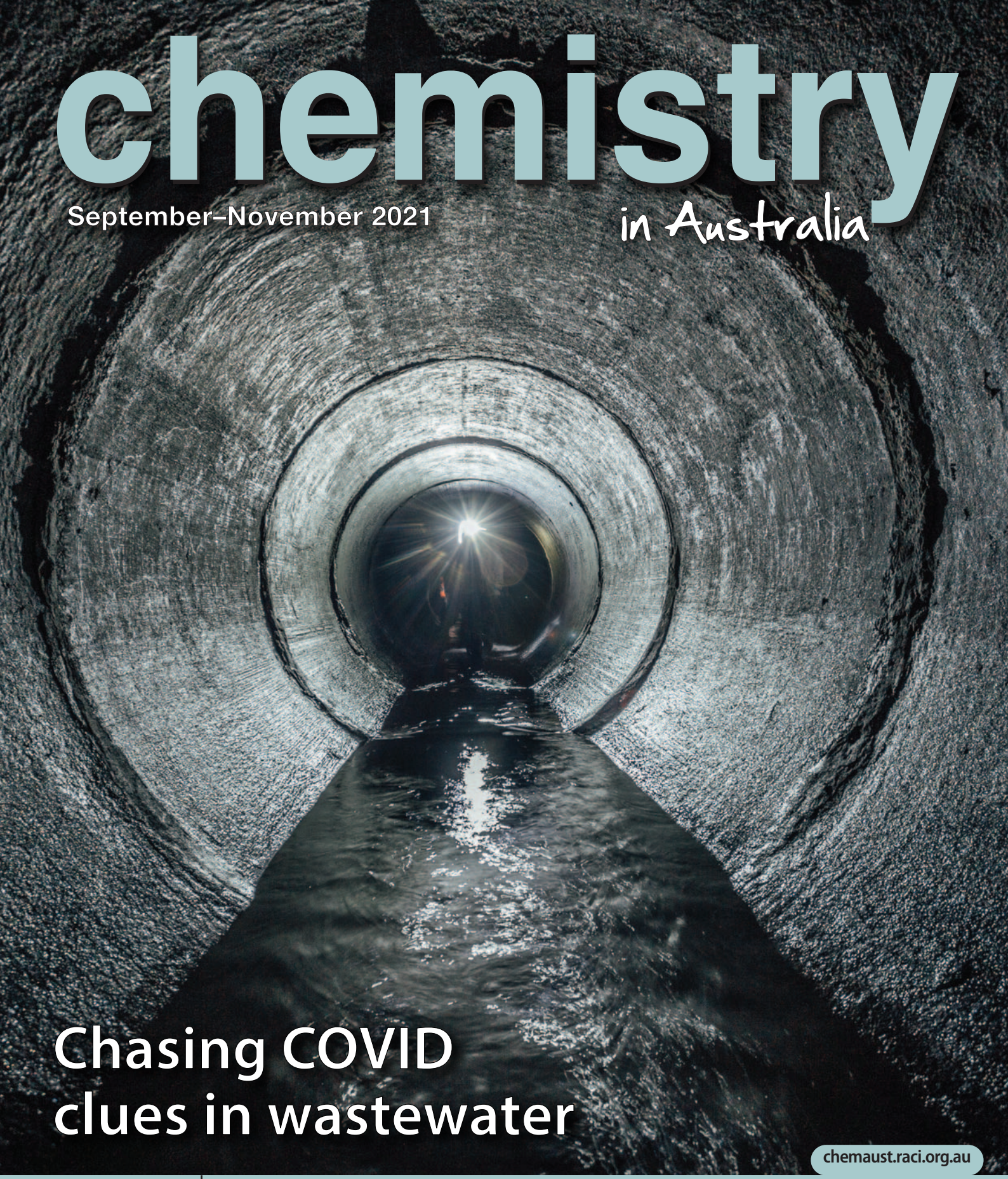
# chemistry in Australia

September–November 2021



## Chasing COVID clues in wastewater

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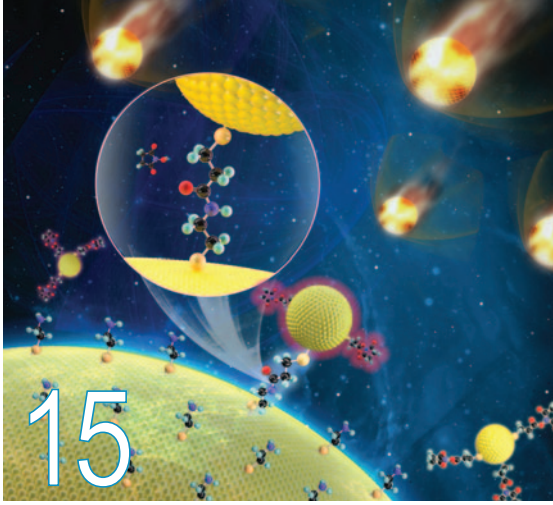


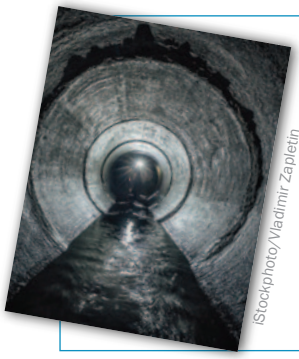
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## cover story

### Collaborating against COVID

Scientists worldwide have stepped up to challenges posed by COVID-19. In Australia, water researchers have a critical surveillance role: detection of viral fragments in wastewater.

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# Communication in a time of COVID

Science communication is facing one of its biggest challenges. As I write, New South Wales is in lockdown, and several other states are moving into or out of restrictions. In Japan, Olympic athletes have been competing in almost-empty stadiums.

Fragments of COVID-19 have been detected in wastewater in many regions, including the Northern Rivers region in New South Wales, which includes tourist hotspots such as Byron Bay. Health authorities are particularly concerned about detecting the virus in certain parts of that region because rates of childhood vaccination are low, vaccine-hesitancy and anti-vaccination sentiment have been historically high, and regional areas have limited health resources.

Understandably, the public have many questions about wastewater detections – why are there fragments in the water, are the fragments harmful and what do they tell us about when infectious people have been in a community? On page 19, Dave Sammut and Chantelle Craig discuss Water Research Australia's sewage surveillance project, ColoSSoS, and the important work of the scientists who develop testing methods, and who test and analyse COVID fragments in wastewater.

People I know who are vaccine hesitant or opposed to the COVID vaccine no longer watch mainstream news – or any news – because they mistrust it or find it overwhelming. A vaccine-hesitant friend asked me if mRNA vaccines could affect DNA. Although I knew the answer, it was a challenge to explain this in an accessible way. I sent her a link to a Q&A explanation of the science, without any alarming pandemic context. I hope I was able to reassure my friend without bamboozling or alienating her, but it reminded me of how different people's perspectives and understandings can be.

Earlier this year I moved from Victoria, where the communication about COVID at daily press conferences was largely comprehensive, clear, carefully worded and consistent, to New South Wales, where it can be repetitive, long-winded, often ambiguous and sometimes incomprehensible. Journalists here sometimes struggle to convey the press conference messages to an English-speaking readership, so I can only imagine the difficulties of trying to relay information in Auslan and/or to people with culturally and linguistically diverse backgrounds. Making things worse are those journalists who distort or misinterpret data (unintentionally or otherwise). Even scientifically literate people might need to brush up on terms such as *efficacy*, *efficiency* and *relative risk* (ab.co/37l0UjC), and be alert to the context (such as disease severity and infectivity, subpopulations, type of vaccine and type of virus strain) and the statistics (identifying skewed data, or small or unrepresentative samples), and to plain old pseudoscience.

Professor Brian Oliver leads the Respiratory Molecular Pathogenesis Group at the University of Technology Sydney and the Woolcock Institute. In a recent news release from the Australian Science Media Centre, he said that confusion relating to the Delta strain of COVID-19 is largely due to people associating data from one area with another context, using old data, misquoting other people or not understanding a data source (e.g. whether it was a clinical trial or a real-world population).

I have begun an online course developed by American graphics guru Edward Tufte about analysing and presenting information. In the presentation and the five books that accompany it, Tufte is quick to make the point that, just like language, graphics can be abused, through intention or ignorance.

In his book *Visual explanations*, Tufte describes the 'cognitive paradise of explanation, a sparkling and exuberant world, intensely relevant to the design of information'. This is clearly Tufte's true love, and he has transformed thinking about graphic presentation in many organisations, with clients having included IBM, Bose and NASA.

Phill Jones writes in The Scholarly Kitchen blog about the effects of a 'mangled press conference on COVID' in the UK, stressing the need for 'good data storytelling' (bit.ly/3x1SXKT). He gives an example of some particularly confusing PowerPoint slides as part of a government COVID briefing, saying the biggest crimes weren't the poor layout or legibility, but 'that nobody had taken the time to understand all the different sources of data and synthesize them into a coherent story'. He refers to *Visual representations*, where Tufte posits that the disastrous outcome of the 1986 *Challenger* launch may have been avoided if data relating to O-ring damage had been presented in graphic form and in context. (For more about this, see data visualisation designer Luuk van der Meer's blog post at bit.ly/2TwBPit.)

There's no denying that science communication can be difficult at the best of times. The COVID crisis underscores that we must continue to train scientists in public-facing roles in science communication, and to offer quality courses in science journalism.

The Australian Bureau of Statistics says that this year's census will mine valuable data about the impacts of COVID in Australia. I wonder if the ABS has considered seeking out the masterful and magical talents of Tufte?

**Sally Woollett**
(editor@raci.org.au)

## Plastics' Frontiers: spread the word

The RACI Industrial Division is to be commended in presenting its webinar series 'Plastics' Frontiers'. Given that the subject of plastics is one that has generated a great deal of heat and very little light in the public and political arenas, it is indeed timely that such a detailed discussion should take place. My concern is that the information being imparted during the webinar episodes may not reach the widest possible audience, and I am not sure if the webinar format is entirely suitable in such a role.

My limited experience with webinars is that they can be an ephemeral experience. Frequently, there is no post-webinar material available for either later viewing or reading. Further, it could be argued that the two-hour sessions in an after-dinner evening time slot may be a disincentive to people otherwise interested in the subject matter. The material being presented is too important to fade in the memories of the relative few who will view the episodes. If it has not been thought of already, I would like to propose that the presenters of the episodes consider preparing companion articles that could be published in *Chemistry in Australia*. I would also suggest that these articles could be collated in the form of a white paper, which could be published and made available to science educators, science journalists and scientific advisors to governments. I would be happy to purchase such a document. The most important points could be summarised and published as press releases, to ensure that information is properly presented and to minimise chances of misrepresentation.

I can understand the reluctance of the RACI to get drawn into the public political arena, but the subject of plastics is one of great importance to our society. It is inconceivable that our society can do without products in which plastics are used. At present, anti-plastics activists, who may have other motives, are dominating the public media space. The opportunity to present a balanced, unbiased appreciation of plastics in society should not be missed.

**Tom Smith** FRACI CChem

## 'Your say' guidelines

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

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**EDITOR**
Sally Woollett
Ph 0406 321 312
wools@westnet.com.au

**PRODUCTION EDITOR**
Catherine Greenwood
catherine.greenwood@bigpond.com

**ADVERTISING SALES**
Mary Pappa
Ph/fax (03) 9328 2033/2670
mary.pappa@raci.org.au

**PRODUCTION**
Control Publishing
publishing@control.com.au
www.control.com.au

**BOOK REVIEWS**
Damien Blackwell
damo34@internode.on.net

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

**EDUCATION RESEARCH HIGHLIGHTS**
Reyne Pullen
reyne.pullen@sydney.edu.au

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

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# New chief scientist for CSIRO

Professor Bronwyn Fox FRACI CChem has been appointed as CSIRO's Chief Scientist, close to 30 years after she began her career with CSIRO as a research assistant.

Fox, CSIRO's fourth female Chief Scientist, joins the agency from Swinburne University of Technology, where she is Deputy Vice-Chancellor (Research and Enterprise).

CSIRO Chief Executive Dr Larry Marshall said Fox brings great depth of scientific experience to the role.

'Bronwyn exemplifies the CSIRO way – driven to deliver, brilliant but humble, leading by listening, and a generous collaborator', Marshall said.

'She has a long history of bringing together researchers from across multiple scientific domains and institutions, leveraging digital science, and helping industry to translate brilliant ideas into real-world solutions.

'Her sustained commitment to supporting the growth of the manufacturing industry in Australia strongly supports our purpose to deliver solutions from science that drive Australia's economic recovery and resilience.'

As a materials and engineering scientist, Fox was the founding Director of Swinburne's Manufacturing Futures Research Institute, with a mission to support the transition of Australia's manufacturing sector to Industry 4.0 – the fourth industrial revolution.

Fox said she had worked with CSIRO scientists for close to 30 years.

'It is wonderful to return to CSIRO as Chief Scientist after starting as a 22-year-old research assistant, and to be able to champion science research and capability, working with industry and fostering STEM careers', Fox said.

'The depth of scientific research at CSIRO and its committed people are a unique and special national treasure and I look forward to taking up the role.'

Fox is Chair of the Australian Academy of Technology and Engineering (Victorian Division), a Fellow of the Academy of Technological Sciences and Engineering, and a graduate of the Australian Institute of Company Directors.

CSIRO

Professor Bronwyn Fox

# Sunscreen recalled over benzene concerns

The Therapeutic Goods Administration (TGA) has announced that Johnson & Johnson Pacific is recalling all batches of Neutrogena Ultra Sheer Body Mist Sunscreen Spray SPF 50+, AUST L 202301, after benzene was detected in some batches. Benzene is classified as a human carcinogen, a substance that could potentially cause cancer depending on the level and extent of exposure. Benzene is not an ingredient in this product but is sometimes used in medicine manufacturing processes. Exposure to benzene in this sunscreen product, at the levels detected, would not be expected to cause serious adverse health effects, according to the TGA.

The TGA has limits on these types of solvents, and benzene must be below a concentration of 2 ppm in medicines. This includes sunscreen products that are listed medicines in Australia.

Johnson & Johnson Consumer Inc product testing detected benzene at concentrations less than 3 ppm in two of the 17 batches supplied in Australia. Johnson & Johnson Pacific is recalling all batches of the affected product supplied within Australia. All batches with an expiry date of 30 August 2023 or earlier should not be used due to possible health risks linked to benzene. Consumers should discard the products and visit www.neutrogena.com.au to request a refund. All unsold product will be removed from the market.

People with any concerns or questions about this issue are advised to speak to a health professional or contact the Johnson & Johnson Pacific Pty Ltd Consumer Care Centre on 1800 789 348.

Consumers and health professionals are encouraged to report problems with medicines or vaccines to www.tga.gov.au/reporting-problems. These reports contribute to TGA's monitoring of these products.

Australian Government Department of Health

# COVID-19 lockdown highlights ozone chemistry in China

In early 2020, daily life in Northern China came to a sudden halt as the region entered a strict period of lockdown to slow the spread of COVID-19. Emissions from transportation and industry plummeted. Emissions of nitrogen oxides ($NO_x$) from fossil fuels fell by 60–70%.

And yet, environmental researchers noticed that ground-level ozone pollution in Beijing and the Northern China Plain dramatically increased during this period, despite the decrease of $NO_x$, a component of ozone.

The region is no stranger to severe ozone pollution but until about five years ago, most ozone events occurred during the summer. Recently, the ozone season in China has been getting longer, spreading into early spring and late winter. As it turns out, the COVID-19 lockdown can help explain why.

Researchers from the Harvard John A. Paulson School of Engineering and Applied Sciences (SEAS) and the Nanjing University of Information Science & Technology (NUIST) have found that another component of ozone, volatile organic compounds (VOCs), may be to blame for the increase in winter ozone.

The research is published in the *Proceedings of the National Academy of Sciences* (doi.org/10.1073/pnas.2015797118).

Ozone is formed through a series of chemical reactions, starting with the oxidation of VOCs. This reaction forms chemical radicals, which drive reactions between $NO_x$ and VOCs to produce ozone in the presence of sunlight. In a previous study, researchers from SEAS and NUIST found that in the summer, particulate matter (PM2.5) acts like a sponge for the radicals needed to generate ozone pollution, sucking them up and preventing them from producing ozone.

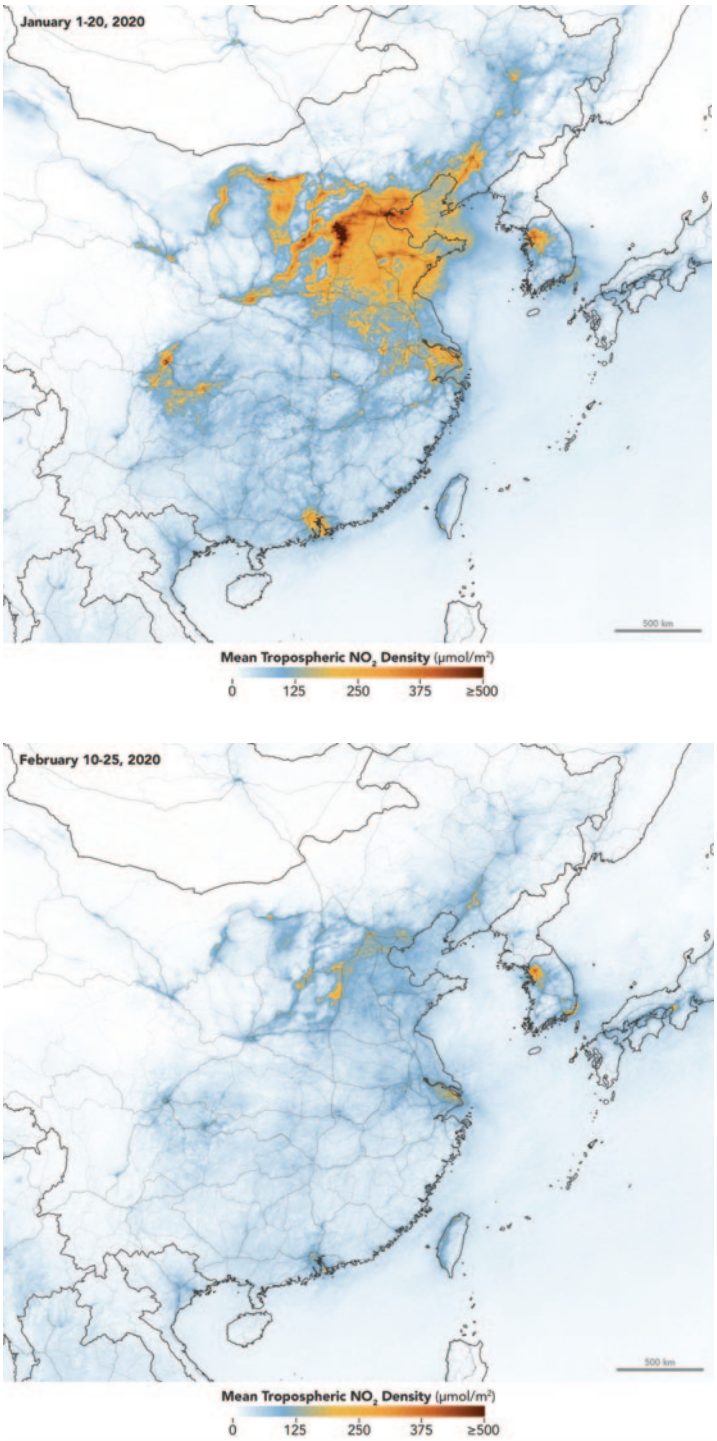
In that paper, the researchers found that air pollution policies instituted by the Chinese government that reduced PM2.5 were causing an increase in harmful ground-level ozone pollution, especially in large cities.

