A closer look at contrails  • Studying over the summer months
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This year in chemistry
In this final issue for 2015, we take a look back at some events and activities in chemistry and other science.

cover story
Contrails: the making of a chemical cocktail
Researchers have been studying contrails since the world wars. What do we know about this very visible phenomenon of physical chemistry?
Science as a state of mind

Although I have spent the vast majority of my professional time in publishing, I still think of myself first and foremost as a scientist. Science research filled my working hours for just a few years, so why do I persist in seeing myself in this light? The answer is in my way of thinking. To me, the mindset of science reaches beyond profession; it’s a way of looking at everything.

Science and me

I like working with information, not equipment. My mind is far more at home amongst words and pictures than amidst laboratory apparatus. So in the mid-1990s I left my lab life as a research chemist to move into publishing. I switched to science editing, so it stands to reason that I took my knowledge of science along with me.

In this new career, however, I found that I continued to do something often attributed to scientists – the habit of asking: ‘Why?’ ‘How?’ and ‘What if?’ A publishing colleague once complimented me on my ‘fine analytical mind’ – I am good at figuring out why a manuscript is or isn’t working, what is missing and how the different parts can best be arranged. This ‘science thinking’ came along for the ride and it continues to serve me well.

Science sticks – so do stereotypes

What my colleague recognised as an asset – and it certainly is in publishing – can also be a liability. Some people can see me as doubting or untrusting, because I might not take something at face value; I want to get to the bottom of things. At times I tame this tendency in ‘polite’ company, reining in my questioning where it might not be welcomed. It would be nice if more people could understand where I’m coming from.

Compounding this problem is that the stereotype of scientists as boring or aloof is alive and well. My partner and I are both sciencey people, and we’re both familiar with the awkward silence that follows your admission at a social gathering that you’re a scientist.

It seems odd then that we, and not our non-sciencey friends, are the ones asking ‘Why?’ and ‘How?’ in the course of conversation. We are breaching our ‘boring’ stereotype. They are clever, well-educated and articulate, but they’re just not that curious about how the natural world works.

Is this questioning frame of mind the font of science? Yes – but I think that it’s not, nor should it be seen as, exclusive to science.

Critical thinking – nature or nurture?

Critical thinking needs to be rebagged to reflect what it really is, to demystify it and to decouple it from science. Calling it creative thinking, questioning or knowledge-seeking might give it a better chance of success. (I think we’d best avoid ‘scepticism’, which is often assumed to be a negative thing these days, even though scientific scepticism is at the core of scientific method.)

My bet is that a tendency to think like this is a mixture of genetics and environment.

Fostering life-long curiosity

Children are innately curious; they test things out and over time, they increase and modify their knowledge and understanding. As they grow we can foster this habit and show them that what they are doing is not just about science. Scientist or not, they will develop a mindset that affords immense freedom (except, perhaps, at dinner parties).

My daughter says to me that she wants to be a naturalist when she grows up. I look at her, and her passion for observing nature, and tell her that she is a naturalist already. I really hope she believes me.

This article was originally published at Women in Science Australia. Read the original article at www.womeninscienceaust.org.

Sally Woollett (editor@raci.org.au)
For particle physics this was a historic discovery. Its standard model of the innermost workings of matter had been incredibly successful, having resisted all experimental challenges for more than 20 years. However, as it requires neutrinos to be massless, the new observations had clearly shown that the standard model cannot be the complete theory of the fundamental constituents of the universe.

The discovery rewarded with this year’s Nobel Prize in Physics has yielded crucial insights into the all but hidden world of neutrinos. After photons, the particles of light, neutrinos are the most numerous in the entire cosmos. The Earth is constantly bombarded by them.

Many neutrinos are created in reactions between cosmic radiation and the Earth’s atmosphere. Others are produced in nuclear reactions inside the Sun. Thousands of billions of neutrinos are streaming through our bodies each second. Hardly anything can stop them passing; neutrinos are nature’s most elusive elementary particles.

