

chemistry

May 2017

in Australia



**Using biology
to make
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- Trump's Order and the threat to scientific exchange
- New developments in helium microscopy
- Turning yoghurt waste into new products



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cover story

Directed evolution: following nature's lead

Dave Sammut speaks to Caltech professor Frances Arnold, who is 'using biology to do chemistry'.

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20 13769: Trump's Order and the threat to scientific exchange

The US Presidential Order imposing travel restrictions is of deep concern to the international scientific community.



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Facing facts and their ‘alternatives’

At a recent science communicators’ conference, the audience was set a challenge. We were asked to think of ways to convince the arachnophobic delegates in the room to each keep a pet huntsman in their car for a month.

Having arachnophobic tendencies myself (for the larger varieties, at least), I was really struck by the futility of confronting irrational thoughts with facts. It doesn’t matter a jot how much research is behind those facts, or how many genuine experts support them – think climate change and vaccination – those facts are unlikely to sway convictions based on beliefs or emotion.

Scientists taking a stand

1958: A petition calling for an end to nuclear weapons testing and signed by more than 11 000 scientists is presented to the United Nations by Linus Pauling and his wife.

2010: About 2000 scientists attend the Science is Vital rally in London, protesting research funding cuts.

2012: A mock funeral for British science is held outside London’s Houses of Parliament by physical scientists in protest of funding reforms.

2013: Scientists across Canada rally in protest of cuts by the Harper government to scientific programs and the ‘muzzling’ of federal scientists.

2014: More than 19 000 people sign an open letter to national governments and the European Parliament and Commission, as ‘a wake-up call to policy makers to correct their course, and to researchers and citizens to defend the essential role of science in society’.

2015: Several thousand Russian scientists gather in Moscow to protest government research reforms.

2015: Indian scientist Pushpa Mittra Bhargava returns his prestigious Padma Bhushan, awarded by the Indian government, in protest of ‘active promotion of irrational and sectarian thought by important functionaries of the government’.

2016: Almost 3000 scientists sign an open letter to CSIRO and to the Australian government, raising concerns over the effects of job cuts in climate research. Rallies are held in several capital cities.

2016: Scientists of the American Geophysical Union rally in San Francisco to call for Donald Trump to acknowledge and address climate change.

2016: Italian physicist Giorgio Parisi writes a letter, co-signed by 69 other researchers, urging the European Union to put pressure on governments to ‘[keep] their research funding above subsistence level’. Accompanying the letter is a petition signed by 50 000 people.

22 April 2017: March for Science in Washington, DC, with ‘sister’ marches around the world.

29 April 2017: People’s Climate March in Washington, DC, with ‘sister’ marches around the US.

A new phrase surfaced in White House circles this year: ‘alternative facts’. Falsehoods such as White House Press Secretary Sean Spicer’s statement about the attendance at Donald Trump’s inauguration can now be rebranded, thanks to Counselor to the President, Kellyanne Conway. The tweet by Donald Trump, in 2012, that ‘The concept of global warming was created by and for the Chinese in order to make US manufacturing non-competitive’ was apparently his ‘alternative’ to solid, extensive and longstanding scientific evidence.

It’s one thing to dismiss the anti-science feeling of a small minority, but quite another matter when this attitude is coming from a position of immense power and authority. Scientists and the broader community have been joining in protest of bans and restrictions on US government scientists, but the sentiment is mixed. Should the message be pro-science or anti-Trump? In February, shortly after confirmation of Scott Pruitt as the new head of the US Environmental Protection Agency, scientists and others gathered in protest in Copley Square in Boston. Pruitt is said to be a ‘climate change doubter’ (<http://econ.st/2mD0YFD>). The previous day, in the same city, Gretchen Goldman, Research Director of the Union of Concerned Scientists, addressed the annual meeting of the American Association for the Advancement of Science, entitled ‘Defending science and scientific integrity in the age of Trump’. ‘They’re looking to dismantle the very process by which we use science to inform decision-making’, she said of the Trump administration.

Dominique Brossard, a specialist in public attitudes on scientific issues at the University of Wisconsin in Madison, can understand the dilemma. Speaking about the March for Science on 22 April she said, ‘If the event is interpreted as “These people who like science are marching against Trump”, it could politicise science even more and potentially hurt public trust in science as an institution’ (<http://bit.ly/2LBVsnf>).

I was heartened to read about the 1000-strong Science Solidarity List in Brittany Howard’s feature this month about US Presidential Order 13769, ‘Protecting the Nation from Foreign Terrorist Entry into the United States’ (p. 20). The list was formed by the European Molecular Biology Association, and US-based scientists stranded abroad can search the site for offers of bench space, resources and accommodation in their current location. At the time of printing, there were 50 offers in Australia. It’s good to see scientists getting together to help others.

And what was the proposal most popular with the arachnophobes at the science communicators’ conference? Talk to them, listen to their concerns – and then ask them to consider the consequences of their actions and attitudes for their children.



Sally Woollett (editor@raci.org.au)

Centenary of death of chemistry laureates

It was interesting to read in Sally Woollett's editorial in the March issue (p. 4) of the several Nobel laureates in chemistry who were born in 1917, the centenary year of the RACI. To that might be added the fact that 1917 is the year of the deaths of two of the early Nobel Prize winners in chemistry.

One is Adolf von Baeyer, who died in August that year at age 81. He received the prize in 1905 'in recognition of his services in the advancement of organic chemistry and the chemical industry, through his work on organic dyes and hydroaromatic compounds'.

The other is Eduard Buchner, who received a Nobel Prize in 1907 'for his biochemical researches and his discovery of cell-free fermentation'. At the beginning of World War I, Buchner entered the German Army, and he died in action in August 1917 at age 57.

In spite of taking an interest in such matters for very many years, I was unaware until I read Sally's piece that the organic chemists J.W. Cornforth and R.B. Woodward had been born in the same year. The latter predeceased the former by 34 years.

Clifford Jones FRACI CChem

RACI and overseas membership

The following may sound like a provocative question, but is meant as an honest question: as a chemist permanently based in Europe, is there any point maintaining my membership of the RACI?

I should stress that I have no intention of leaving the RACI, but the question occurred to me here over Christmas. Let me explain my background. I obtained my BSc(Hons) and PhD (organic chemistry) at the University of Sydney. After five years in postdoctoral positions at the Centre for Drug Discovery and Development (now part of the IMB) at the University of Queensland, I obtained a three-year postdoctoral position at the University of Cambridge. Since then, I have held positions within the pharmaceutical industry in Denmark (largely as a process chemist). With that as my background, I believe it is

relevant to consider both (a) the relevance of the RACI to me at present, and (b) my relevance to the RACI.

The relevance of the RACI to me for the last 20 years is essentially negligible. There is no similar institution in Denmark, and the title Chartered Chemist has no weight whatsoever in Denmark. Yes, I appreciate that chemistry (and science in general) needs a voice in Australia, and that the RACI helps to supply such a voice, but I have not been able to vote in Australia for many years, and (and this hurts when I say it) it is unlikely that I will be permanently based in Australia in the future (for many different reasons).

What is my relevance for the RACI? Pretty similar, I feel, i.e. negligible. Yes, one more person in the statistics, but no other relevance. I am not part of any local group (since I am not 'local'), so I am not able to contribute in any meaningful manner. Taking part in working groups and such like is similarly more or less excluded, in part because I lack 'local knowledge', and partly because I cannot physically be there. I have always felt it very important to encourage and help the next generation of chemists, but I cannot do this for Australian chemists, since I am geographically remote (as an example, the University of Sydney's mentoring program requires, reasonably enough, that the mentors live in Australia).

To summarise, I have difficulty seeing how I am relevant to the RACI, and, similarly, I see very little relevance of the RACI in my professional life. So therefore the question: is there any point maintaining my membership of the RACI? I would be very happy to discover that there are important points that I have overlooked.

Robert Dancer MRACI CChem

Editor's note: A copy of this letter has been forwarded separately to the RACI Board. The Board recently embarked on a strategic planning exercise in an effort to turn around declining membership. They have identified five key areas that need to be addressed and are asking for member assistance. Suggestions about how the RACI can improve interactions with international members are welcome. See www.raci.org.au/raci-news/plan.

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ISSN 0314-4240 e-ISSN 1839-2539



Laser tool reveals helium secrets

Curtin University researchers have for the first time been able to visualise where helium atoms are trapped within individual mineral grains, providing information that can help to determine the geological history of the Earth's crust and assist in monitoring natural hazards such as earthquakes and volcanic eruptions.

The researchers, led by Professor Brent McInnes of Curtin's John de Laeter Centre, teamed up with Canberra-based high-technology instrument manufacturer ASI Pty Ltd to create a new laser microanalysis instrument, the RESOchron™, capable of measuring helium at high resolution – to one-tenth the width of a human hair.

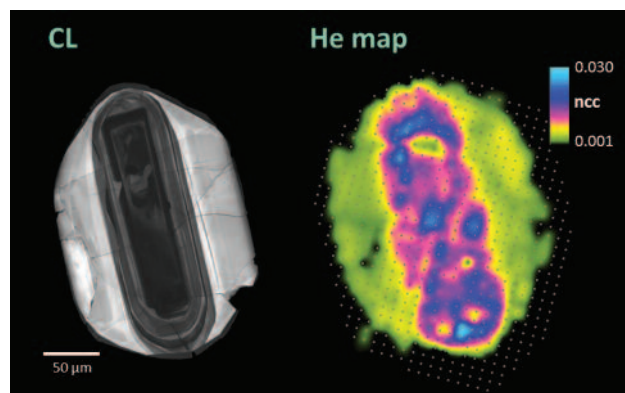
Dr Martin Danišik, lead author of a paper on the research published in *Science Advances* (doi: 10.1126/sciadv.1601121), said helium – generated over long periods of time in uranium- and thorium-bearing mineral crystals – was a highly sought-after commodity used in medical and industrial applications. It has also been used by geoscientists to date rocks.

'Scientists have been using the helium-dating technique to determine the age of minerals for over 100 years, but until now, nobody has been able to observe the actual distribution of helium within the crystal structure,' Danišik said.

Danišik said that by using the RESOchron to repeatedly raster a laser across a zircon crystal's surface, the team was able to create the first helium abundance map.

'We then used numerical simulations to determine how thermal events in the Earth's crust influenced helium abundance patterns in the crystal over geological time,' Danišik said.

'By matching measured and simulated helium distributions, we were able to decipher the mineral's geological history.'



Cathodoluminescence image of zircon (left) and corresponding helium distribution map (right) showing excellent correlation between uranium and helium content. Curtin University

McInnes, who conceived the instrument concept and assembled the project team, said the ability to measure radiogenic helium distributions in individual grains could help scientists understand more about the timing of fault movement, volcanic eruptions and mountain-building processes, as well as assist in the exploration for mineral and petroleum deposits.

'We were surprised to discover extremely high concentrations of helium in cavities within crystals, and speculate that this could be useful in earthquake monitoring, because the crushing of minerals during fault motion should break open these cavities and release a flux of helium gas that can be detected at surface,' McInnes said.

'Our team has previously demonstrated that minerals in diamond-bearing kimberlite pipes have uniquely low abundances of helium, and this technology can be used to rapidly scan exploration samples to both detect kimberlitic zircon and identify the age of the kimberlite pipe.'

Curtin University

Soil linked to antibiotic-resistant bacteria

Soils containing even small amounts of metals are more likely to contain strains of antibiotic-resistant bacteria, according to new research from Edith Cowan University.

Antibiotic-resistant bacteria pose one of the world's most pressing health issues. The researchers found that soils containing even small amounts of lead, manganese or aluminium contained bacteria with antibiotic resistance.

Researcher Dr Annette Koenders said previous studies carried out overseas had shown a link between high levels of metal contamination in soil and antibiotic-resistant bacteria.

'But our study, undertaken in Western Australia, shows that even low concentrations of metals are correlated with increased antibiotic resistance in bacteria,' Koenders said.

'This antibiotic resistance in bacteria occurs as part of a naturally occurring response to protect from pollutants or stress, especially toxic metals.'

Soil samples were collected from 80 sites on residential properties around the state. The samples were analysed for the

presence of 14 different metals.

The DNA of the bacteria in each soil sample was analysed for the presence of genes associated with antibiotic resistance.

Koenders said the results showed that an assessment of the metals present in soil should form part of environmental approvals for new developments.

'This is particularly important when developing aged-care facilities or schools and childcare centres and where people grow their own food', she said.

'This is because as well as being more vulnerable to bacterial infection, children and older people, on average, are in contact with soil more often because children are crawling and playing on the ground, whereas for older people they are likely to spend more time gardening and growing home-grown produce.'

The study was recently published in *Environmental Science and Pollution Research* (doi: 10.1007/s11356-016-7997-y).

Edith Cowan University

High cobalt levels in Queensland turtle blood

Cobalt, a naturally occurring mineral that can also be an environmental pollutant, has been recorded in the blood of Queensland turtles at potentially harmful levels

Researcher C. Alex Villa from the Queensland Alliance for Environmental Health Services (QAEHS) – a partnership between the University of Queensland and Queensland Health – was lead author of a study on metals in coastal green sea turtles published in *Environmental Pollution* (doi: 10.1016/j.envpol.2016.10.085).

Turtles in the Howick Group of islands in far north Queensland's Great Barrier Reef, removed from localised human-caused pollution, served as a baseline to which researchers compared populations from Cleveland Bay, Upstart Bay and Shoalwater Bay.

'The turtles tested at Cleveland Bay and Upstart Bay looked healthy on the outside but their blood cobalt levels were very high in comparison to the Great Barrier Reef metal baseline levels,' Villa said.

'At Upstart Bay we found green turtles had cobalt blood levels 4–25 times higher than the baseline established by our research.'

Levels of other metals well above the baseline were also observed in turtles along the Queensland coast, including molybdenum, manganese, magnesium, sodium, arsenic, antimony and lead.

Queensland is one of the world's largest cobalt exporters, given its close association with copper and nickel ores.

Environmental levels can be increased well beyond normal if cobalt is released by industrial, agricultural or other human activities; however, sources at the study sites were unknown.

Veterinarian and co-author Dr Mark Flint at the University of Queensland's Vet-MARTI unit said 44% of tested Upstart Bay turtles indicated signs of a systematic stressor and an active inflammatory response.



One of the Great Barrier Reef turtles with an eye lesion. Christine Hof/WWF

He said elevated levels of cobalt, antimony and manganese correlated significantly with clinical markers of inflammation, and markers indicating stress on turtle organs needed for expelling toxins.

A quarter of the 161 turtles examined at Upstart Bay this year had mild to severe eye lesions.

'We don't know why this is occurring. The infection appears to be bacterial and not a virus, so it could be another indication that this is a population under pressure,' Flint said.

Co-author Dr Caroline Gaus released findings last year showing green turtles from Queensland's nearshore habitats were exposed to thousands of chemicals, the effects of which remain unknown.

She said recent findings supported the notion metal exposure is having an impact on the health of coastal populations of sea turtles; however, the exact effects and extent require closer

examination.

Although Upstart Bay is located on a rural coastline, the Burdekin River has one of the highest discharge volumes of any river in Australia, and encompasses a catchment of 130 000 km².

Cleveland Bay is adjacent to Townsville, where metal processing is a key industry, while Shoalwater Bay is a military area that has intermittent underwater demolition and explosives disposal.

The report was based largely on data from the Rivers to Reefs to Turtles project, a partnership between QAEHS, UQ School of Veterinary Science's Vet-MARTI unit, WWF-Australia, Queensland Government's Department of Environment and Heritage Protection, Griffith University, and James Cook University with support from the Great Barrier Reef Marine Park Authority, and funding from Banrock Station Environmental Trust.

University of Queensland

Turning yoghurt waste into new products

With exploding consumer demand for Greek yoghurt, production is up. That's great for food companies' bottom lines, but it also leaves them dealing with a lot more acid whey, a problematic by-product of the Greek yoghurt-making process.

Acid whey, if not properly disposed of, can cause environmental problems. Currently, companies typically pay to landspread it on farmers' fields or dump it down the drain. Some plants are starting to send it to anaerobic digesters, where it's fermented to produce methane.

Scientists at the University of Wisconsin-Madison, US, are developing a better option – one that will transform this trash into treasure.

'The whole goal is to take this problematic mixture of stuff – acid whey – and isolate all of the various components and find commercial uses for them,' said Dean Sommer, a food technologist with Wisconsin Center for Dairy Research (CDR) in the UW-Madison College of Agricultural and Life Sciences.

That's no easy task.

Food companies have been separating the components of sweet whey – the by-product of cheese production – for more than a decade, extracting high-value whey protein powders that are featured in muscle-building products and other high-protein foods and beverages.

However, acid whey from Greek yoghurt is harder to work with. Similar to sweet whey, it's mostly water – 95% – but it

contains a lot less protein, which is considered the valuable part. Some of the other 'solids' in acid whey, which include lactose, lactic acid, calcium, phosphorus and galactose, make it more difficult to process. For instance, galactose and lactic acid turn it into a sticky mess when it's dried down.

Instead of drying it, CDR scientists are developing technologies that utilise high-tech filters, or membranes, to separate out the various components.

'We're taking the membranes that are available to us and stringing them together and developing a process that allows us to get some value-added ingredients out at the other end', said dairy processing technologist Karen Smith, who is working on the project.

At this point, the CDR has set its sights on lactose, an ingredient that food companies will pay good money for in food-grade form.

'It's the lowest-hanging fruit, the most valuable thing in there in terms of volume and potential worth', said Sommer.

A number of companies are already implementing lactose-isolating technology in their commercial plants.

Isolating the other components will come later, part of the long-term vision for this technology. When it's perfected, explained Sommer, acid whey will be stripped of its ingredients until there's nothing left. 'It will just be water', he said.

Nicole Miller, University of Wisconsin-Madison



University of Wisconsin-Madison Center for Dairy Research food technologist Dean Sommer showing a beaker of acid whey. The high-tech filters used to separate the various components are inside the metal pipes. UW-Madison College of Agricultural and Life Sciences

New theory explains how Earth's inner core remains solid despite extreme heat

Even though it is hotter than the surface of the Sun, the crystallised iron core of Earth remains solid. A new study from KTH Royal Institute of Technology, Sweden, may finally settle a longstanding debate over how that's possible, as well as why seismic waves travel at higher speeds between the planet's poles than through the equator.