In this research, the team found that $NO_x$ plays a similar role during winter, scavenging radicals and preventing them from forming ozone. As $NO_x$ levels decrease, either suddenly with lockdown or gradually with air pollution controls, more radicals are available for VOCs to react with. This enhanced oxidation of VOCs by radicals would amplify by producing more radicals themselves, and this process optimises the ozone production efficiency of $NO_x$.

The research highlights the need to better understand the sources and species of VOCs and regulate their emissions.

'VOC emission controls would stop the spread of the ozone season and have major benefits on public health, crop production, and particulate pollution,' said Hong Liao, Professor at NUIST and co-corresponding author of this work.

Harvard John A. Paulson School of Engineering and Applied Sciences




**$NO_2$ values across China 1–20 January 2020 (before the quarantine) and 10–25 February (during the quarantine). The data was collected by the Tropospheric Monitoring Instrument on ESA's Sentinel-5 satellite.** NASA

# Microalgae identified as clean source of hydrogen

**Microalgae cultures in the CSIRO Microalgae Collection laboratory.** CSIRO/CC BY 3.0

A new method of producing hydrogen and methane from renewable sources, namely microalgae, has been uncovered by researchers at Monash University, IITB-Monash Research Academy Mumbai, and The Indian Institute of Technology Bombay.

Using reactive flash volatilisation (RFV), the researchers have found that the greenhouse gas emissions from hydrogen production by microalgae is 36% less than from the steam reforming of methane – the current best practice for hydrogen production. RFV is a gasification process that uses oxygen and steam to convert biomass or fossil fuel-based carbon materials into gases.

With additional renewable energy processes, such as hydro-electricity, integrated with the researchers' hydrogen production process, carbon emissions could drop by as much as 87%.

The research, published in the *Journal of Cleaner Production* (doi.org/10.1016/j.jclepro.2020.123726), also shows that with the prevailing cost of hydrogen at $10/kg, by using RFV, the payback period of initial investment was just 3.78 years with a 22% internal rate of return.

Currently, the production of microalgae does not meet commercial demand. However, microalgae cultivation for energy applications could also provide additional revenue streams for rural communities, potentially making them self-sufficient, researchers say.

'Hydrogen and methane are clean sources of fuel and green chemical synthesis only if they are produced from renewable resources. At present, 96% of hydrogen and all methane is produced using non-renewable resources', said Associate Professor Akshat Tanksale from Monash University and research co-author said.

'Microalgae as a feedstock is attractive due to its high carbon dioxide fixation efficiency, growth rate, photosynthetic efficiency, ability to grow in brackish water – like rivers and lakes – and the ability to cultivate it on land not suitable for agriculture.

'Water and renewable electricity integration with microalgae harvesting can bring down the costs and increase the sustainability of hydrogen production from this process.'

Dr Yogendra Shastri from the Department of Chemical Engineering at IITB-Monash Research Academy Mumbai said climate change concerns have led to an increasing push for cleaner energy options, and microalgae could be a potential candidate to produce renewable fuel.

'Hydrogen is acknowledged as clean fuel since it doesn't lead to the emission of greenhouse gases when used. However, the production of hydrogen also needs to be sustainable,' Dr Shastri said.

'Biodiesel production from microalgae is limited due to low lipid extraction efficiency, less than 20%, and the high cost of microalgae harvesting and drying.

'Furthermore, microalgae-based hydrogen and methane production haven't yet been commercialised due to expensive pre-treatment, such as harvesting, drying and lipid extraction; low carbon conversion efficiency; and tar accumulation.'

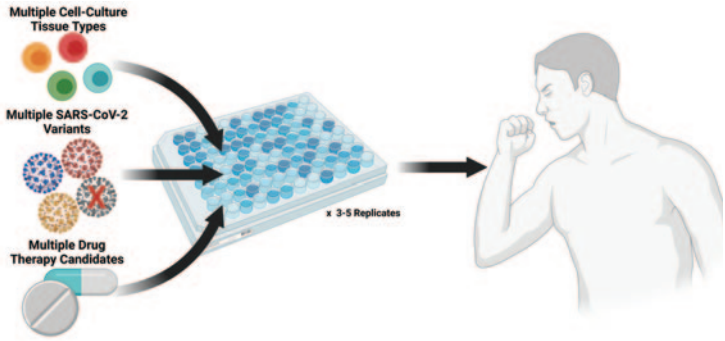
Researchers performed the RFV of microalgae at 550–650°C, using steam as the gasifying agent. This meant dewatering or drying of microalgae was not required and significantly reduced energy consumption.

Using India-based JSW Steel as a case study for their source of $CO_2$ for microalgae cultivation, the research team estimated that just under 12 800 kg/h of microalgae would be available for hydrogen production at a rate of 1240 kg/h.

Although it is expensive to develop infrastructure to cultivate microalgae and then refine it into hydrogen and methane, the overall return on investment in the long term could make hydrogen and methane cost-effective and environmentally friendly fuel sources.

Monash University

# New funding to fast-track COVID-19 treatments




Scientists will develop a faster, smarter way of rapidly screening existing drugs and advancing those that can be used to treat COVID-19 and aim to have identified three suitable TGA- or FDA-approved drug candidates to progress to phase 2–3 human clinical trials within a year.

Led by researchers at CSIRO's Australian Centre for Disease Preparedness in Geelong, the project received $1 million in funding from the Australian Government's Medical Research Future Fund (MRFF), with the remaining contributed by CSIRO.

CSIRO scientist and project leader Dr S.S. Vasan said in addition to vaccines, there was an urgent need for safe, effective and affordable COVID-19 treatments that specifically targeted the virus.

'A great strategy to find potential COVID-19 treatments is to repurpose drugs already approved for other diseases, but the current methods to do this are expensive, time-consuming and not fit for purpose', Vasan said.

'The MRFF funding will enable us to develop a multi-tissue drug screening tool, tailored for infections by SARS-CoV-2 and all its variants of concern, which could help fast track drugs for phase 2–3 human clinical trials and minimise the need for animal trials.'

The scientists will use four types of clinically relevant human tissues – lower respiratory tract, lung, neural and cardiac tissues – specifically selected based on how SARS-CoV-2 infects people.

Barwon Health's Director of Infectious Diseases and project collaborator Professor Eugene Athan said the lower respiratory tract and lung models are appropriate because they play a key role in severe infections.

'The neural and cardiac tissues are highly relevant because this disease is now known to cause neurologic disorders, heart dysfunction and damage in some patients', Athan said.

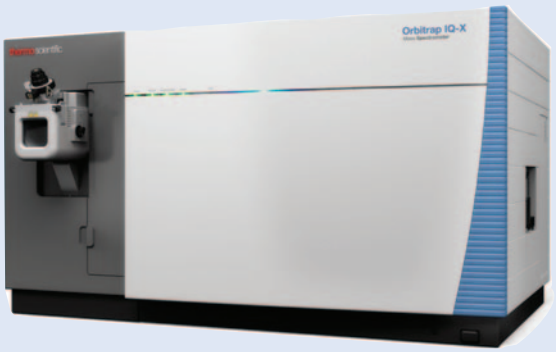
The scientists will use novel systems biology (a biomedical approach to understand the bigger picture) and machine-learning methods to differentiate between healthy and diseased states of key human tissues, which will enable additional ways to determine if a drug is able to reliably restore a diseased tissue to a healthier state.

CSIRO

# New mass spectrometer from Thermo Fisher

The new Thermo Scientific Orbitrap IQ-X Tribrid mass spectrometer is designed specifically for small-molecule structural elucidation of metabolites and unknown compounds.

With this new, intelligent mass spectrometer, small-molecule researchers can now reveal complex chemical structures with confidence, ease and experimental versatility. The wide range of applications includes metabolomics and lipidomics research, leachable/extractable impurities identification and forensic toxicology.




**Enhanced: Differential ion mobility interface for higher productivity and data quality.** The Thermo Scientific FAIMS Pro Duo interface builds upon the foundation of the Thermo Scientific FAIMS Pro interface to support biological mass spectrometry and extend differential ion mobility to a broader range of applications, including proteomics, plasma profiling and targeted small-molecule quantitation. The differential ion mobility interface increases productivity and data quality for qualitative and quantitative workflows.

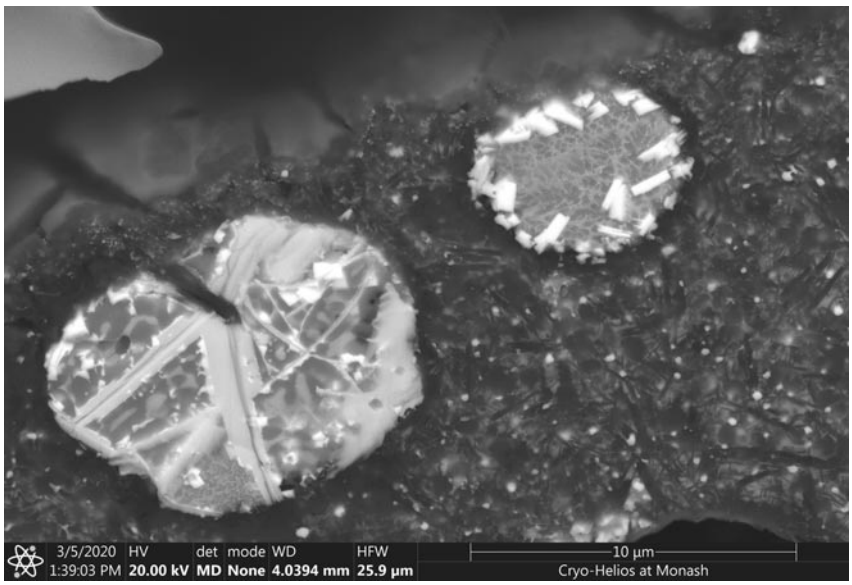
The FAIMS Pro Duo interface easily integrates with Thermo Fisher's next-generation mass spectrometers, including the Thermo Scientific Orbitrap Tribrid, Thermo Scientific Orbitrap Exploris, Thermo Scientific TSQ Altis triple quadrupole, and Thermo Scientific TSQ Quantis triple quadrupole mass spectrometers.

**Enhanced: Gas chromatography headspace autosampler.** The Thermo Scientific TriPlus 500 Headspace Autosampler is now available with a new version featuring an external transfer line that can be connected to the GC inlet, supporting those analytical set-ups where a direct column connection is not possible. A relevant example is the analysis of dissolved gases in transformer oil according to the method ASTM D-3612C, which implies the connection of the headspace autosampler to a transformer oil gas analyser.

For any testing laboratory conducting volatiles analysis, static headspace-gas chromatography, with its simplicity and broad applicability, is one of the most reliable and robust techniques. The headspace autosampler is popular within analytical testing and QA/QC laboratories in pharma, forensic, food packaging and environmental fields.

To speak to a sales specialist about these products, please email us at CMD.APACMARKETING@thermofisher.com.

# Radioactive particles from British nuclear testing still in outback Australia




**Electron microscopy image of a complex hot particle from Maralinga, consisting of two quenched polymetallic melts. The dark areas correspond to an Fe–Al rich melt, and the lighter 'globules' are an immiscible melt rich in Pu–U–C with varying amounts of Fe–Al (accounting for the different grey shades).**

More than 100 kg of highly toxic uranium and plutonium was dispersed in the form of tiny 'hot' radioactive particles after Britain detonated nine atomic bombs in remote areas of South Australia, including Maralinga between 1953 and 1963.

Scientists have new evidence to show these radioactive particles persist in soils to this day, more than 60 years after the detonations. Previously, we had limited understanding of how plutonium was released from these 'hot' particles into the environment for uptake by wildlife around Maralinga.

But a study published in Nature's *Scientific Reports* (doi.org/10.1038/s41598-021-89757-5), and led by Monash University researchers, warns that the hot particles are much more complex and varied than previously thought.

Currently, there are no international best practice standards for the environmental impact or risk assessment of Pu–U-rich hot particles released during nuclear testing.

This study provides the first mechanism for future modelling to predict the environmental life cycle of plutonium from hot particles, including how they are slowly broken down in the environment over a long period, and potentially exposed to animals and humans through inhalation, soil or ground water.

'The resulting radioactive contamination and cover-up continues to haunt us', said lead study author Dr Megan Cook, from the Monash University School of Earth, Atmosphere and Environment.

'The results of our study profoundly changes our understanding of the nature of hot particles at Maralinga – despite the fact that those were some of the best studied particles anywhere in the world.'

The research team used synchrotron radiation at the Diamond Light Source near Oxford, UK, to decipher the physical and chemical make-up of the particles.

At Monash University, they dissected some of the hot particles by using a nano-sized ion beam, and further characterised the complex make-up of these particles down to the nano-size in exquisite details.

'Our observations of the hot particles from the Maralinga provide a clear explanation for the complex and variable behaviour of different hot particles with respect to the chemical and physical weathering that has hindered predictive modelling to this day', said study co-author Associate Professor Vanessa Wong.

'This study provides a mechanistic foundation for predicting the future evolution of hot particles from high-temperature nuclear events and the likely exposure pathways.'

The researchers demonstrated that the complexity of the hot particles arose from the cooling of polymetallic melts from thousands of degrees Celsius in the explosion cloud during their formation.

'We found that the particles contained low-valence plutonium–uranium–carbon compounds that are typically highly reactive – which is unexpected for particles that survived for over 30 years in the environment,' said corresponding author Dr Barbara Etschmann.

Between 1950 and 1988, there were more than 230 recorded nuclear weapon accidents, including at least 10 with documented release of radioactive particles into the environment. The risks of such incidents are only increasing as international treaties such as the Intermediate-Range Nuclear Forces Treaty were cancelled.

'Our study invites a revisit of the implications of earlier results for the fate of plutonium at Maralinga,' said study co-author Professor Joël Brugger.

'Understanding the fate of hot particles in the arid environment setting of the Australian outback is critical for securing Australia in case of nuclear incidents in the region, and returning all the native land affected by the British tests to the traditional Anangu owners of the Maralinga Tjarutja lands.'

Monash University

# Solving intergenerational challenges with science

Australia must 'level up' on our outlays in income-generating R&D and research translation to tackle the vast structural economic, social and budget challenges ahead, Science & Technology Australia has said.

Science & Technology Australia Chief Executive Officer Misha Schubert said the Intergenerational Report's forecasts made an urgent case for STEM investment.

'A slowing economy, a major productivity challenge, a dropping birth rate, and a long-term COVID hangover sharpen the imperative for clever investments now to put Australia on a path to become a global science and technology superpower', she said.

'The clear message from this report is that Australia needs to level up its investments in future income-generating R&D and research translation to tackle the challenges ahead. Science and technology are the answer to every one of them.'

'In a world advancing technologically at breakneck speed, the key to future prosperity for Australia will be our ability to be at the forefront of the big advances in science, engineered solutions and the emerging technologies of AI and quantum.'

'Nailing those capabilities will help Australia to solve the big social, economic and budget challenges coming our way – including in health care and aged care.'

Science & Technology Australia's recent policy vision – Australia as a STEM Superpower – contains many of the answers on how the nation can meet the challenges highlighted in June's Intergenerational Report.

'An ambitious strategy to level up Australia's R&D investment should begin with a new $2.4 billion research translation and commercialisation fund and a national R&D target of 3% of GDP to peg ourselves to key global rivals.'

Science & Technology Australia

**Key science and technology measures announced in 2021 Budget**

- $206.4 million in tax incentives with a 'patent box' to strengthen sovereign manufacturing of Australian-patented technologies
- $42.4 million over seven years to support 230 women in STEM with higher education STEM scholarships, including industry placements
- $300 million for the Square Kilometre Array giant telescope in regional Western Australia
- $116.7 million to upgrade waste storage and maintenance of equipment at ANSTO
- $13.3 million over four years for the Australian Space Agency to boost regulatory and technical capabilities
- A commitment to develop onshore mRNA vaccine manufacturing capability
- $10.4 million over four years to extend the national partnership agreement on clinical trials and introduce mitochondrial donations into medical research
- $26.8 million over four years for a national soils science challenge
- Streamlining visas to target highly skilled individuals
- $643.4 million over four years to develop clean energy technologies
- $43.8 million over three years to expand the cyber security skills innovation fund
- $22.6 million over six years for 234 scholarships in next-generation emerging technologies (such as AI)
- $1.2 billion for digital economy transformation in measures announced last week
- $52.4 million over four years for global science and technology collaborations and diplomacy

# From physicist to German Chancellor: final term for Angela Merkel

After almost 16 years as German Chancellor, Dr Angela Merkel will not seek a fifth term ahead of the country going to the polls in late September.

Germany's first female Chancellor, Merkel studied physics at Karl Marx University in Leipzig, later studying and working at the Central Institute for Physical Chemistry of the Academy of Sciences in Berlin-Adlershof. She was awarded a doctorate in quantum chemistry in 1986. In July this year, Merkel was awarded a Johns Hopkins Doctorate of Humane Letters by Johns Hopkins University 'in recognition of her principled and courageous global leadership'.

Merkel's husband, Joachim Sauer, also a quantum chemist, is professor emeritus of physical and theoretical chemistry at the Humboldt University of Berlin. Sauer was an invited speaker at the International Symposium on Relations between Homogeneous and Heterogeneous Catalysis hosted in 2018 by the RACI and the Catalysis Society of Australia.

*Physics World*, in a policy piece published when Merkel was seeking her third term in office, reported, 'Thomas Mannel, a theoretical particle physicist at the University of Siegen, says that one of Merkel's most significant contributions is her support for the Excellence Initiative, which is designed to produce internationally recognized universities in Germany that can match rivals in the UK and US.'

Speaking in Berlin earlier this year at her final federal summer press conference, Merkel addressed the tragedies of the recent floods in Germany and the COVID pandemic, saying 'The more who are vaccinated, the freer we will be again'.

Avi Richards/Unsplash

# Climate change widespread, rapid and intensifying – IPCC

Scientists are observing changes in Earth's climate in every region and across the whole climate system, according to the latest Intergovernmental Panel on Climate Change (IPCC) report. Many of the changes observed in the climate are unprecedented in thousands, if not hundreds of thousands, of years, and some of the changes already set in motion – such as continued sea level rise – are irreversible over hundreds to thousands of years.

However, strong and sustained reductions in emissions of $CO_2$ and other greenhouse gases would limit climate change. Although benefits for air quality would come quickly, it could take 20–30 years to see global temperatures stabilise, according to the IPCC Working Group I report, *Climate change 2021: the physical science basis*, approved by 195 member governments of the IPCC, through a virtual approval session that was held over two weeks starting on 26 July.

The Working Group I report is the first instalment of the IPCC's Sixth Assessment Report, which will be completed in 2022. 'This report reflects extraordinary efforts under exceptional circumstances', said Hoesung Lee, Chair of the IPCC. 'The innovations in this report, and advances in climate science that it reflects, provide an invaluable input into climate negotiations and decision making.'

The report provides new estimates of the chances of crossing the global warming level of 1.5°C in the next decades, and finds that unless there are immediate, rapid and large-scale reductions in greenhouse gas emissions, limiting warming to close to 1.5°C or even 2°C will be beyond reach. The report shows that emissions of greenhouse gases from human activities are responsible for approximately 1.1°C of warming since 1850–1900, and finds that averaged over the next 20 years, global temperature is expected to reach or exceed 1.5°C of warming. This assessment is based on improved observational datasets to assess historical warming, as well as progress in scientific understanding of the response of the climate system to human-caused greenhouse gas emissions.