The experiments continue and intense activity is underway worldwide in order to capture neutrinos and examine their properties. New discoveries about their deepest secrets are expected to change our current understanding of the history, structure and future fate of the universe.
Physiology or Medicine: transforming treatment of parasitic disease

The Nobel Assembly at Karolinska Institutet has decided to award the 2015 Nobel Prize in Physiology or Medicine with one half jointly to William C. Campbell and Satoshi Ōmura for their discoveries concerning a novel therapy against infections caused by roundworm parasites and the other half to Youyou Tu for her discoveries concerning a novel therapy against malaria.

Diseases caused by parasites have plagued humankind for millennia and constitute a major global health problem. In particular, parasitic diseases affect the world’s poorest populations and represent a huge barrier to improving human health and wellbeing. This year’s Nobel Laureates have developed therapies that have revolutionised the treatment of some of the most devastating parasitic diseases.

William C. Campbell and Satoshi Ōmura discovered a new drug, avermectin, the derivatives of which have radically lowered the incidence of river blindness and lymphatic filariasis, as well as showing efficacy against an expanding number of other parasitic diseases. Youyou Tu discovered artemisinin, a drug that has significantly reduced the mortality rates for patients with malaria.

These two discoveries have provided humankind with powerful new means to combat these debilitating diseases that affect hundreds of millions of people annually. The consequences in terms of improved human health and reduced suffering are immeasurable.

We live in a biologically complex world, which is populated not only by humans and other large animals, but also by a plethora of other organisms, some of which are harmful or deadly to us.

A variety of parasites cause disease. A medically important group are the parasitic worms (helminths), which are estimated to afflict one-third of the world’s population and are particularly prevalent in sub-Saharan Africa, South Asia and Central and South America. River blindness and lymphatic filariasis are two diseases caused by parasitic worms. As the name implies, river blindness (onchocerciasis) ultimately leads to blindness, because of chronic inflammation in the cornea. Lymphatic filariasis, afflicting more than 100 million people, causes chronic swelling and leads to life-long stigmatising and disabling clinical symptoms, including elephantiasis (lymphedema) and scrotal hydrocele.

Malaria has been with humankind for as long as we know. It is a mosquito-borne disease caused by single-cell parasites, which invade red blood cells, causing fever, and in severe cases brain damage and death. More than 3.4 billion of the world’s

Satoshi Ōmura searched for novel strains of Streptomyces bacteria as a source for new bioactive compounds. He isolated microbes from soil samples in Japan, cultured them in the laboratory and characterised many thousands of Streptomyces cultures. From those, he selected around 50 cultures that appeared most promising, and one of these cultures later turned out to be Streptomyces avermitilis (pictured), the source of avermectin.

About the Nobel laureates

**Takaaki Kajita** was born in 1959 in Higashimatsuyama, Japan. He holds a PhD (1986) from the University of Tokyo, where he is the Director of Institute for Cosmic Ray Research and Professor.

**Arthur B. McDonald** was born in 1943 in Sydney, Canada. He holds a PhD (1969) from California Institute of Technology. He is Professor Emeritus at Queen’s University, Kingston, Canada.

**William C. Campbell** was born in 1930 in Ramelton, Ireland. After receiving a BA from Trinity College, University of Dublin, Ireland, in 1952, he received a PhD from University of Wisconsin, Madison, USA, in 1957. From 1957 to 1990 he was with the Merck Institute for Therapeutic Research, from 1984 to 1990 as Senior Scientist and Director for Assay Research and Development. Campbell is currently a Research Fellow Emeritus at Drew University, Madison, New Jersey.
most vulnerable citizens are at risk of contracting Malaria, and each year it claims more than 450,000 lives, predominantly among children.

After decades of limited progress in developing durable therapies for parasitic diseases, the discoveries by this year’s Laureates radically changed the situation.