Spinning within Earth's molten core is a crystal ball – actually a mass formation of almost pure crystallised iron – nearly the size of the moon. Understanding this strange, unobservable feature of our planet depends on knowing the atomic structure of these crystals – something scientists have been trying to do for years.

As with all metals, the atomic-scale crystal structures of iron change depending on the temperature and pressure the metal is exposed to. Atoms are packed into variations of cubic, as well as hexagonal, formations. At room temperatures and normal atmospheric pressure, iron is in a body-centred cubic (BCC) phase, which is a crystal architecture with eight corner points and a centre point. But at extremely high pressure, the crystalline structures transform into 12-point hexagonal forms, or a close-packed (HCP) phase.

At Earth's core, where pressure is 3.5 million times higher than surface pressure – and temperatures are some 6000°C higher – scientists have proposed that the atomic architecture of iron must be hexagonal. Whether BCC iron exists in the centre of Earth has been debated for the last 30 years, and a 2014 study ruled it out, arguing that BCC would be unstable under such conditions.

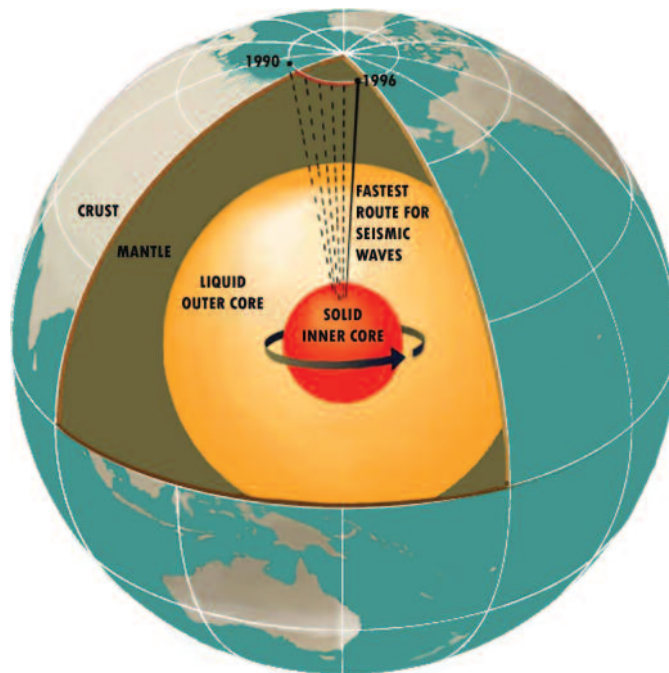
However, in a recent study published in *Nature Geosciences* (doi: 10.1038/ngeo2892), researchers at KTH found that iron at Earth's core is indeed in the BCC phase. Anatoly Belonoshko, a researcher in the Department of Physics at KTH, said that when the researchers looked into larger computational samples of iron than studied previously, characteristics of the BCC iron that were thought to render it unstable wound up doing just the opposite.

'Under conditions in Earth's core, BCC iron exhibits a pattern of atomic diffusion never before observed', Belonoshko said.

Belonoshko said the data also shows that pure iron likely accounts for 96% of the inner core's composition, along with nickel and possibly light elements.

Their conclusions are drawn from laborious computer simulations performed using Triolith, one of the largest Swedish supercomputers. These simulations allowed them to reinterpret observations collected three years ago at Livermore Lawrence National Laboratory in California.

At low temperatures, BCC is unstable and crystalline planes slide out of the ideal BCC structure. But at high temperatures, the stabilisation of these structures begins much like a card game – with the shuffling of a 'deck'. Belonoshko said that in



Earth's inner core spins at its own rate, as much as 0.2° of longitude per year faster than the Earth layers above it. Earth's magnetic field comes from the outer core's ocean of iron, which is an electrically conducting fluid in constant motion. The magnetic field waxes and wanes, the poles drift and, occasionally, flip. Included in the diagram is the movement of magnetic north from 1900 to 1996.

NASA/Dixon Rohr

the extreme heat of the core, atoms no longer belong to planes because of the high amplitude of atomic motion.

Such a shuffling leads to an enormous increase in the distribution of molecules and energy – which leads to increasing entropy, or the distribution of energy states. That, in turn, makes the BCC stable.

Normally, diffusion destroys crystal structures, turning them into liquid. In this case, diffusion allows iron to preserve the BCC structure. Belonoshko said, 'The instability kills the BCC phase at low temperature, but makes the BCC phase stable at high temperature'.

This diffusion also explains why Earth's core is anisotropic – that is, it has a texture that is directional – like the grain of wood. Anisotropy explains why seismic waves travel faster between Earth's poles, than through the equator.

The prediction opens the path to understanding the interior of Earth and eventually to predicting Earth's future, Belonoshko said. 'The ultimate goal of Earth sciences is to understand the past, present and future of Earth – and our prediction allows us to do just that.'

David Callahan, KTH Royal Institute of Technology

New helium microscope reveals startling details without frying the sample

When using an electron microscope, having your samples fried or explode isn't quite the result one wants.

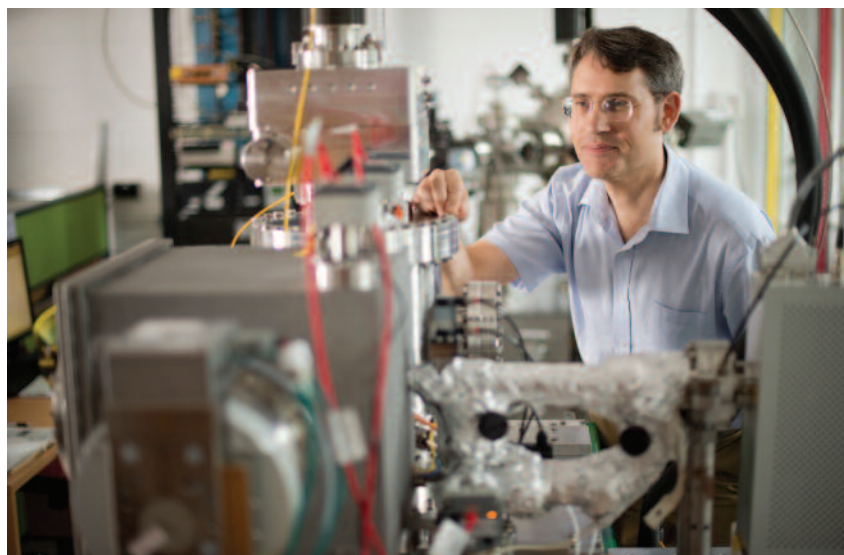
But for Professor Paul Dastoor, this was an all-too-common problem. In his work on organic and polymer electronics, conventional electron microscopes were a no-go zone because much of his sample would either boil or blow up under the microscope he was using.

However, an alternative is now available in the form of a new prototype helium-based microscope, developed by Dastoor and his team at the University of Newcastle, in New South Wales, with collaborators at the University of Cambridge in the UK.

Eye of the needle

Inspired by the classic design of a pinhole camera, the team developed technology that uses a beam of neutral helium atoms to form images.

The prototype scanning helium microscope (SHeM) offers a more delicate



Professor Paul Dastoor with the scanning helium microscope. University of Newcastle

touch than electron microscopes, and thus doesn't cause any damage to samples.

Dastoor's team have used the SHeM prototype to image fine details such as distinct flakes of chitin on a butterfly's wing that resemble plated armour as well as the curve of a spider's fang.

As an added advantage, the helium atom beam can also potentially reveal the chemical content of the surface being imaged.

Dastoor said scientists have worked for decades on developing helium microscopy.

'It's been going on for a very long time. I've been working in the area of helium atom scattering for more than 20 years and there were many people trying to do this research before us', he said.

The challenge lay in wrangling the helium atoms into a single beam before they could be used to capture images.

That's how the design of the pinhole camera inspired the team's breakthrough. In the SHeM, the gas was passed through an aperture to a vacuum chamber. There, the helium atoms form a beam before landing on the sample surface.

'By shining the helium through a pinhole, we simplify the optics of the

system and we can create images of the sample', Dastoor said.

Lobbing a softball

But why use helium, which is the second lightest element after hydrogen? Dastoor explained that the stable nature of helium atoms made the gas suitable for the job.

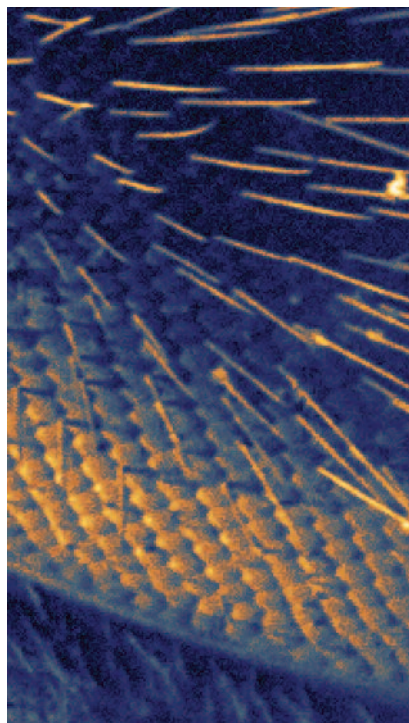
'One, helium atoms are not electrically charged. Helium's full electron shell means it is inert, so it isn't going to undertake any chemical reactions with other surfaces. The second advantage is that they are very low energy', he said.

That latter advantage was key to Dastoor's decision to develop the SHeM.

The helium atom beam's energy is less than 0.1 electronvolts, far lower than the 100 000-electronvolt beam used by electron microscopes and the roughly 1-electronvolt energy of a typical chemical bond.

'Imagine the helium atoms as a great big soft ball that bounces off the outermost electrons on the sample surface. It doesn't get close to the atom core through the first layer', Dastoor said.

If the beam has too much energy, it runs the risk of breaking chemical bonds



Detail of a honey bee's eye imaged by the scanning helium microscope.

University of Newcastle

and damaging the sample. This is why many samples can only be viewed once, or very few times, under a conventional electron microscope.

More than just a pretty picture

As the sample is moved in front of the beam, the helium atoms bounce off the sample and are measured by the detector. The researchers then use software to map the scattered intensity as a function of position.

‘We put the sample in front of the beam, and it hits a different pixel on the surface. And with each pixel, we get a certain number of counts, and then we create an image’, Dastoor said.

How they bounce and reflect off the sample also depends on the chemistry of the surface.

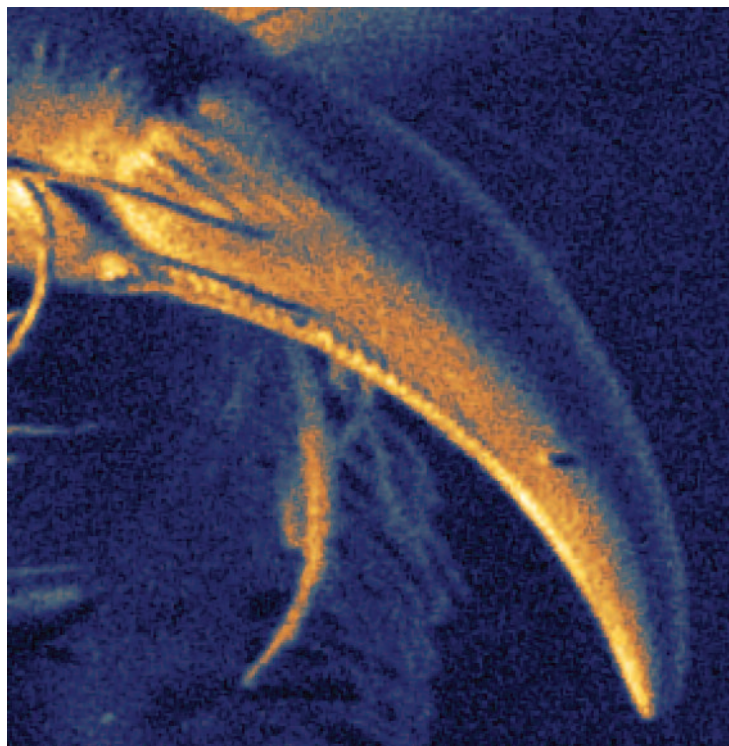
Steven Moody, a scanning electron microscope specialist from the University of Sydney, who was not involved in the study, said this is not the first instance of imaging instruments using helium.

Moody added that the key difference in SHeM is the ‘pinhole’ design, giving it greater resolution, but at the cost of signal.

‘The advantage this contrast offers is the potential to improve our understanding of surface phenomena. It certainly presents an interesting opportunity to help further our understanding of surface physics, which is critical because that’s where most of the action is’, he said.

‘The main limit at this point appears to be signal. This means that as a general imaging tool, other methods are much more time efficient.’

The next step in the development of the SHeM prototype is to downsize it. So far SHeM is limited to imaging with a resolution of up to a micron, with plans for the next version to proceed to the nanometre range.



Close-up of spider's fang imaged by the scanning helium microscope.
University of Newcastle

In addition, Dastoor said that he plans to adapt the entire SHeM system to be smaller, so it can eventually fit on a laboratory bench top.

‘At the moment, it is a large prototype. We are already designing the next version for construction so it is quite encouraging’, he said.

Ivy Shih, Editor, *The Conversation*. First published at <https://theconversation.com>.

New president of Australian Institute of Physics

The Australian Institute of Physics (AIP) has announced that the Director of the Australian Synchrotron, Professor Andrew Peele, is its new President.

The new appointment recognises Peele's leadership in the science sector, and will see him take a key role in supporting physics in research, education, industry and the community.

Peele has been Director of the Synchrotron since 2013, and came to the role after working as Head of Science and Professor of Physics at La Trobe University.

Peele said he is greatly looking forward to this additional role, and to enhancing the opportunities made available to the Australian physics community.

Peele's own research improved the versatility and quality of X-ray imaging, including new methods in phase imaging and coherent diffractive imaging, with applications such as tomographic imaging of cells and materials to better understand them.

He has published over 100 refereed articles and has served as Victorian Branch Chair of the AIP and Co-Chair of the AIP National Congress in 2010.

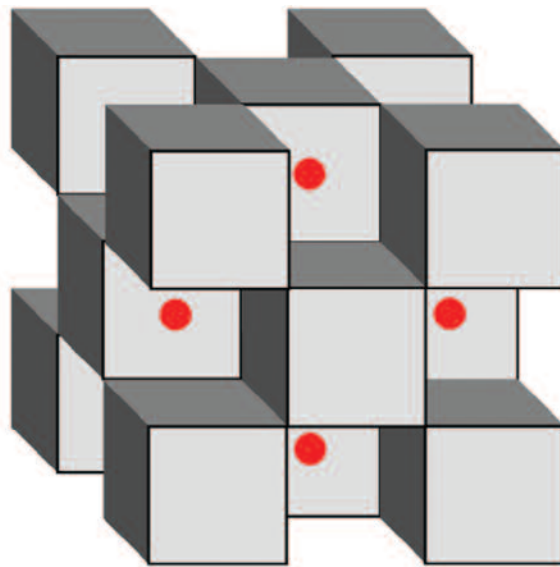
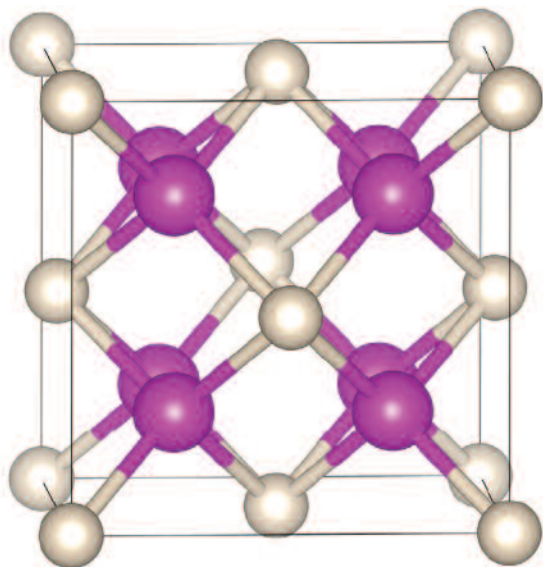
His appointments have included leading the X-ray Science group in La Trobe University's Department of Physics, a Queen Elizabeth II Research Fellowship held at the University of Melbourne and La Trobe University, and postdoctoral research at NASA's Goddard Space Flight Center.

ANSTO



Professor Andrew Peele,
AIP's new director.

Sodium bonds with helium under pressure



Crystal structure of Na_2He at 300 GPa. Left: ball-and-stick representation (pink and grey atoms represent Na and He, respectively); right: polyhedral representation, where half of the Na_8 cubes are occupied by He atoms (shown as polyhedra) and half by two electrons (shown as red spheres). Ivan Popov

Can helium bond with other elements to form a stable compound? Students attentive to Utah State University Professor Alex Boldyrev's introductory chemistry lectures would immediately respond 'no'. And they'd be correct – if the scholars are standing on Earth's surface.

But all bets are off if the students journey to the centre of the Earth, à la Jules Verne's Otto Lidenbrock, or if they venture to one of the solar system's large planets, such as Jupiter or Saturn.

'That's because extremely high pressure, like that found at the Earth's core or giant neighbours, completely alters helium's chemistry,' said Boldyrev.

It's a surprising finding, he said, because, on Earth, helium is a chemically inert and unreactive compound that eschews connections with other elements and compounds. The first of the noble gases, helium features an extremely stable, closed-shell electronic configuration, leaving no openings for connections.

Further, Boldyrev's colleagues confirmed computationally and

experimentally that sodium readily bonds with helium under high pressure to form the curious Na_2He compound. These findings were so unexpected that Boldyrev and colleagues struggled for more than two years to convince science reviewers and editors to publish their results.

Persistence paid off. Boldyrev and his doctoral student Ivan Popov, as members of an international research group led by Artem Oganov of Stony Brook University, US, published the findings in *Nature Chemistry* (doi: 10.1038/nchem.2716).