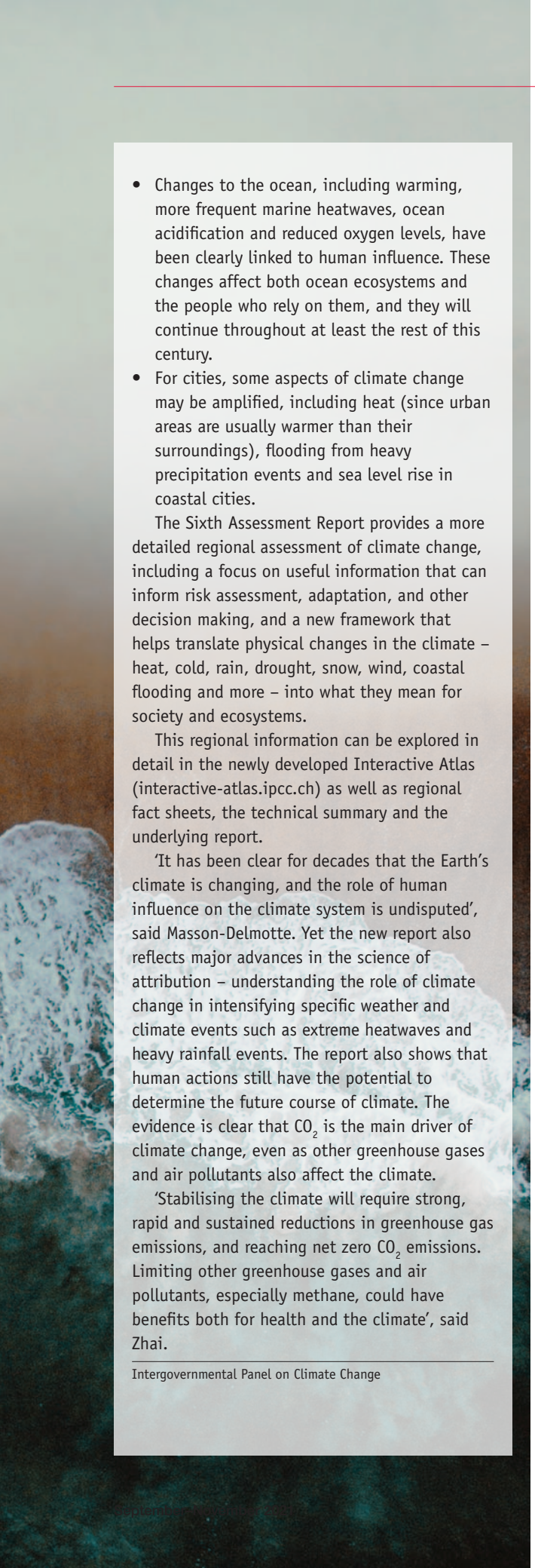
'This report is a reality check', said IPCC Working Group I Co-Chair Valérie Masson-Delmotte. 'We now have a much clearer picture of the past, present and future climate, which is essential for understanding where we are headed, what can be done, and how we can prepare.'

Many characteristics of climate change directly depend on the level of global warming, but what people experience is often very different from the global average. For example, warming over land is greater than the global average, and it is more than twice as high in the Arctic. 'Climate change is already affecting every region on Earth, in multiple ways. The changes we experience will increase with additional warming', said IPCC Working Group I Co-Chair Panmao Zhai.

The report projects that, in the coming decades, climate changes will increase in all regions. For 1.5°C of global warming, there will be increasing heatwaves, longer warm seasons and shorter cold seasons. At 2°C of global warming, heat extremes would more often reach critical tolerance thresholds for agriculture and health.

But it is not just about temperature. Climate change is bringing many different changes in different regions – which will all increase with further warming. These include changes to wetness and dryness, to winds, snow and ice, coastal areas and oceans. For example:

- Climate change is intensifying the water cycle. This brings more intense rainfall and associated flooding, as well as more intense drought in many regions.
- Climate change is affecting rainfall patterns. At high latitudes, precipitation is likely to increase, while it is projected to decrease over large parts of the subtropics. Changes to monsoon precipitation are expected, which will vary by region.
- Coastal areas will see continued sea level rise throughout the 21st century, contributing to more frequent and severe coastal flooding in low-lying areas and coastal erosion. Extreme sea level events that previously occurred once in 100 years could happen every year by the end of this century.
- Further warming will amplify permafrost thawing, and the loss of seasonal snow cover, melting of glaciers and ice sheets, and loss of summer Arctic sea ice.



- Changes to the ocean, including warming, more frequent marine heatwaves, ocean acidification and reduced oxygen levels, have been clearly linked to human influence. These changes affect both ocean ecosystems and the people who rely on them, and they will continue throughout at least the rest of this century.
- For cities, some aspects of climate change may be amplified, including heat (since urban areas are usually warmer than their surroundings), flooding from heavy precipitation events and sea level rise in coastal cities.

The Sixth Assessment Report provides a more detailed regional assessment of climate change, including a focus on useful information that can inform risk assessment, adaptation, and other decision making, and a new framework that helps translate physical changes in the climate – heat, cold, rain, drought, snow, wind, coastal flooding and more – into what they mean for society and ecosystems.

This regional information can be explored in detail in the newly developed Interactive Atlas (interactive-atlas.ipcc.ch) as well as regional fact sheets, the technical summary and the underlying report.

'It has been clear for decades that the Earth's climate is changing, and the role of human influence on the climate system is undisputed', said Masson-Delmotte. Yet the new report also reflects major advances in the science of attribution – understanding the role of climate change in intensifying specific weather and climate events such as extreme heatwaves and heavy rainfall events. The report also shows that human actions still have the potential to determine the future course of climate. The evidence is clear that $CO_2$ is the main driver of climate change, even as other greenhouse gases and air pollutants also affect the climate.

'Stabilising the climate will require strong, rapid and sustained reductions in greenhouse gas emissions, and reaching net zero $CO_2$ emissions. Limiting other greenhouse gases and air pollutants, especially methane, could have benefits both for health and the climate', said Zhai.

Intergovernmental Panel on Climate Change

## Robot chemist offers insight into origins of life

A robotic 'evolution machine' capable of exploring the generational development of chemical mixtures over long periods of time could help cast new light on the origins of life, scientists say.

Chemists from the University of Glasgow, Scotland, developed the robot, which uses a machine-learning algorithm to make decisions about which chemicals from a selection of 18 to combine in a reactor, and how to set conditions under which the reaction occurs. The robot can run the experiments on its own, with minimal human supervision.

The process aims to provide new insight into how Earth's complex organic life developed from its simple, non-living chemical origins by allowing the machine to run experiments over the course of several weeks.

Measuring the mass index of the product of each experiment teaches the robot something new about the complexity of molecules produced by each reaction. That information helps it learn how to vary the experiment to create a more complex molecule in subsequent reactions – a digital version, the team hopes, of the natural selection for complexity that gave rise to organic life.

In a paper published in *Nature Communications* (doi.org/10.1038/s41467-021-23828-z), the research team describes how the robot carried out hundreds of experiments across six batches of tests over four-week periods.

Over this time, the team found not only that complex molecules were created, but that some of these new molecules were persisting over many cycles despite dilution. This indicates that other processes, such as catalysis and replication, may be occurring.

The system builds on previous research led by the University's Regius Professor of Chemistry, Lee Cronin. Researchers from his group developed the chemical robot and launched a 'Spotify for chemistry' to allow researchers to download chemical formulas to use in their own chemical robots.

They have also recently published a paper on assembly theory, which quantifies the complexity of molecules and could be used to identify the tell-tale signs of the chemical building blocks of life.

Cronin said, 'The work we've been doing over the last decade or so has in many ways been leading up to this. Our chemical robot has really expanded the horizons of what is possible in the lab by automating basic tasks and allowing them to be done over and over again across long periods of time.

'Very few chemical experiments last longer than a few days, but the natural development of chemical biological systems took place over millions of years. Allowing the robot to carry out dozens of recursive experiments over the span of weeks, and then eventually to months and even years. opens up new opportunities to learn how chemical complexity began at the dawn of life.

'As robot chemists become more common in labs around the world, and the digital democratisation of chemistry becomes more widespread, we're hoping that other researchers will get on board and use the platform we've developed to make their own contributions.'

University of Glasgow

# RSC Robert Boyle Prize for Analytical Science to chemical engineer

**Kourosh Kalantar-zadeh with the ingestible human gas capsule based on 2D material sensoring technology.** RMIT

Professor Kourosh Kalantar-zadeh, chief investigator at the ARC Centre of Excellence in Future Low-Energy Electronics Technologies (FLEET Centre) at the University of New South Wales, Sydney, has been awarded the 2020 Robert Boyle Prize for Analytical Science by the Royal Society of Chemistry.

Kalantar-zadeh is recognised for his significant influence across many fields of engineering. His research has produced innovative pollution sensors, transistors, medical devices and optical systems.

Many of these devices are already commercially available and positively affecting peoples' lives worldwide – such as highly sensitive immunosensors, new materials for smart windows and reactors for the deposition of atomically thin electronic materials. Other innovations are in the final stages of commercialisation, such as ingestible gas-sensing capsules used for diagnosing gut disorders.

Although Kalantar-zadeh is internationally recognised in materials sciences, electronics and transducer research – in particular for his work on liquid metals and 2D semiconductors and sensors – one of his most satisfying discoveries has been the invention of an ingestible chemical sensor: the human gas-sensing capsule.

'A highlight of my scientific career was seeing the first signals from the ingestible gas-sensing capsule that I had swallowed in response to ingredients of an ice cream that I had eaten,' said Kalantar-zadeh.

The Robert Boyle Prize for Analytical Science is awarded for outstanding contributions to analytical science. Awarded biennially, the Prize awards the winner £5000 and a medal, and (usually!) is accompanied by a UK lecture tour. Robert Boyle (1627–1691) is widely regarded as being the first modern chemist and a pioneer of the modern scientific method.

Within FLEET, Kalantar-zadeh's team at UNSW with collaborators at RMIT develop the fabrication techniques necessary for advanced devices, using electron and ion beam lithography and other tools.

Kalantar-zadeh is a 2018 Australian Research Council (ARC) Laureate Fellow and a professor of chemical engineering at UNSW, Sydney, where he directs the Centre for Advanced Solid and Liquid based Electronics and Optics. Formerly, he was a Distinguished Professor of Electronic Engineering at RMIT in Melbourne.

ARC Centre of Excellence in Future Low-Energy Electronics Technologies

# ACS Priestley Medal to molecule designer

Caltech Office of Strategic Communications

**Peter Dervan**

The American Chemical Society (ACS) has awarded Peter Dervan, the California Institute of Technology's (Caltech's) Bren Professor of Chemistry, Emeritus, the 2022 Priestley Medal, the Society's highest honour.

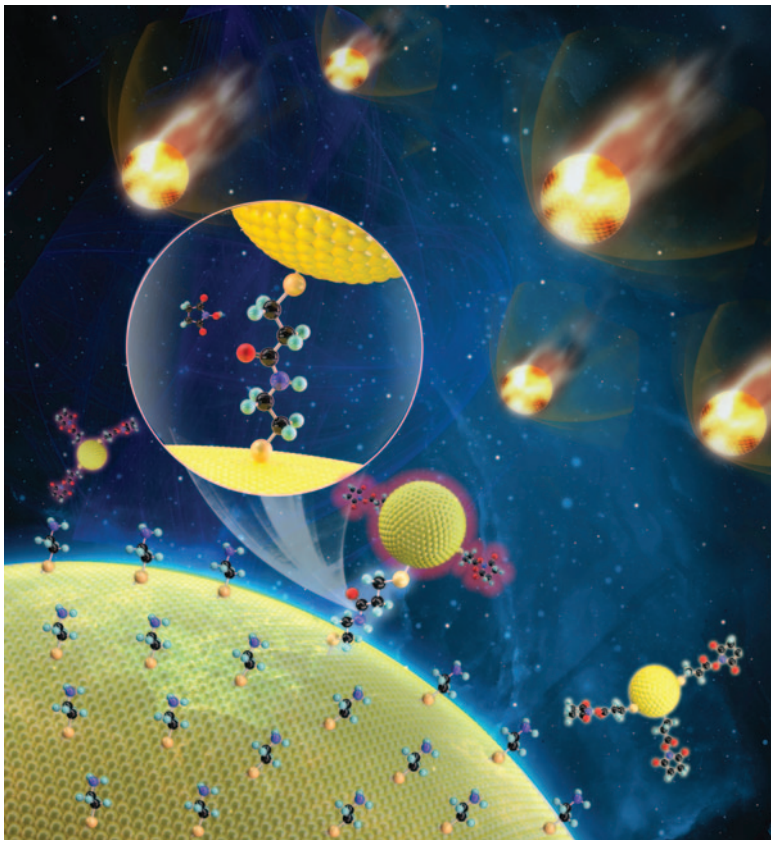
ACS awards the Priestley Medal annually to an individual for distinguished services to chemistry. Dervan is being honoured for his pioneering contributions in rational design of molecules that bind sequence-specifically to DNA, work that has been foundational at the chemistry–biology interface.

Dervan's research has focused on chemical biology. He has developed several synthetic molecules that bind to specific DNA sequences and can regulate gene expression.

Dervan has served as the chair of the scientific advisory board at the Welch Foundation, a non-profit organisation that provides funding to chemistry researchers.

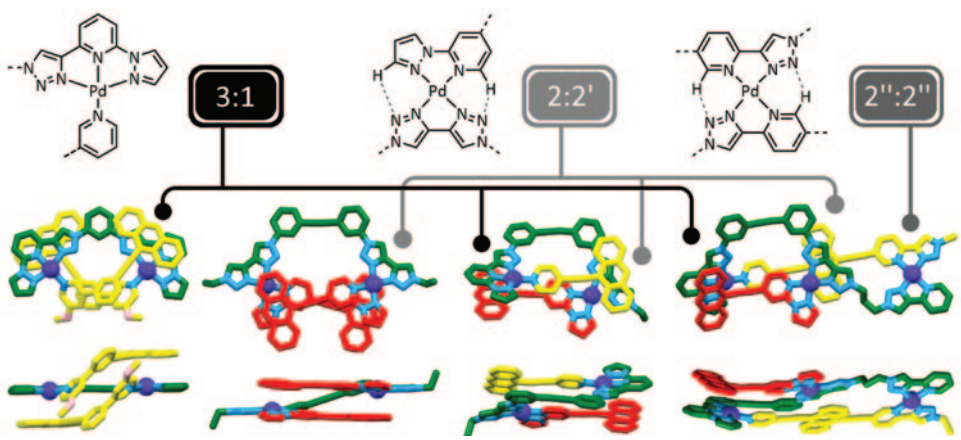
American Chemical Society

## Seeing is believing: direct observation of single-molecule amide bond formation



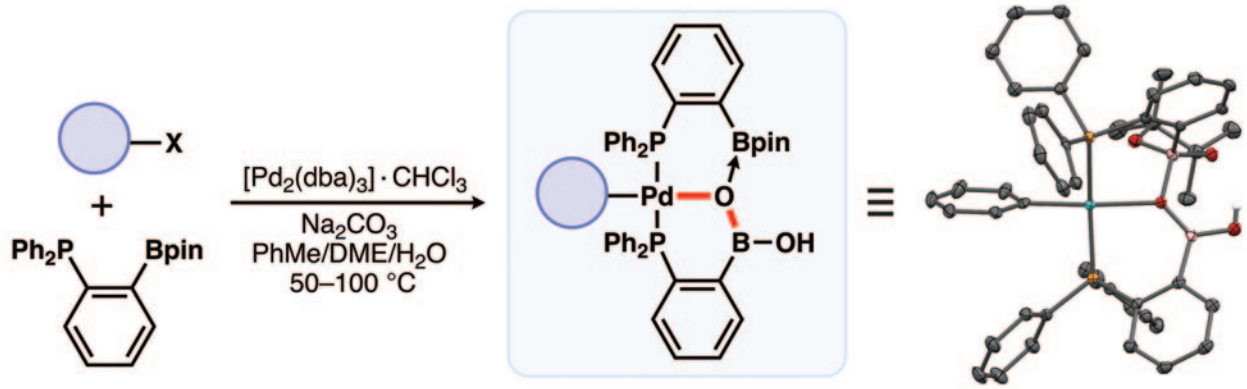
Direct observation of bond formation during a chemical reaction has been a grand challenge for chemists. Although remarkably sophisticated techniques for monitoring chemical reactions have been developed, the ability to detect and observe the formation of a chemical bond at the single-molecule level has remained an elusive goal. Amide bond formation is one of the most frequently used reactions in organic and biomolecular chemistry, including one-quarter of reactions reported in small-molecule pharmaceutical patents. Recent advances by a team from Deakin University and Florida International University (USA) have enabled the mapping of single-molecule amide coupling reactions (Kong N., Guo J., Chang S., Pan J., Wang J., Zhou J., Liu J., Zhou H., Pfeffer F.M., Liu J.Q., Barrow C.J., He J., Yang W.R. *J. Am. Chem. Soc.* 2021, **143**, 9781–90). Amide bond formation of an aminolysis reaction at the single-molecule level was directly probed in a plasmonic nanocavity, which was initiated by single nanoparticle collision events between functionalised free-moving gold nanoparticles and a gold nanoelectrode in an aqueous buffer.

## Self-assembling metallo-sequences that fold into persistent conformations




Foldamers adopt conformations in solution that depend on the identity and ordering of the components that comprise their sequence. Their conformational persistence is key to their function in biological molecules such as proteins, as well as synthetic analogues. To maintain sequence integrity and conformational control, these sequences are generally constructed using irreversible bond formation. Thermodynamic sequence formation using coordination bonds would be attractive synthetically and provide modular capability, but to accomplish this goal, strategies to maintain specific sequence ordering would be required. Dan Preston, a DECRA fellow at the Australian National University, has developed such a system for forming specific sequences under thermodynamic control (Preston D. *Angew. Chem. Int. Ed.* 2021, https://doi.org/10.1002/anie.202108456). The system uses orthogonal combinations of complementary ligand pairings around square planar palladium(II), exploiting sites of different denticity and/or hydrogen bonding capability. These combinations are shown in the image as 3:1 (tridentate to monodentate pairing), 2:2′ (bidentate hydrogen bond acceptor to bidentate hydrogen bond donor pairing) and 2′′:2′′(bis-bidentate mixed hydrogen bond donor–acceptor pairing). Through this approach, metallo-sequences are formed as thermodynamic products, and affinity between electron-rich and -deficient aromatic regions of the combined components then drives folding into defined conformations, due to complementary π–π interactions.