Satoshi Ōmura, a Japanese microbiologist and expert in isolating natural products, focused on a group of bacteria, *Streptomyces*, which lives in the soil and was known to produce a plethora of agents with antibacterial activities (including streptomycin discovered by Selman Waksman, Nobel Prize 1952). Equipped with extraordinary skills in developing unique methods for large-scale culturing and characterisation of these bacteria, Ōmura isolated new strains of *Streptomyces* from soil samples and successfully cultured them in the laboratory. From many thousand different cultures, he selected about 50 of the most promising, with the intent that they would be further analysed for their activity against harmful microorganisms.

William C. Campbell, an expert in parasite biology working in the US, acquired Ōmura’s *Streptomyces* cultures and explored their efficacy. Campbell showed that a component from one of the cultures was remarkably effective against parasites in domestic and farm animals. The bioactive agent was purified and named avermectin, which was subsequently chemically modified to a more effective compound, ivermectin. Ivermectin was later tested in humans with parasitic infections and effectively killed parasite larvae (microfilaria). Collectively, Ōmura’s and Campbell’s contributions led to the discovery of a new class of drugs with extraordinary efficacy against parasitic diseases.

Malaria was traditionally treated by chloroquine or quinine, but with declining success. By the late 1960s, efforts to eradicate malaria had failed and the disease was on the rise. At that time, Youyou Tu in China turned to traditional herbal medicine to tackle the challenge of developing novel malaria therapies. From a large-scale screen of herbal remedies in malaria-infected animals, an extract from the plant *Artemisia annua* emerged as an interesting candidate. However, the results were inconsistent, so Tu revisited the ancient literature and discovered clues that guided her in her quest to successfully extract the active component from *Artemisia annua*. Tu was the first to show that this component, later called artemisinin, was highly effective against the malaria parasite, both in infected animals and in humans. Artemisinin represents

**Satoshi Ōmura** was born in 1935 in the Yamanashi Prefecture, Japan, and is a Japanese citizen. He received a PhD in Pharmaceutical Sciences in 1968 from University of Tokyo and a PhD in Chemistry in 1970 from Tokyo University of Science. He was a researcher at the Kitasato Institute, Japan from 1965 to 1971 and Professor at Kitasato University, Japan from 1975 to 2007. Since 2007, Satoshi Omura has been Professor Emeritus at Kitasato University.

**Youyou Tu** was born in 1930 in China and is a Chinese citizen. She graduated from the Pharmacy Department at Beijing Medical University in 1955. From 1965 to 1978 she was Assistant Professor at the China Academy of Traditional Chinese Medicine, from 1979 to 1984 Associate Professor and from 1985 Professor at the same Institute. From 2000, Tu has been Chief Professor at the China Academy of Traditional Chinese Medicine.
a new class of antimalarial agents that rapidly kill the malaria parasites at an early stage of their development, which explains its unprecedented potency in the treatment of severe malaria.

The discoveries of avermectin and artemisinin have fundamentally changed the treatment of parasitic diseases. Today the avermectin-derivative ivermectin is used in all parts of the world that are plagued by parasitic diseases. Ivermectin is highly effective against a range of parasites, has limited side effects and is freely available across the globe. The importance of ivermectin for improving the health and wellbeing of millions of individuals with river blindness and lymphatic filariasis, primarily in the poorest regions of the world, is immeasurable. Treatment is so successful that these diseases are on the verge of eradication, which would be a major feat in the medical history of humankind. Malaria infects close to 200 million individuals yearly. Artemisinin is used in all malaria-ridden parts of the world. When used in combination therapy, it is estimated to reduce mortality from malaria by more than 20% overall and by more than 30% in children. For Africa alone, this means that more than 100,000 lives are saved each year.

The discoveries of avermectin and artemisinin have revolutionised therapy for patients suffering from devastating parasitic diseases. Campbell, Ōmura and Tu have transformed the treatment of parasitic diseases. The global impact of their discoveries and the resulting benefit to mankind are immeasurable.

