many have already been attacked by water, air and even microbial life for centuries. The researchers knew that the spots were left by microbes that also caused the top layer of the document to splinter off. Using genetic techniques, the researchers were able to identify exactly what kind of bacteria were leaving the stains, and hope that this will allow them to restore other documents damaged in this manner.

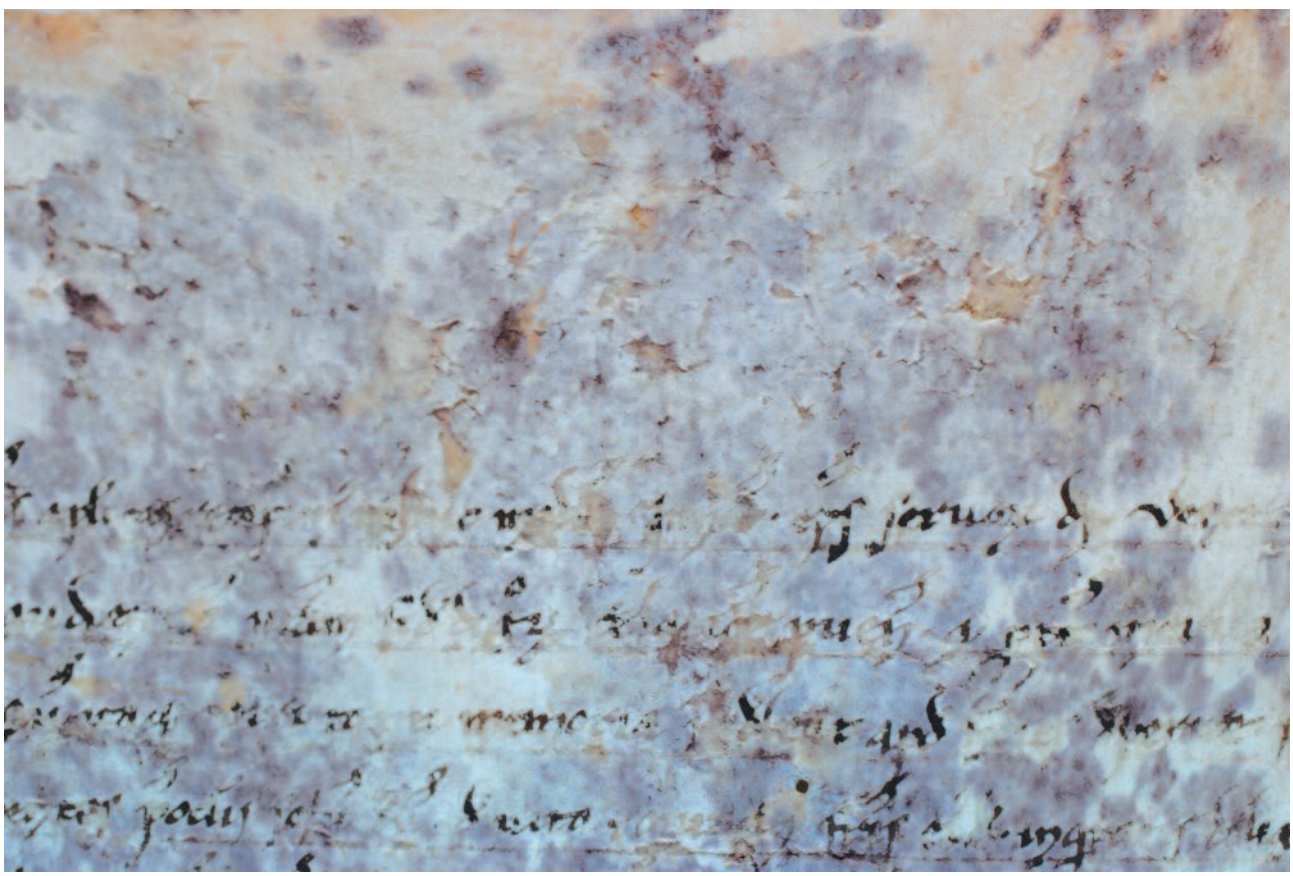
The microorganisms responsible for purple spots on a 13th-century scroll have been identified in a study in *Scientific Reports* (https://doi.org/10.1038/s41598-017-05398-7). Ancient parchments are commonly attacked by microbes, resulting in purple spots and the detachment of the superficial layer of the document, which affects the readability. The authors hope that their findings may help in the restoration and conservation of ancient parchments.

The five-metre long parchment, A.A. Arm. I-XVIII 3328, written in 1244 for a canonisation inquiry, tells the story of a young soldier called Laurentius Loricatus who killed a man by accident. To make amends for his crime, he retired to a cave near Subiaco, Italy, for the next 34 years. However, the document is covered in purple spots, with damage to the collagen structure significantly affecting its readability. The damage is most likely to have occurred prior to the scroll being moved to the Vatican Secret Archive at the end of the 18th century, where it is now kept under controlled environmental conditions.

By performing a genetic analysis of the microbial communities colonising the scroll, Luciana Migliore and colleagues found that *Gammaproteobacteria* were present in the purple spots but absent in the undamaged areas of the parchment. The authors suggest that deterioration of the parchment occurred during a process of microbial succession, in which *Halobacteria* – responsible for the rhodopsins that produce the purple spots – were replaced by *Gammaproteobacteria*, only leaving the purple stains behind. The authors suggest that further studies could help identify the exact sequence of microbes that produced the rhodopsins responsible for the spots and may reveal new approaches to aid in the restoration of documents damaged in this manner.

Springer Nature

G. Vendittozzi



Small technology to clean huge volume of wastewater

Researchers from Edith Cowan University have developed a way to modify the atomic structure of iron to create a metal that can strip impurities from water in just a few minutes.

The breakthrough, recently published in *Advanced Functional Materials* (http://doi.org/10.1002/adfm.201702258), offers new applications in the mining, textile and other industries where large amounts of wastewater are produced.

Associate Professor Laichang Zhang from ECU's School of Engineering was able to change the atomic structure of iron to form what is known as metallic glass.

Metallic glass gets its name not from the fact that it is transparent and can be used in windows, but because its atomic structure resembles that of glass.

Whereas the atomic structure of traditional metals is very ordered, with the atoms forming a grid-like structure, metallic glass atoms have a much more disorganised composition.

'It is this disordered atomic structure that gives metallic glass its very interesting and useful characteristics', Zhang said.

A thin strip of the iron-based metallic glass developed by Zhang can remove impurities such as dyes or heavy metals from even highly polluted water in just minutes.

'It works by binding the atoms of the dye or heavy metals to the ribbon, leaving behind useable water', Zhang said.

'This offers a number of benefits compared to the current method of using iron powder to treat wastewater. Firstly, using iron powder leaves you with a large amount of iron sludge that must be stored. Secondly, it is expensive to produce and can only be used once.

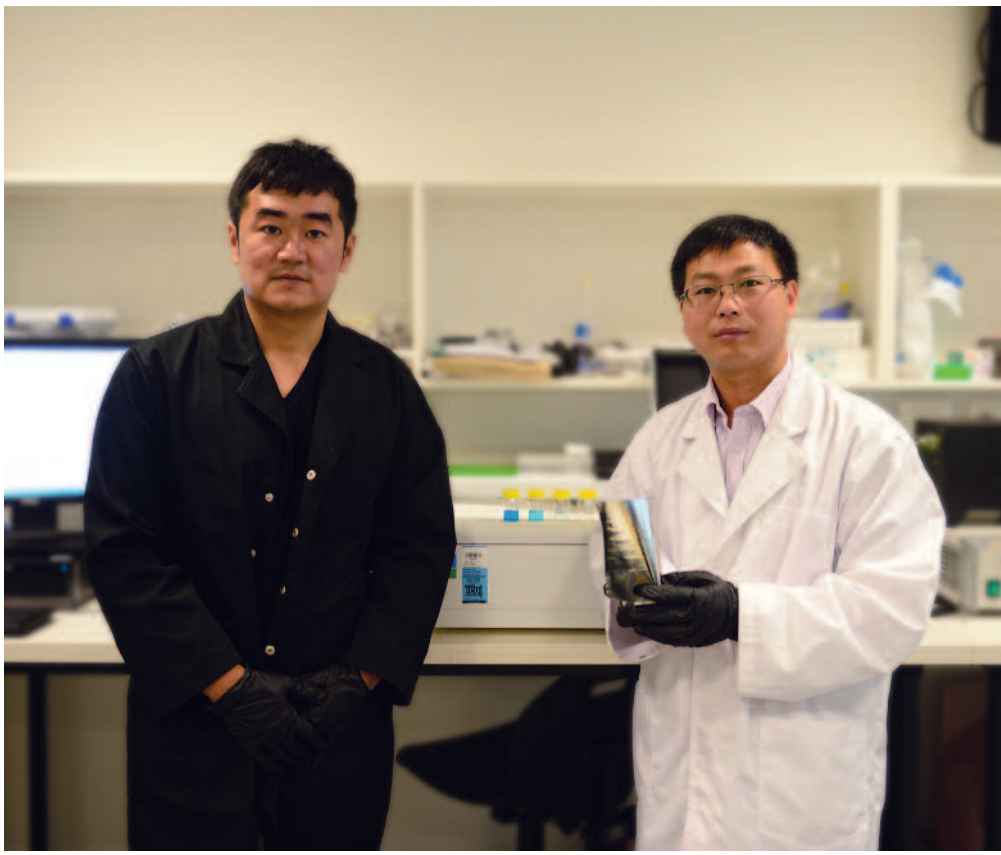
'In contrast, the iron-based metallic glass we have developed can be reused up to 20 times, produces no waste iron sludge and can be produced as cheaply a few dollars per kilogram.'

Zhang said the technology could have significant applications in the textile and mining industries.

'Mining and textile production produces huge amounts of water that is contaminated with heavy metals and dyes respectively', he said.

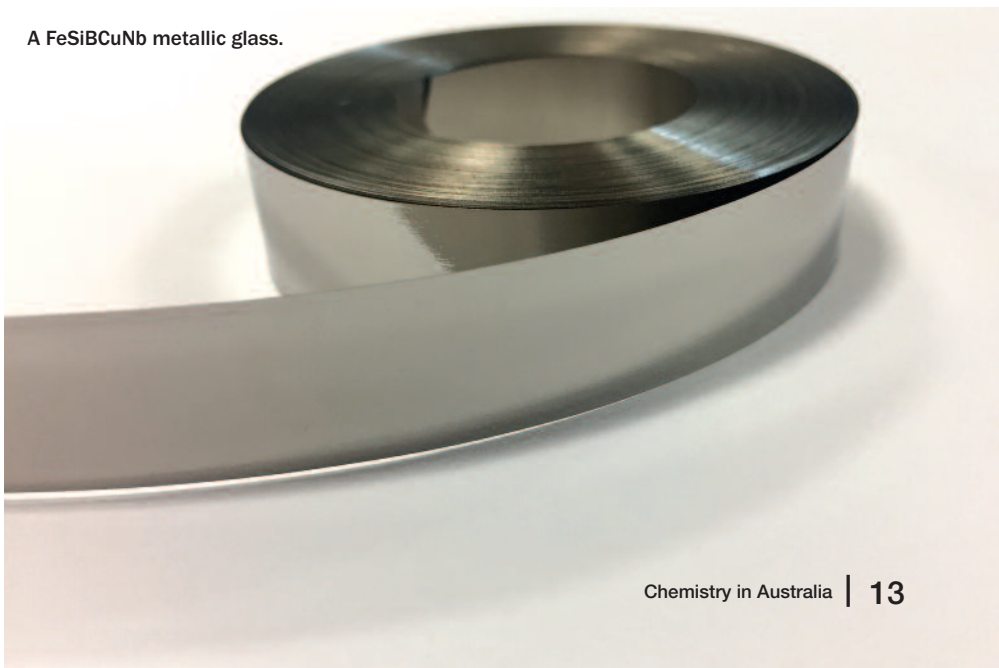
'We have already had significant interest from companies in both China and Australia who are keen to work with us to develop this technology, including Ausino Drilling Services, whose clients include Rio Tinto and the Aluminium Corporation of China.'

Edith Cowan University



Professor Laichang Zhang (right) and PhD student Zhe Jai (left).

A FeSiBCuNb metallic glass.



Methane from tundra, ocean floor didn't spike during previous natural warming period

Researchers sample along a transect at Taylor Glacier in Antarctica, with Friis Hill on the left and the Asgard mountain range in the background. Courtesy Hinrich Schaefer

Scientists concerned that global warming may release huge stores of methane from reservoirs beneath Arctic tundra and deposits of marine hydrates – a theory known as the 'clathrate gun' hypothesis – have turned to geologic history to search for evidence of significant methane release during past warming events.

However, a study published in *Nature* (http://doi.org/10.1038/nature23316) suggests that the last ice age transition to a warmer climate some 11 500 years ago did not include massive methane flux from marine sediments or the tundra. Instead, the likely source of rising levels of atmospheric methane was tropical wetlands.

While this certainly is good news, the study also points at a larger role of humans in the recent methane rise.

'Our findings show that natural geologic emissions of methane – for example, leakage from oil seeps or gas deposits in the ground – are much smaller than previously thought', said Edward Brook, co-author and Oregon State University paleoclimatologist. 'That means that a greater percentage of the methane in the atmosphere today is due to human activities, including oil drilling, and the extraction and transport of natural gas.'

The study suggests that human emissions of geologic methane may be as much as 25% higher than previous estimates. Although not as abundant as carbon dioxide, methane is a much more powerful greenhouse gas and therefore the rising levels are an important contributor to global warming.

'This means we have even more potential to fight global warming by curbing methane emissions from our fossil fuel use', said lead author Vasilii Petrenko, an associate professor of earth and environmental sciences at the University of Rochester.