## Structure of pre-transmetallation intermediates in Suzuki–Miyaura reaction

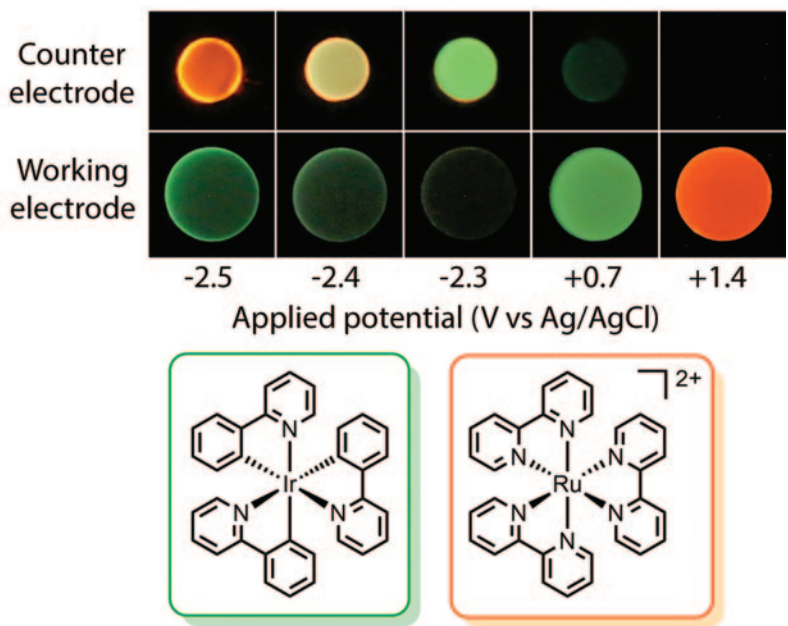



Although palladium(II) boronates are generally accepted to be fundamental pre-transmetallation intermediates in the Suzuki–Miyaura cross-coupling, they are typically fleeting at or above ambient temperature in this reaction because of their kinetic instability. For this reason, these species have been described as being 'on the borderline of existence' (*J. Am. Chem. Soc.* 2017, **139**, 3805–21).

Researchers from the University of Tasmania and the University of Otago (New Zealand) have recently addressed this issue by exploiting a simple strategy to develop a general method to synthesise a family of palladium(II) boronates that are kinetically stable by design (Olding A., Ho C.C., Canty A.J., Lucas N.T., Horne J., Bissember A.C. *Angew. Chem. Int. Ed.* 2021, **60**, 14897–901). These elusive species were prepared in only one synthetic step from readily accessible compounds, almost all of which are commercially available. This allowed their structures to be secured for the first time by single-crystal X-ray crystallography. The contributions of the first author of this work, Angus Olding, were supported by the 2019 RACI Masson Memorial Scholarship Prize.

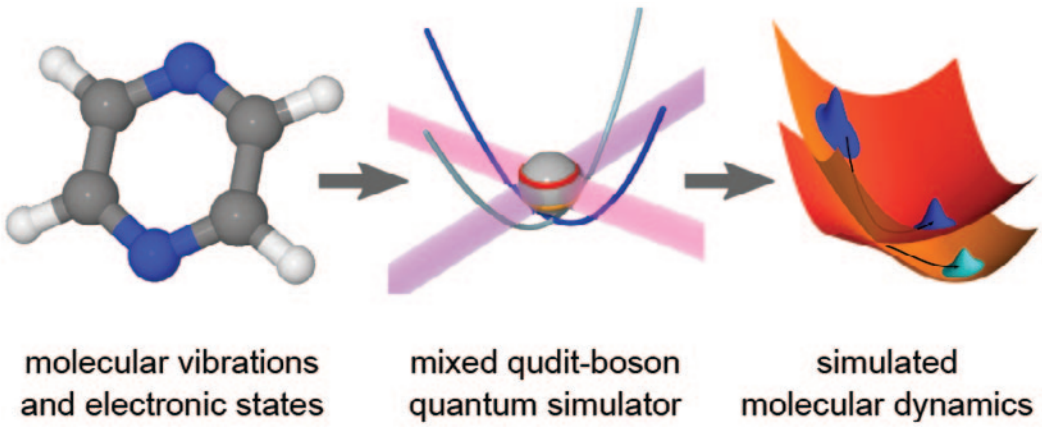
## Shedding light on electrochemiluminescence

Electrochemiluminescence (ECL) is a process in which electronically excited species that emit light are formed in reactions between electrochemically generated intermediates. The extensive use of ECL in commercial immunodiagnostic systems has been limited to a single metal complex luminophore, tris(2,2′-bipyridine)ruthenium(II) ($[Ru(bpy)_3]^{2+}$), but the past decade has seen the emergence of ECL systems involving multiple luminophores that can be discriminated by their redox potentials or emission colours. Researchers at Deakin University, La Trobe University and the University of Strathclyde (UK) have introduced a new experimental approach to characterise these reactions (Adamson N.S., Theakstone A.G., Soulsby L.C., Doeven E.H., Kerr E., Hogan C.F., Francis P.S., Dennany L. *Chem. Sci.* 2021, **12**, 9770–7). This method involves simultaneous measurements of potentials at the working and counter electrodes, the current between these electrodes, and the emission over cyclic voltammetric scans, coupled with photographic imaging of the ECL at the electrode surfaces. The researchers used this technique to provide a mechanism-based rationalisation of the interactions of several metal-complex luminophores and insight into concomitant ECL processes occurring at the counter electrode, which revealed a heretofore unknown ECL pathway from the electrochemical reduction of the tris(2-phenylpyridinato)iridium(III) ($Ir(ppy)_3$) complex.



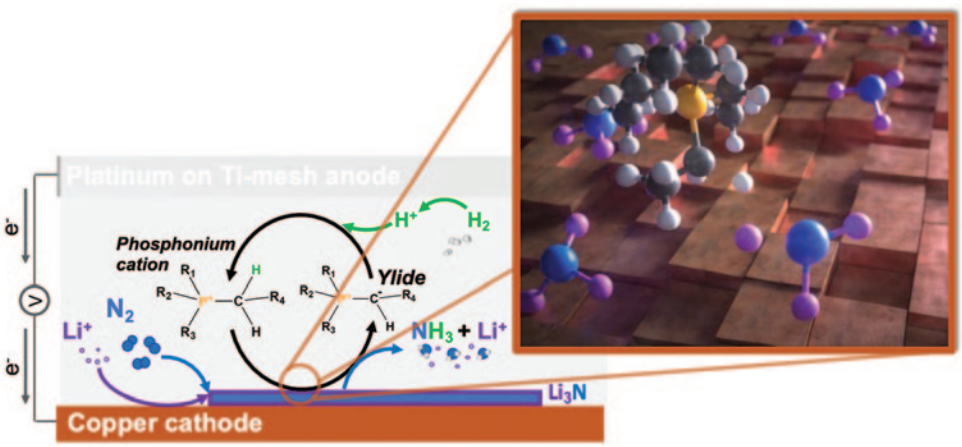
## Simulating chemical reactions on quantum computers

Ordinary computers have a hard time simulating the fully quantum-mechanical motion of nuclei and electrons that takes place during a chemical reaction. The problem is particularly acute for photochemical processes, for which the Born–Oppenheimer approximation can break down, leading to complicated entanglement between nuclear and electronic degrees of freedom. While it has been known for some time that quantum computers could make short work of quantum-chemical calculations, the quantum algorithms involved are usually complicated and would require large quantum computers to run successfully. Now, researchers at the University of Sydney have shown that dramatically smaller quantum devices could simulate chemical reaction dynamics (MacDonell R.J., Dickerson C.E., Birch C.J.T., Kumar A., Edmunds C.L., Biercuk M.J., Hempel C., Kassal I. *Chem. Sci.* 2021, **12**, 9794–805). Their approach uses analogue simulation: instead of ordinary digital calculations, they propose a quantum device tailored for simulating chemical dynamics by exploiting vibrations present in several different quantum technologies. For example, if an ion trap were used as the quantum simulator, the vibrations of the trapped ions would simulate molecular vibrations. The researchers expect their approach will allow existing quantum hardware to carry out chemical calculations that are intractable with ordinary supercomputers.

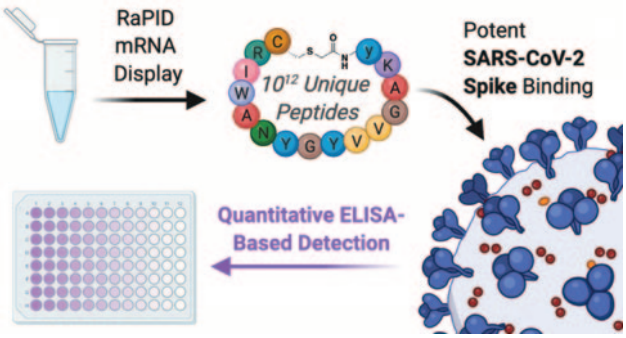



## Phosphonium cations the key to electrochemical ammonia production

Ammonia ($NH_3$) is poised to play a crucial role as a green fuel in a world combating climate change. Although ammonia synthesis is making exciting progress towards full decarbonisation, new plants are still based on traditional Haber–Bosch technology and thus restricted to mega-scale operations, which struggle with the intermittent nature of renewable energy. To overcome these limitations, a team at Monash University, in partnership with the ARC's Centre of Excellence for Electromaterials Science (ACES) and spin-out company Jupiter Ionics, have been developing lithium-mediated electrochemical technology for sustainable ammonia synthesis (Suryanto B.H.R., Matuszek K., Choi J., Hodgetts R.Y., Du H.-L., Bakker J.M., Kang C.S.M., Cherepanov P.V., Simonov A.N., MacFarlane D.R. *Science* 2021, **372**, 1187–91). The highlight of this research is the team's success in replacing ethanol (commonly used as a sacrificial proton source) with an ionic-liquid-based phosphonium proton 'shuttle'. This shuttle is a replenishing proton source, delivering protons from hydrogen gas split at the anode to lithium nitride ($Li_3N$) waiting at the cathode, before returning to collect a new proton. The performance of this system is front running in the literature: the rate of production is 53 nmol $s^{-1}$ $cm^{-2}$ at 69% faradaic efficiency. Additionally, three-day experiments demonstrate longer term stability. Jupiter Ionics is scaling up the technology towards commercial units.

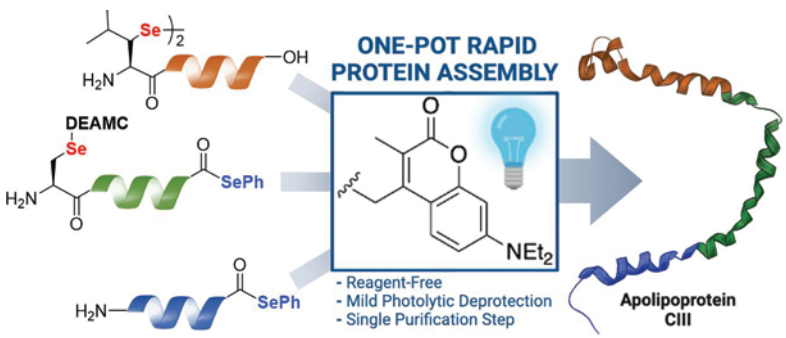


## Novel affinity ligands for SARS-CoV-2 spike




The COVID-19 pandemic has been responsible for many deaths as well as global disruption since the first reported SARS-CoV-2 infection in late 2019. Entry of the SARS-CoV-2 virus into cells is orchestrated by the viral spike protein binding to a receptor on the surface of human cells called angiotensin-converting enzyme 2 (ACE2). Given the importance of the SARS-CoV-2 spike protein for infection, affinity ligands to the spike protein have the potential for applications as antivirals and diagnostic reagents. In recent work from a team at the University of Sydney and the Kirby Institute, several high-affinity cyclic peptides with dissociation constants against the receptor binding domain of the spike protein in the nanomolar range (15–550 nM) were discovered through the use of mRNA with genetic reprogramming (Norman A., Franck C., Christie M., Hawkins P.M.E., Patel K. Ashhurst A.S., Aggarwal A., Low J.K.K., Siddiquee R., Ashley C.L., Steain M., Triccas J.A., Turville S., Mackay J.P., Passioura T., Payne R.J. *ACS Cent. Sci.* 2021, **7**, 1001–8). A co-crystal structure of the highest affinity cyclic peptide bound to the receptor binding domain demonstrated that it binds to a cryptic binding site where it is capable of mimicking the C-terminus of the viral proteins. This cyclic peptide was also used as an affinity reagent to detect the spike protein using an enzyme-linked immunosorbent assay (ELISA)-based system and may find future use for diagnostic applications.

## Light switch for protein synthesis




Researchers at the University of Sydney have developed a novel coumarin-based photolabile protecting group for the 21st amino acid selenocysteine (Sec) in order to facilitate the total chemical synthesis of proteins through iterative peptide-ligation reactions (Kambanis L., Chisholm T.S., Kulkarni S.S., Payne R.J. *Chem. Sci.* 2021, **12**, 10014–21). This 7-diethylamino-3-methyl coumarin (DEAMC) protecting group could be rapidly and efficiently deprotected within minutes using visible-light irradiation without any deleterious side reactions such as elimination and radical deselenisation that plague other protecting groups. DEAMC-protected Sec was subsequently employed as a linchpin in iterative diselenide–selenoester ligation reactions to rapidly and efficiently assemble proteins in 'one pot'. For example, the 60- and 80-residue fragments of the tumour-associated glycoprotein mucin 1 were assembled in 2–3 hours from three- and four-fragment assemblies, respectively, with only a single purification step. The utility of the photolabile DEAMC group, coupled with the efficiency of the diselenide–selenoester ligation chemistry at low concentrations, was also showcased in the total chemical synthesis of the poorly aqueous-soluble and aggregation-prone protein apolipoprotein CIII in just 4 hours with only a single purification step. The new methodology may find use in the future in the chemical synthesis of other poorly soluble proteins, including lipoproteins.

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.

# Collaborating against COVID

Ivan Bandura/Unsplash

BY **DAVE SAMMUT** AND **CHANTELLE CRAIG**

**Scientists worldwide have stepped up to challenges posed by COVID-19. In Australia, water researchers have a critical surveillance role: detection of viral fragments in wastewater.**

Since early last year, every one of us has benefited in some way from researchers' achievements in relation to vaccine development, diagnostic tests, test kits, hand sanitisers, masks, treatments and more. But few of us will be aware of the achievements of ColoSSoS: Collaboration on Sewage Surveillance of SARS-CoV-2.

Led by Water Research Australia (WaterRA), the ColoSSoS project brings together a broad community of research organisations, water authorities and state health departments. It involves national experts in health, microbiology, laboratory testing, wastewater-based epidemiology and policy communication, and links to global expertise through the Australian Water Association, Global Water Research Coalition and the US Water Research Foundation.

It has been known for roughly 75 years that sewage wastewater can be used to provide critical signals about infection rates in populations. This has been demonstrated for several enteric viruses such as norovirus, hepatitis A virus and poliovirus.

'The ColoSSoS Project leverages the 20+ years of health and water-based research undertaken by WaterRA and its predecessor – the CRC for Water Quality and Treatment', says ColoSSoS project director Dr Kelly Hill.

As far back as 1996, research was shared among WaterRA members through their publication *Health Stream*, covering the topic of water, waste and wellbeing. A project funded by the Cooperative Research Centre for Water Quality and Treatment aimed to investigate and document a variety of existing surveillance systems relating to the detection of gastrointestinal disease in the community and assess the feasibility of linking these with water quality data. Such information assistance is similar to what is currently being used in the ColoSSoS project to support the national pandemic response.

While diagnostic testing can detect infection in individuals, wastewater-based epidemiology can provide a great deal of information for public health experts on communities, the prevalence of viruses, trends, and the occurrence of otherwise undetected infection. It can provide a particularly effective early warning of disease outbreaks.

For example, an outbreak of a wild poliovirus type 1 was detected during surveillance of the sewerage system in Israel in February 2013. At this point, no cases of acute infection had been detected, yet an emergency immunisation drive was initiated, in which more than one million children under nine were re-vaccinated. Reports estimate that although up to 60% of susceptible individuals became infected within six months, not one child was left paralysed because of the outbreak (bit.ly/3eZqKOz).

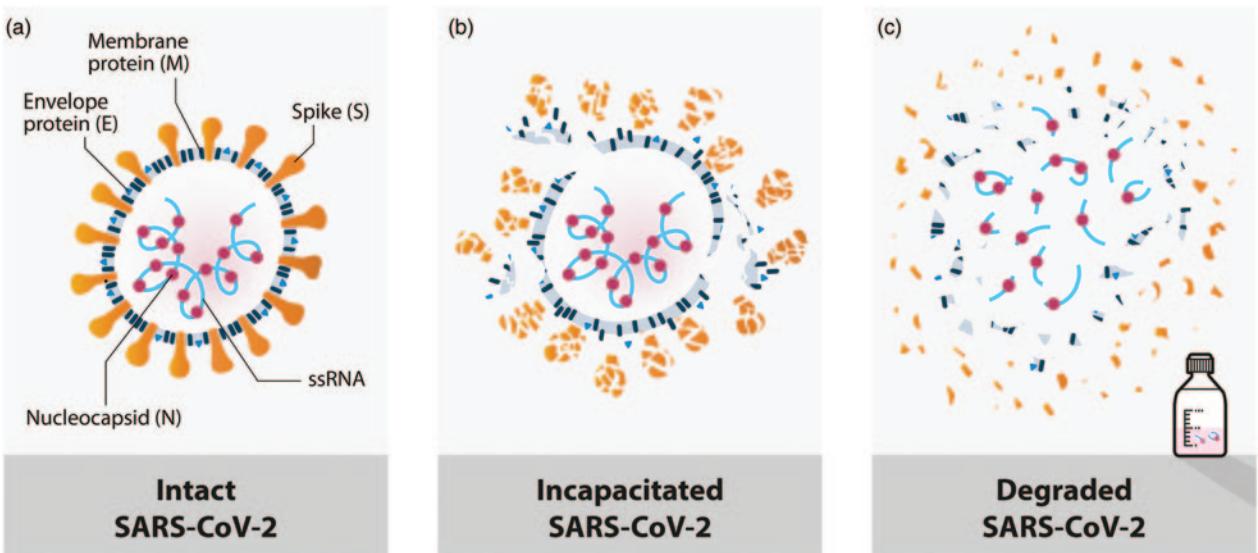
The first cases of COVID-19 in Australia were identified in late January 2020. By March, numbers had spiked to several hundred cases a day. The ColoSSoS initiative was established that same month to rapidly develop an effective analytical tool for detecting SARS-CoV-2 fragments in wastewater, building upon the systems already in place at wastewater treatment plants.

**... wastewater-based epidemiology ... can provide a particularly effective early warning of disease outbreaks.**

'The ColoSSoS program is a global first for leading the sewage surveillance initiative in close collaboration with health departments. This program is one-of-a-kind as it is driven and informed by jurisdictional health departments every step of the way', says Hill.

What makes ColoSSoS so interesting – and so successful – is the principles on which it was founded: that all participants must 'adopt the collaborative framework, conduct all research and activities in a direct response to end-user needs to support public health decision making, to openly share ideas and thoughts, and openly share learnings, work conducted in this program will not be used for commercial gain, or unduly delayed in the pursuit of publication' (bit.ly/3y8koTQ).

From the outset, Hill and her colleagues adopted a four-step expert working group approach: developing a sound sampling strategy, laboratory testing, interpretation and epidemiology, and communication. She directly attributes the success of the initiative to the experts who formed




**SARS-CoV-2 (a) key structure (includes the nucleocapsid, spike, membrane and envelope proteins, and RNA); (b) incapacitation process and (c) degradation. The subsequent analysis of SARS-CoV-2 RNA (typically after conversion to DNA) may follow RNA extraction from intact, incapacitated or degraded virus and combinations thereof.** From Hill K., Zamyadi A., Deere D. et al., *Water Quality Research Journal* 2021, vol. 56(2), pp. 57–67.

each of the working groups – national and international experts across water utilities, research, consultancies and, most importantly, the health agencies.