Nobel Media

Probing the reaction between carbon dioxide and water

Scientists at the US Department of Energy have characterised the structure of carbon dioxide in water and found that the dissolved carbon dioxide bonds only very weakly to the...
surrounding water, but creates a cylindrical cavity in the liquid (Chemical Physics Letters 2014, 614, 282–6; 2015, 633, 214–17). Identifying the structure of dissolved carbon dioxide provides the starting point for all research around this important reaction.

Carbonic acid plays a central role in the acidity of aqueous systems because it is the most common environmental source of protons. When carbon dioxide dissolves in water, carbonic acid forms, which has a very short lifetime – typically around 30 picoseconds – before dissociating into protons and bicarbonate ions. To understand how this reaction occurs, it is crucial to fully characterise each of the species involved in the reaction, including aqueous carbon dioxide and aqueous carbonic acid.

Previously, these researchers at the Lawrence Berkeley National Laboratory (LBNL) and the University of California Berkeley determined the structure of solvated carbonic acid. Following that discovery, they set their sights on the structure of solvated carbon dioxide itself, with the goal being to characterise both the ‘starting’ and ‘ending’ species of the reaction. To accomplish this feat, a unique liquid microjet injector system was used for X-ray absorption spectroscopy (XAS) at the Advanced Light Source at LBNL. The acquired XAS spectrum was then combined with molecular dynamics simulations and theoretical calculations performed at the Molecular Foundry and the National Energy Research Scientific Computing Center.

The amalgamation of these techniques provided a fully characterised structure, one in which the dissolved carbon dioxide acts as a hydrophobe, having formed only very weak hydrogen bonds to the surrounding water molecules. The result of such interactions is the formation of a cylindrical cavity in the liquid water, setting the stage for the subsequent proton transfer chemistry. The results of this study will serve as the foundation for future research into this crucial chemical reaction.

3D-printed antimicrobial teeth could replace fillings

By Peter Dockrill

Nobody likes going to the dentist. No matter how much effort you put into keeping your teeth clean, you could always be doing more – according to your dentist, at least. And they’re quite happy to threaten you with fillings (or worse) if they don’t get what they want.

But the current status quo of dental fillings and implants could face a significant overhaul in the coming years, thanks to the advent of 3D printing, and one new concept tooth in particular.

Researchers in the Netherlands have successfully created a 3D-printed tooth implant (pictured) made from an antimicrobial resin that kills harmful bacteria in the mouth. In other words, this is a tooth that effectively cleans itself.

The plastic used in the tooth incorporates antimicrobial quaternary ammonium...
RACI members shine at chemical engineering awards

The annual ANZ Federation of Chemical Engineering Awards of Excellence were presented at the Gala Dinner of the Asian Pacific Confederation of Chemical Engineering (APCChE) Congress held in Melbourne in October.

These awards showcase outstanding achievement in the field of chemical engineering or industrial chemistry. The RACI Industrial Chemistry Division, Engineers Australia Chemical College, Institute of Chemical Engineers (IChemE) in Australia and New Zealand and the Institute of Professional Engineers NZ (IPENZ) in partnership with corporate sponsors, have instituted these awards to encourage and recognise excellence and to highlight the contributions made by Australian and New Zealand Chemists and Chemical Engineers to the community.

Professor Suresh Bhargava FRACI CChem (RMIT University) was awarded the Chemeca Medal for a life-long achievement of developing sustainable partnerships to nurture innovative industrial chemistry solutions by linking academia with industry. The Chemeca medal is the most prestigious award in the chemical engineering or industrial chemistry profession in Australia and New Zealand. It is awarded to a prominent Australian or New Zealand chemical engineer or industrial chemist who has made an outstanding contribution, through achievement or service, to the practice of chemical engineering or industrial chemistry in its widest sense and who continues to serve the profession.