Anthropogenic methane emissions are the second largest contributor to global warming after carbon dioxide, but there has been uncertainty as to the source of that methane and whether it has changed over time, Brook noted. The new study sheds light on the issue by analysing levels of atmospheric methane from the last deglaciation in air bubbles that have been trapped in pristine ice cores from Antarctica's Taylor Glacier.

The researchers were able to estimate the magnitude of methane emissions from roughly 11 500 years ago by measuring radioactive carbon isotopes in methane, which decay fairly rapidly. Methane released from those marine hydrates and permafrost is old enough that any ^{14}C originally present has now decayed away.

They found that the amount of methane from ancient '^{14}C-free sources'

... a greater percentage of the methane in the atmosphere today is due to human activities, including oil drilling, and the extraction and transport of natural gas.

was very low – less than 10% of the total methane – during the entire range of sampling, from 11 800 to 11 300 years ago.

'A lot of people have painted the Arctic as a methane time bomb', Brook said, 'but this shows that it may be more stable than we thought. Past performance isn't always a predictor of the future, but it is a good analogue. We should be more concerned about anthropogenic sources of methane into the atmosphere, which continue to increase.'

The levels of ^{14}C in the ice cores suggest that the increase in methane during the last deglaciation had another source – likely from tropical wetlands, said co-author Christo Buizert, Oregon State University.

'Methane is not stored in the tropics for long periods of time, but produced every day by microbial activity in wetlands', Buizert said. 'We know from other studies that rainfall increased in the tropics during the last warming period, and that likely created more wetlands that produced the additional methane.'

Atmospheric methane has increased from 750 ppb in the year 1750 to more than 1800 ppb today – mostly from anthropogenic sources, especially leakage from fossil fuel production, the creation of rice paddies, and cattle ranching, the researchers say.

'All of the natural gas that we mine is very old and leaking inevitably occurs during that process', Brook said. 'Natural gas is considered a cleaner energy source than coal, but it can be a significant problem depending on how much of the methane is leaking out.'

The key to documenting the source of atmospheric methane is the pristine ice cores of Taylor Glacier in Antarctica, where dry, windy conditions have allowed this ancient ice to be slowly brought to the surface. One reason scientists had yet to pin down the sources of methane during the last ice age is that the amount of ^{14}C is so small, it takes enormous amounts of ice to get enough air to measure the isotope.

It takes some 900 kilograms of ice, running a melting instrument over three days, to get enough air to produce one sample of measurable ^{14}C. Drilling down in the centre of the ice sheet to find that much ice from the end of the last ice age would be prohibitively costly and labour-intensive, but the unique conditions at Taylor Glacier – pushing that old ice toward the surface – made it possible.

By Mark Floyd, Oregon State University

ChemRN – a new network dedicated to chemistry

Elsevier has announced that SSRN, its working paper repository and preprint server, has launched the Chemistry Research Network – ChemRN.

The launch of ChemRN follows hot on the heels of the launch in June 2017 if BioRN, SSRN's new network dedicated to biology and its first outside the social sciences. BioRN already has nearly 5000 papers live from approximately 6500 authors.

Gregg Gordon, Managing Director of SSRN, said: 'The launch of ChemRN is part of our strategy to extend the expertise and knowledge we have in building community-driven networks to benefit even more people in the research community.'

Chemistry researchers can share ideas and other early stage research, including posting preprints and working papers on ChemRN. Users can quickly upload and read papers for free, across all of chemistry, including the fields of energy, environmental and materials sciences. It allows users to quickly upload and read abstracts and full text papers, free of charge.

A preprint is the author's own write-up of research results and analysis that has not been peer-reviewed, nor had any value added to it by a publisher (such as formatting, copy-editing and technical enhancements). A preprint server, or working paper repository as they are also known, allows users to share these documents.

SSRN has been serving the research community since 1994 and was acquired by Elsevier in May 2016. Since joining Elsevier, SSRN has completely redesigned its website, making it cleaner and easier to use. It has also launched full-text search. SSRN is now working towards deeper integration with Elsevier's other research products, particularly Mendeley's reference management software and Pure's research management system.

Google Doodle honours Australia's Nobel Prize-winner in Chemistry

Australia's only Nobel Prize-winner in Chemistry, Sir John Cornforth, died four years ago, the year after his wife Rita, also a University of Sydney chemistry alumnus, passed away – and to mark what would have been his 100th birthday, Google created a 'Doodle'.

The Doodle was developed for the homepage of Google.com.au and was also run in various countries around the world; beyond Australia, countries that opted in saw the Doodle from 12 am to 12 midnight in their local time on 7 September 2017.

Going deaf from an early age, John Cornforth replaced lectures with textbooks and relied on Rita to lip-read and assist communication in sign language.

University of Sydney historian, Associate Professor Julia Horne, said much had been written about Sir John's achievements, and the important role of his wife and fellow researcher, Lady Cornforth, was also acknowledged: 'Some awards have recognised his wife also, for example the University-wide Rita and John Cornforth Medal', Horne said.

Sir John was an inspired science communicator and gained his Nobel Prize for his work on the stereochemistry of enzyme-catalysed reactions, contributions which, as the *Guardian* stated, stimulated studies on the mechanism of a variety of enzyme-catalysed reactions, many of which are important targets in drug discovery.

University of Sydney Vice-Chancellor and Principal Dr Michael Spence said the Cornforths personified the university's tradition of life-long learning and research excellence.

'The Cornforths made a remarkable contribution to the world and it was perhaps Sir John's determination to consult primary sources, and celebrate science as an ongoing endeavour, that made his work so precise and compelling', Spence said.

Head of the School of Chemistry Professor Philip Gale said he first became acquainted with Sir John's earlier work as a young student at Oxford.

'As a young DPhil student at the University of Oxford, I was aware of Sir John's work early work on phenol-formaldehyde macrocycles. It's a great honour to lead the School of Chemistry at the University of Sydney which provided Sir John with his first experiences of organic chemistry', Gale said.

Dean of the Faculty of Science Professor Trevor Hambley said: 'Having had the good fortune to be present at Sir John's lecture to mark the 75th anniversary of the RACI, I can attest to what an extraordinary intellect he was.'

Rita and John Cornforth. University of Sydney

Sydney biologist Dinah Hales remembers Sir John as a remarkable uncle whose career took him, along with Rita as postgraduates on scholarships, to Oxford University: 'He was a very active man … he liked to bushwalk, climb mountains and was also a chess champion', said Hales, who has retired from her role as associate professor at Macquarie University.

'He also helped me in my research, sending me samples of compounds and explaining aspects of steroid biology and chemistry', Hales said.

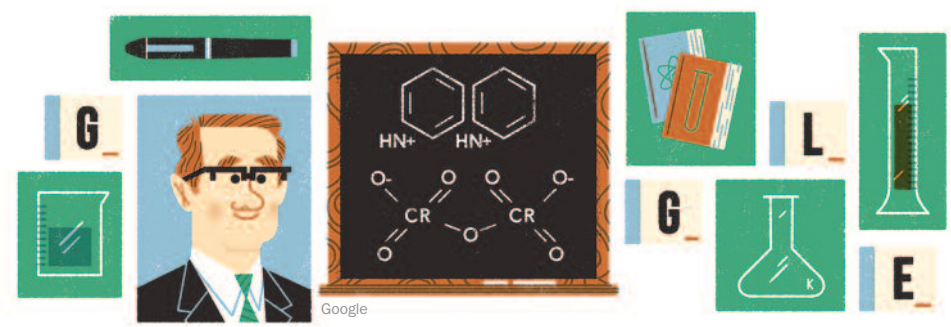
John Cornforth Jnr, a retired engineer living in Switzerland, previously described in a speech to the Royal Society of Chemistry how his father's scientific training permeated other aspects of his life.

'He had a somewhat scientific attitude to gardening – he would always read the literature and then experiment himself … his interest in garden produce tended to stop at the kitchen door (but resume at the dining table).'

Eldest daughter Brenda Osborne, a retired general practitioner from the UK, added that her father was a loving family man who also had a great passion in poetry: 'He had a gift of being able to read a poem perhaps only once and be able to recite it thereafter word perfect.'

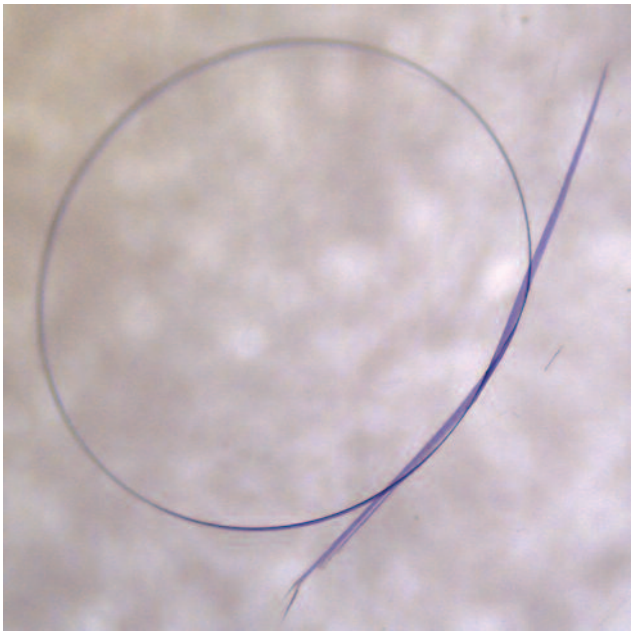
Sir John and Lady Cornforth are survived by their children John Cornforth Jnr, Philippa Cornforth and Brenda Osborne.

University of Sydney



Google

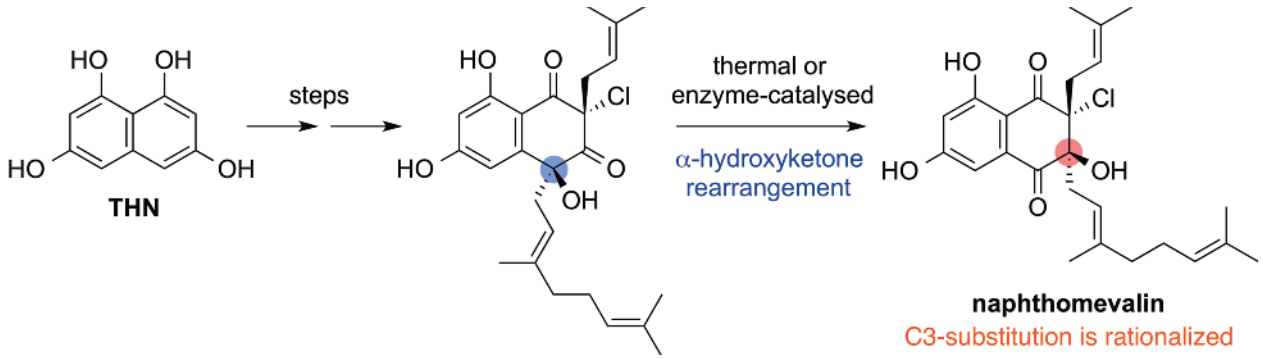
Flexible crystals tie current thinking in knots



Single crystals are typically brittle inelastic materials: when struck or bent, they usually crack, shatter or deform irreversibly. Now, researchers at the Queensland University of Technology and the University of Queensland have grown single crystals of a well-known coordination compound, copper(II) acetylacetonate, that are flexible enough to be reversibly tied into a knot while maintaining crystallinity (Worthy A., Grosjean A., Pfrunder M.C., Xu Y., Yan C., Edwards G., Clegg J.K., McMurtrie J.C. *Nat. Chem.* 2017, https://doi.org/10.1038/NCHEM.2848). Mechanical measurements indicate that the crystals exhibit an elasticity similar to that of soft materials such as nylon, and thus they display properties associated with both hard and soft matter. Using the Australian Synchrotron, the researchers mapped the changes in crystal structure that occur on bending, and determined with atomic precision the mechanism that allows the crystals to bend. Under strain, the molecules in the crystal reversibly rotate, and thus reorganise to allow the mechanical compression and expansion required for elasticity while maintaining the integrity of the crystal structure. Six other examples of flexible crystals were also identified.