Boldyrev and Popov's role in the project was to interpret a chemical bonding in the computational model developed by Oganov and the experimental results generated by Alexander Goncharov of the Carnegie Institution of Washington. Initially, the Na_2He compound was found to consist of Na_8 cubes, of which half were occupied by helium atoms and half were empty.

'Yet, when we performed chemical bonding analysis of these structures, we found each 'empty' cube actually contained an eight-centre, two-electron

bond', Boldyrev said. 'This bond is what's responsible for the stability of this enchanting compound.'

Their findings advanced the research to another step.

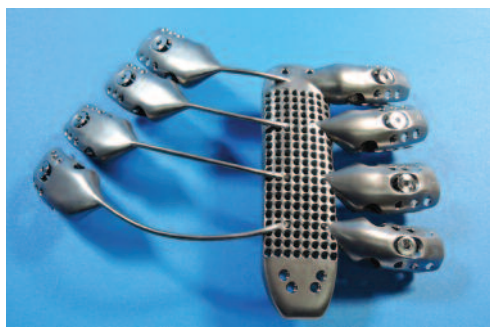
'As we explore the structure of this compound, we're deciphering how this bond occurs and we predicted that, adding oxygen, we could create a similar compound', said Popov.

Such knowledge raises big questions about chemistry and how elements behave beyond the world we know. Questions, Boldyrev said, Earth's inhabitants need to keep in mind as they consider long-term space travel.

'With the recent discovery of multiple exoplanets, we're reminded of the vastness of the universe,' he said. 'Our understanding of chemistry has to change and expand beyond the confines of our own planet.'

Utah State University

3D-printed sternum in world-first surgery



3D-printed titanium sternum and ribs.

© www.anatomics.com

CSIRO has teamed up with Melbourne medical implant company Anatomics and UK doctors to carry out world-first surgery to implant a 3D-printed titanium and polymer sternum into a British patient.

Designed by Anatomics and printed at CSIRO's Lab 22 facility in Melbourne, the sternum was implanted into 61-year-old Daniel Evans, who had previously had his sternum removed due to a rare infection.

Mr Evans has since made a successful recovery.

It is the first time that a titanium sternum combined with a synthetic polymer has been used to replace bone, cartilage and tissue in a patient.

The operation is the latest success story for the CSIRO–Anatomics partnership.

In 2015, a Spanish cancer patient was the recipient of a 3D-printed titanium-only sternum and rib implant that was designed and manufactured by CSIRO and Anatomics.

That life-saving operation followed on from the production of a 3D-printed titanium heel bone that prevented an Australian cancer patient from having his leg amputated in 2014.

CSIRO's Manufacturing business unit has led the collaboration with Anatomics.

'I'm proud of our cutting-edge work with Anatomics that has enabled patients around the world to regain the ability to walk, to sit up and lead normal lives', Director of CSIRO Manufacturing Dr Keith McLean said.

'Here in Melbourne, we have quietly been developing what we believe is one of the world's most advanced capability in reconstructive prosthetics, and this recent success in the UK demonstrates that.'

CSIRO

Next-gen steel under the microscope



Eastern span replacement of the San Francisco–Oakland Bay Bridge.

CC BY-SA 3.0/Frank Schulenburg

Next-generation steel and metal alloys are a step closer to reality, thanks to an international research project involving a University of Queensland scientist.

The work could overcome the problem of hydrogen alloy embrittlement that has led to catastrophic failures in major engineering and building projects.

UQ Centre for Microscopy and Microanalysis Director Professor Roger Wepf said the problem had been recognised for almost 140 years.

'The current generation of these metals can suffer hydrogen embrittlement, where they become brittle and fracture due to the accidental introduction of hydrogen during manufacture and processing', he said.

'A major example of alloy embrittlement occurred in 2013, when bolts in the eastern span of the San Francisco–Oakland bridge failed tests during construction.'

Wepf said hydrogen was extremely volatile and diffused quickly.

'Our research collaboration has, for the first time, localised and visualised hydrogen in steels and alloys', he said.

'This is essential for the development of new alloys with greater endurance.'

'We have shown that it's possible to localise hydrogen at atomic resolution – at the scale of a single atom – or at a nanometre (less than one-billionth of a metre) scale by combining different technologies in a closed and protected workflow.'

'These include state-of-the-art cryo electron microscopy freezing techniques, low-temperature sample preparation in a cryo focused ion beam microscope, and inert cryo-transfer.'

The research, published in *Science*, involved scientists from Oxford and Sheffield universities in the UK and ETH Zurich in Switzerland.

University of Queensland

Protein sheds light on Parkinson's, stomach cancer, melanoma

Collaboration across the Tasman has enabled Australian and New Zealand researchers and scientists to shed light on a protein involved in diseases such as Parkinson's disease, gastric cancer and melanoma.

The Australian Synchrotron in Melbourne was used by researchers from the University of Otago, in collaboration with Australian scientists, with the results published in *PNAS* (www.pnas.org/cgi/doi/10.1073/pnas.1620813114).

The team of researchers, led by Otago Department of Biochemistry's Dr Peter Mace, studied a protein called apoptosis signal-regulating kinase 1 (ASK1).

Mace said the protein plays an important role in controlling how a cell responds to cell damage, and can push the cell towards a process of programmed cell death for the good of the body, if damage to a cell is too great.

'We now know a lot more about how ASK1 gets turned on and off – this is important because in diseases such as Parkinson's, stomach cancer and melanoma, there can be either too much or too little ASK1 activity', he said.

The ASK1 protein gets its name from an Ancient Greek word meaning 'falling off' – apoptosis – and is used to describe the process of programmed dying of cells – of the body actively killing them – rather than their loss by injury.

The researchers found that ASK1 has unexpected parts to its structure, which help control how the protein is turned on, and that an entire family of ASK kinases share these features.

Mace said that the new findings add to our understanding of how cells can trigger specific responses to different threats or damage encountered, such as oxidants, which damage the body's tissues by causing inflammation.

He added that kinases are excellent targets for developing new drugs because they have a 'pocket' in their structure that such compounds can bind to, but to develop better drugs we need to understand far more about how they are controlled. This is the goal of several projects in his lab, he said.

The research team determined ASK1's molecular structure through crystallography studies and performed other biochemical experiments to better understand the protein.

Dr Tom Caradoc-Davies, a principal scientist at the Australian Synchrotron, helped to collect data critical to the project.

'Using the Synchrotron's MX beamlines, we collected data from difficult samples, to help solve questions the research team had about the structure of the protein', Caradoc-Davies said.

The study is a collaboration between Otago researchers and scientists at the Walter and Eliza Hall Institute in Melbourne, and at the Australian Synchrotron.

Australian Synchrotron

Organo-metal compound seen killing cancer cells from inside

Researchers at the University of Warwick, UK, have witnessed – for the first time – cancer cells being targeted and destroyed from the inside, by an organo-metal compound.

Professor Peter J. Sadler, and his group in the Department of Chemistry, have demonstrated that organo-osmium FY26 kills cancer cells by locating and attacking their weakest part.

This is the first time that an osmium-based compound – which is 50 times more active than the current cancer drug cisplatin – has been seen to target the disease.

Using the European Synchrotron Radiation Facility (ESRF), researchers analysed the effects of organo-osmium FY26 in ovarian cancer cells – detecting emissions of X-ray fluorescent light to track the activity of the compound inside the cells.

Looking at sections of cancer cells under nano-focus, it was possible to see an unprecedented level of minute detail. Organelles such as mitochondria, which are the 'powerhouses' of cells and generate their energy, were detectable.

In cancer cells, there are errors and mutations in the DNA of mitochondria, making them very weak and susceptible to attack.

FY26 was found to have positioned itself in the mitochondria – attacking and destroying the vital functions of cancer cells from within, at their weakest point.

Researchers were also able to see natural metals such as zinc and calcium, which are produced by the body moving around the cells. Calcium in particular is known to affect the function of cells, and it is thought that this naturally produced metal helps FY26 to achieve an optimal position for attacking cancer.

More than half of all cancer chemotherapy treatments currently use platinum compounds, which were introduced nearly 40 years ago, so there is a need to explore the benefits that other precious metals could bring.

Although this research was conducted on ovarian cancer cells, the results are applicable to a wider range of cancers.

FY26 has been shown to be more selective between normal cells and cancer cells than cisplatin – having a greater effect on cancer cells than on healthy ones.

Sadler said 'Cancer drugs with new mechanisms of actions which can combat resistance and have fewer side-effects are urgently needed.

'The advanced nano-focused X-ray beam at ESRF has not only allowed us to locate the site of action of our novel organo-osmium FY26 candidate drug in cancer cells at unprecedented resolution, but also study the movement of natural metals such as zinc and calcium in cells. Such studies open up totally new approaches to drug discovery and treatment.'

The research is published in *Chemistry – A European Journal* (doi: 10.1002/chem.201605911).

University of Warwick

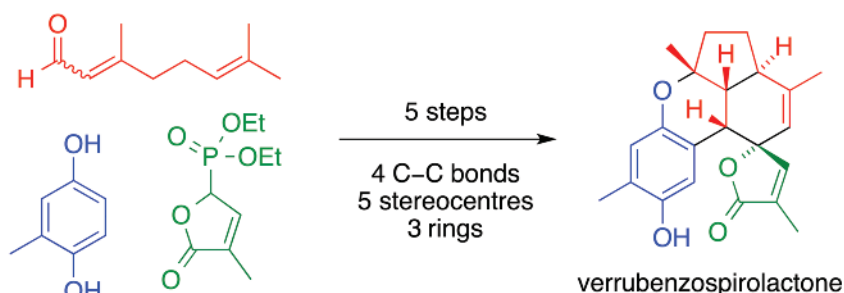
Cascade reactions inspired by nature

Cascade reactions are chemical processes that feature at least two consecutive reactions, with each subsequent reaction occurring solely due to the chemical functionality formed in the previous step. Natural products are a great source of inspiration to organic chemists in the development of cascade reactions for the rapid generation of molecular complexity.

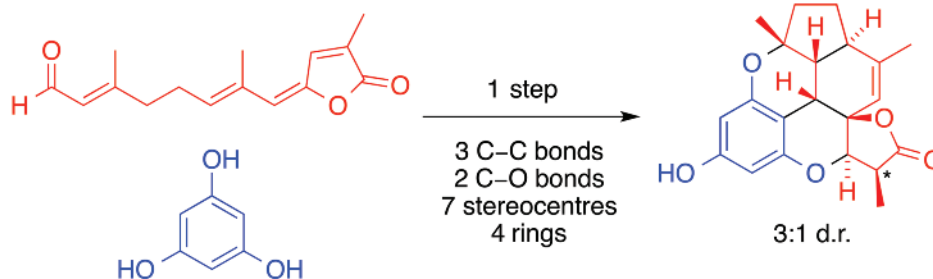
Verrubenzospirolactone is a pentacyclic meroterpenoid natural product recently isolated from the soft coral *Sinularia verruca*. Researchers at the University of Adelaide (Lam H.C., Pepper H.P., Sumby C.J., George J.H. *Angew. Chem. Int. Ed.* 2017, doi:

10.1002/anie.201700114) have completed a concise total synthesis of verrubenzospirolactone in just five steps from simple starting materials, with the final step consisting of a biomimetic intramolecular Diels–Alder reaction of a 2*H*-chromene that forms two rings and four stereocentres. This


Biomimetic total synthesis



Bio-inspired cascade reaction



Diels–Alder reaction occurs spontaneously at 30°C ‘on-water’, so it is likely to be non-enzymatic in Nature. The structure of verrubenzospirolactone was later used to inspire a spectacular cascade reaction that generates seven stereocentres, four rings, three C–C bonds and two C–O bonds in one step.




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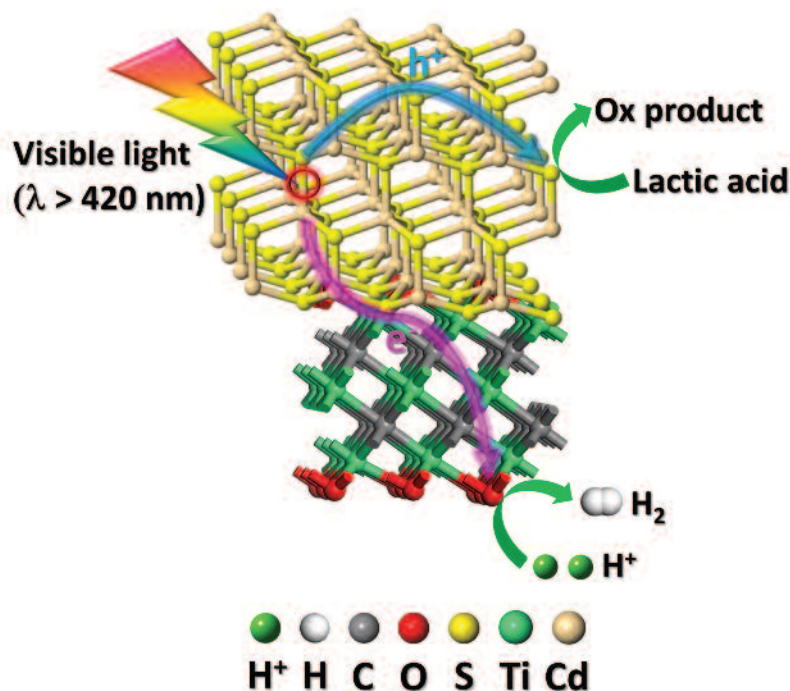
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New MXene material boosts photocatalytic hydrogen production

Scalable and sustainable solar hydrogen production through photocatalytic water splitting requires highly active and stable earth-abundant co-catalyst to replace expensive and scarce platinum. To address this issue, Professor Shi Zhang Qiao at the University of Adelaide and co-workers have employed density functional theory calculations to direct atomic-level exploration, design and fabrication of a MXene material, Ti_3C_2 nanoparticles, as a highly efficient co-catalyst (Ran J., Gao G., Li F.-T., Ma T.-Y., Du A., Qiao S.Z., *Nat. Commun.* 2017, **8**, 13 907). Ti_3C_2 nanoparticles were rationally integrated with cadmium sulfide via a hydrothermal strategy to induce an impressive visible-light photocatalytic hydrogen production activity of $14342 \mu\text{mol h}^{-1} \text{g}^{-1}$ and an apparent quantum efficiency of 40.1% at 420 nm. This high performance arises from the favourable Fermi level position, electrical conductivity and hydrogen evolution capacity of the Ti_3C_2 nanoparticles. Furthermore, Ti_3C_2 nanoparticles also serve as an efficient co-catalyst on ZnS or $\text{Zn}_x\text{Cd}_{1-x}\text{S}$. This work demonstrates the potential of earth-abundant materials of the MXene family to create high-performance and low-cost photocatalysts and photoelectrodes.

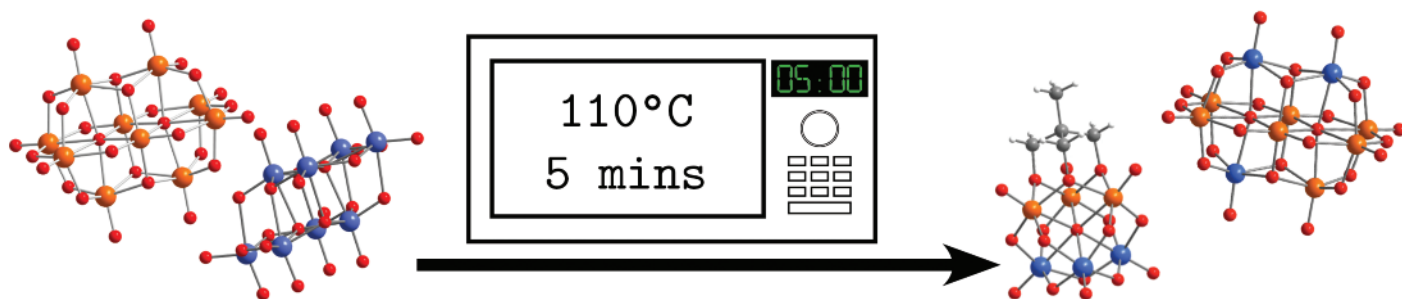


Six of one, ten of another

Polyoxometalates are an expansive class of molecular metal oxides predominantly synthesised in aqueous media by acid-driven condensation of early transition-metal oxyanions in their high oxidation states. In a collaborative project involving researchers from the University of Melbourne, Monash University, Umeå University and CSIRO, non-aqueous, microwave-assisted reaction conditions were used in the targeted synthesis of two novel molybdovanadates from metastable

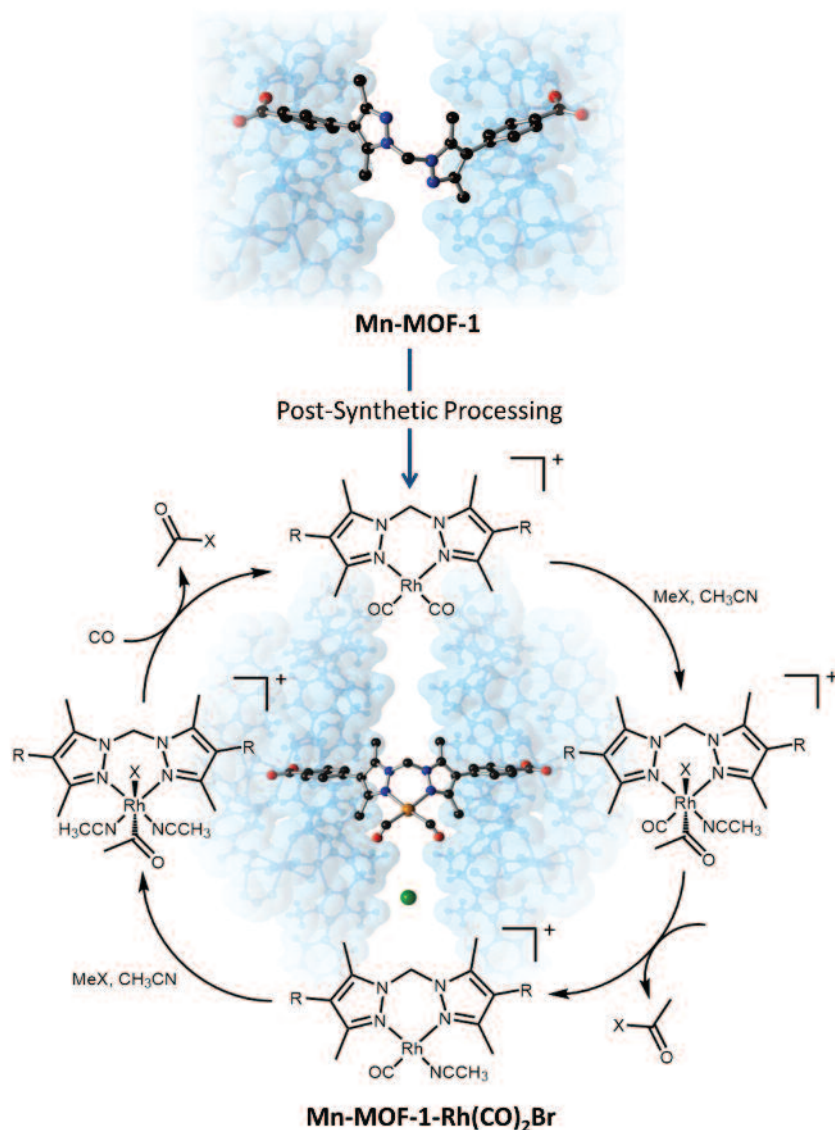
octamolybdate and decavanadate precursors (Spillane S., Sharma R., Zavras A., Mulder R., Ohlin C.A., Goerigk L., O'Hair R.A.J., Ritchie C. *Angew. Chem. Int. Ed.* 2017, doi: 10.1002/anie.201608589). An extensive experimental investigation revealed preferential substitution patterns of vanadium and molybdenum within $[\text{V}_7\text{Mo}_3\text{O}_{28}]^{3-}$ and $[\text{V}_3\text{Mo}_3\text{O}_{16}(\text{C}_5\text{H}_9\text{O}_3)]^{2-}$, with the relative population of structural isomers supported by dispersion-corrected DFT

calculations. The excellent agreement between experiment and theory in the study of $[\text{V}_3\text{Mo}_3\text{O}_{16}(\text{C}_5\text{H}_9\text{O}_3)]^{2-}$ is proposed to be due to a 'locking mechanism' by which condensation of the tripodal ligand to the polyanion surface prevents dynamic post-synthesis solution chemistry. Ongoing research includes elaboration of the pendant organic functionality of these molecules for their incorporation into advanced materials for a variety of applications.