Professor Greg Qiao FRACI CChem (University of Melbourne) was awarded the ExxonMobil Award, which recognises significant ongoing contributions to chemical engineering or industrial chemistry through innovations or a series of related publications over a number of years. Qiao received the ExxonMobil award for his outstanding contributions in the area of synthetic polymer science and engineering including development of pioneering platform technologies in the controlled synthesis of star-polymers, nano-engineered thin films and novel gas membranes. These novel polymeric...
Architectures have applications in nano-engineered drug delivery, surface modifications, tissue engineering and carbon dioxide separations.

Qiao is Professor, an Australian Research Council’s professorial Future fellow and Assistant Dean (Research) in the Melbourne School of Engineering at the University of Melbourne. He is currently the chair of the RACI Polymer Division.

In addition to the Federation Awards the Gala Dinner also provides the opportunity for the hosts of the evening to present their institutional awards. Specifically the RACI Industrial Chemistry Division announced the winner of the 2015 R.K. Murphy Medal – the Division’s most prestigious award.

Dr Ian R. Harrison FRACI CChem (Alcoa) was awarded the 2015 R.K. Murphy Medal from the RACI Industrial Chemistry Division. Harrison received the award in recognition of his outstanding contributions to global alumina production processes, including the development of many successful strategic alliances with key research agencies based in Australia. Harrison currently holds the position of Director, Research and Development for Alcoa Global Refining and is responsible for the development and delivery of technology for Alcoa’s global refining system.

RACI INDUSTRIAL CHEMISTRY DIVISION

Chubb welcomes next Chief Scientist

Professor Ian Chubb has welcomed the announcement of Dr Alan Finkel AO as Australia’s next Chief Scientist.

‘Dr Finkel’s appointment is a testament to his great vision for Australia, pursued with energy, insight and imagination over many decades,’ Professor Chubb said.

‘He is a businessman with the insights of a researcher, and an outstanding advocate for science and technology, demonstrating in his own career the breadth of the innovation agenda and the opportunities it can open for Australians.

‘As Chancellor of Monash University, and President of the Australian Academy of Technological Sciences and Engineering, he has engaged collaboratively and constructively in the policy debate.

‘He comes to the role of Chief Scientist with that rare blend of passion, patience and persistence the position demands.’

Chubb praised Finkel’s longstanding commitment to science communication and literacy across the community.

‘Dr Finkel has called in recent days for Australian governments to “wrap their arms around the future”. As Chief Scientist, he will encourage all of us to embrace a bolder vision of the century ahead.’

Chubb commenced as Chief Scientist in May 2011 and his appointment will conclude at the end of 2015.

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Workplace exposure standards for hazardous chemicals

Safe Work Australia’s Chief Executive Officer, Michelle Baxter, is urging interested parties to express their views about exposure standards for hazardous chemicals used in workplaces in a public consultation process.

Exposure standards refer to the airborne concentration of individual chemicals in the worker’s breathing zone, which, according to current knowledge, should not cause adverse health effects or undue discomfort to nearly all workers.

Exposure standards are specified in the model Work Health and Safety Regulations as mandatory legal limits to protect the health of workers and minimise exposure to chemicals in the workplace. There are some 644 exposure standards, as listed in Workplace exposure standards for airborne contaminants.

‘Safe Work Australia is holding the public consultation process to examine the role of workplace exposure standards and how they could be reviewed and maintained,’ said Baxter.

‘All interested parties are encouraged to express their views about exposure standards by making a submission in response to The role of chemical exposure standards in work health and safety laws: discussion paper.

‘This is an excellent opportunity for workers and businesses using, storing, handling and generating hazardous chemicals, and any other interested stakeholders, to comment. We want to hear your thoughts on the use of exposure standards, the impacts of compliance, their role in the regulatory framework and how they can best be reviewed and maintained.

‘The input received through this public consultation process will help inform policy options for the regulation of workplace exposure standards,’ said Baxter.

The public consultation period is open for six weeks from 9 November 2015 until 18 December 2015. Submissions close at 5.30 pm AEDT, Friday 18 December 2015.