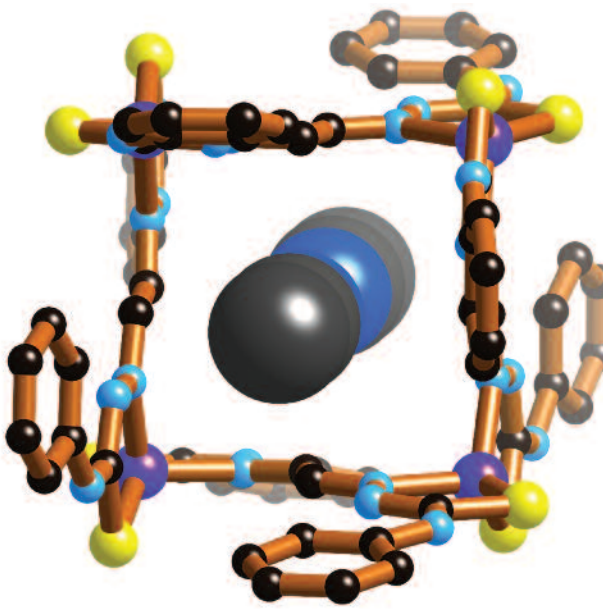
Paradigm shift in marine natural product biosynthesis

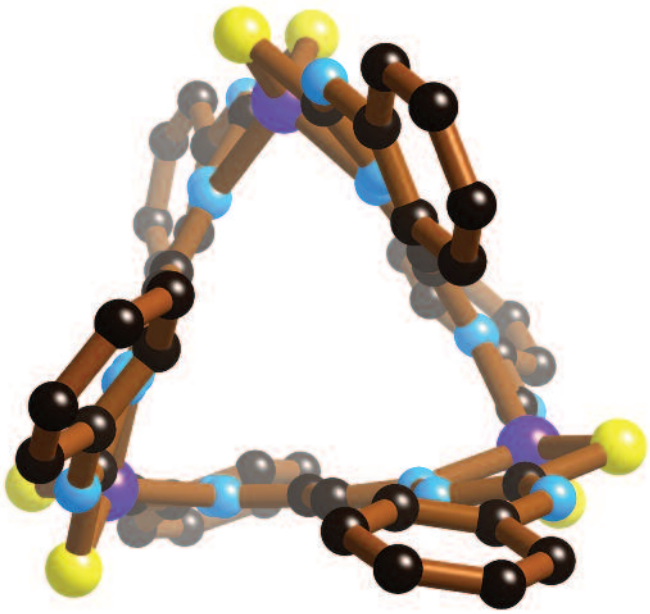
A large family of naphthoquinone meroterpenoids with potent antibiotic activity, including the napyradiomycins, are biosynthesised from tetrahydroxynaphthalene (THN) by marine bacteria. However, the prenyl substitution pattern of the napyradiomycins, such as naphthomevalin, contradicts the expected nucleophilic reactivity of THN. Intrigued by this, researchers at the University of Adelaide and the Scripps Institution of Oceanography, UC San Diego, USA, collaborated to investigate the biogenesis of the napyradiomycins and discovered a biosynthetically unique α-hydroxyketone rearrangement that explains the unusual substitution pattern (Miles Z.D., Diethelm S., Pepper H.P., Huang D.M., George J.H., Moore B.S. *Nat. Chem.* 2017, https:/doi.org/10.1038/NCHEM.2829). First, a thermal α-hydroxyketone rearrangement was developed by organic chemists at the University of Adelaide in a biomimetic total synthesis of naphthomevalin. This total synthesis provided access to proposed biosynthetic intermediates, which aided the discovery by biochemists at the Scripps Institution of Oceanography of a bacterial enzyme that catalyses the 1,2-shift. Computational studies were also conducted to give further insight into this mechanistically and biosynthetically interesting rearrangement.



Templating coordination nanotube assembly

Molecular structures with 1D channels, known as nanotubes, have potential applications in gas sorption, separation and storage. Recently, Brett Paterson, Brendan Abrahams, Paul Donnelly and colleagues from the University of Melbourne used host–guest interactions to direct the assembly of coordination complexes into nanotubes that can act as hosts for small molecules (Paterson B.M., White K.F., White J.M., Abrahams B.F., Donnelly P.S. *Angew. Chem. Int. Ed.* 2017, **56**, 8370–4). Two different Zn^{II} complexes of glyoxal-bis(4-phenyl-3-thiosemicarbazone) were prepared from the same starting materials by altering the synthetic conditions. When the complex was prepared in dimethylsulfoxide, a triangular prism structure formed, involving three Zn^{II} centres and three bridging ligands. In contrast, discrete square coordination nanotubes with four Zn^{II} centres bridged by four ligands were formed by simply adding the linear small molecules acetonitrile (CH_3CN), carbon dioxide (CO_2) or carbon disulfide (CS_2). The linear molecules template the formation of the square coordination nanotubes and are included as guests within the channels. The template can be removed and the hollow nanotubes can adsorb two molecules of CO_2. These approaches could be useful for selective molecular recognition and capture.





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.

The editors' experiences (part 1): (lack of) author ethics in journal publishing

After more than 18 months in the role of editors-in-chief of *Australian Journal of Chemistry* and handling a large number of submissions, we have been periodically both startled and bemused by fortunately rare examples of poor behaviour on the part of authors. The pressure to publish in a Western journal of established international repute remains very high for many scientists, but particularly for those hailing from countries where research funding and defined career paths remain difficult. This has led to recourse by some authors to dubious or unethical means to have their submissions accepted and CVs correspondingly enhanced. Here are some examples that one or the other of us has had to deal with (including with other journals that we are associated with).

- *Authorship changes after provisional acceptance of a paper.* On more than one occasion, after the corresponding author has been notified of provisional acceptance of their manuscript subject to revision, the revised manuscript is eventually returned together with a covering letter outlining the minor editorial changes and corrections that have been made. These have been accompanied by a statement that the changes have necessitated the addition of one or more authors. It is nearly always clear to us that the manuscript changes were so minor as to make it impossible that any new contribution was provided by the proposed new author(s). There have been reports of some authors making the provisional acceptance letters an opportunity to sell co-authorship places on revised manuscripts (M. Hvistendahl, *Science* 2013, vol. 342, pp. 1035–1039). We usually refuse to accommodate such requests unless major revisions were undertaken in which additional studies were indeed performed and reported by the new authors.
- *Withdrawal of an accepted manuscript.* After much effort has been spent in sourcing suitably qualified reviewers, who, themselves, then spend a great deal of time preparing comprehensive assessments together with a recommendation of provisional acceptance subject to revision, the corresponding author then notifies us that a decision has been made by their department to send the revised (and now scientifically much-improved and fully English-edited) work as a new manuscript to another journal, often one with a higher impact factor. This is despite agreeing at the time of the original submission to have the work published in our journal (subject, of course, to suitable revision and acceptance). Such behaviour is particularly galling, given the waste of the editors' and reviewers' considerable efforts during the manuscript handling process. Naturally, the authors are blacklisted from making future submissions.
- *Simultaneous submissions to journals*. On one occasion, a referee in Japan notified us that a manuscript he had agreed to review was identical to another by the same authors that he was reviewing for a different journal. On questioning the corresponding author, the excuse was given that it was the result of a 'clerical error' by the department's secretary, who sent the manuscript simultaneously to different journals. It was evident that, in this case, a multiple submission was an effort to increase the chances of acceptance of the manuscript by any forum. Needless to say, it was rejected by our journal and the authors are now permanently blacklisted.

Fortunately, *Australian Journal of Chemistry* has a very efficient publishing office (CSIRO Publishing), which, together with its vigilant editorial board, continues to be wise to these unethical efforts to secure publication in our journal. Yet, we will undoubtedly continue to be surprised by original efforts to 'bend' the author submission procedures.

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

IUPAC's centenary

Creating the common language of chemistry

Preparations for the centenary of IUPAC in 2019 are already under way, reports Mary Garson.

The RACI's centenary this year is a milestone – a unique opportunity to recognise what RACI has accomplished and to acknowledge its ongoing role and responsibility in the future of chemistry, both nationally and internationally.

In 2019, the International Union of Pure and Applied Chemistry (IUPAC) will likewise celebrate 100 years. The Union was formally registered on 28 July 1919. A steering committee set up by the IUPAC Bureau has outlined the following vision for the centenary, providing the following background and offering initial ideas. Subsequently, a formal IUPAC100 management committee has been established. Members at large, including individuals and national adhering organisations such as RACI, are invited to become involved in the various events and activities that are planned.

Background

As the curtain rose on the 20th century, chemistry was already a mature science and a thriving industry. But communication within the industry was difficult. There were few generally accepted norms for the naming of chemical compounds and chemists routinely did so according to their own personal preferences, resulting in multiple names for a single, unique compound. This lack of a universally accepted language in chemistry created a major barrier to the sharing of information, ultimately hindering efficient research and the rapid advancement of scientific discovery. Aware of this major barrier to the growth of scientific knowledge, a group of eminent chemists and visionaries from France, Belgium, Italy, the UK and the US gathered in 1919 to create IUPAC.

The IUPAC founders were also aware that chemical instrumentation and methodologies were continuously evolving towards greater precision and that more tools were being developed to assess the chemical and physical properties of substances. Therefore, IUPAC was given the charter not only to create a nomenclature that would facilitate communication within the chemistry community, but also to develop standards and norms for the calibration and normalisation of chemical substances.

What in 1919 perhaps seemed a distant and unachievable goal is today a reality. Thanks to the efforts of a legion of chemists over many decades, advances in scientific research have

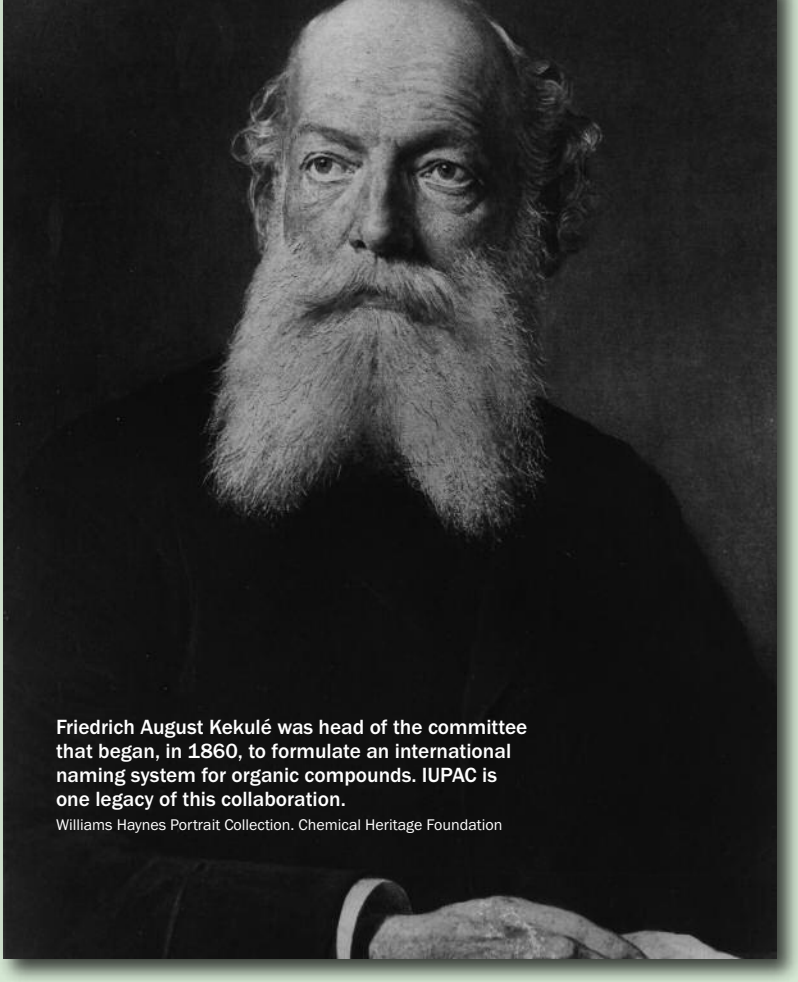
escalated due to the creation of universally accepted standards, terms and nomenclature.

IUPAC as a creator of the common language of chemistry

Conceived as an international organisation, IUPAC was born in the aftermath of World War I – an event that negatively affected the public's perspective of science in general, and of chemistry in particular, leading them to question the peacetime role of chemistry and the societal benefits that it provides. Through the organisation of regularly scheduled scientific meetings worldwide, IUPAC has nurtured an international community that has dealt with all aspects of chemistry, pure as well as applied.

One hundred years later, IUPAC and the field of chemistry jointly face many interwoven challenges such as globalisation, the energy crisis, climate change and other environmental challenges. The IUPAC Centenary offers an opportunity not only to commemorate this century-old organisation, but also to rethink how IUPAC can better promote and advance the evolving field of chemistry, particularly as we move into the era of 'big data'. It is an opportune time to take a critical and ambitious look at IUPAC in order to prepare the global chemistry community for the future, and to engage effectively with the next generation of chemists who will lead our science forward.

Chemistry is a major contributor to the well-being of humankind, from the ongoing evolution of better and more effective medicines to the production of safe, clean water. Some of its major breakthroughs such as the fixation of nitrogen to make fertiliser or the synthesis of nylon as a new material have greatly contributed to health and security, but there are still major challenges to be met. From societal challenges such as climate change to alternatives to fossil fuels, chemistry has a significant role to play in the invention of new solutions for a better and more sustainable future for all. Today's United Nations Sustainable Development Goals (https://sustainabledevelopment.un.org/sdgs) are both a call to and a source of inspiration for chemists. IUPAC, as the international organisation of chemistry, should play a major role in creating the platform providing the resources and the network for delivering the needed solutions more effectively and in a



Friedrich August Kekulé was head of the committee that began, in 1860, to formulate an international naming system for organic compounds. IUPAC is one legacy of this collaboration.
Williams Haynes Portrait Collection. Chemical Heritage Foundation

IUPAC's early history

IUPAC was formed in 1919 by chemists from industry and academia, who recognised the need for international standardisation in chemistry.

The standardisation of weights, measures, names and symbols is essential to the well-being and continued success of the scientific enterprise and to the smooth development and growth of international trade and commerce.

This desire for international cooperation among chemists and facilitation of the work of the international, but fragmented, chemistry community were the earliest characteristics of the Union. Even before the creation of IUPAC, a predecessor body, the International Association of Chemical Societies (IACS), had met in Paris in 1911 and produced a set of proposals for the work that the new Association should address.

These included:

- nomenclature of inorganic and organic chemistry
- standardisation of atomic weights
- standardisation of physical constants
- editing tables of properties of matter
- establishing a commission for the review of work
- standardisation of the formats of publications
- measures required to prevent repetition of the same papers.

Although 1911 might now seem an early date for chemists to start talking about the possibility of and need for international collaboration and standardisation, the first international attempt at organising organic chemical nomenclature – the Geneva Nomenclature of 1892 – grew out of a series of international meetings, the first of which was organised by Kekulé in 1860.

iupac.org

iStockphoto/rglinsky

Inaugurated in 1974, the Palais des Congrès de Paris is the venue for the 2019 World Chemistry Congress and General Assembly of IUPAC.

collaborative and open manner.