Coronaviruses (named for their round appearance and spiked surfaces) are a very large and diverse family of 'enveloped RNA' viruses. Unlike 'naked' viruses, they have a lipid envelope around the surface of the virus, the structure of which holds the membrane, envelope and spike proteins together. This actually makes them more fragile than other viruses, because the virus loses its ability to infect human host cells if the lipid envelope is destroyed.

Like other coronaviruses, SARS-CoV-2 is sensitive to ultraviolet light and chlorine disinfection, and is rapidly broken down by the detergents commonly found in sewage. For this reason, it is not believed to survive for long in raw sewage, and scientists therefore look for genetic fragments, rather than the active virus, in wastewater. (This also means that drinking water is believed to be safe from SARS-CoV-2 because of the treatment measures already in place for our water supply.)

ColoSSoS researchers initially focused on the sampling locations and methods. Water utilities already kept detailed maps of their infrastructure, pumping stations and network points, together with the catchment areas for each. These digital maps were enhanced with other potentially important sampling locations, such as hospitals and aged-care facilities, to design a flexible and appropriate sampling protocol that can be adapted as needed in the event of an outbreak.

'The optimal location for sampling is determined by several factors and groups', says Hill. 'It is led by health departments who have the information of clinical case numbers, and expert knowledge of at-risk locations and communities to test. This is combined with water agencies who have expert knowledge of the sewer network and ''peak'' timings for collection of samples.'

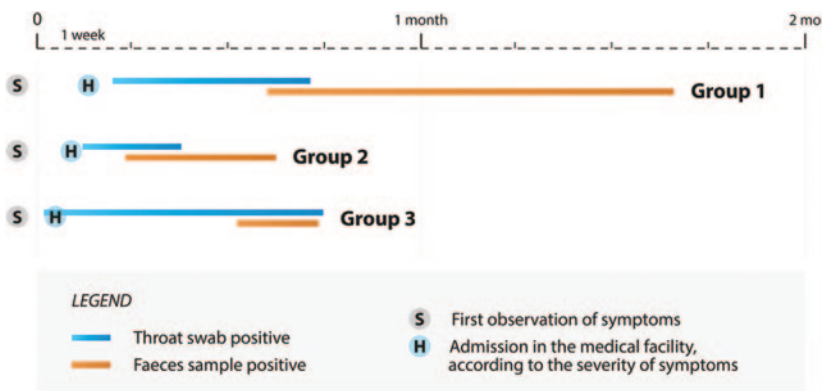
One of the interesting findings from the design of these protocols is how COVID-19 is changing national behaviours. Water authorities have long known about the influence of the 'first flush' in the morning, when the volumes and make-up of sewage are significantly different from the rest of the day. This is important to sample planning, because the sputum and phlegm from toothbrushing, nose blowing and face washing contain much more SARS-CoV-2 'shedding' than stools. So, by planning to sample during the first flush period, the analysis can be more sensitive to SARS-CoV-2 traces in the source population – but during lockdown, that first flush is coming 30–60 minutes later than normal.

For each sample, a worker in full PPE collects 500 millilitres of wastewater. The bottle is put on ice to keep it at less than 10°C, so that the sample is not compromised. The bottle is shaken and the contents are adjusted to pH 3, the iso-electric point at which the virus will become positively charged. The sample is filtered through a negatively charged membrane to capture the virus.

The negatively charged membrane-filtration method for virus recovery identified by Sydney Water microbiologist Sudhi Payyappat is considered the most effective (ab.co/3y9Srfd), and is now common practice among nine of the participating laboratories that took part in the ColoSSoS interlaboratory proficiency study (undertaken by the National Measurement Institute).

The membrane is chopped up and put in a tube containing glass beads. The tube is put in a vibrating 'bead beater', releasing the viruses from the membrane. 'Everything inside the cell comes out', said Payyappat to the ABC. 'It is washed, the acid is separated and put in a tube with pure water.'

The genetic code for SARS-CoV-2 having been used to identify key target gene sequences, the sample is subject to reverse transcriptase–quantitative PCR (RT-qPCR) to multiply the fragments, and then measured. However, this is not completely straightforward. Wastewater is a highly complex analytical matrix – both chemically and biologically. According to Erica Donner and colleagues in a paper published this year in *Microbiology Australia*, 'a ''typical'' urbanised community may be releasing tens of thousands of different chemical pollutants from their everyday activities in homes, hospitals, commercial and industrial settings. Some of these decrease the … sensitivity, for example, by accelerating the decay of SARS-CoV-2 shed from infected people, or by inhibiting the polymerase chain reaction (PCR), a method that typically enables very low concentrations of the virus to be detected' (bit.ly/3i5N4YC).




**The extended duration of the virus in faecal samples versus symptom observation and throat swab test results.** From Hill K., Zamyadi A., Deere D. et al., *Water Quality Research Journal* 2021, vol. 56(2), pp. 57–67; adapted from Wu Y., Guo C., Tang L., et al., *The Lancet Gastroenterology & Hepatology* 2020, vol. 5(5), pp. 434–5.

**The negatively charged membrane-filtration method for virus recovery ... is considered the most effective, and is now common practice among nine of the participating laboratories that took part in the ColoSSoS interlaboratory proficiency study**

**Sydney Water microbiologist Sudhi Payyappat loading samples for polymerase chain reaction (PCR) amplification to detect SARS-CoV-2.** Sydney Water

Donner and her colleagues went on to state that 'Researchers involved in this process noted that the openness in sharing protocols and ideas was essential for the rapid national response and operationalisation. Rapid publication turnaround by dedicated academic reviewers and journal editorial teams, and the increasing availability of pre-print publications was also instrumental'.

Through the ColoSSoS expert working groups, the participating laboratories were using some common standards. However, the methods and detailed protocols from each laboratory are slightly different. 'This is not unusual', explains Hill, as various methods are validated and approved around the world for similar testing on wastewater for polio virus. Testing protocols across the ColoSSoS laboratory testing expert working group are summarised in a WaterRA report (2021) (bit.ly/3moqflv).

The third step in the ColoSSoS project planning was evaluating the data to make it most useful for health authorities. As noted by Hill and colleagues in a paper published early this year in *Water Quality Research Journal*, 'Back-calculating from the observations at the end of the wastewater catchment to population-relevant information is promising but still under development' (bit.ly/3f52870). Data is still being gathered on the key factors for this calculation: '(a) shedding rates and duration, (b) links between the genetic signal and the infection prevalence and (c) fate within wastewater and how this changes with wastewater characteristics (e.g. dilution, temperature, retention time, percentage trade waste, etc.) that may vary with time and season'.

In the meantime, very useful insights can be drawn from trend detection (single-direction, up or down) and changes in trend (up or down). The simple detection of SARS-CoV-2 fragments in wastewater does not necessarily denote the onset of a new health emergency. A patient recovering from COVID-19 can continue to shed virus in their stool for weeks after they are no longer infectious, or a person with the infection might have simply travelled through the catchment. Trend data can give insights on this.

WaterRA, through the ColoSSoS project, supported the undertaking of a proficiency program through the National Measurement Institute to consider the various laboratory protocols and the data being produced, particularly with regard to reproducibility and limit of detection. Hill explains: 'understanding the quality of data being reported to health departments is particularly relevant when qualitative data is being reported in a low-case setting, such as Australia's'.

The final key question is: 'How should a positive detection be managed in terms of the public health response?' The limitation in back-calculation is problematic for some audiences, given that politicians and the community struggle with the basic principles of scientific uncertainty.

'The task is very complex, with multiple phases', says Hill. 'You need to start with rapid development of

reliable methods, followed by a scale-up, and all of these need to be well informed by your health department' (bit.ly/3iSNtNn).

'A large focus was put on building a team comprised of health department personnel, utilities communications and utilities experts, as well as expert science communicators', says Hill. 'The team have developed a communications plan (which includes a risk analysis and mitigation strategy), an immediate action plan (for example, for briefings to ministers), as well as key messages for utilities, and a communications matrix [outlining] the type of communication, objective audience, frequency, desired goals and who the task manager might be.'

In November 2020, traces of SARS-CoV-2 were detected in sewage at two local pumping stations from a population of 18 500 people in Sydney's north-west. With a large local Indian community, local leaders help spread the message about testing, and diagnostic testing numbers were boosted significantly on the back of that community response. Since that time, detection of SARS-CoV-2 fragments in various communities has been a regular feature of news reports, and of the associated health response. The successful outcomes from the ColoSSoS project are evident. Hundreds of samples are being analysed per month, feeding critical data to our health systems. Sampling can be broad, or it can be targeted at key communities, such as individual hospitals and aged-care facilities. It may in future be able to contribute to the maintenance of a society that lives with COVID-19, for example in the analysis of wastewater (such as from cruise ships) to detect emerging variants from overseas and provide an early warning of potential outbreaks.

This work is science at its best – pure of purpose, open and collaborative in nature, swiftly achieving outcomes for the good of all society.

**Dave Sammut** FRACI CChem and **Chantelle Craig** are the principals of DCS Technical, a boutique scientific consultancy providing services to the Australian and international minerals, waste recycling and general scientific industries.

# Borodin

# Scientist and Sunday composer

BY **DAVID EDMONDS, ALF LARCHER** AND **RICHARD THWAITES**

**Although best known as a composer, Borodin first trained as a medical doctor and then became an eminent chemist, describing himself as a Sunday composer only: 'Science is my work and music is my fun'.**

**Alexander Borodin, c. 1865.**
Wikicommons

Alexander Porfiryevich Borodin was born in November 1833 in St Petersburg, Russia, son of 62-year-old Georgian nobleman Prince Luka Stepanovitch Gedianishvili and his 25-year-old servant Avdot'ya Konsantinova Anonova. The nobleman had Alexander registered as the son of one of his valets, Porfiry Borodin, and the valet's wife, Tatiana, hence Borodin's Russian name.

The young Borodin was integrated into the royal house's servant staff and classed as a serf, according to the social structure of the time. He called his biological mother 'Auntie Tetushka' and it is not clear whether he knew who she really was. The double whammy of illegitimacy and serfdom did not provide the precocious Borodin many opportunities, but this was overcome

by his 'auntie', who rallied tutors from both inside and outside of the household to provide tutelage on a wide variety of subjects. He learned to play the flute, cello and piano and studied several foreign languages – French, German and English. At age six, he was freed from serfdom after his mother married in 1839. He started writing music when he was nine and built a home laboratory to produce fireworks when he was 13.

Avdot'ya Anonova tried unsuccessfully to enrol Borodin at St Petersburg University when he was 17 but pulled a few strings to get him enrolled at the Medico-Surgical Academy in the same city in 1850. He graduated in 1856 'with exceptional distinction'. Although qualifying as a doctor and surgeon and becoming a house surgeon at the second military hospital from 1856 to 1859, Borodin became interested in chemistry under the influence of Professor Nikolai Zinin, who was the first to synthesise aniline, the basis of the synthetic dye industry.

Borodin received a doctorate of medicine in 1858 for his thesis 'On the analogy of arsenic and phosphoric acids in chemical and toxicological behaviour' but then abandoned his medical career in 1859 to concentrate on chemistry and music.

Subsequently, funded by the Medico-Surgical Academy, Borodin travelled extensively and lived in Western Europe, working in the laboratories of Bunsen and Erlenmeyer in Heidelberg with other Russian and German scientists. Dimitri Mendeleev was also there, being a dominant member of the so-called Heidelberg Circle of chemists, the members of which would discuss their research and the world in general, including the formation of a Russian Chemical Society. Borodin and Mendeleev seem to have hit it off immediately, spending much time together, including dining together most evenings. Writing to his mother, Borodin told her of his new friendship and how he had visited Mendeleev's laboratory, which he had

**St Petersburg Medico-Surgical Academy. Borodin graduated from here in 1856 with exceptional distinction.** Александров, CC BY-SA 3.0

**Borodin and Mendeleev seem to have hit it off immediately, spending much time together, including dining together most evenings.**

## Borodin and Mendeleev – two Russians at large

In October 1860, Borodin decided to go to Italy with Mendeleev, travelling to Venice, Verona and Milan. The two seemed to want to get away from the formalities and stuffiness of Heidelberg and the very recent Karlsruhe Conference, and let their hair down, with them 'dressing like artists' to blend into the Italian population. The plan worked a little too well, as near Verona their train was searched by Austrian police for an escaped Italian political prisoner (since at the time Austria controlled much of northern Italy and a resistance movement was well under way). The actual escaped prisoner was on the train, but the police mistook Borodin, because of his Italian 'countenance' for the fugitive. Borodin and Mendeleev were searched, questioned and nearly arrested before convincing the police that they were two harmless Russian chemists. When they finally crossed the border into Italy, everyone in the rail car embraced and kissed them, shouting 'Viva', the reason being that the political fugitive was sitting in the same rail car all the time, with the police not noticing him. Borodin and Mendeleev seemed to have enjoyed their new fame and the rest of their stay in Italy.

The careers of both men progressed, with them both attaining academic positions in St Petersburg. Both were influenced and inculcated by Professor Voskresenskii of St Petersburg University on the importance of teaching, which Borodin put into practice when working in the Medico-Surgical Academy. Mendeleev always spoke highly of his friend, once stating that when travelling internationally people would often ask 'What has your Borodin done that is new?'

established in his (Mendeleev's) apartment (see November/December 2019 issue, p. 16).

They both travelled to the Karlsruhe Congress in 1860, a critical event in the history of chemistry, where Borodin was particularly inspired by the many brilliant lectures given and ideas presented. After the Congress, Borodin and Mendeleev returned to Heidelberg, during which they no doubt richly discussed all that had transpired at the Congress. This period included journeys with Mendeleev to Italy (see box p. 25), Switzerland and France, attending a Papal mass in Rome, visiting Pasteur (among others) and lecturing in Paris.

Borodin proposed to Russian pianist Katerina S. Protopopova in 1861, and they married in 1863. Because of her poor health, they relocated to Pisa for some time, and while in Pisa Borodin worked on fluorine compounds with Sebastian de Luca and Paola Tessinari.

In 1862, Borodin returned to St Petersburg Medico-Surgical Academy and, in 1864, replaced Zinin as Professor of Chemistry. Borodin lived in the grounds of the Academy for the rest of his life with Katerina, their two adopted daughters, a number of cats and itinerant family members. He continued to travel around Europe, representing the Academy at important international meetings and conferences.

Among his other achievements, Borodin, together with Sergey Botkin, Ivan Sechenov and other professors, founded the first medical course for women in Russia, commencing with obstetrics, in 1872. He completely redesigned the archaic chemistry courses and included more equipment and demonstrations, wooing a greater number of students to them. During the period of Mendeleev's time teaching, the abolition of serfdom brought greater social freedoms, with Borodin particularly championing the education of women, notwithstanding the discomfort of the Czarist government.

Borodin became the Director of the Medico-Surgical Academy Laboratories in 1874 and was the chair of the Governing Board of St Petersburg Music Lovers from 1879 to 1880.

In February 1887, aged only 53, Borodin collapsed suddenly and died from a heart attack at a fancy-dress party in the Academy. After his untimely death, a group of female doctors he had trained placed a silver wreath on his grave, thanking him on behalf of 10 graduations of women.

**Some of Borodin's contributions to the chemistry literature**

| Year | Short English title |
|---|---|
| 1858 | On the action of ethyl iodide on benzoylanilide |
| 1862 | Contribution to the history of benzil |
| 1862 | Data for the history of fluorides |
| 1864 | On the action of sodium on valeraldehyde |
| 1867 | Research on Bukhara opium |
| 1869 | Condensation products of aldehydes |
| 1870 | Condensation products of valeraldehyde |
| 1872 | On condensation products of common aldehydes |
| 1873 | On the action of ammonia on cuminol |
| 1876 | On a new method for the quantitative determination of urea |
| 1884 | On the relationship of hydrogen peroxide toward lower organisms and the importance of ozonised oils for disinfection |
| 1884 | On the composition of brick tea |

From George B. Kauffman's 'Complete list of Borodin's chemical and musical works' (bit.ly/3iek017). The source of each publication can be found here.

## Borodin's chemistry

Borodin's contributions to chemistry were substantial. From 1858 to 1886, he authored or co-authored some 40 papers of extraordinary diversity. His first paper was: 'On the action of ethyl iodide on hydrobenzamide and amarine and the constitution of these compounds'.

Illustrating both the range and depth of Borodin's chemistry interests and expertise, the table below contains just a few examples of his work. In most cases, Borodin co-authored the publication with one or more collaborators.

A colleague* has suggested that the most significant papers produced by Borodin include those on the preparation of benzoyl fluoride (during his stay in Pisa in 1862), the polymerisation and condensation of aldehydes (in St Petersburg in the period 1864–1873) and the determination of urea in urine, also in St Petersburg from 1875 onwards.

$$CH_3COOAg + Br_2 \rightarrow CH_3Br + CO_2 + AgBr$$

**Borodin first observed silver salts of carboxylic acids reacting with a halogen to produce an organic halide (now called the Hunsdiecker–Borodin reaction) in the early 1860s.**

Borodin's early work in St Petersburg involved elucidating the mechanisms of several organic reactions, but also included work on the analysis of mineral water found in springs at the health resort of Soligalich, well known for its therapeutic properties.

In Pisa, Borodin collaborated with de Luca and Tessinari, producing several papers on the production of benzoyl fluoride and similar compounds. Back in St Petersburg, much of Borodin's work was on the polymerisation and condensation of aldehydes. He ruffled the feathers of prominent German organic chemist

* Our sincere thanks to Professor Ian Rae for providing his published papers on Borodin and for his ongoing advice on the life, chemistry and times of Borodin.

August Kekulé during this period because Kekulé regarded work on aldehydes as his own territory and resented others intruding on his patch.

Borodin's work on the development of analytical techniques for the determination of urea was extremely important at the time because it involved the production of nitrogen gas, which enabled very low concentrations of urea to be determined.

Other studies included work on disinfectants (which would have been particularly relevant to the operation of the Medico-Surgical Academy where Borodin worked and lived) and analyses to determine the composition of types and grades of tea compressed into bricks, quite popular in various parts of Asia at the time.

In February 1871, work was reported on studies performed under Borodin's guidance by assistant Dr Krylov. They expected analysis of the fat in heart muscles affected by fatty degeneration to yield glycerol. Instead, they found cholesterol, first reported 1789 but the structure not verified until 1932. (The importance of this discovery was not realised until the 1910s, when German chemist Adolf Windaus noted cholesterol in the atherosclerotic plaques of human aortas.)

## Borodin's music

Borodin's musical output was minuscule compared with other composers of note, yet his legacy is firmly established. Some works, such as his masterpiece opera *Prince Igor* and third symphony, were completed by other composers. Borodin's major works include:

- the opera *Prince Igor*, commenced in 1869, completed by Rimsky-Korsakov and Glazunov
- three symphonies 1865, 1877, 1886–7 (third symphony completed by Rimsky-Korsakov and Glazunov)
- the tone poem *In the Steppes of Central Asia*, 1880
- chamber works, including the popular second string quartet, 1882
- 16 solo songs.

Borodin first met composers Mily Balakirev and Modest Mussorgsky around 1862. Balakirev became Borodin's musical mentor. Five Russian composers of the late 19th century became known as the 'Mighty Handful', all being well-known musicians and composers in their spare time, having at least initial careers outside music. These were Mily Balakirev (mathematician), Nicolai Rimsky-Korsakov (navy officer), Modest Mussorgsky (army officer), Cesar Cui (engineer and army officer) and Alexander Borodin (surgeon and chemist).