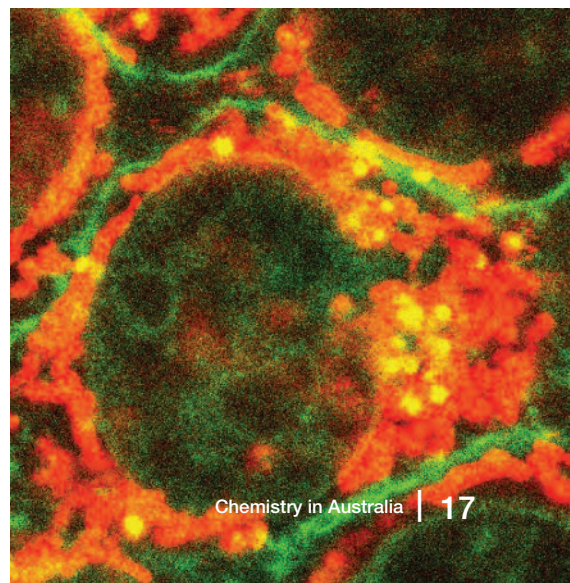
Charting catalytic cycles in a metal–organic framework

Previously, University of Adelaide researchers had shown that it was possible to use X-ray crystallography to capture snapshots of metal-centred reactions taking place inside the pores of a metal-organic framework (MOF) (*Nat. Chem.* 2014, **6**, 906–12). Now, in collaboration with colleagues from Kyoto University, they have revealed that it is possible to follow entire catalytic cycles within this MOF and to shed light on the reactivity of particular chemical species (Burgun A., Coghlan C.J., Huang D.M., Chen W., Horike S., Kitagawa S., Alvino J., Metha G.F., Sumbly C.J., Doonan C.J. *Angew. Chem. Int. Ed.* 2017, doi: 10.1002/anie.201611254). In this latest contribution the team examined carbonylation of haloalkanes and determined that catalytic competency of a Rh-metallated MOF relies upon having both structural flexibility and the requisite space around the metal-based catalytic centre. For instance, in the reductive elimination step of the catalytic cycle, it was observed that only less sterically demanding reagents could rearrange to facilitate elimination, whereas bulky ligands trapped the catalyst mid-cycle. The research highlights that MOFs offer the precise control of single-site catalysis particular to homogeneous systems while overcoming issues such as product separation, reusability and catalyst aggregation.



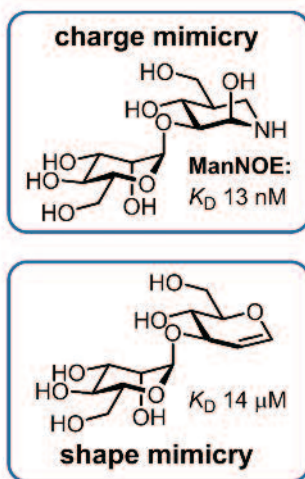
Watching nanoparticles move through a cell

To design nanoparticles for targeted drug delivery, it is important to understand how they move through a cell. Traditional fluorescence microscopy methods, however, only provide information about the number of nanoparticles and not whether they are moving. Now, researchers from the Australian Centre of NanoMedicine at the University of New South Wales have adapted a fluorescence microscopy method known as pair-correlation analysis to monitor the movement of fluorescent nanoparticles through the cell (Hinde H., Thammasiraphop K., Duong H.T.T., Yeow J., Karagoza B., Boyer C., Gooding J.J., Gaus K. *Nat. Nanotechnol.* 2017, **12**, 81–9). This method can measure how many particles are moving, how fast they move and whether they can cross intracellular barriers. Using polymeric nanoparticles that assemble into different shapes depending on their molecular weight but otherwise have identical chemistry, the team showed why high-aspect-ratio rod-shaped nanoparticles were superior cancer-cell killers than spherical nanoparticles. The rods can move through the nuclear membrane and deliver the anticancer drug directly into the nucleus, whereas spheres are stopped at the nuclear envelope. The method can be adapted to understand the movement of any fluorescent nanoparticle and is thus a useful tool for designing nanoparticles for drug delivery and diagnostics.

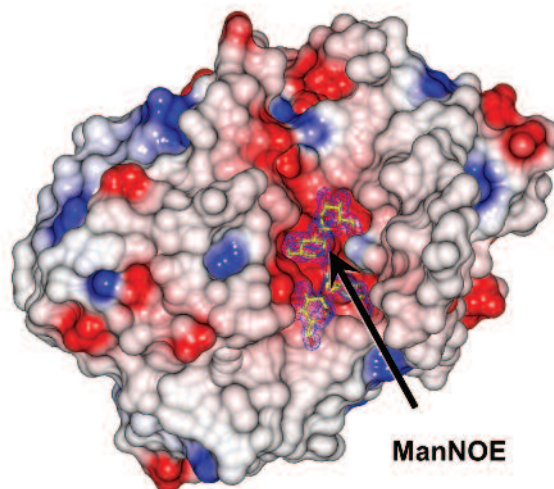


Charge trumps shape for glycosidase inhibition

Sugar-derived heterocycles are widely used as glycosidase inhibitors owing to their ability to mimic the partial positive charge of the reaction transition state and to match the shape of the substrate. However, the preference for shape versus charge mimicry for inhibition of a particular glycosidase must be determined on a case-by-case basis. A collaboration between the group of Professor Spencer Williams at the University of Melbourne and colleagues from Spain, France and the UK has used an integrated synthetic, crystallographic and quantum mechanical approach to assess the contributions of shape and charge to inhibition of a glycosidase involved in degrading complex



carbohydrates attached to proteins. Neutral molecules designed to imitate the distorted shape of the transition state were less effective inhibitors than molecules that imitated the charge of the transition state but with poor shape mimicry. This discovery inspired the design and synthesis of mannosyl-neuromycin (ManNOE), the most potent inhibitor yet reported for this enzyme,



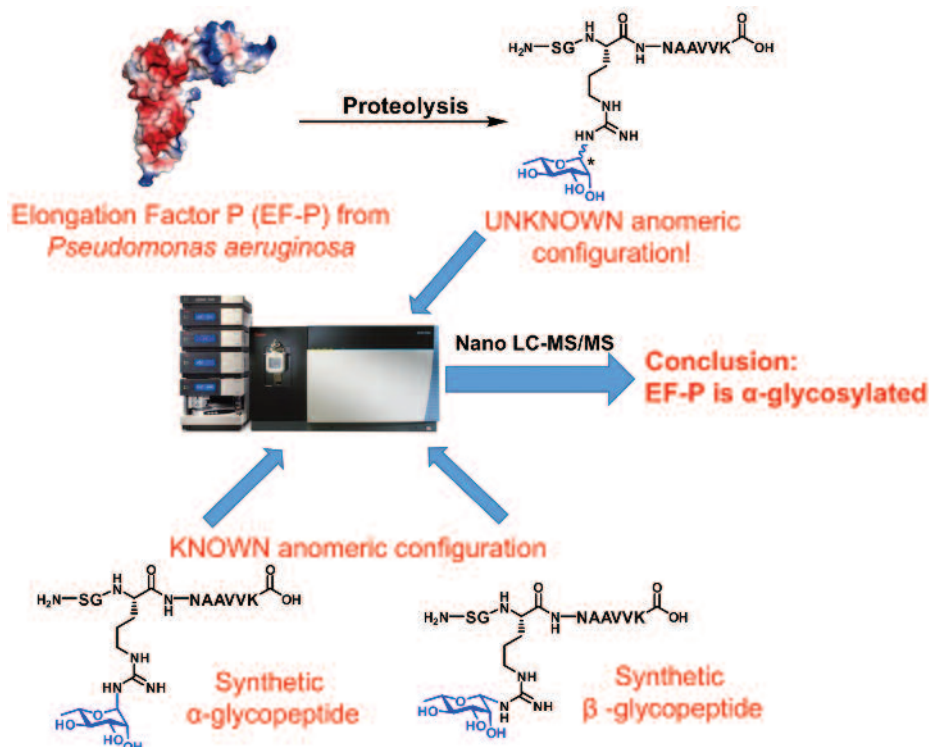
which achieves its inhibition by optimising polar and ionic interactions with the enzyme (Petricevic M., Sobala L.F., Fernandes P.Z., Raich L., Thompson A.J., Bernardo-Seisdedos G., Millet O., Zhu S., Sollogoub M., Jiménez-Barbero J., Rovira C., Davies G.J., Williams S.J. *J. Am. Chem. Soc.* 2017, **139**, 1089–97).

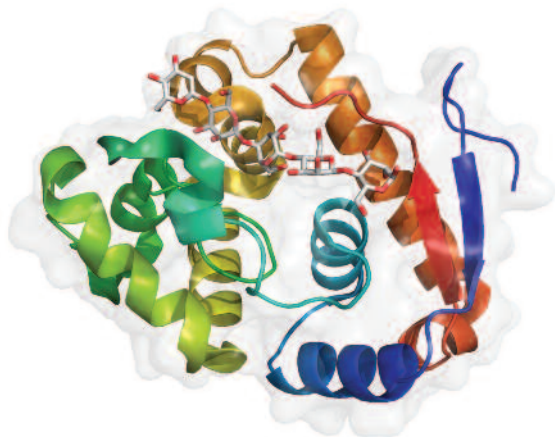
Stereochemistry of a new bacterial carbohydrate modification

Until recently, glycosylation was considered a post-translational modification exclusive to proteins of higher eukaryotic organisms. However, a number of studies have now established that bacterial proteins can also possess covalent carbohydrate modifications on amino acid side chains. In 2015, a new modification – L-rhamnosylation of Arg residues – was discovered on bacterial translation elongation factor P (EF-P), a protein required for preventing ribosome stalling when translating polyproline motifs (Jung K. et al. *Nat. Chem. Biol.* 2015, **11**, 266–70). The rhamnosylation was demonstrated to be critical for EF-P function in several pathogens, including *Pseudomonas aeruginosa*, suggesting that the glycosylation machinery is a potentially novel antimicrobial target. However, the anomeric stereochemistry of L-rhamnose appended to the side chain of the arginine residue was undisclosed. Researchers at the University of Sydney in collaboration with the Walter and Eliza Hall Institute and Ohio State University have now resolved this question (Wang S., Corcilus L., Sharp P.P., Rajkovic A., Ibba M., Parker B.L., Payne R.J. *Chem. Sci.*

2017, **8**, 2296–302). The team synthesised suitably protected rhamnosylated arginine amino acids with both α - and β -configuration and incorporated them into EF-P standards. By analysing glycopeptide standards bearing both rhamnosyl

configurations using 1D and 2D NMR as well as nano liquid chromatography coupled to tandem mass spectrometry, the researchers unequivocally determined the anomeric configuration of the rhamnose moiety on EF-P to be α .





A mannanase that has left the fold

Mannans are polysaccharides present within the plant cell wall and endosperm. Their degradation is catalysed by β -1,4-mannanases and assorted auxiliary enzymes, which act in concert to liberate D-mannose. β -Mannanases are of growing industrial significance in the food, detergent and biofuels industries, which process β -mannan-rich plant material, and in the oil and gas industry, which deploys β -1,4-mannans to modulate fluid rheology in the fracking process. The groups of Dr Ethan Goddard-Borger (Walter and Eliza Hall Institute), Professor Spencer Williams (University of Melbourne) and European colleagues, have reported on the structure and mechanism of a newly described family of β -mannanases (family GH134) that, unusually, adopts a fold closely related to hen egg white lysozyme (the first enzyme to have its three-dimensional structure determined) (Jin Y., Petricevic M., John A., Raich L., Jenkins H., Portela De Souza L., Cuskin F., Gilbert H.J., Rovira C., Goddard-Borger E.D., Williams S.J., Davies G.J. *ACS Cent. Sci.* 2016, **2**, 896–903). A combined theoretical and experimental approach was used to show that the enzyme performs catalysis with inversion of anomeric configuration and a ‘southern hemisphere’ conformational itinerary involving a ring-flipped pyranose conformation.

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

Len Lindoy – special 80th birthday issue

The May issue features a tribute to Professor Leonard (Len) Francis Lindoy, who turned 80 in April. Len earned his MSc and PhD at the University of New South Wales under Stanley Livingstone. After postdoctoral research at the Ohio State University with Daryle H. Busch, he was appointed to the newly established James Cook University in 1970. Len became an international leader in macrocyclic chemistry, and his laboratory at JCU, where he worked closely with the late George Meehan, became a centre for measurements of stability constants. With low numbers of postgraduate students, Len pursued external collaborations vigorously. He was awarded the first personal chair at JCU, a DSc from UNSW, and the RACI Burrows Medal. He became Chair of the ARC Chemistry Panel, President of the Australian Institute of Nuclear Science and Engineering, and a Fellow of the Australian Academy of Science (AAS) before moving to the University of Sydney as Chair of Inorganic Chemistry in 1996. Subsequently, he received the David Craig Medal (AAS), the Leighton Memorial Medal (RACI), and the Centenary Medal of the Australian Government. He has held a number of international guest professorships and received several honorary doctorates. Although formally retired from the university in 2005, he still publishes prolifically and constantly travels and attends conferences all over the world, together with his wife Fay.

The special issue contains articles from many former students, collaborators and friends from around the world, including Karsten and Kerstin Gloe and Jan Weigand (Dresden) (complexes of hexadentate ligands), Peter Comba (Heidelberg), a long-standing friend of Australia (cobalt(II) bispyridines), and Peter Tasker (Edinburgh), who reports on solvent extraction properties of simple ligands – an area in which Lindoy, Tasker and the Gloes have collaborated extensively. Ed Constable and Catherine Housecroft (Basel) describe ferrocene-functionalised terpyridines, Shim Sung Lee (Korea) (Ag^{I} complexes), Keisuke Ohto (Japan) and Yang Kim (Korea) (derivatives of *p*-*t*-octylcalix[4]arene and its extraction properties), Yang Kim with collaborators Shinya Hayami (Japan) and Jack Harrowfield (Strasbourg) (a heterometallic luminophore). Harrowfield, Brian Skelton and the late Allan White (University of Western Australia) also report on cobalt(III) cation with lanthanate(III) anion, and the Hayami group describes spin-crossover in cobalt(II) complexes.


Many of Len’s connections with China were established with the help of his former postdoc Gang Wei, now at CSIRO. Minbo Lan and Gang report on free radicals in mice liver, Yuan Zeli and Gang on oxovanadium(IV) compounds, and Zhu Tao and Gang on supramolecular assemblies of cucurbit[10]uril.

Studies on metal–organic frameworks are reported by J.J. Vittal (Singapore), Christian Doonan and Chris Sumby (University of Adelaide), and Suzanne Neville (University of Sydney) and co-workers. Stuart Batten, Keith Murray, David Turner and Glen Deacon (Monash University) report on thiocyanate transition metal complexes and their magnetic susceptibilities.

Peter Junk (JCU) reports on rare earth complexes. Deanna D’Alessandro (University of Sydney) (PhD at JCU with Richard Keene) contributes a spectroelectrochemical investigation of Ru^{II} complexes, and Roger Bishop (UNSW) discusses substances with weak molecular forces but high melting points.

Suzanne Smith and Nadine DiBartolo, both former students of Len’s from JCU, report on ^{64}Cu PET-imaging in continuation of earlier work with Len. David Schilter, a former honours student, reports from Ulsan, Korea, on NiFe-hydrogenase models. Former postdoc Feng Li (Western Sydney University) reports on hexadentate Schiff-bases. Former masters student Jon Beves (UNSW) and PhD student Jason Price report on hydrogen bonding in crystal engineering. Former PhD student Jack Clegg (University of Queensland) discusses halogen bonding with former postdoc John McMurtrie (QUT), and with Jason Price he reports on 2,2’-bipyridine-containing macrocycles.