IUPAC's legacy is very rich and one that should be celebrated. After a century of activity and growth, IUPAC has helped to shape a very dynamic field of knowledge. Chemistry has reinvented itself several times since 1919, reorganising its structure through the creation of new subdisciplines, fostering new topics at the crossroads of well-rooted specialties, and forging multidisciplinary communities for the resolution of contemporary problems, such as the creation of new materials and environmental studies. Along with its constant effort to shape and constantly improve the language of chemistry to reflect new developments, IUPAC has also been instrumental in the support of education and in the global growth of chemistry. IUPAC remains an indispensable resource for chemistry.

After a century of activity and growth, IUPAC has helped to shape a very dynamic field of knowledge.

Events and activities

IUPAC has made a formal submission to UNESCO to request the inclusion of 28 July in their calendar of anniversary dates for 2019; the executive board of UNESCO will advise its decision on this anniversary date during October 2017.

In July 2019, the global chemistry community will meet in Paris for the World Chemistry Congress (WCC) and General Assembly of IUPAC. This is not a coincidence! When offering the venue, French colleagues made the point of wanting to celebrate IUPAC's centenary in the City of Light. The organisers of the 2019 WCC plan several events to celebrate the IUPAC Centenary, including sessions focused on IUPAC's role in the evolution of chemistry, the revolution of instrumentation in chemistry, education and training in chemistry, and some of the scientists who have worked for IUPAC.

Other activities and events that are planned include:

- *the celebration of IUPAC's role in creating the common language of chemistry*: This is envisaged as a key theme of the Centenary activities. Since the 150th anniversary of Mendeleev's periodic table will also take place in 2019, this will also be highlighted in the celebration. An online global competition centred on periodic table trivia is planned and will reach a global audience of young students in a way that will be attractive to them, and that will give visibility to the work of IUPAC over the last 100 years.

IUPAC President, Natalia Tarasova, says, 'In 2019, we will pause to celebrate our successes and give serious deliberation as to how IUPAC can best continue in the years ahead to serve as an advocate for the free exchange of scientific information for the benefit of humankind worldwide. While this celebration is just one moment in time, we hope that it will have a lasting impact through events that will advocate the value and importance of science literacy to students worldwide, inspire younger generations of men and women to become the innovative chemists of the 21st century and beyond, and have a positive influence on the public's perception of science in general and chemistry in particular.'

Courtesy IUPAC

- *a video to gather, share, and visualise the history of IUPAC*: This will document the many contributions made by this international organisation in creating a common language for chemistry, providing objective scientific expertise, and developing the essential tools for the application and communication of chemical knowledge for the benefit of humankind and the world.
- *web stories*: A series of 25 web stories will further highlight some of the essential tools and activities that have been created by IUPAC, and will highlight how these tools are currently being used by scientists around the world every day. Typical examples include InChI identifiers, Commission II – Atomic Weights, the various 'colour' books such as the Green Book on quantities, symbols and units used in physical chemistry.
- *interactive periodic table*: A group of young chemists will work under the IUPAC banner to increase the participation of early career chemists in IUPAC through stories of 100 influential chemists (from high school to established career scientists). One idea they have, again linked to the 150th anniversary of the periodic table, is to create an interactive periodic table organised by 'jobs' related to chemistry. Each 'element' will be a portrait of a person who works within the field of chemistry, and will address the diversity of chemists and/or students of chemistry worldwide.
- *social media outreach*: The young chemists group, working in association with IUPAC, also aims to increase the use of social media as an outreach tool within IUPAC and similar chemistry organisations, and to increase the awareness of the general public of how chemistry is intrinsically part of their everyday life. More than ever, global organisations such as IUPAC need to engage better with the community of chemists who represent the future of the discipline.
- *logo competition*: Prior to the Centenary, students worldwide were invited to design a logo as part of the celebration, and the successful entry was then reworked by a graphic designer (see image on page 20).
- *virtual handshake*: Using social media, IUPAC members and chemists worldwide will create a virtual handshake during a global breakfast to be held in May 2019 as a prelude to the main celebrations in July. In this activity, 'Women Celebrating a Chemical Moment in Time', women chemists and chemistry students from around the world will network by VOIP, Skype, social media and/or blogs. Some breakfasts will choose to have panel discussions or guest speakers. A website with the video on the history and language of IUPAC, and also for sharing footage, photos and stories post-events, will provide information for organisers of the various individual breakfast events.
- *education and professional development*: If funding can be obtained, a summer school in 2019 aims to teach green chemistry to young postgraduate and graduate chemists from the developing countries, in particular from Africa.

The way forward

The website for the IUPAC100 Celebrations (www.iupac.org/iupac100) will be launched during the latter part of 2017. The IUPAC100 celebrations will provide a unique opportunity for IUPAC and all its members to highlight the importance of chemistry in an international setting, and to preview the role of chemistry in the next 100 years. It will be excellent if Australian chemists joined in! How will you celebrate?

This article contains content originally published in the September–October 2016 issue of *Chemistry International*, and has been updated with content provided by individual members of the IUPAC100 Management and Planning Committee; this committee is chaired by Professor Mary Garson FRACI CChem, University of Queensland, together with Dr Laura McConnell, Bayer Corp., USA.

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Chemical companies fail to comply with EU regulations

BY **JOHANNE UHRENHOLT KUSNITZOFF** AND **IDA ERIKSEN**

Chemical companies are required to document that their chemicals are safe but the majority withhold or submit incomplete information to the European authorities, allowing dangerous substances to stay on the market.

For the past ten years, it has been the responsibility of European chemical companies to ensure that their products do not contain substances that are harmful to human health or to the environment. To a large extent, the system depends on trust and now it appears that this trust has been misplaced. Chemical companies in Europe do not adequately report the harmful effects that their products could inflict on people and the environment. This means that we may be exposed to various types of dangerous substances, such as endocrine disrupting chemicals – substances that may interfere with the

In 2016, an ECHA test revealed that 72% of company reports were missing important information on substances that they produce or import.

hormone system with negative side-effects for people and the environment.

So says Henrik Holbech, from the European Chemicals Agency's (ECHA) expert group on endocrine disruptors. The information that chemical companies are obligated to submit to the agency about harmful substances in their products is often missing or wrong, he says.

'Unfortunately I can't give concrete examples since the expert group's work is confidential. But overall a lot of statutory data are missing. There's also examples of data sitting with the chemical companies from studies that they conducted, but haven't shared before we force them to do so. It's very frustrating and a big problem for regulating harmful substances', says Holbech.

In 2016, an ECHA test revealed that 72% of company reports were missing important information on substances that they produce or import. Screening by German authorities in 2015 showed that just one of 1814 so-called 'data packs' that companies had submitted met the authority's requirements.

'An obstacle to protecting public health'

The situation is so bad that the director of ECHA, Geert Dancet, sent an email to the chemical industry in April 2017, demanding an immediate improvement so that the authorities could do their job.

Dancet wrote that 'the failure of companies to comply with the requirements of EU chemicals legislation is a fundamental obstacle to ECHA's efforts to protect public health.'

If companies do not improve, then this will have severe consequences, he warns.

'The current data is simply insufficient to make a well-founded assessment of the risk of a chemical. This has two significant consequences: we waste our time hunting harmless substances and, far worse, may not prioritise the most worrying substances.'

The extent of this lack of information on chemicals in the market place surprises the Danish Consumer Council THINK Chemicals.

'It's unacceptable that companies report insufficient information on any effects of these substances, as the spot check shows. This must be the foundation of the EU's work on chemicals, and it's the companies' responsibility. They owe us consumers, who eventually buy their goods, to live up to that responsibility', says project manager Stine Müller.

Scientific data omitted

European companies have been obligated to submit all available and relevant scientific data to ECHA since 2007. This applies to chemicals that they produce themselves or import from other parts of the world.

But when the experts, including Holbech, reviewed the data packs it seemed that 'very often' crucial scientific data on chemicals are missing.

'In the meantime we see that such data already exists, but the companies don't share it, and this is especially problematic if they show harmful effects', says Holbech.

'I don't think that chemical manufacturers are trying to put harmful substances out into the market place. It's probably more about taking advantage of the political uncertainty that still exists around many of these potential endocrine disrupting substances', he says.

Danish Environment Agency: it does not look like an honest mistake

The Environment Agency in Denmark is well aware of the problem, says Marie Louise Holmer, who works with endocrine substance regulation in Denmark.

Chemical companies regularly try to avoid testing their chemicals by posting earlier decisions for other substances.

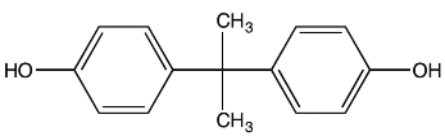
Her colleague, Magnus Løfstedt, who is responsible for the Danish Environment Ministry's adoption of REACH legislation, suggests that some of the failures may be honest mistakes, but this is still problematic.

'I don't want to argue that the rules are clear and we certainly find companies that trade in good faith, despite not complying with all the rules. But from this study on the quality of the data packs that they must submit, many companies clearly evade the rules regarding standard information requirements', says Løfstedt.

Many companies do their best

Chemical manufacturers and importers in Denmark are aware that data packs are not as good as they could be. But this does not mean that people are cheating the system, says Karin Klitgaard, head of environmental policy from the Confederation of Danish Industry.

'It's not our experience that the data packs are deliberately neglectful. Our



For endocrine disrupters such as bisphenol A (pictured), companies are obligated to conduct a single test if they produce or import more than 1000 tons of the substance a year. Therefore, it is important that companies reveal all existing scientific data on the effects of endocrine disrupters.

Changes to ECHA Candidate List

The European Chemicals Agency (ECHA) has added the substance perfluorohexane-1-sulfonic acid to the Candidate List of substances of very high concern (SVHCs). Entries for bisphenol A and four phthalates have been updated to include endocrine-disrupting properties for human health. The Candidate List now contains 174 substances.

Perfluorohexane-1-sulfonic acid belongs to the group of per- and poly-fluoroalkyl substances (PFASs). This identification is part of a regulatory activity, targeting this large substance group with the aim of clarifying the concerns and regulating the substances, as necessary. The aim is also to avoid undesired substitution with other PFASs. Several PFASs have already been identified as SVHCs, one group (PFOA and related substances) is now restricted, one restriction is under preparation and many assessments are underway.

The bisphenol A entry was updated to reflect an additional reason for inclusion due to its endocrine-disrupting properties having adverse effects on human health. Bisphenol A was included in the Candidate List in January because of its toxicity to reproduction.

The entries for benzyl butyl phthalate, bis(2-ethylhexyl)phthalate, dibutyl phthalate and diisobutyl phthalate were also updated because the European Commission has decided on their endocrine-disrupting properties.

ECHA headquarters in Helsinki. Kaihsu Tai/CC BY-SA 3.0

The Candidate List is a list of substances that may have serious effects on human health or the environment. Substances on the Candidate List are also known as 'substances of very high concern'. The aim of publishing such a list is to inform the general public and industry that these substances are candidates for possible inclusion in the Authorisation List. Once they are on the Authorisation List, industry will need to apply for permission to continue using the substance after the sunset date.

Companies may have legal obligations resulting from the inclusion of the substance in the Candidate List. These obligations may apply to the listed substance on its own, in mixtures or in articles. In particular, any supplier of articles containing a Candidate List substance above a concentration of 0.1% (weight by weight) has communication obligations towards customers down the supply chain and consumers.

In addition, importers and producers of articles containing the substance have six months from the date of its inclusion in the Candidate List (7 July 2017) to notify ECHA. Information on these obligations and related tools are available on ECHA's website.

The Candidate List is a list of substances that may have serious effects on human health or the environment.

European Chemicals Agency. A table of changes is available at https://echa.europa.eu.

members spend an enormous amount of energy correctly registering and reporting substances. No one wants to make mistakes and send harmful substances out into the market place', she says.

In fact, companies want more control over the data packs, says Klitgaard.

'Those who don't do it right undermine the entire system and make the rest look bad. So we want ECHA to reveal the data packs that don't meet their requirements and enforce the rules better', she says, and adds that REACH legislation was designed to prevent substances being sold if there was not enough information regarding their effects.

Only 5% of data have been checked

Right now, ECHA cannot do much to encourage companies to improve their data reporting, says Holbech.

ECHA have spot checked just 5% of company reports and so there are probably many more undetected incidences. By the time ECHA becomes aware of any potential harmful effects, the products are already on the market, he says.

Hence, the Danish Consumer Council THINK Chemicals would also like to see the rules tightened, though they regret that such steps are necessary.

'The REACH requirements should certainly be met and if they're not, then the EU should have tools to ensure that they are. But it is of course sad that our authorities need to use extra time and resources to control rather than work more pro-actively for consumer safety', says Müller.

Johanne Uhrenholt Kusnitzoff and **Ida Eriksen** are regular contributors to ScienceNordic. Originally published as part of a series on endocrine-disrupting chemicals: http://sciencenordic.com/endocrine-disrupting-chemicals. Reused with permission.

The **RACI Centenary Congress** was a confluence of chemistry, creativity and camaraderie. It was also a time for colour, collaboration and celebration.