Borodin organised to blend his scientific and musical travels, trying to ensure that science and musical meetings and events coincided at the same dates and locations. For example, while in Germany he met Franz Liszt in Weimar, where together they played piano duets of Borodin's music.

A number of Borodin's major works are readily available on recordings and YouTube clips. A recommended introduction would be to listen to the Polovtsian Dances from the opera *Prince Igor* about 10 minutes duration. Further recommended are the second symphony, tone poem *In the Steppes of Central Asia* and the second string quartet.

To hear some of Borodin's best tunes given Broadway interpretation, listen to a recording of the musical *Kismet*, which was produced with acclaim on Broadway and the West End of London in the mid-1950s.

## Further reading

- A more complete biography and detailed description of his music is found in Sadie S., Tyrrell J. *The New Grove Dictionary of Music and Musicians*, 2nd edn, Grove, New York, 2001.
- For an overview of Borodin's life and details of chemistry, see Kauffman G.B., Rae I.D., Solov'ev Yu I. 'Borodin, composer and chemist', *Chemical and Engineering News*, 1987, vol. 65(7), pp. 28-35.
- For chemistry specifics, see Rae I.D. 'The Research in Organic Chemistry of Aleksandr Borodin', *AMBIX*, Vol. 36, Part 3, November 1989.

**David Edmonds** FRACI CChem is a past President of the RACI. Now retired, he worked in various technical roles in the therapeutic goods industry and is passionate about live and recorded classical music.
**Alf Larcher** FRACI CChem is a petroleum, environmental and industrial chemist with an occasional urge to write science articles.
**Richard Thwaites** FRACI CChem retired from full-time employment in the chemical industry in 2008. He is a former RACI Victorian Branch President and Qualifications & Accreditation Committee Chair. He is a member of the *Chemistry in Australia* Management Committee. His interest in Borodin started at a music camp, in his youth, when he played the cello part in a performance of the overture to *Prince Igor*.

A Riefler clock
NIST

# From 1901 to 2021

## NIST measurements then and now

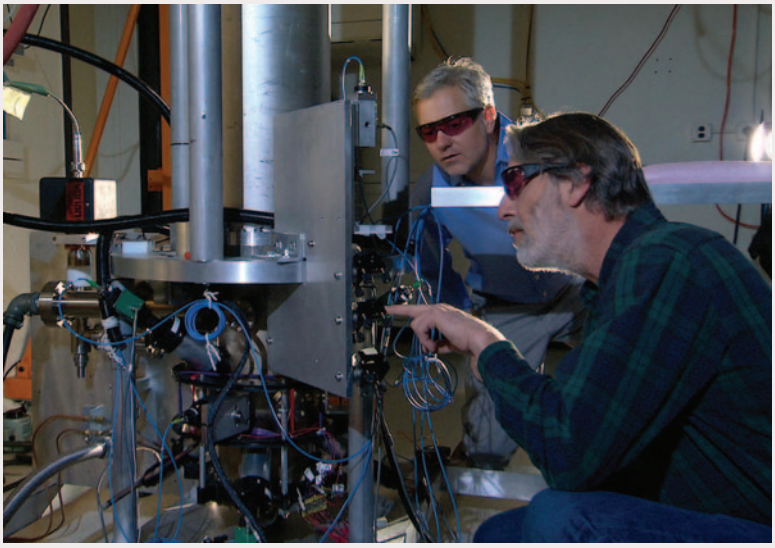
BY **MARK ESSER**

A lot has changed at the US National Institute of Standards and Technology (NIST) in the past 120 years. For one thing, we were known as the National Bureau of Standards for the first 87 years of our existence. Then, in 1988, we became the National Institute of Standards and Technology (NIST), to reflect our agency's expanding mission and a renewed emphasis on boosting the competitiveness of American industry. But as much as things change, they also stay the same. While much of our early work has been baked into the American economy, NIST continues to be a world leader in advancing measurement science. We still provide many of our original services, though the techniques and technologies have evolved.

## Time

NIST didn't build its own clock at the very beginning. One of the first purchases NIST made was a Riefler clock (see main image) in 1904 from the Clemens Riefler firm in Germany. The Riefler clock was a highly stable pendulum clock that achieved accuracies to within one-hundredth of a second per day, about 3.5 seconds per year.

Today, using technology made possible by the Nobel Prize-winning work of NIST's Bill Phillips and his colleagues, we use atomic fountain clocks to define the second as the time it takes for 9 192 631 770 cycles of radiation to be emitted from a specially energised caesium atom. The most advanced caesium clock, the NIST-F2, is so accurate that it would neither gain nor lose one second in about 300 million years.



**NIST physicists Steve Jefferts (foreground) and Tom Heavner with the NIST-F2 caesium fountain atomic clock.** NIST

## Electricity

The ampere that our founders were using in 1901 was not the same unit of electric current that we use today. In fact, it wasn't even quite one ampere! Back then, the ampere was practically defined as the current that would electrically deposit a small amount of silver on a negatively charged surface using a device known as a silver voltmeter. That voltmeter in turn had to be calibrated using a standard Weston cell, a type of battery that reliably produced a steady voltage for a reasonably long time.

Now, the workhorse of precise and accurate primary realisations of the volt the world over is the Josephson junction, only made possible by quantum phenomena that were discovered decades after NIST was founded. A Josephson junction is made from two layers of superconducting materials separated by a layer of atomically thin insulating material. When bathed in a particular frequency of microwave radiation, a quantum mechanical phenomenon known as electron tunnelling causes the junction to generate a proportional voltage. NIST now makes Josephson junctions that offer accuracies of better than one part per billion and don't need to ever be calibrated. The standards are used to calibrate voltmeters – devices important to the manufacture of consumer and industrial electronics and even the operation of the electric grid.

**Scientist F.A. Wolff (right) operates an oil bath while watching a temperature gauge in order to measure the temperature response of several Weston cells, used to calibrate voltmeters in 1903. His colleague on the left appears to be crafting the mercury thermometers used in the experiment.** NIST

**... the workhorse of precise and accurate primary realisations of the volt the world over is the Josephson junction ...**

Early reference materials. NIST

## Standard reference materials

NIST has been producing standard reference materials (SRMs) since 1905. First, we produced standard samples of iron for the American Foundrymen's Association to aid in metallurgical analysis and quality control. Before long, NIST was making 'standard samples' (our original name for SRMs) for hundreds of products and materials. Now, NIST produces more than 1000 different types of SRMs, each of which has thoroughly measured properties.


A Rueprecht balance. NIST Digital Archives

Today, we have SRMs for things that people 120 years ago might not have imagined. For instance, our monoclonal antibody reference material. Many of today's top drugs are based on monoclonal antibodies, customisable proteins that can block pathways for disease and seek out specific cells, such as cancer cells, and deliver chemicals or radiation to them. NIST's reference material provides a common benchmark that drugmakers can share to verify and improve their methods for quality control.

## Mass

When NIST was founded, we had our own precision balances constructed for comparing and calibrating masses against the US copies of the International Prototype Kilogram, a small cylinder of platinum and iridium that served as the world's standard of mass. Those balances would have looked a lot like this Rueprecht balance, which was built in 1901 and bought by NIST in 1945. It was used for primary mass comparisons until 1960, when it was replaced by a NIST-improved version.

Now, the ultimate standard of mass is no longer a physical object. It's defined in terms of an unchanging number in quantum physics called the Planck constant, which, through a couple of mathematical steps, can convert a certain amount of the energy in electromagnetic radiation to its equivalent in mass. In the laboratory, the kilogram is measured by the electrical energy it takes to hold that mass against the force of Earth's gravity. We measure that electrical energy using a new kind of balance called a Kibble balance, a technology that NIST and its colleagues at the National Physical Laboratory in the UK improved and refined for use to redefine the kilogram.

## Lighting

Shortly after its founding, NIST was put to work testing some of the products the government bought to see if they were up to specifications. One problem that plagued the government was how quickly the light bulbs it bought were burning out. At that time, the government was buying one million incandescent light bulbs per year. NIST tested a selection of commercially available bulbs, and its work showed that many bulbs didn't conform to the manufacturer's

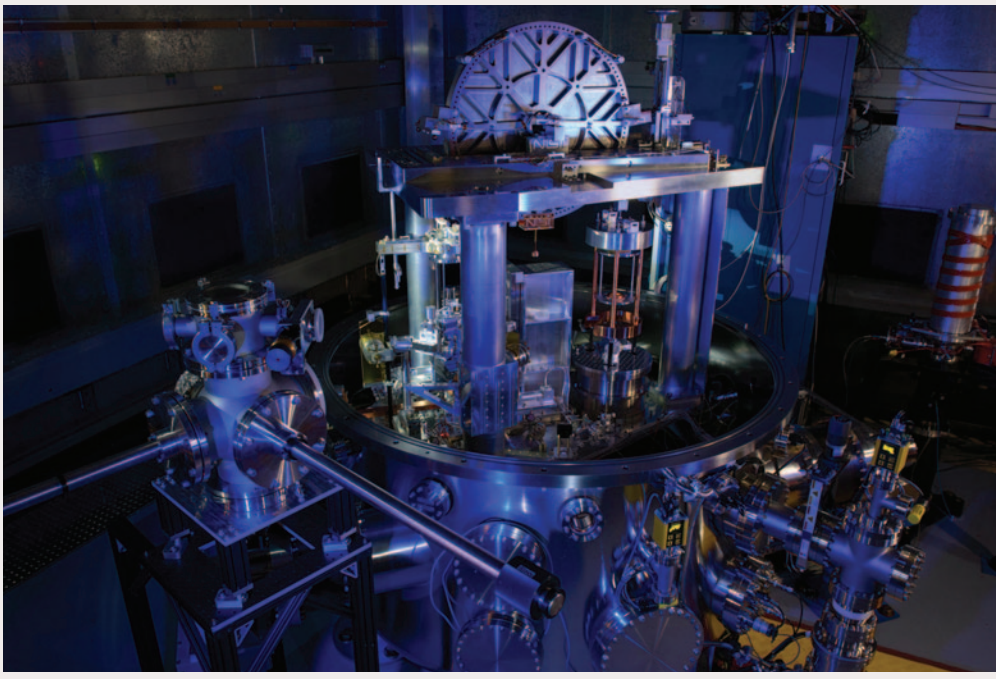
standards or federal specifications. Because the government bought so many products, testing helped improve the quality of not just light bulbs, but countless products from entire industries that wanted to sell to the government.

NIST is still gathering test data on lighting products. One of the major differences is that it's no longer incandescent light bulbs, but LEDs. We've all heard that LEDs are supposed to be able to burn for 50 000 hours or more, but how do we know that? Industry tests don't often simulate the way LEDs are used in real life, so NIST set up a test bed for LEDs to gather data to help improve models of their performance, leading to better products in the real world.

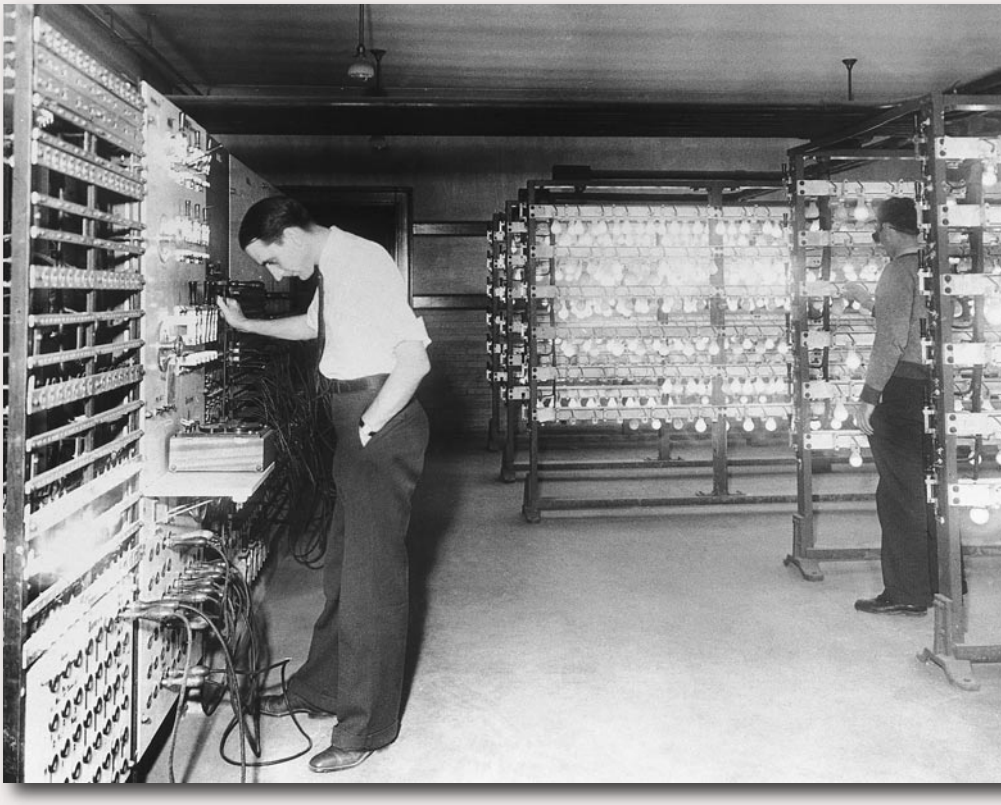
## Looking ahead

NIST's impact on the past 120 years has been considerable. Now a major thrust of NIST's work is to move NIST measurements out of our labs and put them directly in the hands of industrial and scientific researchers in the form of chip-based standards for not only voltage and electric current, but also time and temperature and a host of other quantities. The NIST on a Chip program promises to revolutionise the way standard measurements are made. Who knows? Perhaps this could be another turning point in NIST's history?

**Mark Esser** is a writer in the NIST Public Affairs Office and contributing editor of the blog Taking Measure. Reproduced from the NIST blog, www.nist.gov/blogs/taking-measure/1901-2021-measurements-then-and-now.



**The NIST-4 Kibble balance.** J. Lee/NIST



**An early NIST light bulb testbed.** NIST

# RACI members receive Queen's Birthday Honours

Two RACI Fellows were recently recognised in the 2021 Queen's Birthday Honours List: Emeritus Professor John B. Bremner and Professor Hugh J. Cornell.

John Bremner

Emeritus Professor John B. Bremner was awarded a Member of the Order of Australia (AM) for significant service to tertiary education, and to biomolecular science. A past President of the RACI Tasmanian Branch, he has held the position of emeritus professor at the University of Wollongong since 2008. His many areas of specialisation include organic and medicinal chemistry, the molecular basis of dyeing, and anti-cancer agents. He is also a current member of the University's Cancer Drug Research Team. He is involved as well in the development of a new anti-cancer drug formulation (Deflexifol), which is currently in the clinical trials phase.

Bremner received the RACI Adrien Albert Award in 2001 and was made a Distinguished Fellow in 2011. He is also a Fellow of the Royal Society of Chemistry (UK).

Bremner has been involved in research initiatives with many students and staff over the years and he is especially pleased to acknowledge all their terrific work and contributions. Chemistry is such an exciting area in which to work in both teaching and research and the frontiers are continuing to expand, particularly in cross-disciplinary contexts like medicinal chemistry.

He is continuing with other chemistry research collaborations and research writing, including a recently published book on multiple action-based design approaches to antibacterials. His other involvements cover the coordination and teaching of English as a second language through a long standing and free community-oriented activity of Corrimal Region Uniting Church. He has also assisted with extensive tutoring of students sitting for Occupational English Tests.

Hugh Cornell at RMIT University during the 1990s.

Honorary Life Member Professor Hugh Cornell was awarded an Order of Australia medal (OAM) for his contribution to research and education in the field of biochemistry. He has gained an international reputation in gluten toxicity in coeliac disease with his 42 papers in international journals. He is best known for his elucidation of the peptides from wheat protein A-gliadin, which are toxic to people with coeliac disease.

In 2001, he enlisted the aid of veterinary pathologist Dr Teodor Stelmasiak because he was interested in studying the digestive enzymes in animals that may provide the basis for enzyme therapy in people with coeliac disease. At the time, Teodor established the company Glutagen Pty. Ltd. with a view to commercialising products using the principle of enzyme therapy. Working with the plant enzyme caricain (from *Carica papaya*) was the next stage in development of Gluteguard, which was launched by Glutagen in 2016. Gluteguard is a supplement designed to guard against inadvertent gluten ingestion by gluten-sensitive individuals on a nominal gluten-free diet. It is enjoying much successs, with almost all users reporting a high degree of protection against gluten.

Together with Stelmasiak, Cornell has established enzyme therapy as a principle for better management of patients with sensitivity to gluten.

Cornell became an Associate member of RACI in 1952 and a Fellow in 1979, after obtaining his PhD from the University of Melbourne in 1972. He was promoted to associate professor when RMIT became a university in 1991 and upon retirement in 1997 became an adjunct professor. He extends his best wishes to all officials and members of RACI and at 90 years of age remains dedicated to his research and believing strongly that the profession of chemistry has served people and the planet very well. The cereal chemists of the Division of Cereal Chemistry are testimony to that!

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**Call for Abstracts open**

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## New Fellow

**David Hansen** is Head of Global Quality and Research and Development at SunRice, a leading Australian-owned rice food business. In this role, he is responsible for a number of technical functions, including food safety and quality, R&D, packaging technology, regulatory affairs and the SunRice corporate laboratory.

Hansen completed a BSc(Hons) in food science and technology at the University of New South Wales. His fourth-year project, supervised by Professor Ken Buckle, examined potential applications for high-protein fortification with flour from pigeon pea (*Cajanus cajan*). He later completed an MEngSc in manufacturing engineering also at the University of New South Wales and an MBA at Charles Sturt University, graduating with distinction.

Following graduation, Hansen commenced work at Sanitarium's Research and Development Centre, working in food microbiology and researching isolation of flat sour bacteria in low-acid foods before moving into product development. His work on UHT soy beverage products pioneered various novel functional ingredients, leading to the UP&GO beverage range.

Several positions in the food industry then followed, including quality, operations and supply chain management roles at Kellogg, Goodman Fielder, Dairy Farmers and General Mills. During a subsequent supply chain role at CHEP, Hansen completed the 18-month Brambles Executive Development Program at CEDEP (The European Centre for Executive Development) Fontainebleau, France.

Particular areas of professional interest include:

- operational risk and application of risk-based methodologies to food safety and quality risks
- food contaminants and control strategies
- principles of hygienic design and good manufacturing practice standards in food manufacturing
- food security, particularly enabling rice supply through the COVID-19 pandemic to Pacific markets.

Hansen has been a member of the RACI since 1994. He is passionate about encouraging STEM studies in schools and participated in the CSIRO Scientists in Schools program. He has also participated in NAWO (National Association of Women in Operations) events and has actively mentored many younger science and engineering graduates.

In 2004, David and his wife Kate, a public health physician, co-founded CLAN (Caring and Living as Neighbours) Child Health, a not-for-profit organisation focused on improving quality of life for children living with chronic health conditions in resource-poor settings (www.clanchildhealth.org).

# Congress 2022 Update

## Call for abstracts

On behalf of the Organising Committee, it gives me great pleasure to invite you to be part of the 2022 RACI National Congress, which will be held in Brisbane 3–8 July 2022.