Jon Beves MRACI, **Jack Clegg** MRACI CChem, **Richard Keene** FRACI CChem, **Yang Kim** and **Curt Wentrup** FAA, FRACI CChem



13769: Trump's Order and the threat to scientific exchange

BY **BRITTANY HOWARD**

The US Presidential Order imposing travel restrictions is of deep concern to the international scientific community.

Many expressions of concern emerged from the scientific community in the wake of Presidential Executive Order 13769, 'Protecting the Nation from Terrorist Entry into the United States', signed by President Donald J. Trump on 27 January 2017. Among them was a statement on 3 February issued by the American Chemical Society, discussing the 'chilling effect this order may potentially have on the freedom of scientific exchange among scientists

and students worldwide'. RACI President Peter Junk has stated that 'RACI, as a scientific community, supports the ACS's view that scientists should be able to operate without restrictions to travel to enable continuing collaboration, attend scientific conferences and meetings and interact openly with other nations.'

As a result of the Order, severe travel restrictions were imposed on citizens of seven Muslim-majority countries – Iraq, Syria, Iran, Libya, Somalia, Sudan and Yemen. Allegedly,

there was little or no consultation with the Department of Homeland Security in respect of preparing drafts, publication and signing of the Order. It is, therefore, perhaps of little wonder that the Order resulted in mass confusion across US borders, with the relevant authorities themselves appearing confounded as to its actual implementation.

The Order was shortly thereafter blocked by the 9th Circuit Federal Appeals Court. However, this relief was only temporary. A revised Order was unveiled on 6 March, and is set to be effective from 16 March. The revised Order has removed Iraq from the list of countries to which the travel restrictions apply. Several states (including Hawaii, Washington, Oregon, Minnesota and New York) have since challenged the revised Order by filing suits to federal judges (bit.ly/2nbsl7p).

Following the rollout of the initial Order, the international scientific community rallied to support those immediately affected by the travel restrictions. The European Molecular Biology Organisation (EMBO) formed the Science Solidarity List, which assisted scientists outside of the US to offer assistance to those US-based scientists temporarily stranded abroad. As at 24 February, more than 1000 offers of assistance had come from far and wide, including many from Australia, offering desk space and lab benches, internet and library access, accommodation and even 'a warm welcome' (bit.ly/2len6Gz).

Editors of the *British Medical Journal* responded to the travel restrictions by publishing an article that stressed that President Trump's immigration policies could 'disrupt the flow of scientific ideas and knowledge'. Further, the authors stated that they were concerned that the administration was 'acting in ways that will suppress research and limit communication on scientific topics that it deems politically inconvenient'. Undoubtedly, the travel restrictions will also hinder the

The sentiment put forward in the open letter may perhaps be attributed to President Trump's overarching attitude towards science – at least as it has been conveyed by the media – in which he appears to show a general misunderstanding.

recruitment of talented scientists to American institutions (bit.ly/2ltisQj).

Prior to the Presidential Executive Order, Forbes published 'An Open Letter to President Trump From 500 Women Scientists', which in hindsight pre-empted many of these exact issues that have since come to the fore under the Trump administration. The penned letter stated that 'science progress is built on diversity and innovation and only works when we encourage openness and contribution from everyone – scientists of different genders, races,

classes, creeds, cultures, and perspectives. Encouraging such inclusivity ensures that scientific research is critically evaluated from every angle' (bit.ly/2maD57P).

The sentiment put forward in the open letter may perhaps be attributed to President Trump's overarching attitude towards science – at least as it has been conveyed by the media – in which he appears to show a general misunderstanding. President Trump, himself, has previously been reported as propagating the myth that vaccines cause autism and has used his Twitter platform to deny the existence of climate change. In perhaps what has been the most telling sign, the topic of science did not once feature in President Trump's inaugural address. In contrast, scientists hold fond memories of Barack Obama's pledge in 2009 to 'restore science to its rightful place'.

At the time of writing, President Trump was yet to appoint a scientific advisor, a position that carries the more formal title of the Director of the Office of Science and Technology Policy. The level of stature and access that is afforded to the position is at the full discretion of President Trump. The scientific advisor bears the key role of consulting with scientists both internal and external to the government, to ensure the President is being provided with the best available information – scientific facts – for making key decisions on any science-related policy.

The Science Solidarity List: 1000 and counting

'Desk space, lab space, internet access, help with housing.' (Australia)

'Cancer Research lab, desk space, computer access, friendly environment.' (Spain)

'Bench space, internet access and science chat without boundaries. RNA biology.' (England)

'Organic chemist here, I could potentially offer temporary accommodation and internet access.' (UK)

'Laboratory bench, desk, help with housing and visa and staying permit issues, access to laboratory equipment including mass spectrometry for up to 1–2 people.' (Italy)



AAAS Chief Executive Rush Holt Jr (pictured here with school children in his district and USDA administrator Pat Dombroski) was a professor of physics and public policy before serving as a US Senator in the Democratic Party. USDA/CCA-2.0

The White House has not provided any indication of who may be appointed to the role of scientific advisor; however, rumours circulating Capitol Hill would lead us to believe that several controversial candidates are in the running. One such scientist is William Happer, a Princeton University physicist, immigrant and registered Democrat, who has previously stated that he does not agree with 'all the hysteria about climate change'. Also rumoured to be in the running is Yale University computer scientist David Gelernter, who has also denied the existence of climate change. Either of these scientists would seem to be a good fit with the Trump administration, given President Trump has previously alleged that climate change is nothing more than a Chinese hoax created to damage US manufacturing (<http://theatlntc/2IVcmLW>).

In late January, the media reported that the Trump administration had enforced blanket bans on government scientists of at least the Environmental Protection Agency (EPA), the Interior Department, the Department of

Agriculture and the Department of Health and Human Services.

The Trump administration moved swiftly to block the EPA from issuing grants and contracts to study environmental issues. In addition, any EPA studies that are conducted must be reviewed and approved by White House officials before they are released. It is understood that the restrictions also include a temporary blackout on media releases and social media activity. Doug Ericksen, the Communications Director for the Trump transition team at the EPA, has stated that the blackout extends to content on the EPA website, including details of scientific evidence showing that the Earth's climate is warming, and that anthropogenic carbon emissions are to blame (bit.ly/2mfBDBK).

Similarly, scientists at the US Department of Agriculture were allegedly banned from releasing any 'public-facing documents', and comparable restrictions are believed to have been forced upon the Department of Health and Human Services (<http://ti.me/2ltgSxP>).

The restrictions are viewed by many as an attempt to muzzle scientists, and a means to prevent critical research and hard facts from being disseminated to the public.

The restrictions are viewed by many as an attempt to muzzle scientists, and a means to prevent critical research and scientific facts from being disseminated to the public. The American Association for the Advancement of Science (AAAS) has responded to the restrictions by warning against censorship and intimidation, issuing a statement by Chief Executive, Rush Holt Jr, that 'As the AAAS Council stated in 2006, censorship, intimidation, or other restriction on the freedom of scientists employed or funded by government organisations to communicate their unclassified scientific findings and assessments not only to each other but also to policymakers and to the public is inimical to the advance of science and its appropriate application in the policy domain'. The US Director of the World Resources Institute also called for the restrictions to be lifted, and stated that 'these actions will stem the free flow of information and have a chilling effect on staff in these agencies ... The administration should lift these bans as soon as possible and ensure that the role of science is respected within our government agencies' (<http://ind.pn/2IY4VSx>).

The flow of scientific information from government research institutes and organisations to the media and

general public has varied between recent presidencies. For example, Bill Clinton and Barack Obama adopted more expansive definitions of freedom of information. In contrast, George W. Bush sought to restrict it. Most recently, the EPA enacted a scientific integrity document during the Obama administration, which detailed that scientific studies were to be conducted and reviewed by the agency, and that the studies should eventually be communicated to the public 'uncompromised by political or other interference' (<http://ti.me/2mGP3Ee>). It seems the scientific integrity document is of little assistance under the Trump administration. In fact, President Trump's restrictions on scientific authorities fly in the face of Article 19 of the Universal Declaration of Human Rights – one's right to freedom of speech.

However, the imposition of such restrictions is not an unprecedented act. Remarkably, Canadian scientists have only recently had such restrictions lifted following the commencement of the Trudeau government. Previously, former Canadian Prime Minister Stephen Harper, who was in office from 2006 to 2015, prevented government scientists from speaking with media and discussing their research. The focus of the Harper restrictions was in relation to information that highlighted undesirable consequences of industrial development, including climate change. The government policies saw Canadian scientists don their white lab coats and march in protest. A mock funeral procession was held in the streets to mourn the 'death of scientific evidence', and included eulogies that took aim at the years of escalating hostility between Canadian scientists and the Canadian government. It was in these protests that the catchphrase 'no science, no evidence, no truth, no democracy' was coined. The Harper government also eliminated the position of National Science Advisor.

Trump administration moves to muzzle scientists, block research

WASHINGTON (24 January 2017) – It's the first full week of President Trump's administration and attacks on science are already underway. In a memo to Environmental Protection Agency staff, the Trump transition team ordered a freeze on grants and contracts and imposed new restrictions on EPA scientists. At the US Department of Agriculture, scientists at the agency's main research arm have been barred from any public communication about their work. This undermines vital public health and environmental protections, erodes public trust and violates the basic principles of science, according to the Union of Concerned Scientists (UCS).

Below is a statement by Andrew Rosenberg, director of the Center for Science and Democracy at UCS.

'These actions don't just threaten scientists – they threaten everyone in the country who breathes air, drinks water and eats food. These agency scientists carry out research in support of policies that protect our health and safety and help farmers, and it makes no sense to put up walls between them and the public, or unilaterally halt the work they do.

'Both the EPA and the USDA have developed scientific integrity policies that, among other things, protect scientists' right to speak out about their work. The American people deserve to know the results of taxpayer-funded research.

'Halting the EPA's grants and contracts is equally short-sighted and destructive. As we saw in past government shutdowns, you can't just turn scientific research on and off like a switch. We know that scientists can lose years of work, businesses can see investments lost and communities can be deprived of information they need to make good decisions. EPA grants and contracts include efforts like water safety testing and hazardous waste disposal – work that you can't just walk away from without exposing communities to preventable risks.

'If you care about clean air, clean water and policies that actually protect people, you need the best independent science – and actions like this make it harder for Americans to benefit from science. That the administration has moved so quickly to clamp down on scientists shows that the Trump administration is more focused on lifting rules on polluters than keeping our air and water clean.

'The scientific community is ready to fight back against any efforts to marginalise or suppress science and undermine science-based policies and research people depend on. More than 5500 scientists have come together to say that President Trump must respect the role of science. These actions are the clearest sign yet that he isn't living up to that standard.'

Union of Concerned Scientists





President Trump speaking about his immigration policy in Phoenix, Arizona, on 31 August 2016. Gage Skidmore/CC BY-SA 2.0

The Harper restrictions were extraordinarily effective in restricting the dissemination of research and its outcomes to the public. A 2013 survey reported that a quarter of Canadian government scientists had been asked to exclude or alter scientific information for non-scientific reasons, and 90% considered they were not able to discuss their research freely with the media. A leaked internal Environment Canada document revealed that the restrictions had reduced the department's engagement with media on climate change by a staggering 80%. The Trudeau government has since lifted the restrictions, and last year Canadian scientists, with the support of their union, worked to ensure their contracts would permanently enshrine their right to discuss their research with the media and public (bit.ly/2ltisQj).

When it comes to the dissemination of research and innovation to the public, the patent system is one of the oldest and most successful means for doing so. Most certainly, the primary premise of the patent system is to reward inventors through the grant of an exclusive monopoly in exchange for disclosing the invention to the community in the form of a published patent document. As of yet, the Trump administration is yet to release any policy papers or give any indication of what is in store for the current US patent system, and the intellectual property regimes in general. In any event, any changes implemented by President Trump must strike the delicate balance of affording commensurate intellectual property rights to an inventor. If the afforded rights are considered too weak, the incentive to seek patent protection will be lacking, resulting in the invention

not being published and therefore not disclosed to the public.

Much of what will eventuate from the Trump administration remains to be seen. Many consider that the restrictions have had severe implications on scientific collaborations, including preventing travel between collaborating research groups and to international conferences to present findings, and have prevented many talented scientists from entering the US. Undoubtedly, it is in the best interests of everyone, including President Trump himself, that he and his administration are armed with scientific facts.

Brittany Howard MRACI completed a PhD in medicinal chemistry at the Monash Institute of Pharmaceutical Sciences before undertaking a postdoctoral position with the National Institutes of Health (US). She is currently a patent attorney with FB Rice Patent and Trade Mark Attorneys.

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Directed evolution

DNA polymerase, the enzyme that synthesises DNA molecules.

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Following nature's lead

Dave Sammut speaks to Caltech professor Frances Arnold, who is 'using biology to do chemistry'.

If DNA is a language of life, we have so far only learned the alphabet, and to read and write the simplest sentences. Designing and synthesising known sequences of DNA is one thing; predicting the function of the resulting proteins is quite another. Thus, tailoring biochemical agents for desired functions is a significant challenge. Evolution has the answer.

In February, I spoke with Frances Arnold, the Dick and Barbara Dickinson Professor of Chemical Engineering, Bioengineering and Biochemistry at the California Institute of Technology, US. She will be a plenary speaker at the RACI Centenary Congress later this year.

'How a protein sequence encodes what the protein does remains an open question'

Arnold has been awarded the 2016 Millennium Technology Prize (€1 million) for her work in a different approach to the design-function problem. 'I don't want to insult computational [scientists], but we cannot design enzymes in any reliable fashion, especially when it comes to the functions that are really unique to chemistry, to how enzymes make new molecules. We cannot predict what amino acid sequence would give rise to a desired function. But we would not be talking to one another unless there were a reliable design process for

making them – that process is evolution.'

Arnold uses the science of 'directed evolution' to create improved proteins in the laboratory, with specific outcomes in mind. In a 2015 lecture at Oak Ridge National Laboratory (bit.ly/2lrXLHI), Arnold stated that: 'DNA code was solved even before I was born – how DNA encodes a protein sequence, but how a protein sequence encodes the folded protein structure remains an open question. And that's not even the question that matters. It's "How does the sequence encode function?" Those are two big questions that I don't have time to wait for people to solve'. Arnold instead elected to use nature's own processes to solve real human problems.

'To me, the greatest engineer of all time is nature'

Arnold's point is that nature has already evolved immensely powerful tools to drive efficient, selective and renewable chemistry. 'To me, the greatest engineer of all time is nature', she says. Arnold's vision is to use nature's existing materials and inventive processes to efficiently produce chemicals in a sustainable fashion: 'Life is poised to do chemistry that we never dreamed of. We are using biology to do chemistry that human chemists thought only they could do, and more'.

Arnold's vision is to use nature's existing materials and inventive processes to efficiently produce chemicals in a sustainable fashion.



Frances Arnold

Of course, humans have been utilising nature's processes for some time to build new biological variants. The chihuahua is a long process of selective breeding away from the wolf. After generations of selection, staple crops and grains have yields far beyond their early agricultural ancestors, and with modern genetic techniques we are experimenting with other properties such as pest protection.

Directed evolution's different approach is to use the empirical 'better or worse' selection from evolutionary processes, rather than more theoretical methods of protein design. In Arnold's words: 'Chemistry is hard to design, but easy to evolve'.

'Nothing comes from nothing'

Arnold emphasises that 'nothing comes from nothing'. The starting point to approach any new chemical function is to find some biological agent – a protein – that does the desired job to some extent, no matter how infinitesimally small.

Take Arnold's recent work on creating enzymes that catalyse the formation of a carbon–silicon bond, a bond nature is not known to make (Kan et al., *Science* 2016, vol. 354, pp. 1048–51). Human chemists have never made such organosilicon compounds using iron-based catalysts. Arnold's co-workers started by screening haem proteins to find ones that functioned even at extremely low levels. From these, they knew that the chemistry

was at least possible. 'Planning is important. Choosing where to start is a rational, knowledge-based process.'

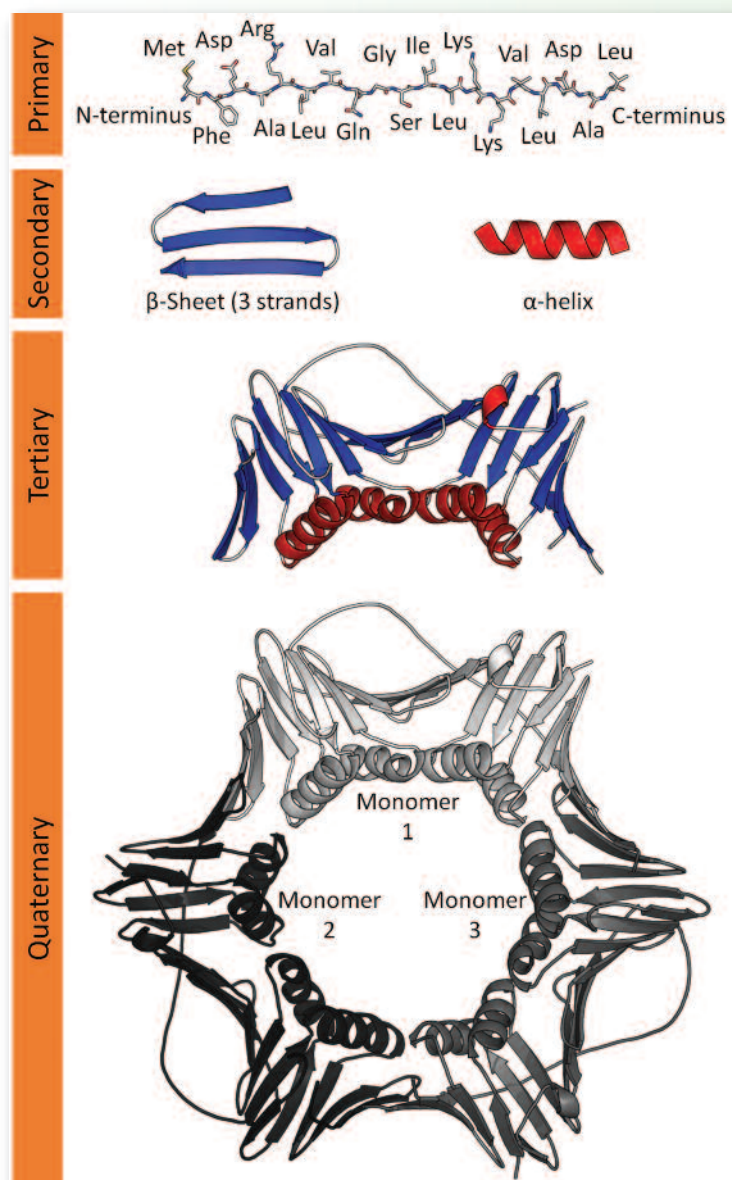
Next, Arnold applied processes for directed and random mutation of the proteins (for example, controlled mutation using the polymerase chain reaction), creating hundreds of physical samples that they screened by well-established analytical methods for improved activity in the new reaction. The genes encoding the improved proteins were recombined or mutated again to enable beneficial

mutations to accumulate. The evolved enzyme they reported formed organosilicon compounds inside bacterial cells, essentially 'bringing silicon to life' for the first time.