23-28 July 2017 | Melbourne

raci 100 Centenary Congress

Professor Mark Buntine, Centenary Congress chair, speaking at the welcome reception. Photographer at Large

The opening ceremony, in one of the plenary halls. Photographer at Large

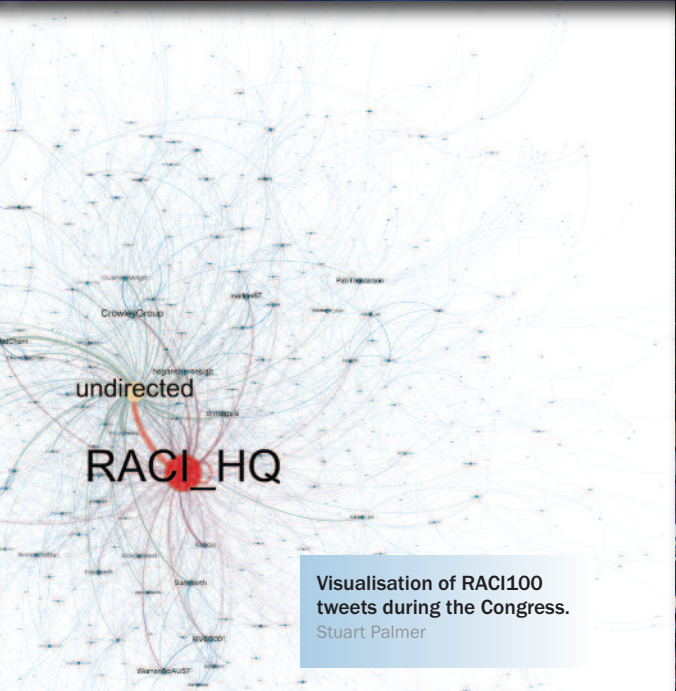
The first female presidents of the Asian Federation for Medicinal Chemistry. Associate Professor Renate Griffith (right), AFMC president in 2016 and 2017, and chair of the organising committee for AIMECS2017 at the Centenary Congress, is handing over the flag to the next president, Professor Esin Aki-Yalcin from Turkey. Esin will become president of AFMC next year and organise AIMECS2019 in Turkey. Courtesy Renate Griffith

Professor Frances Arnold, plenary speaker: 'This was a great meeting – I really enjoyed being in Melbourne, and the science was super. Here's a photo of three of your plenary speakers (from left): Dr Laura Kiessling, Professor Frances Arnold, Professor Molly Stevens) enjoying dinner at Il Cantuccio on my birthday!' Courtesy Frances Arnold

Michael KAssiou

A winter theme at the Centenary Congress Celebration dinner.

Photographer at Large



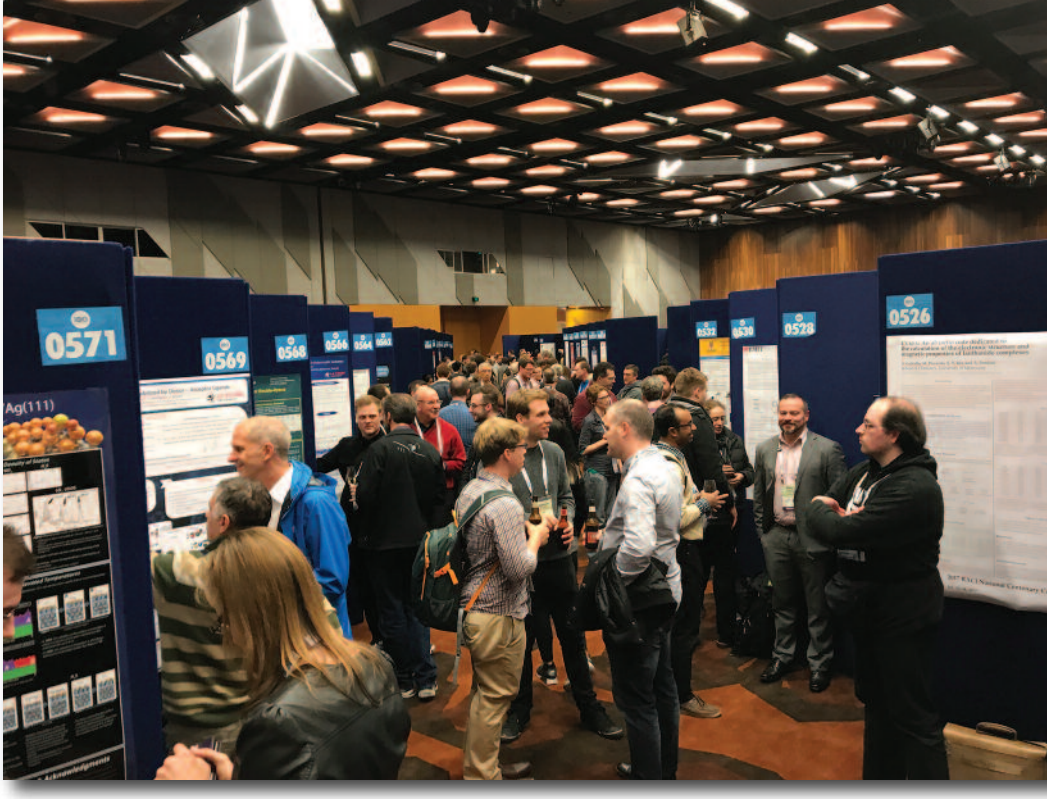
Visualisation of RACI100 tweets during the Congress.
Stuart Palmer

Chemistry goes on ice for an evening. Photographer at Large

The perfect complement to a conference. Photographer at Large

The first female president of RACI's first 100 years, Dr Doreen Clark (right), with Dr Vicky Gardiner, who will be the first female president of RACI's second 100 years. Courtesy Vicki Gardiner

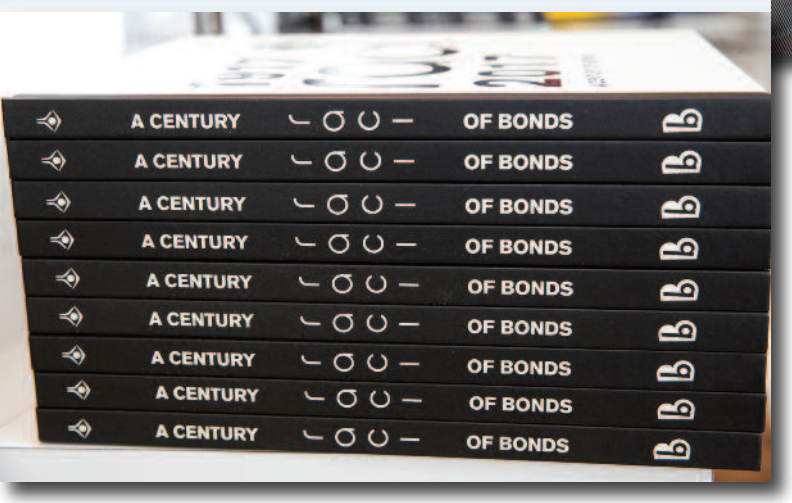
One of the awards presented at the Academic Sharp Brain event. Photographer at Large



Student and poster sessions attracted plenty of interest.
Oliver Jones

How many Fellows can you fit on an escalator? Photographer at Large

RACI: a century of bonds, published as part of centenary celebrations and given to Congress delegates. Photographer at Large



Professor Martyn Poliakoff (at the Melbourne Museum), keynote speaker: 'Great conference, fantastic organisation but I only saw one kangaroo!'
Martyn Poliakoff

Supporting women in chemistry

Guests at the RACI Congress Women in Chemistry dinner, held at South Wharf.

Guests for the 'Supporting Women in Chemistry' panel event, joined by members of the WinC committee. Back (from left): Yvonne Mah, Marguerite Evans-Galea, Annabella Newton, Amy Heffernan, Katherine Locock. Front (from left): Belinda Abbott, Susan Northfield.

The RACI Victorian Branch's Women in Chemistry (WinC) committee is one of the most active groups of the branch, regularly running networking and career development events throughout the year. At the recent RACI Centenary Congress in Melbourne (23–28 July 2017), WinC had an active presence throughout the conference. They held two events over the course of the week, and found the engagement with local, interstate and international colleagues to be highly rewarding.

The first event was a dinner on the Monday night of the conference, held at a local South Wharf restaurant along Melbourne's Yarra River. More than 50 guests joined WinC for the evening, with special presentations from five of the congress' plenary and keynote speakers: Laura Kiessling (University of Wisconsin), Sally Brooker (University of Otago), Vivian Yam (University of Hong Kong), Andrea Robinson (Monash University) and Zaiping Guo (University of Wollongong). Each of the speakers provided anecdotes of their research experiences, highlighting 'not to give up too easily or too early', 'be passionate' and the 'importance of a supportive network'. Overall, it was an enjoyable and inspiring night for all in attendance, and a fantastic networking opportunity for the students and early career researchers, who spent the evening in conversation with both the speakers and members of the WinC committee.

The second WinC event was a 'Supporting Women in Chemistry' discussion panel, held on the Thursday afternoon. Guest speakers on the panel were Dr Marguerite Evans-Galea (Industry Mentoring Network in STEM), Dr Annabella Newton (Victorian WinC committee) and Dr Katherine Locock (RACI Equity Committee). Each of the speakers gave an overview of the activities of their respective support networks, including upcoming events, and then participated in a rigorous Q&A session with the audience. This was the first event for which WinC live-tweeted updates for those who couldn't attend the event in person, which was filled to capacity. In addition to WinC's own online engagement, it was gratifying to see that guests at the panel event also contributed their thoughts using the same hashtag, #supportWinC. Following from this social media success, in future the RACI-VIC WinC committee will continue to use this hashtag to promote their events.

The WinC committee wish to thank the RACI Congress organisers for helping to facilitate inclusion of these two successful events in the program. If you wish to engage with the RACI-VIC WinC committee, keep watch for the hashtag #supportWinC; or if you wish to be added to the WinC mailing list, please contact raci-vic@raci.org.au. To stay apprised of all their upcoming events, visit www.raci.org.au/branches/vic-branch/women-in-chemistry-group. The WinC committee is pleased to welcome all members of the scientific community to attend their events, which are not exclusively aimed at women or chemists.

Dr Susan Northfield MRACI is Secretary for RACI-VIC Women in Chemistry Committee.

What is your best method and is it disclosed in your patent?

Dr David Herman, FB Rice

A requirement for obtaining a valid Australian patent is that the specification must disclose the 'best method' known to the applicant of performing the invention. The purpose of the best method requirement arises from the *quid pro quo* of the patent system – that the applicant must disclose the most effective means of performing an invention for the public to be able to research and develop further following its publication and to be commercially free to use once the granted monopoly expires, and that the applicant does not omit information that gives the best results.

So what does disclose the 'best method' exactly mean? Given failing to do so can render a patent invalid in Australia, it is essential that this requirement is properly understood.

What is the best method?

The best method is related to the nature of the invention. Importantly, the best method is not determined with sole reference to the claims. If the claims of the invention relate to a product *per se* (i.e. a chemical compound), the specification may still need to include the best method for the product's manufacture, along with the applicant's best version of the product.

In particular, if there are numerous possible methods for manufacturing the product, which may vary the properties of the product, the applicant is required to disclose the best method they use to make the product. This may, for example, be a new method of isolating the product *per se*, or could merely be one optimised single step in what otherwise would be a routine procedure; for example, the selection of a specific drying temperature when making pharmaceutical tablets by conventional processes.

There is no need to explicitly state in the patent specification that 'the best method known to the applicant is ...', or if more than one method is included, to indicate which method is the best, provided it is disclosed in some shape or form.

When is the best method assessed?

The best method requirement is assessed on the basis of the applicant's knowledge at the time of filing the complete application. This will include the knowledge of the inventors and any other contributors to the research. Should a better method be developed prior to filing the complete application (i.e. during the priority period), it must be included in the complete specification. The complete specification does not need to be amended if a better method is developed after the complete specification filing date.

Can the best method be added in later?

Australian patent law now prohibits any amendment that extends the disclosure of a patent specification. Put simply, an amendment to include something new about how to perform the invention is not allowable.

Australia is now out of step with other countries on this best method requirement. A common strategy overseas may be to pursue the best product in one patent and its best manufacture method for making it in a separate patent. A best manufacturing method may also wish to be retained as a trade secret or in-house knowledge. However, in view of Australia's requirements, withholding the best method from a patent application runs a risk of it being found invalid.

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

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Distrust of experts happens when we forget they are human beings

In 2016, conservative, pro-Brexit, British politician Michael Gove announced that people in England '… have had enough of experts with organisations from acronyms saying that they know what is best and getting it consistently wrong'.

In the US, Donald Trump famously doesn't believe any expert who doesn't agree with him. Our most recent former Prime Minister Tony Abbott has also been accused of having trust issues.

Growing distrust of experts is linked with changing social and political climates. But it also stems from misunderstandings about what experts are, and what their obligations to society entail.

At their heart, criticisms of experts often imply that they are servants, commodities or so vested in their field they can't relate to reality.

To restore trust in experts, we need to remember they are, first and foremost, human beings.

How detractors define and judge experts

It's probably safe to assume politicians are working from a relatively simple definition of 'expert', such as: 'an expert is a person with specialist knowledge not commonly held, or likely to be understood, by a layman'.

When people like Trump make assertions about the right and proper role of experts in public conversations, they appear to have an implicit list of infringements that experts must never transgress.

Expressing values or opinions

Detractors claim that when speaking as an expert, the things you say in public should be untainted by your values and opinions. In essence, you should be a passive conduit for information or facts.

University of Colorado Professor Roger Pielke offers a subtle disdain for experts occupying this position when he critiques the 'stealth issues advocate', a role 'characterised by the expert who seeks to hide his/her advocacy behind a facade of science, either pure scientist or science arbiter'.

Deviating from the straight and narrow

Critics of experts believe that should you even *appear* to deviate from your role as a neutral presenter of facts (for example, by offering policy advice), you are no longer an expert and/or cannot be trusted.

This is typified by Myron Ebell when he was head of Donald Trump's Environmental Protection Agency transition team. He said:

> […] whenever you hear an environmental expert, think that he is an urban eco-imperialist.