Every five years, the RACI brings together chemistry professionals from across all its divisions, academia, industry and government to showcase the latest breakthroughs in our discipline, to explore new opportunities for collaboration and to network with preeminent members of the international chemistry community. The theme for the 2022 National Congress is 'Chemistry: catalysing solutions to global challenges'. As this indicates, we will engage members from all fields of chemistry in efforts to formulate genuine and sustainable solutions to our biggest global challenges, including alternative energy sources, climate change, food security and antibiotic resistance, through presentations and discussions.

The plenary sessions will include talks by world-acclaimed speakers:

- **Varinder K. Aggarwal**, University of Bristol, England
- **Maria Forsyth**, Deakin University, Australia
- **Sharon Hammes-Schiffer**, Yale University, USA
- **Thisbe Lindhorst**, University of Kiel, Otto Diels Institute of Organic Chemistry, Germany
- **Rodney S. Ruoff**, Institute for Basic Science, Republic of Korea
- **Carl Wieman**, Stanford University, USA
- **Vivian W.-W. Yam**, The University of Hong Kong, China.

**Abstract submissions are open.** I would like to invite you to submit an abstract for consideration as a poster or an oral presentation in one of the symposia.

- Oral presentations – 15 minutes to present and 4 minutes for audience questions.
- Poster presentations – Posters will be on display during the congress, with authors in attendance at a specified day/time.

Abstracts must be submitted by Monday 28 February 2022. For further information on abstract submission, please see the Abstracts page of our website www.raci2022.com or email the congress secretariat on raci2022@expertevents.com.au.

## Super early bird registration opens on 1 September.

We look forward to welcoming you to be part of the RACI National Congress in Brisbane in July 2022. We are sure that it will be an intellectually exciting and enjoyable event for all.

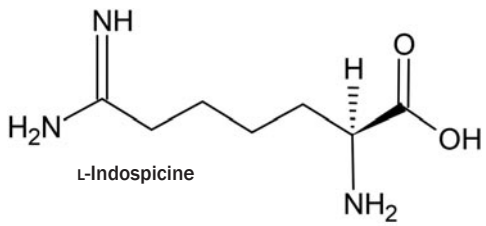
Professor Debra Bernhardt, Congress Chair

# Indospicine – not a dog's best friend

*Indigofera linnaei* Dinesh Valke/CC BY-SA 2.0

On 22 July 2021, *The Age* and some other Australian newspapers reported the death of at least 14 dogs in a region of eastern Victoria, as a result of indirectly ingesting a plant toxin, believed to be indospicine; as many as 45 dogs in the area suffered liver toxicity.

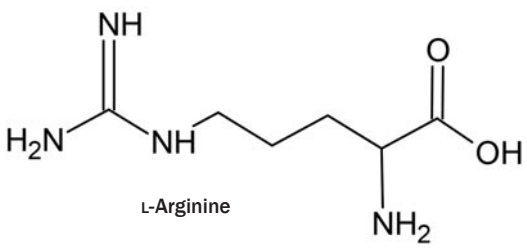
L-Indospicine is a non-proteinogenic hepatotoxic amino acid found in plants of the genus *Indigofera*, which grow in tropical Africa, Asia, Australia and the Americas.




L-Indospicine

*Indigofera linnaei* is native to northern Western Australia, where it is known as Birdsville indigo. *Indigofera australis* is an ornamental leguminous shrub, growing to about two metres, and is widespread in southern Australia and is commonly found in house gardens. It is not clear if it contains indospicine.

L-Indospicine is structurally related to the essential amino acid L-arginine, in which the NH is replaced by a methylene group, making L-indospicine an antagonist of L-arginine.




L-Arginine

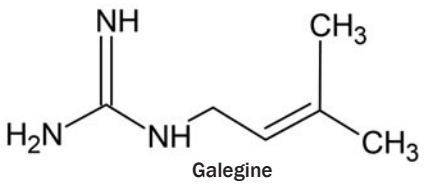
PrimeSafe and Agriculture Victoria scientists subsequently confirmed that indospicine is the toxic substance involved in the deaths and liver toxicity in dogs. Indospicine toxicity has never before been reported in Victoria.

Although dogs are unlikely to eat *Indigofera* plants of any species, they can indirectly ingest indospicine, which accumulates in the flesh of animals grazing on *Indigofera* species, when their meat is fed raw to dogs.

M. Hegarty and his group at the CSIRO Division of Tropical Pastures in Brisbane discovered indospicine in 1968, and explored its toxic effects, publishing their first paper 'Indospicine, a new hepatotoxic amino acid from *Indigofera spicata*' in *Nature* (1968, vol. 217, pp. 354–5).

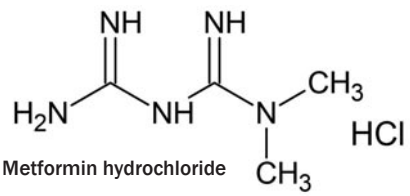
On 30 July, Victorian regulators announced in a joint statement that the indospicine in meat originated in horses that had grazed the toxic plant in the Northern Territory, before they were sent to Gippsland for slaughter. To date, 22 dogs have died and more than 40 dogs have developed serious liver disease.

In his Letter from Melbourne in the June–August issue, Ian Rae wrote about a European plant, *Galega officinalis* (French lilac and other names), the seeds of which contain the substance galegine. Galegine and L-arginine have the same guanidine end group, while indospicine has an amidine end group.




Galegine

Further research led to the pharmacologically more acceptable bisguanides. Metformin, a bisguanide, as the hydrochloride salt, remains the first line of treatment worldwide, for type 2 diabetes.




Metformin hydrochloride

**P.G. Lehman** FRACI CChem

# Unmasking the structure of an azasugar

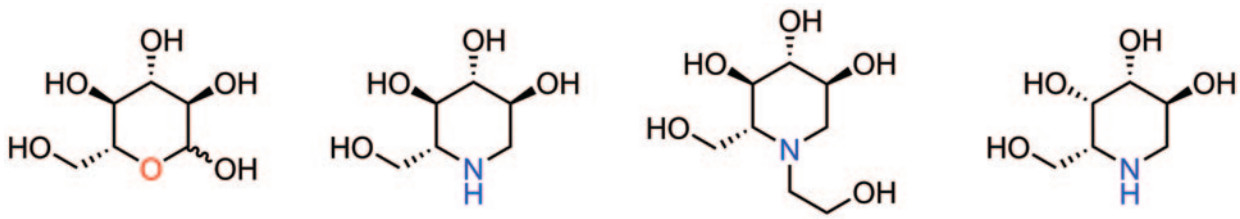

Yuhan Wendy Cun, PhD student, University of Wollongong

Azasugars are a class of organic compounds that are similar in structure to regular carbohydrates, except they have a nitrogen atom in the ring instead of the usual oxygen. This 'similar, but different' structure means that, compared with regular sugars, azasugars often have stronger affinities for glycosidases – enzymes that break glycosidic bonds of complex carbohydrates – because of the potential for protonating the nitrogen atom, affording a stronger interaction with the polar amino acids at the enzyme's active site.

This affinity is the guiding principle behind azasugar-based drugs such as Miglitol and Migalastat. Miglitol is a type 2 diabetes medication that prevents post-prandial blood sugar spikes by slowing the breakdown of complex carbohydrates. Migalastat is a medication for treating a rare genetic disorder known as Fabry's disease, characterised by a mutated form of α-galactosidase A; by binding to the defective enzyme and helping it fold correctly, the azasugar-based drug restores the enzyme's usual function and protects it from the cell's own enzyme mutation defences.

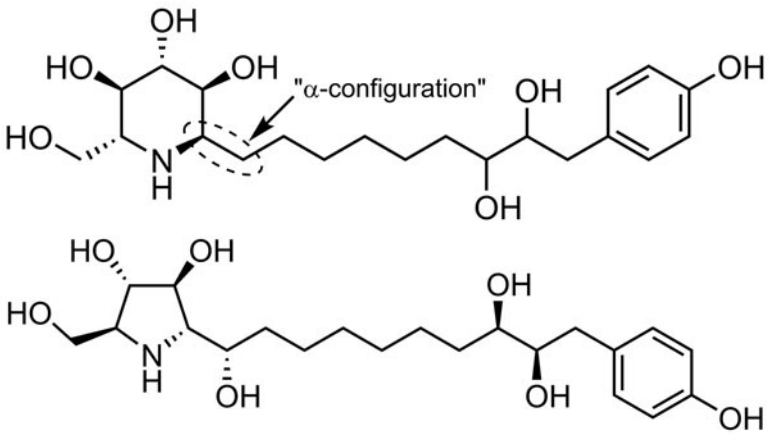
The many functional groups and stereogenic centres of azasugars often make their structures difficult to determine. Such was the case for glyphaeaside C: an azasugar isolated from *Glyphaea brevis*, a small tree native to the tropical regions of Africa (*Phytochemistry* 2015, vol. 109, pp. 76–83). At first, glyphaeaside C was believed to be a six-membered ring azasugar with the same configuration as D-glucose, with one of the hydroxy groups replaced with a long alkyl side chain. The α-configuration of the side chain would lead one to expect strong α-glucosidase inhibition, but glyphaeaside C was instead observed to be a strong β-glucosidase inhibitor. This discrepancy meant that either the side chain was playing an unexpectedly important role in determining the azasugar's enzyme selectivity or the originally proposed structure was incorrect.

Often, just isolating a compound from a natural source does not tell the full story and a total synthesis is required to unmask the compound's true structure. In




**Some examples of azasugars.**

**The many functional groups and stereogenic centres of azasugars often make their structures difficult to determine.**




**Glyphaeaside C structures, initially proposed (top) and corrected (bottom).**

the case of azasugars, their biological activities and basic spectroscopic data can tell us that a ring-bound nitrogen is present, but the carbon atoms that it is bonded to can be harder to deduce. A closer inspection of the NMR spectroscopy data led us to hypothesise that glyphaeaside C was in fact a five-membered ring azasugar. Our proposed structure could be obtained from the original by reattaching the nitrogen to a different carbon, thereby shifting the other carbon from the ring to the side chain, although the two structures cannot be interconverted as simply in practice.

To test our hypothesis, as part of my PhD project, we conducted a total synthesis of the five-membered ring structure by following and adapting procedures used by other groups to prepare related broussonetine azasugars, including a novel epoxide ring-opening reaction using a Gilman-like reagent. As it turns out, the NMR data of our proposed structure was a perfect match with the natural product, although it rotated polarised light in the opposite direction. This suggests that natural glyphaeaside C is the mirror image, or enantiomer, of the compound that we prepared. Like the broussonetines, our synthetic product was a strong β-glucosidase inhibitor, although noticeably weaker than the natural product. Although we are much closer to knowing the true structure of glyphaeaside C, there remains much to be unmasked about its interactions with glycosidases.

**Brendan Byatt** is a PhD student and **Stephen Pyne** FRACI CChem is a professor of chemistry at the University of Wollongong. This research was published in *Organic Letters* 2021, vol. 23, pp. 4029–33.

# An inconvenient pH

The control of the oceans' pH is dominated by that most important buffer bicarbonate, which also controls the pH of your blood and saliva.

## pH in the oceans

The average pH of unpolluted ocean surfaces is about 8.1, having decreased from an estimated 8.2 in pre-industrial times.

A drop in pH of 0.1 might seem trivial but a logarithmic scale such as that used to represent pH distorts by compressing large numbers and expanding small ones. It is needed for scales that cover a range of magnitudes (such as the decibel, lumen, and Richter scales), but for chemical calculations, absolute concentrations are required.

If a decrease in pH of 0.1 in the ocean is reported as a 26% decrease, then lemon juice (pH 2), is 30 000% more acidic than soda water (pH 4.5).

When seawater begins to evaporate at the edge of drying ocean pools, the white stuff that you see is not (as most believe) common salt (the overwhelmingly major solute of oceans); first, it is limestone (when roughly 50% of the water has evaporated) and then gypsum (when 80–90% of the water has evaporated), and only then do lovely clear cubic crystals of common salt form (when 85–95% of the water has evaporated).

Salt from seawater is traditionally purified by evaporating the water from a succession of pumped or gravity-fed pools of increasing salinity to first separate out the less desirable, less soluble salts (see Maxwell I.A., *Chem. Aust.* December 2014–January 2015, pp. 36–37).

## More $CO_2$ in the atmosphere

Increasing atmospheric $CO_2$ from fossil fuels means more $CO_2$ will eventually dissolve in the rivers and oceans. 'Increased acidity' suggests a pH less than 7, so 'reduced alkalinity' is clearer.

Unlike other acids, $CO_2$ has a dual role; it also supplies a common ion, namely carbonate.

### Limestone caves – a freshwater situation

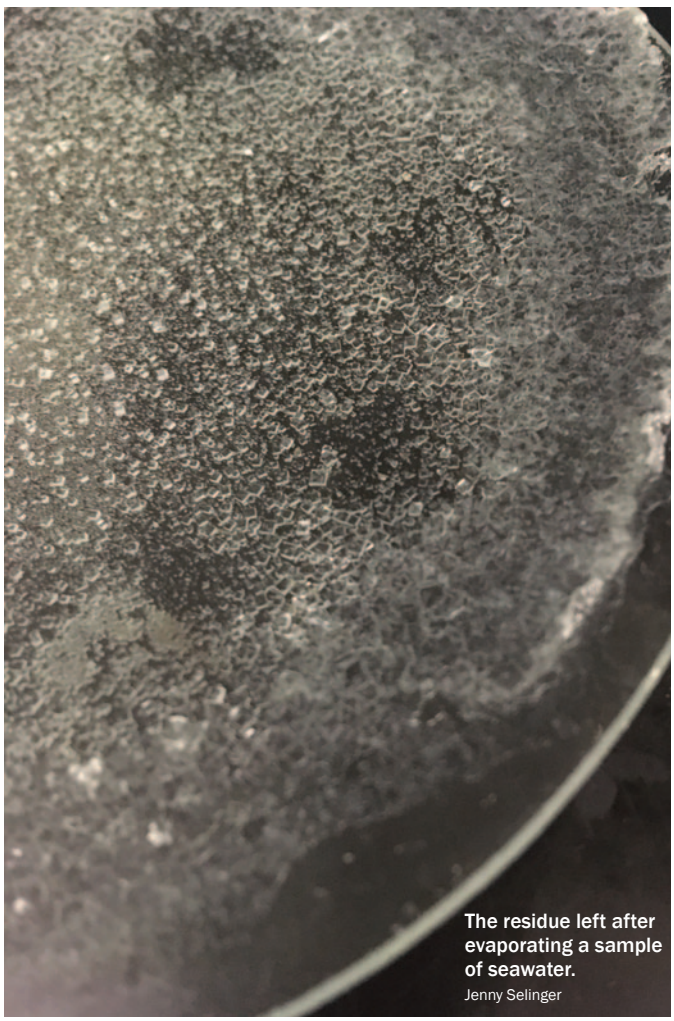
The fresh water that enters limestone caves is initially unbuffered.

This rainwater laden with aqueous $CO_2$ (0.035%, pH around 5.3) percolates through the soil and picks up much more $CO_2$ from plant roots and decaying vegetable matter (0.15–0.65%), becoming more acidic. This brew extracts calcium carbonate and relocates it (via bicarbonate) to the inside of the caves. Stalactites and stalagmites are formed. The newly added bicarbonate buffers the acid, and the pH increases to 7.2–7.8 (bit.ly/3xlfpPe). This water feeds underground rivers and releases $CO_2$ gas. This can accumulate to toxic levels in the bottom of caves.

Lake Nyos in Cameroon had a natural store of water that is supersaturated with $CO_2$ at its base. This $CO_2$ rose to the surface in August 1986, bubbled out and spread overland, killing 1746 people and 3500 livestock.

Fast forward to current experiments with underground storage of $CO_2$ in porous rock (bit.ly/2V1FMg5) ... is it a long-term solution?

Because of a very high concentration of spectator ions such as sodium in seawater, calcium carbonate is at least 60 times more soluble than it is in fresh water.

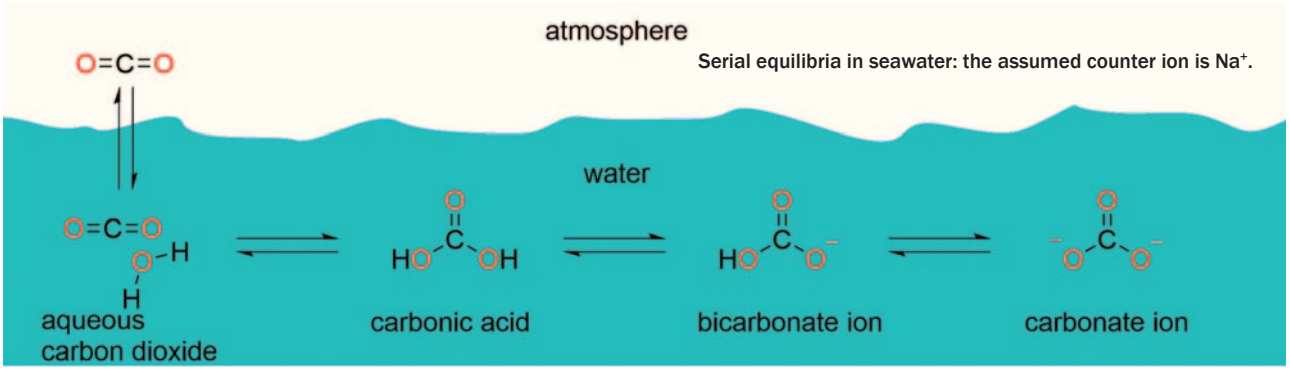


**The residue left after evaporating a sample of seawater.**
Jenny Selinger

## Ocean equilibria

The following diagrams display prevalence of species and serial equilibria in seawater.

What is a common ion? In the top diagram, you can see that adding $CO_2$ shifts the equilibrium to the right but adding carbonic acid shifts the equilibrium to the left. These opposing actions roughly balance until the pH eventually drops to about 7 where bicarbonate buffering fails significantly (see graph).




Serial equilibria in seawater: the assumed counter ion is $Na^+$.

## Activity fudge factors

Because of a multitude of interactions in solution mixtures, chemical species behave experimentally as if they are at a different (often lower) concentration from the actual concentration (bit.ly/37U7Zb8). This is non-ideal.

A century ago, a factor called the *activity*, was introduced; activity is determined experimentally to correct for these 'anomalies' (stanford.io/3rNeJAI). A parallel is suggested for a team sport, where substituting a player of apparent equivalent ability, or changing the nature of the spectators, can unpredictably and mightily, change team dynamics and performance.

Any change in the composition of (sea)water, natural or artificial, changes all the activities, including the solubility of calcium carbonate.

Simple activity calculations predict that the solubility product $K_{sp}(CaCO_3)$ is $5.4 \times 10^{-7}$ in seawater at pH 8.1, but is $8.7 \times 10^{-9}$ in fresh water – about 60 times lower. Kinetic control (e.g. rates of precipitation and dissolution), rather than thermodynamic control, is determinant. Tough stuff.

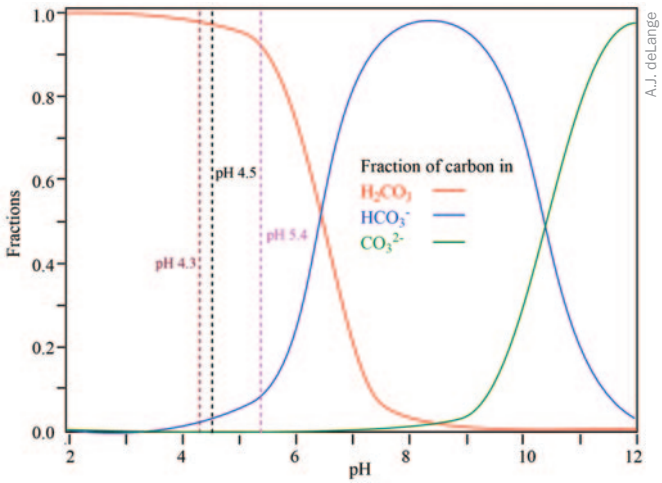
Many other factors, including local pollutants, can play a large (sometimes unintentional) role.