By starting with functional proteins that are homologous or evolutionarily related, Arnold significantly increases the odds of success. With 20 amino acids and at least 400 peptides in a protein chain, that makes for an astronomical number of combinations – at least 20^{400} . Most of these combinations won't be

functional. With more than just two or three random mutations, the probability of creating a functional protein is very low. Arnold's approach allows her to accumulate dozens or sometimes hundreds of mutations while still achieving a reasonable chance of successful variants.

'When we do this, we create so-called "chimeric" structures. What we've learned is that recombination is conservative. When we do this, we can create large numbers of [DNA] sequences. We can synthesise these



Proteins 101

Amino acids: These organic molecules are used by living organisms to make proteins. There are about 20 types of amino acids, which we source by breaking down the proteins in the food we eat.

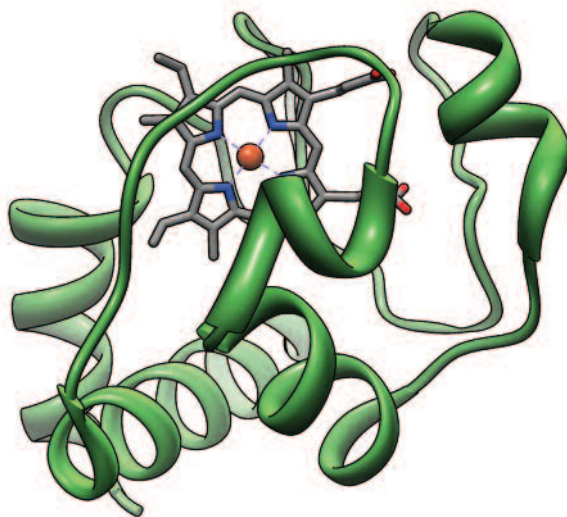
Proteins: These are long chains of amino acids. They are the most diverse group of biologically active substances, and are effectively the central component to life. There are thousands of different proteins just in the human body, with many different types, including structural (such as collagen and keratin), defensive (such as antibodies), transport (such as haemoglobin) and catalysts (such as enzymes).

Making a protein: Via 'transcription', a copy of the DNA (deoxyribonucleic acid) in a cell is created, called RNA (ribonucleic acid). This is something like the 'printer instructions'. Via 'translation', the RNA is transported to a ribosome, something like the 'protein printer'. The ribosome finds a 'beginner' sequence on the RNA called a 'codon', then moves sequentially down the strand of RNA, where every three 'letter' combination represents another amino acid 'peptide' molecule. The ribosome builds a string of peptides, until it finds the 'stop' point on the RNA, and the protein synthesis is complete.

Protein structure: The particular three-dimensional shape of each protein defines its highly specific function. If this shape is altered, the protein becomes denatured and does not function as expected. Four levels of structure are used to describe the protein:

- primary structure – the linear sequence of amino acids
- secondary structure – where hydrogen bonding between amino acids creates three-dimensional geometry, such as an alpha helix or a pleated sheet
- tertiary structure – the overall shape of the protein: globular (such as enzymes) or fibrous (such as muscle tissue)
- quaternary structure – the appearance when a protein is composed of two or more polypeptide chains.

By starting with functional proteins that are homologous or evolutionarily related, Arnold significantly increases the odds of success.



Three-dimensional structure of cytochrome c (green) with a haem molecule coordinating a central iron atom (orange). Frances Arnold's group have discovered 'that haem proteins catalyse the formation of organosilicon compounds under physiological conditions via carbene insertion into silicon-hydrogen bonds' (doi: 10.1126/science.aah6219).

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and put them into bacteria and see who folds and functions.'

'Still, we do it safely. We have a computational algorithm so you can take more disparate sequences. We can choose the recombination cross-over points so as to maximise the number of these that will be folded and functional.'

'A simple process of random uphill walk'

A key point is that, rather than seeking the optimum solution, the process seeks one or more *incrementally better* solutions. According to Arnold, it's 'a simple process of optimisation by a random uphill walk – making mutations over multiple generations and collecting the beneficial effects'.

'The science of molecular breeding is choosing how big a barrier you have to jump in each level of the optimisation. If you choose that properly, you can continually walk uphill to adapt the protein to its new function.'

The surprising outcome is that with just a few generations – not tens or

hundreds – considerable improvements in yield, selectivity and/or other targeted properties can be achieved. 'We can do what nature takes millions of years to do in a matter of weeks. Proteins are very adaptable'.

For this, Arnold explains, the selection of the screening method is absolutely critical. 'You get what you screen for.' Arnold gives the example of a manufacturer who approached her years ago to develop cold-temperature enzymes for laundry detergents. She explained to the manufacturer that while she could definitely develop enzymes that would function well over a wide range of temperatures, the enzymes could easily lose their primary useful function – of taking stains off of clothes – unless she screened them in washing machines.

'Science is a small fraction of commercial success'

Having come to this area from an engineering background, Arnold describes herself as very much an applied scientist. While her laboratory

does a great deal of pure research, she has been involved in 13 start-ups to commercialise technologies arising from her work and others', six of which have gone public. She describes these as 'all great fun', but is particularly enthusiastic about her most recent start-up (Provivi), which is seeking to develop processes for commercial production of insect pheromones that can be safely sprayed onto crops to disrupt pest breeding cycles.

On the topic of commercialising new technologies, Arnold is passionate in the expression of her views: 'Science is a small fraction of commercial success. It takes business skills, timing and a great story'. She says that too many scientists develop a technology, then try to find an application for it. 'First', says Arnold, 'find a problem worth solving'.

Arnold is an engaging speaker, and we'll expect her to be addressing a packed house in July.

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

Friends of Timor Leste Chemistry

I have been to Timor Leste twice, in 2015 and 2016. In 2016, I met with Professor Samuel Venancio de Sousa Freitas, Dean of the Faculty of Science at the National University of Timor Leste. He is a chemist and is keen to form a Timor Leste Chemical Society (TLCS) and to participate in regional activities through the Federation of Asian Chemical Societies. I have been helping him to set up the society. It has a draft constitution based on the RACI constitution and about 50 potential members.

The 2017 RACI Centenary Conference would be a great opportunity for the fledgling society to launch its international interactions.

The 2017 RACI Centenary Conference would be a great opportunity for the fledgling society to launch its international interactions.

To this end, I have formed the Friends of Timor Leste Chemistry to assist the TLCS and help bring someone to the conference. This will cost about \$2000. I have made an initial donation of \$500.

I have been interested in Timor Leste since the time that I was living in Jakarta. I was there in 1999 when the Indonesian Government agreed to hold a referendum in their Timor Timur province to determine whether the population wanted independence. They did, with an overwhelming majority! The Indonesian Army did not accept the decision and civil war broke out. The Australian Defence Force led the international peacekeeping effort and this caused some resentment towards Australian expatriates. Despite this general resentment, our Indonesian hosts were very kind to us.

I returned home in 2001 and followed the progress of the new country, Timor Leste, to full independence in May 2002. In 2004, I was part of a group in Mount Waverley that formed Friends of Vemasse with the aim of supporting the subdistrict of Vemasse. This is a community on the north coast of Timor Leste about 100 kilometres east of Dili. Friends of Vemasse has

devoted its efforts to support education in the subdistrict. For example, we pay the salaries of four teachers in the Senior High School in Vemasse.

On both of my visits to Timor Leste, I have been aware of the important contribution chemistry and chemists will play in the economic and social development of the nation.

Tom Spurling FRACI CChem. To express an interest or to find out more about this initiative, email tspurling@swin.edu.au. To find out how to donate, email roger.stapleford@raci.org.au.



iStockphoto/Phongsiri

In Timor Leste:

GDP per capita (purchasing power parity) is \$4200 compared to \$48 800 in Australia.

38% of children under five are underweight, the highest percentage in the world.

The government is very committed to education and spends nearly 8% of its GDP on education. Australia spends 5.3%.



Professor Samuel Venancio de Sousa Freitas

2017 ACES and GDCh Symposium: functional nanomaterials

On 27 July 2017, the Asian Chemical Editorial Society (ACES) and the German Chemical Society (GDCh) will host the first ACES and GDCh symposium at the biannual Asian Chemical Congress (ACC) in Melbourne. This will take place as part of the centenary celebrations of RACI, an ACES partner. Speakers at the high-level one-day symposium, which will focus on functional nanomaterials, are this year's Ryoji Noyori ACES award winner Chi-Ming Che, University of Hong Kong; Susumu Kitagawa, University of Kyoto; Frank Caruso, University of Melbourne; Bin Liu, National University of Singapore; and Markus Antonietti, Max Planck Institute of Colloids and Interfaces, who will give the GDCh lecture.

The symposium is designed to deepen relationships and foster collaboration between chemists across Asia, Germany and beyond. The biannual Noyori ACES award recognises a top scientist who has made outstanding contributions to the development of chemistry in general and of the ACES journals in particular. It has been initiated by the ACES partners to honour Professor Noyori's instrumental role in nurturing the collaborative ACES spirit in the early days of the organisation and as the founding chairman of the Editorial Board of *Chemistry – An Asian Journal*.

The ACES comprises 13 chemical societies from across Asia and the Pacific who coordinate their publishing activities and foster international cooperation. ACES supports scientific collaboration, which highlights the advantages of exchange and mutual enrichment and helps to break down barriers to the free flow of ideas. It was founded at the 2005 IUPAC Congress in Beijing by the Chinese Chemical Society (CCS), the Chemical Research Society of India (CRSI), the Chemical Society of Japan (CSJ) and the Korean Chemical Society (KCS), and is supported by the Federation of Asian Chemical Societies. At the same meeting, the ACES flagship journal *Chemistry – An Asian Journal* was founded as a sister journal to *Angewandte Chemie* and *Chemistry – A European Journal* with the support of the GDCh. *Chemistry – An Asian Journal*, like the other ACES journals *Asian Journal of Organic Chemistry* and *ChemNanoMat*, is rooted in Asia through its ties to the ACES partner societies. All three ACES journals are nevertheless international in scope and are held in high standing by authors and readers around the world.

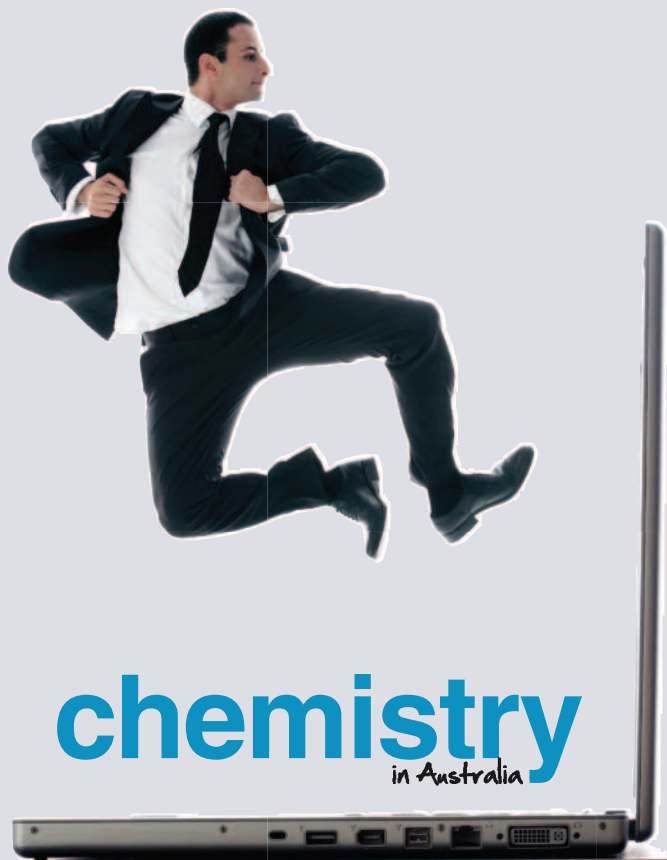
The 12th ACES meeting was held in 2016 in Melbourne, and ACES looks forward to returning there in July 2017 to celebrate 100 years of RACI.

Dr Theresa Kueckmann, Editor, *Chemistry – An Asian Journal*



12th ACES meeting in Melbourne, 2016.

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Bio21 professor to receive IUPAC Distinguished Women in Chemistry award

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

The awards program, initiated as part of the 2011 International Year of Chemistry celebrations, was created to acknowledge and promote the work of women chemists/chemical engineers worldwide. These 12 awardees have been selected on the basis of excellence in basic or applied research, distinguished accomplishments in teaching or education, or demonstrated leadership or managerial excellence in the chemical sciences. The Awards Committee was particularly interested in nominees with a history of leadership and/or community service during their careers.

Other recipients announced by IUPAC were:

- Professor Misako Aida, Hiroshima University, Japan
- Professor Lifeng Chi, Soochow University, China
- Professor M. Concepción Gimeno, Institute of Chemical Synthesis and Homogeneous Catalysis (ISQCH), CSIC-University of Zaragoza, Spain
- Dr Jaqueline Kiplinger, Los Alamos National Laboratory, United States
- Professor Zafra Lerman, Malta Conferences Foundation, United States
- Professor Thisbe K. Lindhorst, Universität Kiel, Germany
- Professor Ekaterina Lokteva, M.V. Lomonosov Moscow State University, Russia
- Professor Yvonne Mascarenhas, University of São Paulo, Brazil
- Dr Veronika Ruth Meyer (retired), Empa St Gallen, Swiss Federal Laboratories for Materials Science and Technology, Switzerland
- Professor Ingrid Montes-González, University of Puerto Rico, Puerto Rico
- Professor Jihong Yu, Jilin University, China

Professor Vanderlan da S. Bolzani, co-chair of the special symposium, remarked: 'We are especially pleased with this year's awardees ... Each year since 2011, the award has gained more attention in the community. During this year's Congress and with the help of IUPAC leadership, we plan to continue this trend. My hope is to make every day International Women's Day!'

International Women's Day is a global day celebrating the social, economic, cultural and political achievements of women. The day also marks a call to action for accelerating gender parity.

An award ceremony will take place during the IUPAC World Chemistry Congress in São Paulo, Brazil, coinciding with the special symposium on Women in Chemistry and reception in honour of the recipients. See www.iupac2017.org for details.

IUPAC

Chemeca's Academic Sharp Brain



To honour the centenary of the RACI, Chemeca 2017 will be held as a partner conference to the RACI Centenary Conference 2017. Nobel laureates will grace the occasion and the number of participants will exceed 4000 to create the largest ever gathering of scientists and engineers held in Australia.

Scientists mix their logic with imagination to create opportunities. Engineers bring change to society and play a major role in the development and application of technology. When we want to bring change, we ask all sorts of questions. This is the easy part; and often, we find theoretical answers. However, the difficult part remains – the implementation. The academic world is moving towards innovation but the challenge remains: how to maintain research excellence with relevance to real-world applications. This can be achieved by rubbing the line between science and engineering to deliver the next age of economic prosperity.

To lead the change towards a better future, we need to involve all those for whom the changes are intended, to create the sense of ownership and responsibility. We need to create a thrilling and exciting landscape that allows everyone to say 'I am a part of the change'. The current generation wants to make a difference. Their participation is vital to create a greater culture of innovation.

Being the 2017 Chemeca Chair, I took the initiative to organise this event in a unique way to showcase innovative research and technology, and to provide inspiration to our emerging professionals as future innovators who fit into the nation's core

How to register

- 1 Download the pitchdeck.
www.racicongress.com/Chemeca2017/academic-sharp-brain.php
- 2 Submit your pitch and a copy of your resumé to:
Dr Neda Mirzadeh, Entrepreneurship Program Coordinator & Organising Committee, Academic Sharp Brain
(nedaossadat.mirzadeh@rmit.edu.au)
- 3 Receive the confirmation of your submission along with some information regarding the next steps.

values. To do so, I have developed an innovative event for the first time: the Academic Sharp Brain. The Academic Sharp Brain is a platform, to not only realise the potential of intelligent minds but to also brighten the future of our professions by bringing innovative ideas to marketplace. The Academic Sharp Brain provides Chemeca participants with the opportunity to pitch their innovative scientific- and engineering-based ideas to the invited experts and potential investors and to attract support and resources to develop business opportunities.

This is the future of the future.

Please accept my invitation to change and my invitation to participate in the Academic Sharp Brain.

Professor Suresh Bhargava, Distinguished Professor, KIA Laureate, Academic Sharp Brain, Founder, Chair & Organiser. For more information on Chemeca, visit www.racicongress.com/Chemeca2017.