Rejection of the 'expertariat': In June 2017, the Trump administration formally advised the United Nations of their intention to withdraw from the Paris Agreement. The Paris Agreement was reached by heads of delegations at the 2015 United Nations Climate Change Conference in Paris (pictured). Presidencia de la República Mexicana/CC BY 2.0

Detractors claim that when speaking as an expert, the things you say in public should be untainted by your values and opinions. In essence, you should be a passive conduit for information or facts.

Making mistakes

Those who criticise experts assert that if you get something wrong, you are no longer an expert and/or cannot be trusted. Myron Ebell referred to experts as 'the expertariat', saying:

> The people of America have rejected the expertariat, and I think with good reason because I think the expertariat have been wrong about one thing after another, including climate policy.

All of these criticisms forget one thing: experts are human beings.

To suggest that the benefits of expertise can be delivered 'value-free' is naive. Like all people, experts are influenced by politics and biases, emotions and beliefs. They are motivated, active agents who create, process and communicate knowledge. Experts are not passive conduits.

The reality of the expert

To consider the role of experts in public debates, I'm drawing on my own area of expertise: science communication. In the spirit of this article, I should note that I claim expertise here based on nearly 20 years of university-based research, practice and teaching as well as my experience providing consultancies in Australia and around the globe.

In my realm, the most interesting grist for discussions around experts and trust turns up wherever science-*related* (but not always science-*based*) assertions are flung around in contests over socially contentious issues.

Climate change action, the acceptance of genetically modified foods, and compulsory childhood vaccination are three classic examples where this regularly plays out in public.

Of course, in examples like these, the role of expertise is not straightforward. For starters, exactly what constitutes pertinent specialist knowledge is itself up for debate.

Scientific aspects of disagreements about climate change, genetic modification or vaccination are regularly accompanied by arguments grounded in social, political, economic and religious concerns. And well they should be – these are not uni-dimensional issues. It's not simply a matter of 'getting some expertise'; it's also about working out which expertise is relevant, and to whom.

In an ideal world, the evidence-based assertions of experts withstand evidence-based challenges, and are modified where they are found wanting. It's through the open, honest, systematic contest of ideas among experts that the best ideas emerge.

Clearly, the place of the expert in public conversations on these issues depends on many factors: the goal(s) of the conversation; the knowledge, interests and positions of the parties involved; and importantly, the types of people who might be 'listening in'.

But more, it should also depend on what the experts themselves want to achieve. Like anyone else, experts have their own motives, even when overtly wearing their expert hat.

Traditionally, an expert's motivation for participating in public conversations as an expert will be rooted in a desire to inform, guide, advise or warn based on their specialist knowledge.

But equally – and often simultaneously – they could be driven to participate because they want to engage, inspire or entertain. They themselves may also hope to learn from their participation in a public conversation.

Or maybe they just want to be noticed (and there's nothing wrong with that).

So, what's the place of experts in public conversations?

Assessing the actions of experts using criteria that downplay, and even ignore, the fact that they are people makes it easier to admonish them and dismiss their expertise because they dare to have opinions, to make mistakes, or to pick a side.

US Navy Professor Tom Nichols says we live in:

> [...] a manic reinterpretation of 'democracy' in which everyone must have their say, and no one must be 'disrespected'.

This is a place where, at the extremes, positions put forward by experts are deemed suspect because they come from experts.

In a world where facts and logic are considered malleable, and where powerful, influential interest groups cast doubt on the notion of expertise *itself*, it's the place of the expert in public conversations to help turn this tide.

It's my opinion that the expert should strive to be seen as *more* human, to embody at every opportunity their position as a part of society, as a person who has interests and opinions *and also* expertise.

How they choose to do this, however, should be up to them.

Rod Lamberts is Deputy Director, Australian National Centre for Public Awareness of Science, Australian National University. First published at www.theconversation.com.

Separating CO_2 in industry

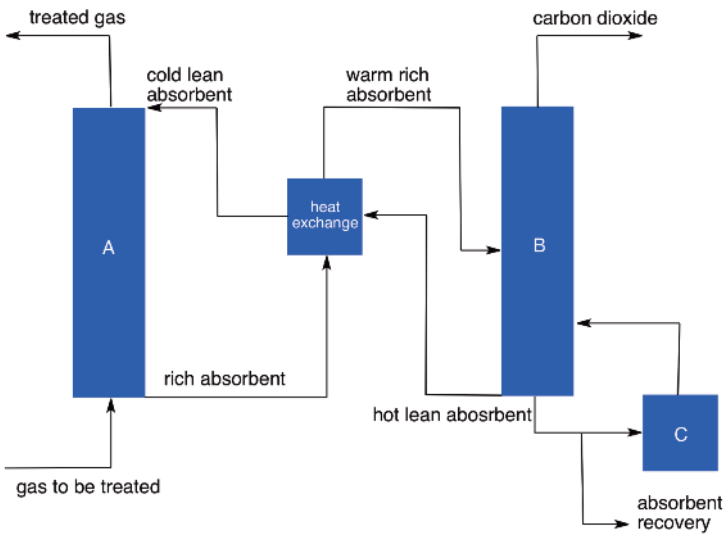
iStockphoto/nielubieklonu

Central to many of the approaches to greenhouse gas mitigation is the removal of carbon dioxide from gaseous emissions so it does not add to the greenhouse burden of the atmosphere. When extracted, the gas can be sequestrated in deep underground storage facilities. In the extreme, there are now several proposals to extract the gas from the atmosphere for geo-sequestration. Here I will discuss the current practice and economics of carbon dioxide separation from streams of mixed gases in industry.

Carbon dioxide is found as a waste (unwanted) gas in a wide variety of streams in the hydrocarbon processing and chemical industry and many different methods are used to remove it. Generally, removal is accomplished by process plant as illustrated below. The gas to be treated flows into the base of tower A at pressure and rises against a descending stream of absorbent. The treated gas (carbon dioxide depleted) exits the top of the tower. Absorbent loaded with carbon dioxide exits the base of the tower and is pumped to a regenerator tower B where the carbon dioxide is desorbed from the absorbent, often by boiling the absorbent by means of a heater C, and exits the top of the tower. Regenerated absorbent is pumped to the top of tower A.

Most commonly, absorbent regeneration is accomplished by heat (boiling the absorbent), and to optimise efficiency of the process the streams passing between the towers pass through heat-exchangers.

The choice of absorbent (process) is determined by the nature of the gas being treated. Some processes use physical absorbents with the rate and efficiency of absorption of carbon dioxide being determined by Henry's law. The table lists common components in gases to be treated, together with their normal boiling points – the value for carbon dioxide is computed. For design purposes, the process is built around the removal of a key gas (carbon dioxide) to a specified level. As a consequence, to a first approximation, gases present with higher boiling point are also removed. For example, in the case



Carbon dioxide removal from industrial gases.

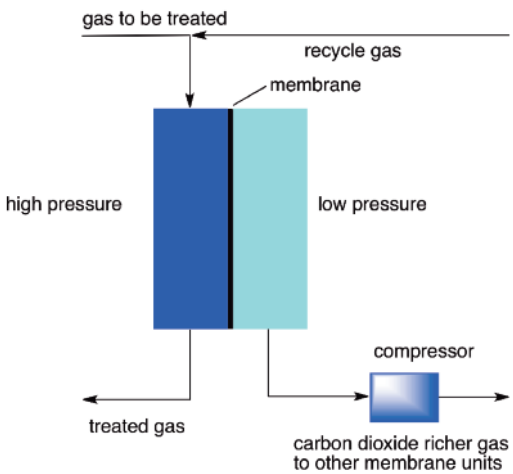
Boiling points of gases pertinent to CO_2 removal

Gas	Boiling point (K)	Gas	Boiling point (K)
H_2	20.4	CH_3SH	279.1
N_2	77.4	NO_2	294.3
CO	81.7	HCN	299
O_2	90.2	i-C_5H_{12}	301
CH_4	112	CH_3CH_2SH	308.2
CO_2 (computed)	**175**	n-C_5H_{10}	309.2
C_2H_6	184.6	CH_3SCH_3	310.5
C_2H_2	188.4	CS_2	319
H_2S	**213.5**	n-C_6H_{14}	341.9
COS	223	C_6H_6	353.2
C_3H_8	231.1	c-C_6H_{12}	353.8
NH_3	240	n-C_7H_{16}	371.6
i-C_4H_{10}	261.4	H_2O	373.2
SO_2	263.2	n-C_8H_{18}	398.8
n-C_4H_{10}	272.7		

of carbon dioxide removal, any hydrocarbons present with a higher boiling point will also be stripped from the gas.

An early process (Rectisol™) uses methanol, which is chilled (to typically –40°C) so the process requires refrigeration plant. This process is good at handling highly fouled gases from gasifiers and the like and is able to strip out high-boiling hydrocarbons and tars. The choice of a low-boiling solvent such as methanol facilitates separation from these materials and methanol recycle. Originally used in coal gasifiers, such a process would be used to clean gases from bio-gasification of renewable feedstock such as wood waste and bagasse. Newer processes use higher boiling solvents to avoid the refrigeration requirement or mixed absorbents to improve selectivity.

To a large extent, membrane processes operate in a similar manner, as shown in the following diagram. High-pressure carbon-dioxide-containing gas enters one side of a unit separated into two by a membrane. Carbon dioxide 'dissolves' in the membrane and passes through the membrane to the low-pressure side of the unit. Adequate separation efficiency is improved by operation of multiple units in series and recompressing and recycling the tail gases. Problems arise when the gas to be treated contains higher boiling compounds that also dissolve and degrade the membrane, such as aromatics. This has occurred in carbon-dioxide-rich natural gas in central Australia.



Membrane processes.

In many instances, hydrogen sulfide removal is also required along with the carbon dioxide. As the table shows, hydrogen sulfide will also be removed with physical absorbents. However, both of these gases are acid gases and there are a large number of processes that use this fact to improve removal efficiency by using an alkaline absorbent. These processes get over the limitations of Henry's law absorption capacity and kinetics by chemically reacting the acid gases. As will be appreciated, the choice of absorbent is limited by the need to form a salt that can be easily reversed in the regenerator:

$$CO_2 \text{ (or } H_2S) + \text{absorbent} \rightarrow \text{absorbent–}CO_2 + \text{heat}$$

Application of heat in the regenerator liberates the acid gases. Alkanol amines are widely used for removing carbon dioxide and hydrogen sulfide from natural gas, heavier hydrocarbons being first removed upstream so they do not interfere with the process.

Another absorbent used is hot potassium carbonate (the Benfield process), which forms a bicarbonate upon contact with carbon dioxide. This process is commonly used in ammonia synthesis plants where ample steam is available for process operation (near 100°C) and absorbent regeneration. Overall, the process is less energy intensive than amine or physical solvent-type processes, and ammonia synthesis gases (nitrogen and hydrogen) are effectively insoluble in the hot potassium carbonate solution, which minimises losses.

The economics of gas treatment and the choice of the process to be used are strongly dependent on the nature of the gases to be treated. At one end of the spectrum is the Rectisol-type process, which can, more or less, treat any gas. Minimising losses and extracting and separating unwanted products such as hydrocarbons and tars requires a lot of process equipment and hence high capital cost. At the other extreme, chemical absorption processes are well established for treating gases with relatively few unwanted species.

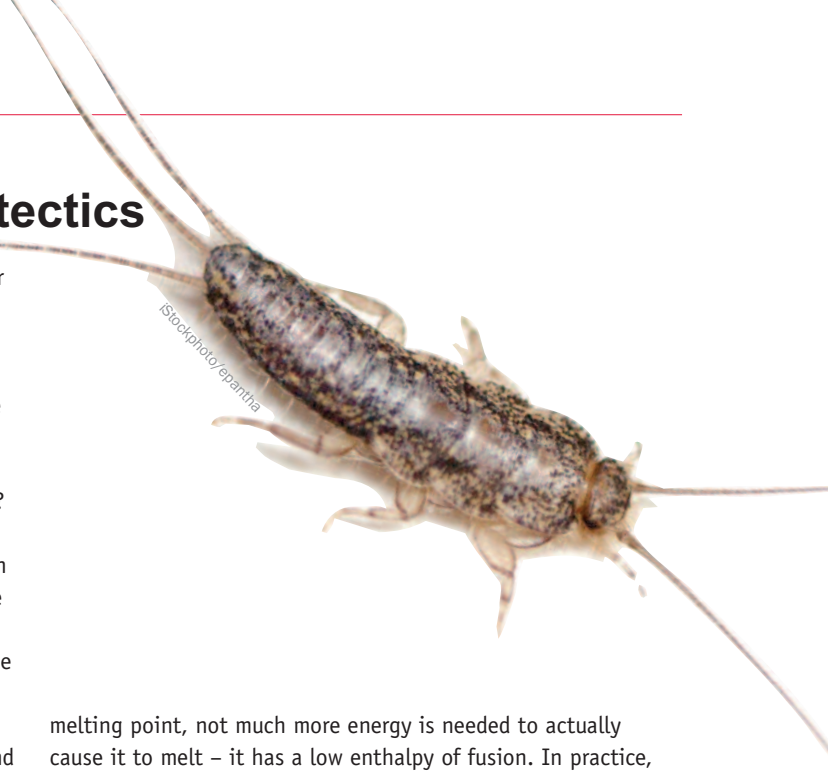
Most natural gas contains some carbon dioxide. This is usually extracted and exhausted to the atmosphere. Only recently as fields higher in carbon dioxide are developed have there been proposals for carbon dioxide geo-sequestration. For example, at the Gorgon field in Western Australia (10–20% carbon dioxide), the developers (Chevron) remove and geo-sequestrate carbon dioxide so that the final gas meets specifications for production of LNG or pipeline transmission to Perth (typically 2% carbon dioxide). However, high carbon dioxide content fields in central Australia (25% or more carbon dioxide) and newer developments in Bass Strait (Kipper >10% CO_2) still exhaust extracted carbon dioxide to the atmosphere.