## Oysters, corals and carbonate

The chemistry of the oceans is very complicated; biochemical processes involving enzyme-mediated reactions are even more complicated. Organisms adapt differently to changing environmental stress; there are winners and losers from Darwinian pressure (bit.ly/3iVNbq6).

In some parts of the ocean, natural pH fluctuates substantially. Some corals can protect themselves from fluctuating pH because they control their internal pH environment, so adding excess $CO_2$ to seawater around these corals has no effect on their survival. A good example is the corals on Heron Island in the Great Barrier Reef (go.nature.com/3jc0v8D). Oysters build their carbonate–protein-layered shells (and pearls) biochemically, from the inside out, while controlling their internal pH at 6.8.

Why would ocean organisms choose the hard-to-get carbonate rather than the dominant highly soluble bicarbonate as their source? This is still being investigated, but it has been reported that some control their internal pH independent of the oceans, as well as utilising both bicarbonate and carbonate (bit.ly/37eEQqR).




A.J. deLange

**Prevalence of species in seawater: fraction of inorganic carbon as aqueous $CO_2$, baking soda and washing soda as a function of pH, based on the buffer equation:**

$$pH = pK_a + \log([\text{basic form}]/[\text{acidic form}])$$

Ocean warming transfers $CO_2$ from the oceans to the atmosphere, which helps the former but harms the latter. Increased temperature *reduces* the solubility of solid calcium carbonate. Increased pressure, as with increasing ocean depth, *increases* its solubility.

The severe negative consequences of increased $CO_2$ in the atmosphere aligns with centuries-old accepted physical chemical principles.

But a hyped threat from a pH drop in the Great Barrier Reef does not make any chemical sense.

Sit, as I have, in a limestone cave and watch the pH 7.6 bicarbonate-buffered water flow down and drip, whereby the formations slowly grow, not shrink.

In the words of US journalist Henry Mencken (1880–1956): 'For any complicated problem there is a simple solution that is wrong'. We ignore basic STEM topics … pH, equilibria, buffers, activity and particularly biology and biochemistry … at our peril.

**Ben Selinger** FRACI CChem is Emeritus Professor of Chemistry at ANU and, along with ANU colleague Associate Professor Russell Barrow, released the sixth edition of *Chemistry in the marketplace* (CSIRO Publishing) in June 2017. For more information, visit www.publish.csiro.au/book/7366. Ben guided at Jenolan (limestone) caves (NSW) in 1961 as a university summer vacation job. This article owes a major debt to Ray Hodges for his industrial experience and support. As always, Ian Rae played his crucial role as devil's chemical advocate. Scott Kable and others watched out for chemical incorrectness. Any misinterpretations are mine.

# Vegan-friendly wines

**Yeast on Pinot Noir grapes.** Mark Smith/CC BY 2.0

Over the last year, I have noticed an increase in the promotion of wines as 'vegan friendly' or 'suitable for vegans'. In a recent tasting that I led on white wines of the Loire Valley, all 12 wines were marked as 'vegan friendly', with the blatant contradiction for one wine that was also described as 'brilliantly paired with foie gras'! It is difficult to determine the size of this market in Australia. It is, however, clear that several of our wine export markets are to countries where there is a marked movement to veganism: see, for example, the article by Ellie Douglas in *Decanter* of January this year (bit.ly/2V7KJ6v).

It may seem surprising at first that not all wines are 'vegan friendly', given that wine is made by fermentation of grapes and finishing up in a bottle, cask or can. The critical point is the use of animal-based protein processing aids to manipulate the taste profile of the wine or to clarify or stabilise the wine. In current winemaking practice, processing aids include gelatine, sourced from either bovine or porcine collagen; isinglass, sourced from fish swim bladder; egg white; and milk, either fresh or powdered casein. One of my old French winemaking books included a recipe for the use of powdered bull's blood, fortunately a procedure that is no longer permitted.

About 40 processing aids and 19 additives are approved for use in Australia (see bit.ly/3eTNHma for the full list). This has raised the question of whether all additives and processing aids used for a particular wine should be included on the label. The only mandatory items to list are allergens, including milk and eggs. An ABC online news article in February this year (ab.co/3eTNE9Y) posed the question of whether all ingredients should be listed. Although there is a need for consumers to be fully aware, winemakers are committed to following the winemaking code. Should a wine company be charged with a breach of the code, this would lead to a loss of consumer confidence in the product and affect market position.

When I started writing this column, I had three strategies in mind to address the concerns of vegans. The first is patience in the winemaking process. If a wine is stored on fine lees, that is after the freshly fermented wine is racked off the larger or gross lees, the wine becomes softer with a fuller mouthfeel. This works well for white wines in particular, allowing clarity of fruit expression. As one Loire winemaker commented, 'we use nine months on fine lees … searching for a pure expression of fruit reflecting the terroir'. No additives are used. However, patience and cash flow, the driving force of company accountants, are in conflict so the process is not widely used.

Plant proteins, as potential replacements for animal proteins, had a slow start in establishing their potential for use in winemaking. However, over the last 20 or so years, there has been extensive work on their suitability in both red and white winemaking. A 2019 review by the oenology group at the University of Padova presents an excellent summary (*Molecules* 2019, vol. 24, p. 2186). Gluten, extracted from cereal, shows some effect for softening red wines by removing phenolic compounds that lead to astringency. Its major limitation is the complex preparation of the gluten and the lack of consistency in its composition. Its use must also be declared as an allergen. Maize zeins and rice proteins have shown promise but have not been widely investigated. Patatin P from potatoes is effective in white wine and is available commercially (bit.ly/3rxWz64). Regulatory approval has been obtained in some countries. Grape seed extract is perhaps the most effective plant-based protein that has been trialled. Despite its 'natural' characteristics, it is not commercially available and lacks approval in many markets.

My third strategy was to suggest natural wines as the way to go for 'vegan friendly'. Natural wines are made with no or minimal intervention in the winemaking process. The classic example is the Pétillant-Naturel (or Pét-Nat) wines that are now readily available in Australia. This style of sparkling wine is made by the Méthode Ancestrale (ancestral method), regarded by many as the oldest sparkling winemaking method. Fermentation commences in a tank, and, at some point, the wine is transferred to bottle to finish. This results in a sparkling, albeit cloudy, wine that can be amazingly refreshing. There is no secondary fermentation and no additives – the yeast is indigenous to the grape. This is pretty much grapes into wine with minimal human intervention.

At a recent tasting that I attended, one participant asked whether yeast is acceptable to vegans. For most vegans, yeast is clearly acceptable. It is a single-celled fungus that is widespread on plants (bit.ly/2W77jfZ). Critical for yeast's acceptance to vegans is that it has no central nervous system, meaning that it cannot experience pain or suffering. There are, however, some vegans, so-called level 5 vegans, who refuse yeast because it is a 'living ingredient' (bit.ly/3zx6s6H). It is a challenge to satisfy everyone.

**Geoffrey R. Scollary** FRACI CChem (scollary45@gmail.com) has been associated with the wine industry in production, teaching and research for the last 40 years. He now continues his wine research and writing at the University of Melbourne and the National Wine and Grape Industry Centre at Charles Sturt University.

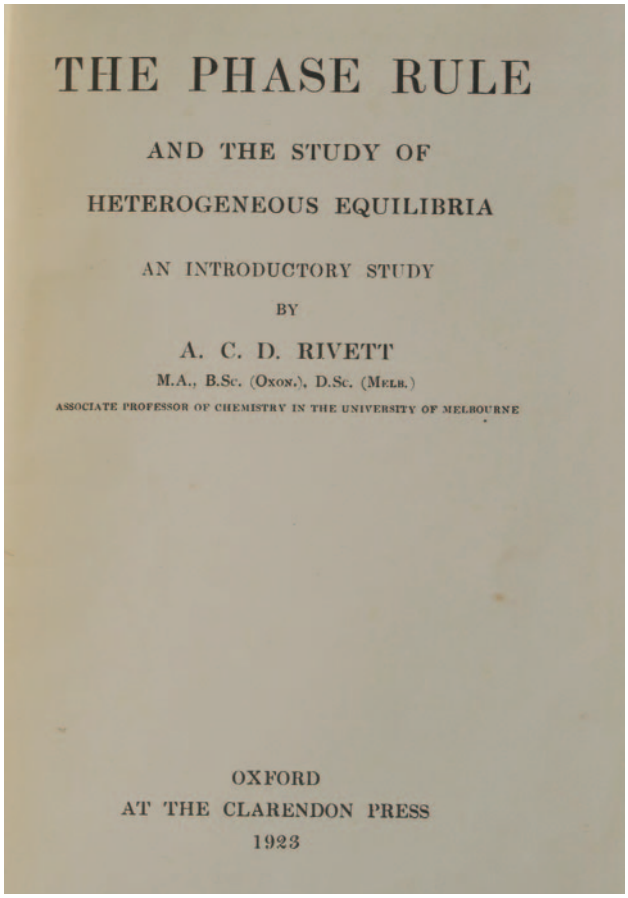
# Learning during lockdown

The lockdowns of 2020 and 2021 put libraries out of reach for weeks on end, and although my local library had a 'mail out' service, and the University of Melbourne did, too, I turned to my own library to re-read some of the volumes on my shelves. There were some books that I'd bought with good intentions but never actually read, an example being *Physical chemistry from Ostwald to Pauling. The making of a science in America*. I had acquired it as a reference work but what I found was a rollicking tale of the transfer of ideas, of personal rivalries and of eccentricity.

The ideas of Ostwald (1852–1932), van't Hoff (1852–1911) and Arrhenius (1859–1927) came together in the theory of electrolytic dissociation of salts in solution, with most of the relevant experimental work being carried out in Ostwald's laboratory in Leipzig. The European founders of this discipline of physical chemistry were known as 'ionists' and their American disciples served under the same flag. Of the more than 40 Americans who came to work with Ostwald, the most prominent was Arthur Amos Noyes (1866–1936), who was there in 1888–89, and who later cemented the trans-Atlantic link by sending many of the students he trained at MIT in Cambridge, Massachusetts, to follow in his footsteps.

The ionists held that dissolving a salt AB gave rise to ions such as $A^+$ and $B^-$, and gave rise to properties that depended on the number of particles in solution, such as osmotic pressure, elevation of boiling point and depression of freezing point, all coming under Raoult's law. This worked well for very dilute solutions, but for stronger solutions the effects were less than simple ionic theory would predict, raising questions about the degree of dissociation and requiring the use of fudge factors such as activity coefficients. Europeans and many American physical chemists accepted the challenge and devised theories to account for the bad behaviour of their solutions. British academic chemists, led by Henry Edward Armstrong (1848–1937), dismissed the whole idea of dissociation as nonsense, so classical physical chemistry was slow to develop in Britain. There was also an alternative stream of thought in the US, championed by Wilder Bancroft at Cornell University, who kept clear of ions to concentrate on the phase rule and colloid chemistry. His bias was evident in the subjects of papers published in the *Journal of Physical Chemistry* that he founded and edited. In 1932, it was taken over by the American Chemical Society and adopted a more catholic editorial stance.

In the first half of the 20th century, chemistry at the University of Melbourne was classical physical chemistry of this type and its influence was still evident when I was an undergraduate there in the late 1950s. David Orme Masson, when he had finished organising science in Australia and retired from the Melbourne chair in 1923, rediscovered his interest in solutions and addressed the 1935 ANZAAS Congress in Melbourne on 'The Molecular Condition of Aqueous Solutions of Acids, Alkalis and Salts'. He addressed the issues of partial ionisation and ionic mobility, two of the grand themes of the previous five decades. Ion mobility led him to consider the idea of 'condensed ions' in solution, such that sodium chloride might give rise to a single chloride ion and the cation $Na_2Cl^+$, only some of which might be completely dissociated. 'Other explanations seem possible', he wrote, 'and this aspect of the problem need not be discussed further at present'.


THE PHASE RULE

AND THE STUDY OF

HETEROGENEOUS EQUILIBRIA

AN INTRODUCTORY STUDY

BY

A. C. D. RIVETT

M.A., B.Sc. (Oxon.), D.Sc. (Melb.)

ASSOCIATE PROFESSOR OF CHEMISTRY IN THE UNIVERSITY OF MELBOURNE

OXFORD

AT THE CLARENDON PRESS

1923

David Rivett, Masson's successor (1923–27), before he went off to head CSIR, was more interested in the phase rule, and he turned his experience of making ammonium nitrate in Britain in the war years, and his subsequent lectures at Melbourne, into a book in which he mentioned in his Introduction the work of many others, including Bancroft. Rivett was succeeded in turn by Ernst Hartung, whose specialties included colloids and the properties of membranes. The phase rule refused to die, however, and when young Bernard Cavanagh was appointed to replace Rivett, he had never heard of the phase rule until he came to Melbourne and did not enjoy the experience of teaching it. Neither did his students, according to Joan Radford's 1978 history of the department. His research on activity coefficients, partition coefficients and potentiometric titrations, however, must have gladdened Masson's heart.

**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 is an editor of *Historical Records of Australian Science*.

## events

For further details, visit raci.org.au/events.

**Careers in Drug Development, Past and Future**
8 September, Sydney, NSW

**RACI Margaret Sheil Leadership Award Lecture**
14 September, webinar

**RACI Mentoring Program**
16 September, webinar
21 October, webinar
18 November, webinar

**Early Career Chemists Events**
23 September, webinar
30 September, webinar
28 October, webinar
25 November, webinar

**The Future of Material Science Festival**
30 September, Adelaide, SA

**Chemraderie**
7 October, webinar
4 November, webinar
2 December, webinar

**Ask Me Anything**
14 October, webinar

**Intensive Careers Workshop**
15–23 October, online workshop

**Careers Hack**
11 November, webinar

**2021 NSW Branch President's Dinner**
19 November, Concord, NSW

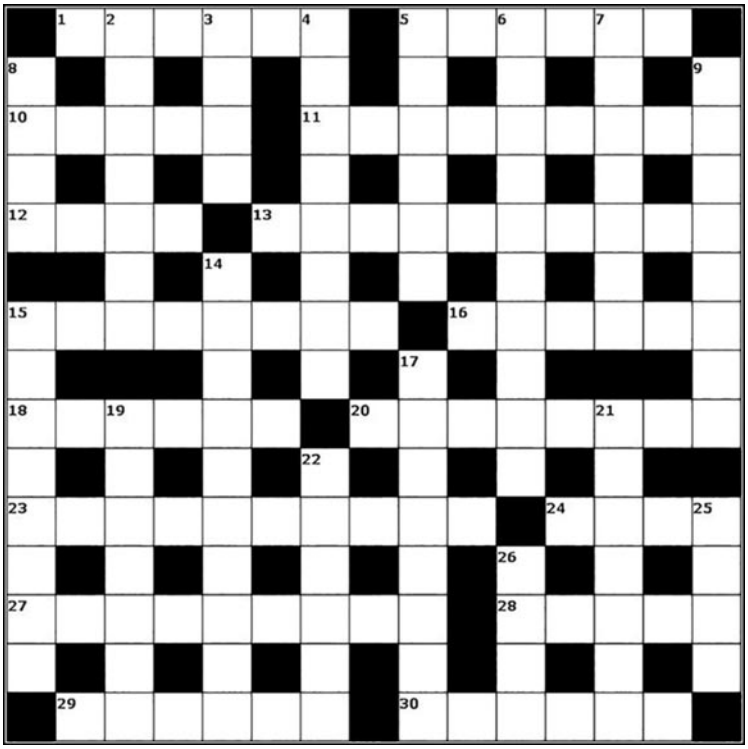
**Intensive Careers Workshop**
26 November – 4 December

**Queensland Annual Chemistry Symposium**
26 November, Gold Coast, Qld

**Chemistry Teachers Professional Development Day**
30 November, Melbourne, Vic.



## cryptic chemistry



**Across**

**1** Bundles 167361916. (6)
**5** Near the end plasma laboratory studied atomic beam frequency seconds. (6)
**10** Second side in hot water. (5)
**11** Clue X-ions bring about separation. (9)
**12 & 25 Down** Authentic role of *a* for the complex number *a* + *bi*. (4,4)
**13** To the hilt, ran zoo flat out. (10)
**15** Novel dye held a common functional group. (8)
**16** Privileged unknown. (6)
**18** The first Occam's Razor yielded a coherent group of tested general propositions. (6)
**20** Rant: visa distributed COVID-19 problems. (8)
**23** Do metallic elements get lined up? (10)
**24** Three elements make move forward. (4)
**27** Spelling out flame roast ring. (9)
**28** Boo-boo in reversing mirror reflection. (5)
**29** Tentatively schedule in return treatment of embolic nephritis. (6)
**30** Reliable shelter, . . . . (6)

**Down**

**2** ... then a research and development start-up, discovered hydrogen peroxide. (7)
**3** 68 megabyte search. (4)
**4** Is sorted for compounds based on the cyclopenta[*a*]phenanthrene carbon skeleton. (8)
**5** Turn shellac for Spooner acid! (6)
**6** True atomic change relating to the reversible interconversion of structural isomers. (10)
**7** See 26 Down.
**8** Consumer addict. (4)
**9** Powerful nucleophiles coming up set alone. (8)
**14** Rich mine to deliver hot electrode emission. (10)
**15** Stuck on new data tech. (8)
**17** Wet rags a product of passing 10 Across over red-hot coke. (5,3)
**19** See pill made using a conic section. (7)
**21** Unaffected organic? (7)
**22** Use the telephone after an intensely radioactive metallic element moves out from the centre. (6)
**25** See 12 Across.
**26 & 7 Down** It could be a better time for carbon-14, as an example. (4,7)

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

# Professional development – message from the Board

We've all enjoyed the professional development activities that COVID-19 has foisted upon us. From expanding our technical knowledge of viruses, testing, and the development of vaccines, through to learning how to communicate remotely, COVID-19 has provided us with an extravaganza of opportunities to learn new skills and take in new information, but it should not stop here. As a professional society, the RACI represents and caters for the needs of all of our members as a priority, whether that's for a first-year graduate or a retiree who still has an active interest in chemistry. Our services and activities range from professional and career development across all chemical sciences and employment sectors, through to regular and engaging networking opportunities, but the opportunity always exist to improve.

That's why we're getting in touch with you. We'd like to hear from you, as one of our members, about what professional development activities you would like the RACI to engage in and deliver. It need not be just about the chemical sciences, but other skills we all have to develop and use, such as business and leadership, entrepreneurship, design thinking, project management, quality management, and digital skills.

Please complete our two-minute professional development survey at www.surveymonkey.com/r/CWCP5ZS and/or send your thoughts to RGStapleford@raci.org.au.

The survey will close on 15 September 2021.

Of course, we know a lot of our members already deliver training in a variety of areas. We're also looking to engage with you about any of your existing professional development offerings that we could deliver in partnership with your organisation to address a membership need.

Please send your ideas to RGStapleford@raci.org.au.

Thank you for continuing to support RACI and we hope you are as excited as we are about this new initiative.

On behalf of the RACI Board,
Roger Stapleford, CEO RACI

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