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books

Bring back the King: the new science of de-extinction

Pilcher H., Bloomsbury Sigma, 2016, hardback, ISBN 9781472912251, 304 pp., \$31.50

'De-extinction' is the idea that we can bring back to life species that have gone extinct – think dinosaurs, mammoths and dodos. As we learn more about DNA and the molecular processes taking place in a growing embryo, the *Jurassic Park* scenario of creating new organisms that replicate their extinct ancestors begins to look feasible.

In *Bring back the King*, Helen Pilcher examines this possibility from many angles, from the science (theoretical and practical) to ethics, politics and potential impacts (both good and bad) if we succeed. It's a fascinating book that fleshes out the scientific concepts with lots of engaging detail. We meet some of the scientists taking small steps towards achieving the de-extinction dream, including Mike Tyler and Michael Archer, who have attempted to re-create the Australian gastric-brooding frog and the Tasmanian tiger, respectively.

We meet the animals as well: Stan the seven-tonne *Tyrannosaurus rex*, Celia the last wild bucardo mountain goat, Martha the last living passenger pigeon, Benjamin the last Tasmanian tiger, and more. The stories of these recent extinctions are poignant, and it's somewhat disheartening that right now human impacts on the environment are causing more extinctions than ever.

Helen Pilcher is a scientist-turned-writer of both science and comedy – a winning combination that ensures the subject is discussed in depth in a very readable way. Even Pilcher's self-declared 'folly' – the chapter on bringing back Elvis Presley (so not re-creating an extinct species as such but cloning 'the King' himself) – illuminates important issues in genetics.

Each chapter, focusing on a different de-extinction candidate, builds up the picture of how the science of cloning and genetic manipulation has developed over the last few decades and what current technology can achieve. Sadly for dinosaur lovers, DNA deterioration rules out cloning *T. rex* à la *Jurassic Park*, even if we were willing to have them roaming the world again.

The science of de-extinction is much more than cloning, although that itself is challenge enough. I appreciated the explanation of the new genome editing technology known as CRISPR, which provides another approach to re-creating extinct species (as well as being a tool for new health therapies).

Bring back the King is an informative and open-minded evaluation of de-extinction. What does de-extinction really mean? Would the re-created organism really be the same as its extinct ancestors? How would it fit into today's environment? Which species should we choose?

In the end, Pilcher turns to the northern white rhinoceros – a subspecies with only three living individuals when the book was published and still with us today. The science of de-extinction may even more appropriately be applied to species (or subspecies) like these, she argues.

De-extinction is still some way off, but it is getting closer. *Bring back the King* has made me excited about the possibilities.

Margie Beilharz



The top chemical inventions that changed our lives

Dr Marcus Caulfield, Partner and Registered Patent and Trade Marks Attorney, FB Rice



We all know, well chemists and patent attorneys know, that chemistry is an enabling science that underpins just about every part of our lives. But are you aware of the top chemical inventions that truly enabled the modern world, and that they were all patented at one stage or another?

1 Penicillin

Penicillin was famously discovered by Alexander Fleming in 1928, who observed that mould growing in a petri dish suppressed the growth of bacteria. Critically, Dr Fleming decided not to patent his invention, falsely believing that this would help get the invention to those most in need, and very little was done with the discovery for over 10 years. It was not until the outbreak of World War II that the Australian pharmacologist Howard Florey and his team of chemists figured out a way to purify penicillin. The rest, as they say, is history. The processes for the production of penicillin were eventually patented, and penicillin went on to save millions of lives.

2 Haber-Bosch process

While the name may not mean much to most people, this 1909 patented invention for the artificial fixation of nitrogen directly led to modern nitrogen fertilisers and the ability to feed billions of people. The so-called 'detonator of the population explosion' enabled the global population to increase from 1.6 billion in 1900 to over 7 billion today. In fact, nearly 80% of the nitrogen found in human tissues originated from the Haber-Bosch process, demonstrating how integral this process is to our modern lives.

3 Polythene

In a story similar to that of penicillin, the German chemist Hans von Pechmann discovered in 1898 that a waxy substance formed at the bottom of his test tubes. His team determined that this substance was made up of very long molecular chains and they called it polymethylene. Professor Pechmann did not seek patent protection for his discovery and no further significant development was made. In the early 1930s, a second team working at the Imperial Chemical Industries (ICI) again, accidentally produced the same waxy substance when oxygen leaked into one of their reaction vessels. Following two years of intense research and development (and several patent applications), their serendipitous discovery was turned into the basis of the modern plastics industry.

4 The Pill

The development of the contraceptive pill in the 1950s arguably led to a social revolution. It had been known since at least the 1930s that hormone-based therapies had the potential to control the menstrual cycle, though there was no way to efficiently synthesise the hormones. This changed in the 1940s and early 1950s. Professor Russel Marker, and later Carl Djerassi, at a small Mexican drug company, Syntex, developed a process for the artificial synthesis of progesterone from compounds isolated from the Mexican yam. Dr Djerassi patented his technology and used the profits to fund his research and development for better and safer versions of the oral contraceptive pill.

To discuss your invention, email mcaulfield@fbrice.com.au.

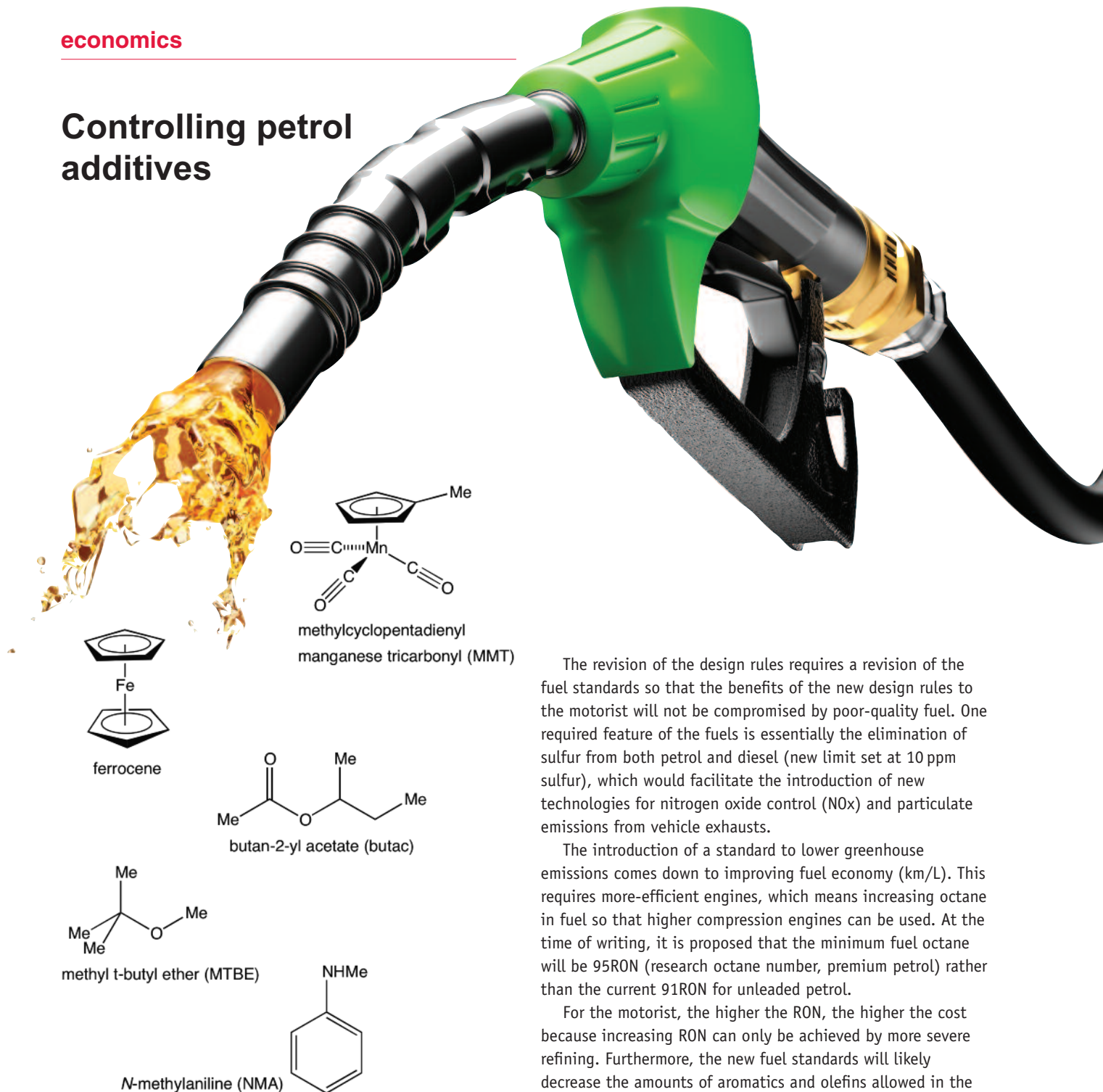
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Controlling petrol additives



The quality of fuel sold in Australia is regulated by the Fuel Standards Act. The Act sets the levels of various components and performance criteria for petrol, diesel, LPG, ethanol fuels and biodiesel. The Fuel Standards Act complements vehicle design rules, which set performance levels for new vehicles sold in Australia, including emission limits. A review of vehicle design rules is currently underway, which will tighten emission standards and extend emission limits to include greenhouse gas emissions. This harmonises Australian design rules with European design rules.

The revision of the design rules requires a revision of the fuel standards so that the benefits of the new design rules to the motorist will not be compromised by poor-quality fuel. One required feature of the fuels is essentially the elimination of sulfur from both petrol and diesel (new limit set at 10 ppm sulfur), which would facilitate the introduction of new technologies for nitrogen oxide control (NO_x) and particulate emissions from vehicle exhausts.

The introduction of a standard to lower greenhouse emissions comes down to improving fuel economy (km/L). This requires more-efficient engines, which means increasing octane in fuel so that higher compression engines can be used. At the time of writing, it is proposed that the minimum fuel octane will be 95RON (research octane number, premium petrol) rather than the current 91RON for unleaded petrol.

For the motorist, the higher the RON, the higher the cost because increasing RON can only be achieved by more severe refining. Furthermore, the new fuel standards will likely decrease the amounts of aromatics and olefins allowed in the fuel. These components are high in octane and the new limits will place further challenges to refiners to achieve the 95RON minimum.

Higher RON can be achieved by using chemical octane boosters. Organometallic additives are very effective but are now banned or opposed by vehicle manufacturers. This includes lead compounds, methylcyclopentadienyl manganese tricarbonyl (MMT) and ferrocene.

Widely used octane boosters are alcohols, especially ethanol, and ethers such as methyl t-butyl ether (MTBE). Ethanol is widely used in Australia but there are issues with vehicle compatibility (especially with old vehicles) and ethanol is not

Higher research octane number can be achieved by using chemical octane boosters.

very compatible with petrol (fungible). Adding ethanol to petrol results in higher vapour pressure, which increases fugitive emissions and it separates from petrol in the presence of water, such as condensation in storage tanks. Although adding ethanol may achieve the 95RON standard, obtaining the higher 98RON grades could be difficult.

MTBE is widely used in Europe, the Middle East and across Asia. In western Europe and Japan, in particular, the ethanol derivative ETBE is used. Australia does not use MTBE for historical reasons to do with leaking storage tanks contaminating ground water. Compared to other petrol components, MTBE has low toxicity but apparently some people can taste MTBE in potable water at the 20 ppb (parts per billion) level, whereas benzene is not detectable below about 150 ppb. In my opinion, the limiting of ethers on this ground is allowing regulatory authorities to ignore leaking tanks in their jurisdictions.

These ethers are very commonly used in refineries in Asia from where increasing volumes of petrol are being sourced for Australian motorists. Having a low limit on MTBE results in Australia having a boutique fuel standard that can only result in higher fuel costs.

Several other octane-boosting components might find their way into Australian petrol. One of the drivers is that sometimes chemical supply can exceed demand and one way of disposing of these chemicals is to mix them with petrol. Some of these compounds may cause long-term damage to vehicles and engines.

The possibility of using furan and substituted furans in petrol is the result of research into producing fuel components from biological sources. These include the mass production of furans from ligno-cellulosic material feedstock (wood waste etc.), which without further treatment would probably prove be too aggressive as solvents for seals in vehicles.

Major research into the lowering or removal of lead from aviation gasoline is developing high-octane petrol formulations containing a diverse range of nitrogen- and oxygen-containing chemicals. These include toxic and dangerous chemicals such as aniline and aggressive solvents such as diethyl carbonate. Whether or not these could be used in transport vehicle fuels is unknown.

N-Methylaniline (NMA) is mainly used as an intermediate in dye manufacture. It would appear to be used fairly widely as an octane booster but is alleged to have caused vehicle problems.

Because it is not an oxygenate, NMA seems to have slipped through several regulatory nets (it is not mentioned in World Wide Fuel Charter, which is the auto industry's view of fuels and fuel additives). NMA is permitted in several jurisdictions (e.g. the US) and banned in others (China, Russia). It is highly toxic and is easily oxidised forming resins. Where it is permitted, NMA usually has to be in association with detergents and fuel combustion modifiers. Whether or not this solves the issue of gum formation is unknown. Industry sources have indicated that NMA has been used on at least one occasion in Australia.

Acetone is a powerful solvent (lacquer removal – nail polish remover) and widely available from local hardware stores. Acetone's main chemical use is in the production of methyl methacrylates (for Perspex etc.) and bisphenol A (used for polycarbonate polymers) with Asia producing over 1 million tonnes per year from more than 20 companies. Currently, supply exceeds demand.

Although most acetone is made by the chemical industry, acetone could be made by renewable methods. Old fermentation routes, now largely obsolete, are known for co-producing acetone, ethanol and butanol. This technology is being revived by genetic engineering methods to ferment sugars to biobutanol.

Internet searches reveal many enthusiastic supporters of using acetone to boost RON to levels of 100 or more. Acetone seems to be widely used by a section of motoring enthusiasts who wish to modify and boost performance of road and racing vehicles. Other members of this community discourage this practice.

Isobutanol produced by genetically modified enzymes is being promoted as an alternative to ethanol by Du Pont, BP and several other companies. It has better fungibility than ethanol, does not have the same level of water uptake and has a lower impact on vapour pressure. It has been suggested as a co-solvent for ethanol.

sec-Butyl acetate (butan-2-yl acetate) (butac) is an industrial solvent widely used in the lacquer and automotive paint industries. Asia produces over 1 million tonnes per year from over 20 companies. Currently, supply exceeds demand. Butac was used in Vietnam where it caused vehicle performance problems, resulting in its ban.

Whatever the outcome of the Fuel Standards review, the Australian motorist is likely to see higher prices for fuel. The demand to increase fuel octane could encourage unscrupulous traders and entrepreneurs to introduce chemicals that boost octane but cause long-term damage to vehicles.

It is important that regulations and regulatory authorities remain in control of additives to petrol and do not inadvertently allow materials into the Australian petrol pool that would damage vehicles and engines.



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

Molecules for food security

Synthetic organic chemists have the ability to create molecules that impact the social and economic aspects of our world – from new medicines, to advances in nanotechnology and plastics.

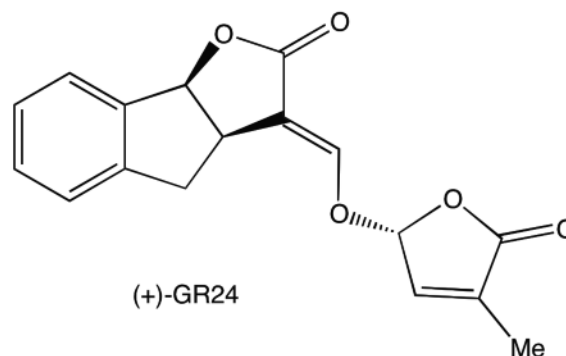
Regardless of the application, advances in these areas have been dependent upon the implementation of new synthetic methods. This is exactly what my research group works hard to achieve, inventing better ways to build life-changing molecules. One of our recent success stories has been in the field of plant-signalling molecules.

Food security looms as a major challenge for society. Cereal crops constitute more than 50% of the calories in human consumption, and the Food and Agriculture Organization of the United Nations predicts that a 60% increase in global production will be required by 2050 to meet the growing need for food. Despite being spectacularly successful, the contribution of synthetic organic chemistry to the agricultural sector has been directed towards crop protection rather than growth promotion (i.e. insecticides and herbicides). Promoting crop growth has traditionally been approached by applying fertilisers. We want to change that. Revolutionary discoveries in 2005 and 2008 mean that we are only just beginning to unravel the complex mechanisms underpinning plant growth and development and a family of plant-signalling molecules called the strigolactones is involved in many of these processes.

... the application of strigolactones can inhibit the accumulation of these ‘stress response’ signalling molecules, which results in continued growth under adverse conditions.

In 2005 strigolactones were identified as the molecules that facilitate plant–fungi communication. Released from the plant’s developing root system into the surrounding soil at picogram concentrations, these compounds cause arbuscular mycorrhizal (AM) fungi to take up residence in plant roots where they provide nutrients (such as phosphates) to the plant while receiving plant-derived carbohydrates in return. This plant–fungi interaction is the most widespread example of symbiosis on the planet, and enhancing this process is an ideal way to promote plant growth and increase crop yields. The stumbling block was accessing the strigolactone molecules.

We rose to prominence in this field by designing and executing an asymmetric total synthesis of a strigolactone signalling molecule called GR24. Before our work, plant researchers used a mixture of compounds in their assays



(+)-GR24 allows plant–fungi symbiosis, enables enhanced nutrient uptake and affects plant growth and development.

because there was no way to control the three-dimensional structure of GR24. We overcame that shortcoming and designed a method to stereoselectively build any GR24 structure (isomer) in just five steps. We currently supply single isomer GR24 molecules to over a dozen research groups worldwide. Our expertise in synthetic organic chemistry allowed us to invent a process that can make hundreds of grams of this molecule in one go, which has enabled its use in field trials in both Canada and China. We are eagerly awaiting the outcome of those trials, but have used the intervening time to take on another strigolactone challenge.