Difficulties of mass carbon dioxide removal are illustrated by the case of the East Natuna gas field in the Indonesian sector of the South China Sea (the West Natuna field provides gas to Singapore). The East Natuna field is one of the largest undeveloped gas fields known. It was discovered in 1973 and is thought to contain over 200 Tcf (trillion cubic feet) of gas, unfortunately with a carbon dioxide content of about 70% (volume), which has so far precluded its development. Proposals to develop the field have gone through many iterations with one proposal to lower the carbon dioxide content by membranes and re-injecting the carbon dioxide requiring double the usual off-shore facilities (dedicated off-shore carbon dioxide removal and geo-sequestration platforms).

In a later issue, I will discuss some matters relating to carbon dioxide removal from flue gas prior to geo-sequestration.

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

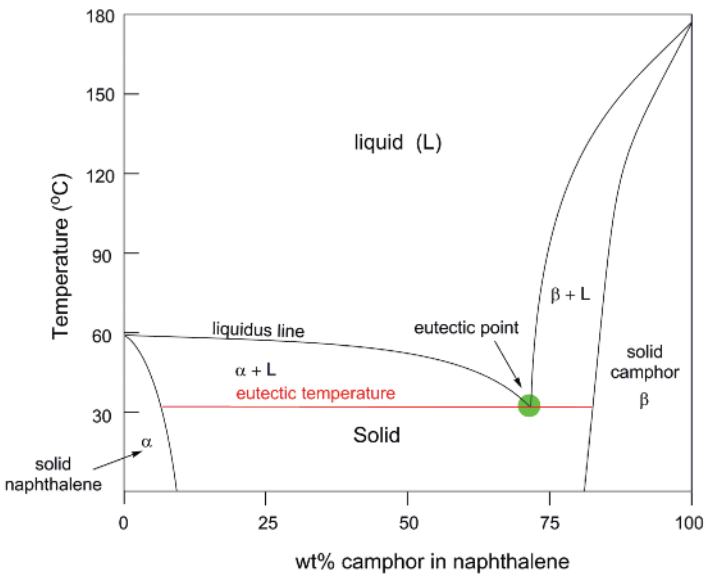
Sublime science meets eutectics



When did you last change those little plastic cages of camphor or naphthalene hanging in the depths of your cupboard? If you've forgotten, chances are they'll be empty, and the moths and silverfish have moved in.

These pure compounds convert readily at room temperature from solid to vapour without forming a liquid; that is, they have a high vapour pressure. This is why they are effective at deterring insects. Why do they have this high vapour pressure? Well, these molecules are compact and globular, and as you raise the temperature they start to rattle around fairly freely in the solid phase. As a consequence, they don't need much more energy to escape as a vapour.

How do we know this? We measure the heat absorbed by the solid as a function of temperature and note how much heat is absorbed as we slowly warm the sample. This tells us at what temperatures different modes of molecular movement start (and thus absorb more energy). When the material reaches its melting point, not much more energy is needed to actually cause it to melt – it has a low enthalpy of fusion. In practice, it is easier to check this by starting from the melt and monitor a cooling curve versus time.



Based on P.M. Robinson, H.J. Rossell and H.G. Scott, Binary phase diagrams of some molecular compounds – I. *Mol. Cryst. Liq. Cryst.* 1970, vol. 10, pp. 61–74.

Camphor belongs to a group of substances called plastic crystals. It is soft and waxy and can be cut with a knife. It was used as a plasticiser for nitrocellulose in producing one of the first mouldable plastics, celluloid. The first movie films were produced on so-called 'nitro' film, which sadly has mostly deteriorated. Celluloid dolls are collectors' items. Celluloid's last major use, for table tennis balls, is also dwindling in favour of polymer balls.

Old camphor packets carried a warning that the camphor should not be used in the presence of naphthalene because it is liable to melt. What is this threatened melting? A eutectic diagram illustrates what happens.

The data for the diagram is obtained by starting with camphor (shown on the right), measuring the melting point and then adding naphthalene, checking the melting point of the mixture after each addition. We see how the melting point decreases. We then do the same with pure naphthalene (shown on the left) and adding camphor.

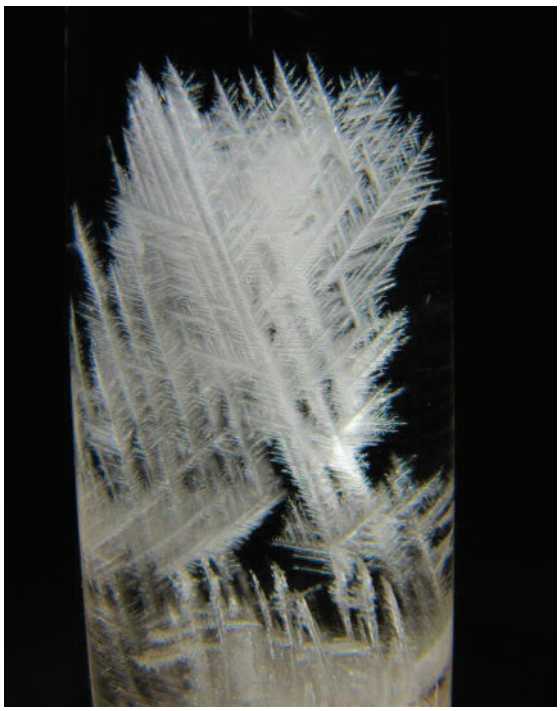
Close to the vertical axes, where the additions are small, the regions are labelled 'α' and 'β' and we are dealing with solid solutions of camphor in naphthalene or naphthalene in camphor of various compositions.

Further out, with more additions, are regions labelled 'α and L', and 'β and L'. The α and β are again solid solutions of

Old camphor packets carried a warning that the camphor should not be used in the presence of naphthalene because it is liable to melt.

In the bad old days, the molecular mass of organic compounds was determined by dissolving a known amount of the compound in molten camphor, freezing it, grinding it, and then measuring the new lower melting point. This is called the Rast method.

The lowering is a colligative property; that is, it depends on the number of moles of the added compound. You know the mass you have added, so you can obtain the molecular mass. The melting point is no longer sharp. Consistency is needed when deciding which point to accept as the melting point because there is a range between first starting to melt and finally all melted.



Admiral Robert FitzRoy, promoting the storm barometer in the 1860s, proclaimed that 'if fixed, undisturbed, in free air, not exposed to radiation, fire, or sun, but in the ordinary light of a well-ventilated room or outer air, the chemical mixture in a so-called storm-glass varies in character with the direction of the wind, not its force, specially (though it may so vary in appearance only) from another cause, electrical tension'.

variable composition but are now mixed with a liquid solution. Above that is a pure liquid solution. These latter curves meet at a fixed point at an intermediate composition called the eutectic point.

Thus there are three compositions with a sharp melting point: pure naphthalene, pure camphor and the eutectic mixture. Below the horizontal line through the eutectic, there is only a mixture of solids.*

The depression of freezing point in the α and β regions is used in a process called the Rast method of determining molecular mass.

If the vapours of camphor and naphthalene came in contact in your cupboard and condensed on your clothes, there would be a low melting point mixture of crystals and liquid. This explains the warning on the old labels. Unlike the natural material, synthetic everyday camphor contains borneol and thus has a lower melting point. This means various melting points can be less than indicated on the diagram.

*For a more detailed interpretation of phase diagrams, see *Chemistry in the marketplace* sixth edition, appendix 5, phase diagrams, and check out the tour of the phase diagram for lead and tin, that in principal is the same as for camphor naphthalene. The latter diagram, shown on page 463, is over-simplified.

Experiment: caged chemicals

- In three narrow, tall jars, place some caged naphthalene, some caged camphor and some caged camphor and naphthalene mothballs together. Seal the jars and place them in the sun for a day or so. Note what you see.
- You should see the sublimation and deposition of crystals on the sides of the glass, different shapes for the two different compounds.
- The jar with both camphor and naphthalene contains a mixture; check the melting point by placing the jar in a larger jar filled with water at around 30°C. The crystals will melt and, on moving out of the sun, may freeze (as a white amorphous solid).

An unrelated question is why the material sublimes from the holders and deposits on the inside of the glass container. Glass is transparent for much of the solar radiation whereas the chemical cages and their contents absorb and will be warmer than the glass walls. This explains the movement and crystal deposition on the inner glass surface. It also shows that garden greenhouses don't work due to the (atmospheric) greenhouse effect. Air inside a car gets hot in the sun but the windscreen doesn't.

A concoction of camphor with additives is the basis of an intriguing 1860s weather forecaster (prognosticator) called a storm barometer or chemical weatherglass, of dubious performance.

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.

Mouthfeel of white wine

I have encountered many different approaches to wine tasting since my first serious involvement after my doctoral studies when the attitude was something like 'cheap is all I can afford, so it must be good'. I did meet one PhD student who tried to quantify this approach by calculating the dollars per each per cent alcohol so that low-priced high-alcohol wines scored well. One winemaker, when discussing whether the 20-point or 100-point scoring scale should be used, claimed that he used a 2-point scale: 1 if the wine went down and 2 if it stayed down!

On the more serious side, I have always been intrigued when, in a tasting session with flavour chemists, their emphasis is only on the aroma of the wine. They spend considerable time trying to identify the aromas and then apply descriptors. They then go on to the next glass without even tasting the first one. When I 'nose' a wine, I am checking to see if the aroma is OK and does not show spoilage characters. Essentially, if it smells like wine, then I taste. If overly spoilt, I generally will not taste because the time required to remove the residual aroma and taste sensations can be too long.

All this is by way of introducing the concept of mouthfeel. Until recently, most of mouthfeel research has focused on red wine, with an examination of the polyphenolic content in relation to astringency and bitterness being one major and ongoing research effort. I suspect that there has been some prejudice towards red wines because these are commonly perceived as more complex than white wines. The opinion of many is that a white wine is what one drinks before red wine! Perhaps the subtlety of good white wines is not apparent to consumers of big red wines (here I am showing my own prejudice).

The state of knowledge on white wine mouthfeel has recently been reviewed by Richard Gawel and Paul Smith from the Australian Wine Research Institute with Sara Cicerale and Russell Keast from Deakin University (*Crit. Rev. Food Sci. Nutr.* 2017, doi: 10.1080/10408398.2017.1346584). Commencing with a summary of the physiology of mouthfeel perception, the review continues with a discussion of the association between mouthfeel and wine composition. Ethanol and pH/acidity are two factors that exert a significant influence on mouthfeel, while a range of medium-to-low-concentration compounds may exert an effect either individually or through interactions with other compounds.

The mouthfeel responses can be broadly classified as warmth, prickling and spritz as well as the tactile sensations of viscosity, astringency and bitterness with sweetness for some styles.

The mouthfeel responses can be broadly classified as warmth, prickling and spritz as well as the tactile sensations of viscosity, astringency and bitterness with sweetness for some styles. Ethanol can produce a warm mouthfeel, changing to prickling as its concentration increases. High acid wines may also exhibit prickling and spritz. Phenolic compounds elicit an astringent response as well as bitterness in some instances. Recent research on polysaccharides indicates that this class of compounds can influence astringency through an interaction with phenolic compounds, although most studies are on red, rather than white, wine. Glycerol, the third most abundant compound in white wine, is often assumed to influence viscosity, although the research is conflicting, perhaps to some extent because of the sweetness of glycerol itself.

Viscosity is a good example of the challenge in linking mouthfeel to wine components. While the physical viscosity of wine can be readily measured, tasters focus on what can be termed 'oral viscosity' as reflected in 'the ease with which the liquid flows between the upper surfaces of the tongue and the palate'. Oral or perceived viscosity generally appears to correlate with a wine's measured physical viscosity (around 0.15 mPa/s). Gawel et al. note that increasing wine pH leads to a higher perceived viscosity. A small pH change is unlikely to change physical viscosity, so the higher mouthfeel viscosity perception would appear to be related to other, not yet, recognised effects.

One of the complexities associated with profiling mouthfeel is the influence of retronasal aroma sensation. Essentially, aromas can be sensed by orthonasal (sniffing in) and retronasal (breathing out) routes (see Shepherd in *Flavour*, 2015, vol. 4, p. 19, doi.org/10.1186/s13411-014-0030-9). This is especially significant in wine because the volatility of several aroma compounds is enhanced by the warmer temperature in the mouth. While detailed studies of the retronasal effect in wine are limited, one by Anthony Sereni, James Osborne and Elizabeth Tomasino from Oregon State University examined the link between retronasal sensing and mouthfeel perception in Chardonnay (*Beverages* 2016, vol. 2, p. 7, doi: 10.3390/beverages2010007). The trick in these experiments is to taste wine in the 'normal way' and repeat the tasting wearing a nose clip, the type of clip used in swimming. The results of the Sereni et al. study showed that there was a definite influence of retronasal aroma on mouthfeel perception, although the nature of the interactions and their link to wine composition remains an open question. There is undoubtedly some great research opportunities here.

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Melville and the Great Honey Hunt

In 1952, the Botanic Garden in Melbourne welcomed an unusual visitor. He was Ronald Melville, a botanist who had recently been appointed to the Australasian Section of the Royal Botanic Garden, Kew, an appointment he held until his retirement in 1968. 'Retirement' did not mean ceasing work as a taxonomist, of course, and he practised his craft until shortly before his death in 1985 at age 82.

During his year in Australia, he was said to have collected more than 20 000 specimens. Many of them must have gone to Kew, but there are 9216 of his specimens in Australian herbaria, 2979 of them Victorian. Only 1716 of the Victorian ones are held here in Melbourne, along with 1675 from other states and territories. I gleaned this information from the wonderful Australasian Virtual Herbarium (https://avh.chah.org.au), to which I was directed by local experts.

Melville had been at Kew, working in the Museum Section, since he was awarded his PhD degree in 1934 for studies on tomato seedlings. His thesis topic is a true indicator that Melville was no mere theorist but, rather, a practical man with wide interests in nutritional and economic botany, as shown in his 1948 book *The story of plants and their uses to man*. Before these interests flowered (pun recognised), however, in the late 1930s he established himself as a specialist on the taxonomy of elms (genus *Ulmus*), starting with those in Britain but ranging further afield to the Eastern Mediterranean and the Himalayas.

During World War II, he was Kew's nominee on several national committees, among them the Vegetable Drugs Committee of the Ministry of Health. Supplies of vitamin C were threatened and so Melville was detailed to work with Dr Magnus Pyke in a search for alternative (to citrus) sources of this essential food component. They examined walnuts, conifer needles and various fruits and edible plants, before concluding that rose hips were the best source. So rosehip syrup was born and its production was undertaken by the Rose Hips Products Association, for whom Melville served on the Scientific Committee.

During the war, Melville also served in the Home Guard, and was a member of the local St John's Ambulance Brigade and secretary of the Twickenham Allotments and Gardens Association and then the Allotments Committee of the Twickenham Borough Council. Home gardens and allotments made valuable contributions to wartime food supplies and the locals would have been delighted to have such an expert in their midst.

As if all this committee work were not enough, Melville served on committees of the Twickenham and Thames Valley Beekeepers Association and took a keen interest in bees and beekeeping. He published several scientific articles on his almost-a-hobby, including one in *Nature* in November 1944 in which he described an investigation into suburban honey that had a strange taste. It came from an apiary in Kensington, not far from Kensington Gardens, and was collected in 1943. 'The

***Ailanthus altissima* flowers.**

first impression on tasting it', he wrote, 'was of a mild floral bouquet, but this was followed by a persistent after-taste reminiscent of cats'. Maybe he meant 'cat's pee'. On diluting the honey and centrifuging, the pollen that the bees had gathered with the nectar settled out, and Melville showed that 44% of the total came from the tree of heaven, *Ailanthus altissima*. The next most abundant contribution was from the sweet chestnut, *Castanea sativa*. On storage, the honey gradually lost the 'cat-like' flavour, and what remained was 'a delicious muscatel flavour'. 'Honey is usually eaten within a short period of its production', the ever-practical Melville wrote, 'but as with wines and cheeses it would pay to store some kinds until the flavour matures'. Among the many constituents of *Ailanthus* that have been identified, the only one that I thought might be responsible was 2,6-dimethoxybenzoquinone.

In the late 1950s, Melville became interested in the development of flowering among Palaeozoic plants, concentrating on *Glossopteris*. This is a 'marker' plant for the Gondwanaland continent and fossil leaf impressions can be found in Southern Australia as well as in South America, India and Madagascar. I remember a geology excursion to Bacchus Marsh, 60 kilometres west of Melbourne, where there are outcrops of Permian sediments bearing *Glossopteris* and *Gangamopteris* leaf impressions.

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

events

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
raci.org.au/events/event/qacs-2017-qld-annual-chemistry-symposium

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.

Christmas HLM Awards and Retirees Lunch
11 December 2017, Graduate House, Carlton, Vic.
raci.org.au/events/event/christmas-hlm-awards-and-retirees-lunch

6th International Conference and Exhibition on Materials Science and Chemistry
17–18 May 2018, Rome, Italy
materialschemistry.conferenceseries.com

ALTA 2018 – Nickel-Cobalt-Copper, Uranium-REE & Gold-PM Conference & Exhibition
19–26 May 2018, Perth, WA
altamet.com.au/conferences/alta-2018

AOCRP-5 – 5th Asian & Ocean Regional Congress on Radiation Protection
20–23 May 2018, Melbourne Vic.
aocrp-5.org

Macro 18 – World Polymer Congress
1–5 July 2018, Cairns, Qld
macro18.org

8th International Conference on Environmental Chemistry and Engineering
20–22 September 2018, Berlin, Germany
environmentalchemistry.conferenceseries.com

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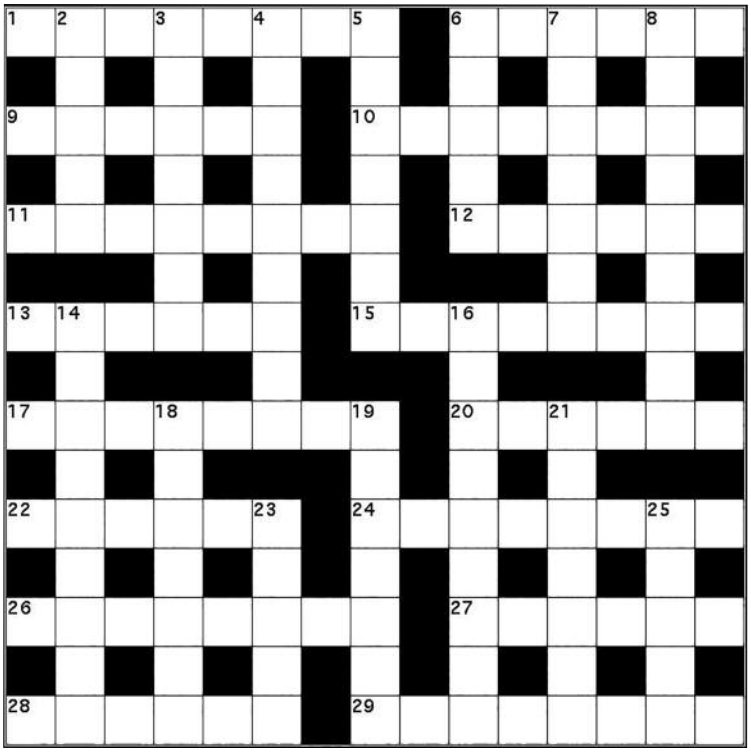

Across

1 Gas centres on leachate enveloping restricted toners. (8)
6 Repair needed after three elements added at the end. (6)
9 Customer holds money over lithium. (6)
10 It's in your DNA; pace, develop. (8)
11 Getting out, paces gin consumption. (8)
12 There's new compounds. (6)
13 Sulfur blends odours. (6)
15 Mixup backed in finding red *rosidae* flowers. (8)
17 Increases loans. (8)
20 Copies pictures. (6)
22 The French pursue a *faux pas* three times. (6)
24 577528616 lights. (8)
26 Human tie to $C_2H_7^+$. (8)
27 $R_2C{=}N\bullet$ found over in northerly Nimitz Glacier. (6)
28 Symbols of carbon bases. (6)
29 Intenser reaction generated intermediates from azides. (8)

Down

2 Maintains grips. (5)
3 Complete in general. (7)
4 Nitric's in 15 Across by its very nature. (9)
5 Promised joke when in troubled need. (7)
6 Afterward could be honest if rhenium is added. (5)
7 More lend support. (7)
8 Meddle to bury two metals. (9)
14 Referee rated room review. (9)
16 One of us cites tin's reaction. (9)
18 Lug in software which pops up. (7)
19 Wise guy weaves on looms. (7)
21 15 Across need in a nucleobase. (7)
23 Vents: bad times! (5)
25 Form of nitrogen in which conduction is due to the movement of electrons rather than positive holes. (1–4)

Graham Mulroney FRACI CChem is Emeritus Professor of Industry Education at RMIT University.
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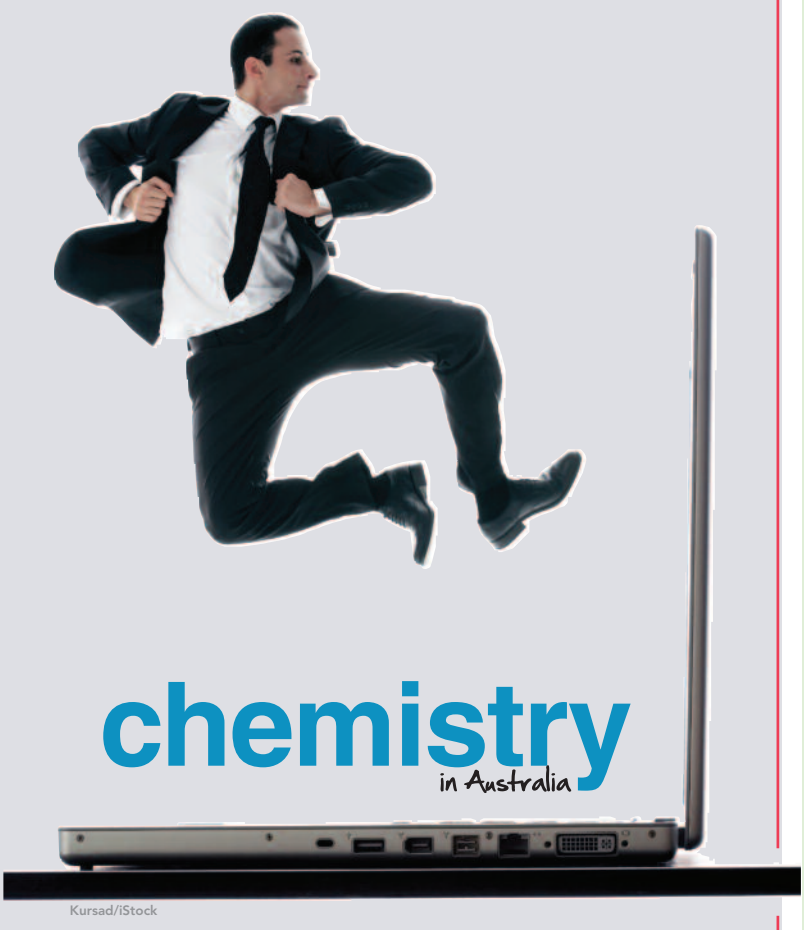

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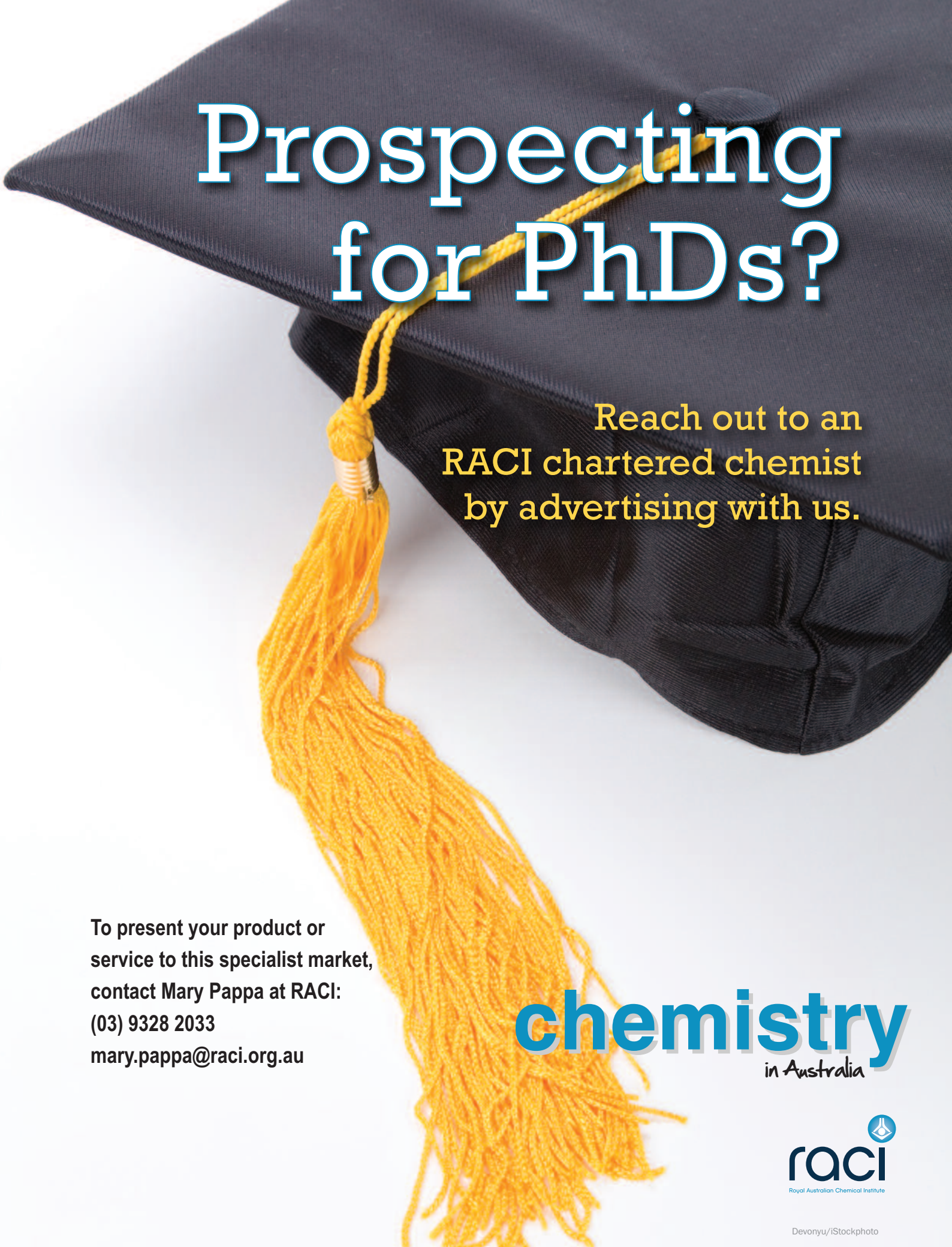

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