We know that strigolactones play vital roles in the growth and development of plants, but we know very little about the mechanisms by which this occurs. In order to see what happens inside a plant, scientists need a fluorescent molecule that behaves just like a strigolactone plant hormone ... so we invented one! This molecule is currently being used by our collaborators to monitor the processes by which hormones influence plant architecture under adverse growing conditions. We know that nutrient and water stress causes plants to accumulate signalling molecules that retard growth and put the plant into ‘survival mode’. This negatively impacts on seed development in cereal crops, the number of seed pods is reduced and the grains do not fully develop. The outcomes are reduced yields and significant devaluation of the harvested grain, which has major financial impacts on the growers, the industry, and the Australian economy. Recently it was shown that the application of strigolactones can inhibit the accumulation of these ‘stress response’ signalling molecules, which results in continued growth under adverse conditions. Using our fluorescent molecule, we can watch what happens inside the plant to stop the stress response. Harnessing this technology for cereal crops would increase crop yields without increasing water and fertiliser inputs.

Organic synthesis sounds a million miles removed from food security, but tomorrow’s food supply is reliant on our ability to build molecules that promote plant growth. My team of dedicated researchers is making great strides to achieve that goal.

Associate Professor Chris McErlean MRACI CChem is in the School of Chemistry at the University of Sydney. This article reused with permission.

Oxygen in red winemaking

There are many options for the fermentation of red wine, ranging from the traditional open fermenter to various stainless steel enclosed fermenters. A&G Engineering, with its home base in Griffith, describes most options available with stainless steel (bit.ly/2lpsmDa). My introduction to winemaking was at Fairfield Winery in Rutherglen where there was in excess of 20 wax-lined concrete open fermenters, and I still retain an attachment to this approach to red wine fermentation. One perceived limitation of open fermenters is the loss of aroma compounds, especially those associated with red fruits: these characters have particular market significance for Australian wine. So closed systems such as rotary fermenters became all the rage.

But nothing is straightforward. Rotary fermenters, as with other closed fermenters, limit or even stop oxygen access during the fermentation and this can lead to the formation of volatile sulfur compounds (VSCs; see April issue, p. 39) that detract from the sought-after fresh fruit aromas. While there are strategies to try and introduce oxygen into the ferment, there has not been a detailed study on a close-to-commercial scale that examines when to add oxygen, how much oxygen may be needed and whether Cu^{2+} additions are sufficient to eliminate the sulfidic off-odours from the VSCs. This is where the chemistry group at the Australian Wine Research Institute comes to the forefront.

In a 2015 review entitled 'Use and impact of oxygen in winemaking', the AWRI chemistry group examined the potential input of oxygen from harvest to the finished wine in relation to chemical composition (Day et al. *Aust. J. Grape Wine Res.* vol. 21, pp. 693–704). While it is clear that too much oxygen can lead to oxidative and microbiological spoilage (for example, Brett character; see September 2014 issue, p. 39), it is now becoming more apparent that targeted amounts of oxygen at specific winemaking points may be beneficial.

The improvement in instrumentation for the reliable measurement of dissolved oxygen (DO) has been a major advantage in allowing winemakers to interpret the link between specific or tailored amounts of oxygen and changes in chemical composition. In particular, the AWRI review refers to oxoluminescent sensors that can be attached to the inside of a wine bottle or into the sight glass on the side of a fermenter or tank. This allows direct in-situ monitoring of DO during fermentation, ageing and bottle development. All this is a far cry from the Clark electrode that I grew up with in my early days of measuring DO in water and trying to use it in wine.

The Day et al. review highlights several studies that need to be performed to increase our knowledge base. One that the authors mention would be to examine the chemical and sensory impacts resulting from the introduction of oxygen into an active fermentation. The AWRI group has followed up the review



Dr Martin Day, AWRI

suggestion and recently published research describing the effect of oxygen treatment during fermentation on the production of the pesky VSCs.

The research utilised the rotary fermenters (see photo) available in the Hickinbotham Roseworthy Wine Science Laboratory at the University of Adelaide (bit.ly/2m00Iyw). Shiraz must was fermented in the rotary fermenters, with each treatment of 730 kilograms of grapes being carried out in triplicate. A control was established by sparging the ferment with nitrogen, with separate samples having Cu^{2+} additions, either early or late in the ferment. Oxygenated ferments were sparged with either 40% oxygen or air. The samples were analysed for VSCs and for fermentation products that contribute to the fruity aroma at two months and again at 12 months after bottling. Sensory analysis for both aroma and palate descriptors was also performed. The results clearly showed the importance of oxygen treatment in reducing VSCs, and the authors developed a relationship between oxygen dose and VSC formation, at least for those VSCs that react with oxygen. Oxygen treatment also improved the aroma profile in terms of enhancing the sensory perception of some characters associated with red fruit aromas. In the non-oxygenated ferments, early Cu^{2+} addition reduced the VSCs.

This work is published in the *Australian Journal of Grape and Wine Research* (2016, vol. 21, pp. 24–35). It is an intensive paper describing a very large study of great significance to the wine industry. The paper, authored by Marilize Bekker, Martin Day, Helen Holt, Eric Wilkes and Paul Smith, was awarded the 2016 best oenology paper award of the Australian Society of Viticulture and Oenology (bit.ly/2l215L8), a richly deserved award. Eric and Paul are members of the RACI and Martin retains his membership of the RSC, all of which goes to show that a background in fundamental chemistry leads to an exciting career in oenological science.



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

The mathematics problem

'I signed up for chemistry, not mathematics' is a common complaint among chemistry students, especially at first-year undergraduate level, but also at senior secondary level and TAFE. Chemistry teachers and educators have observed that today's students have less confidence to handle numerical calculations than their counterparts 20 years ago.

There are several reasons for this. First, a smaller proportion of students are studying mathematics at senior secondary level, and of those students, many are choosing to study 'lower-level' mathematics in the perception that this will result in a higher Australian Tertiary Admissions Ranking (ATAR).

Word problems are the most difficult part of the mathematics curriculum for most students. Regular exercises just ask for some mathematical manipulation, like rearranging an equation, devoid of context. In a word problem, students are presented with a textual description of a scenario. They need to be able to understand and analyse the words to extract the inherent mathematical processes that are involved by translating the words into mathematical relationships. Next, they need to solve the mathematical problem. And finally, they have to translate the mathematical answer back into a word-based answer. This process involves both higher-order thinking skills and mathematical understanding. Every numerical problem or issue in chemistry is equivalent to a word problem in the mathematics curriculum.

Another issue is that numerical questions in chemistry look scarier than equivalent questions in mathematics. For example, a difficult quadratic relationship in a senior secondary mathematics textbook might look like:

$$x^2 + 8x + 13 = 0$$

In contrast, a quadratic relationship in a chemistry textbook might look like:

$$K_a = \frac{[\text{H}_3\text{O}^+][\text{CH}_3\text{CO}_2^-]}{[\text{CH}_3\text{COOH}]} = \frac{(x)(x)}{(0.500 - x)} = 1.8 \times 10^{-5}$$

where $K_a = 1.8 \times 10^{-5}$ is the equilibrium coefficient, 0.500 mol L^{-1} is the initial acetic acid concentration, and x is the numerical value of the final hydronium and acetate concentrations. On rearrangement, this gives the quadratic relationship:

$$x^2 + 1.8 \times 10^{-5}x - 0.9 \times 10^{-5} = 0$$

The quadratic relationship becomes more complicated if there are non-zero initial hydronium and acetate concentrations. Mathematically, the chemistry quadratic relationship is equivalent to the mathematics example, just with different coefficients. With the easy availability of graphics and programmable scientific calculators, these two examples are of the same level of difficulty and both can be solved merely by identifying the coefficients, entering them into the calculator and processing the SOLVE button. The chemistry quadratic relationship looks scary because the coefficients can differ by

several orders of magnitude. This pushes students who might lack confidence into the zone of denial: 'It is too hard, I cannot do it'. Their perception becomes their reality: they cannot do it.

The same is true of graph scales and other representations in chemistry. A mole consists of an unimaginably large number (6.022×10^{23}) of particles, while the size of an atom is extremely small (10^{-10} m). Practising chemists take these numbers for granted, but a novice chemistry learner finds them to be huge obstacles to learning.

The easy availability of smartphones that can do almost everything also contributes to the problem of weak maths skills. It is common to see undergraduate students using smartphones to do numerical calculations in tutorials, seminars, workshops and laboratories. When they come to the examination, they are unpractised in the use of their calculators. Credit and debit cards mean that customers do not practise the ability to quickly estimate if the cash in their wallet is sufficient to pay for their groceries.

Universities have also contributed to this mathematics problem. Most do not require *any* year 12 mathematics as a prerequisite for science degrees. Hence, many university science students, including university chemistry students, have had a minimum of two years without any formal mathematics study. Recently, some undergraduate students said that they had never seen scientific notation (e.g. 1.8×10^{-5}) before, even though scientific notation has been a standard part of the year 8 or year 9 mathematics curriculum for decades. Skills and knowledge become weaker or forgotten through the passage of time unless constant use maintains currency of knowledge. The only part of the senior mathematics syllabus that is used in first-year chemistry at my institution is logarithms. The content knowledge and skills are easily taught. However, the two-year (or more) lack of practice, familiarity and confidence with mathematical skills is harder to remedy, but not insurmountable.

The mathematics problem is not lack of knowledge and skill. The problem is a pessimistic attitude associated with lack of confidence. Yet judgement of proportionality (how much condiment is needed for that recipe) and other mathematical ability is excellent in most students. As educators, we need to help students to recognise the mathematics skills that they do have. Encouraging them to study more senior school mathematics would also help.



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Polarography comes and goes

As the preparation of the Institute's centenary history got under way, it soon became clear that there was far more interesting (interesting to me, anyway) material than could be fitted into the proposed volume. So I'm starting this Letter with the story of a one-day conference on polarography that was held in the chemistry department of the University of Sydney in June 1950. It attracted about a hundred people from industry, CSIRO and academic institutions.

The earliest form of polarography was direct-current polarography, which I knew had been applied to the determinations of heavy metals at very low concentrations by means of the dropping mercury electrode. The unusual electrode system continued to be the basis of the technique, but by 1950 there had been developments in the electronics. Refinements to DC instruments of the type invented by Heyrovsky were described at the conference by H.A. McKenzie (CSIRO Food Preservation Research Laboratory) and A. Millership (Davis Gelatine) while work with the alternating-current technique was presented by S. Hacopian (University of Sydney, Agriculture Department).

There was nothing about heavy metals and instead the experimental papers at the Sydney meeting concentrated on reducible organic substances such as coumarins, benzophenones and azo-proteins. The name of this last group of substances should have been self-explanatory but I had to look up azo-proteins to find that they were proteins that had been modified by attacking them with diazonium salts. The azo linkages so formed are with the tyrosine (phenolic) side chains and they formed points of attachment for dye moieties or ligands for the generation of immune responses. In a more theoretical paper, Lawrie Lyons drew attention to reduction potentials of a range of aromatic hydrocarbons and their calculated electron affinities.

The polarographers gathered again in June 1954 for a two-day meeting in Melbourne where a greater range of topics was presented. Most of the 18 papers (contrast to eight at the Sydney meeting) again dealt with organics, but there were also analytical results for microgram quantities of trace metals in natural products, and calcium in milk and in serum. McKenzie read a paper on the reduction of nitrate ion that had been contributed by J.W. Collat and J.J. Lingane of the Coolidge Memorial Laboratory at Harvard University. All of the authors were from universities or CSIRO, with the exception of W.P. Georgans (BALM Paints, Cabarita, NSW) who described analyses for cobalt (hardening catalyst) and lead in paints, and also pigments and other raw materials characteristic of the industry.

At the conclusion of this second conference, the chairman, Professor D.P. Craig (University of Sydney), said that the keen interest in electrochemistry, and particularly in polarography, suggested that a society should be formed to promote further research work and that a further conference should be held in

about two years' time in Melbourne under the wider title Conference of Electrochemistry.

Accordingly, the next development in the field was a Discussion Meeting on Electrochemistry held at the University of Melbourne in 1956. Polarography results were presented in two of the three sessions but there was strong interest also in electrode processes more generally and the behaviour of ions in solution. This last topic brought to the lectern Dr Michael Spiro, who spoke about transfer numbers of weak electrolytes, a subject that was something of a specialty for the Melbourne department, as I recall from lectures by Spiro and others.

The unusual electrode system continued to be the basis of the technique, but by 1950 there had been developments in the electronics.

The lecturers at the electrochemistry conference were, again, mostly from CSIRO and the universities, with just a sprinkling of industrial chemists. I was struck by some of Australian chemistry's 'big names' – R.H. Stokes (diffusion in concentrated electrolytes), D.O. Jordan (polyelectrolytes) and someone from my ANU past, J.H. Bradbury (dead-stop titrations).

There were other conferences of this type, I believe, but it was nearly a decade before the Electrochemistry Division was formed in 1965, at about the same as Chemical Education and Heterocyclic Chemistry (later subsumed into Organic). By then, the polarograph was a relic of earlier days, its metal work taken over by atomic absorption spectroscopy while cyclic voltammetry and other modern techniques got the rest. Thus removing the need to clean up all that dirty mercury.

Another name from the 1956 meeting to catch my eye was that of Henry Bauer, who spoke about electrode processes in organic polarography. He left Australia (and electrochemistry) soon after to make his career in America where he achieved a sort of fame as a climate sceptic and general denialist. He was the author of *Scientific literacy and the myth of the scientific method* (1992) and (writing as Josef Martin) of an entertaining book about university life, entitled *To rise above principle. The memoirs of an unreconstructed dean* (1988).



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.

11th New Diamond and Nano Carbons Conference

28 May – 1 June 2017, Cairns, Qld

www.ndnc2017.org

3rd International Conference on Organic and Inorganic Chemistry

17–19 July 2017, Chicago, Illinois, USA

<http://organicchemistry.conferenceseries.com>

Vic Branch Centenary Gala Dinner and Ball

22 July 2017, Plaza Ballroom, Melbourne, Vic.

<https://icmsaust.eventsair.com/raci2017/centenary-gala-dinner/ Site/ Register>

6th Modern Solid Phase Peptide Synthesis and its Applications Symposium

12–14 October 2017, Fraser Island, Qld

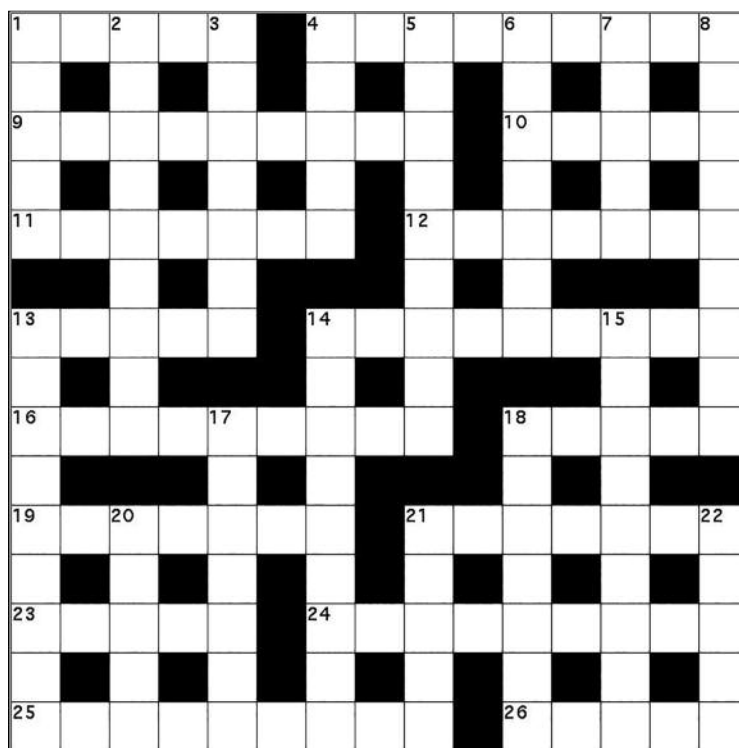
www.solidphase.org

International Conference and Exhibition on Pharmaceutical Nanotechnology

27–29 October 2017, Rome, Italy

<http://nanotechnology.pharmaceuticalconferences.com>

RACI events are shown in blue.



Across

- 1 Appropriate privilege. (5)
- 4 Theft of iridium bred justice newly under control. (9)
- 9 Layabout in something done to add RCO-. (9)
- 10 Crowd push. (5)
- 11 Trucking companies carrying sulfur, aluminium, erbium, hydrogen and uranium! (7)
- 12 Swear and get old and mean. (7)
- 13 Checks bags. (5)
- 14 215316148716 cleavages. (9)
- 16 Put back together cerium/bromine compound. (9)
- 18 Second wet fly. (5)
- 19 Hold back! Don't panic it's aleurone yielding. (7)
- 21 Units 91, 21, 13 and 16. (7)
- 23 HN= discovered in *Weilheim in Oberebayern*. (5)
- 24 Vague little devil! Adding about 65334! (9)
- 25 Roof lifted: four kilograms made into lactose. (4,5)
- 26 Sulfur on argon to measure position under water. (5)

Down

- 1 Get through to land. (5)
- 2 Well known for his work on alcohol-water mixtures from saucy gals. (3-6)
- 3 Sets forth Laser TV revolution. (7)
- 4 Sulfur fixes turns. (5)
- 5 $C_6H_5CONH_2$ vehicle aimed astray. (9)
- 6 Fast flame iron. (7)
- 7 $\theta = 90^\circ$. (5)
- 8 Broken up Reds spied on organisation. (9)
- 13 $RR'R^+C$ to mar Ni cube reorganisation. (9)
- 14 Irritation in volte-face redirection. (9)
- 15 Cutting concern. (9)
- 17 Those chances by Spooner strategies. (7)
- 18 17 Down messy set reacted losing an electron. (7)
- 20 Central to a test team using aluminium. (5)
- 21 Daily report. (5)
- 22 Second pick up is trim. (5)

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

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Medicinal Chemistry



Carbon 2017

World Conference on
Carbon



Chemeca 2017

Australian and New
Zealand Federation of
Chemical Engineers
Annual Conference



GSC8

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Conference on Green and
Sustainable Chemistry



Tetrahedron

18th Asian Edition
Tetrahedron Symposium

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