SAFE WORK AUSTRALIA

on the market

Eliminating time-wasting lab activities

METTLER TOLEDO has released a range of new product upgrades designed to streamline laboratory processes. In addition, METTLER TOLEDO has collaborated with manufacturing consultant and lean laboratory expert Erwin Studer to develop a free Lean Lab Checklist to help improve productivity through the identification and elimination of ‘hidden’ time-wasting activities. Mr Studer shares his expertise in an informative interview.

With many laboratories under increasing pressure to deliver more consistent and predictable performance, optimisation of laboratory processes can contribute significantly to the economic efficiency of an organisation. By employing lean principles, laboratories benefit from a greater understanding of lab capacity and resourcing requirements, bringing about reduced lead times, work-in-progress and costs – and ultimately improved customer service. The questions in the Lean Lab Checklist will not only provide you with an overview of the current status of your lab, but will also highlight where potential improvements can be made.

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Download the free Lead Lab Checklist and watching the interview with Erwin Studer. Additional videos are available demonstrating how the new product developments could revolutionise your lab.

For more information, email branko.radovinovic@mt.com or visit www.mt.com.
Light touch to clicking links
Using visible light to drive cycloaddition reactions offers a simple, inexpensive and green approach to functionalise complex molecules under mild reaction conditions. Of particular interest is the ability to combine such cycloadditions with controlled polymerisation techniques, which allows for precise control over chemical functionality as well as architecture. However, in most cases these reactions rely on the use of complex redox photo-catalysts. The research teams of Dr James Blinco at the Queensland University of Technology and Professor Christopher Barner-Kowollik at the Karlsruhe Institute of Technology in Germany have addressed this issue by discovering an approach for catalyst-free cycloadditions induced by visible light (Mueller J.O., Schmidt F.G., Blinco J.P., Barner-Kowollik C. Angew. Chem. Int. Ed. 2015, 54, 10284−8). The [3+2]-cycloaddition occurs between an electron-deficient alkene and a nitrile ylide, which is released from a stable azirine ring upon photoirradiation. Usually it can only undergo ring opening when irradiated by UV light, but the researchers found that by incorporating a pyrene moiety into the molecular structure, it was possible to trigger the reaction at wavelengths above 400 nm. Irradiation only required low-energy light sources, and efficient small-molecule cycloadditions were achieved with a diverse range of multiple-bond-containing compounds. The method also proved extremely efficient for macromolecules, with quantitative ligation of the azirine with polymers bearing an electron-deficient multiple-bond end-group achieved at ambient conditions after irradiation of only 1 minute. This new methodology constitutes a synthetic platform technology that could affect a broad range of applications, such as biotagging, cell imaging, cell/protein modification, and direct laser writing.

‘True unicorn’ provides insight into natural product biosynthesis
A suite of unusual sesterterpenes found by University of Queensland researchers in Aletris farinosa, or ‘true unicorn’, a North American herb used for centuries in traditional medicine, could provide the key to understanding the biosynthesis of this natural product class (Challinor V.L, Johnston R.C., Bernhardt P.V., Lehmann R.P., Krenske E.H., De Voss J.J Chem. Sci. 2015, 6, 5740−5). Sesterterpenes, more commonly reported from marine organisms, fungi and lichens, are a structurally diverse, yet poorly studied, group of C25 geranylfarnesol-derived terpenoids. In particular, little is known about the mechanisms of sesterterpene biosynthesis, especially in contrast to lower terpenes such as mono- and di-terpenes. The related but unusual structures of the discovered tricyclic sesterterpenes, determined via spectroscopic and computational methods, suggest that subtle differences in the stereochemistry of biosynthetic intermediates might lead to profound differences in the products formed. Quantum chemical calculations revealed that the biosynthetic fate of a key carbocationic intermediate indeed hinges on the configuration of a single stereocentre. Depending on its configuration, this intermediate undergoes either simple elimination or a spectacular cascade of seven 1,2 methyl and hydride shifts to yield the sesterterpenes detected in A. farinosa. These theoretical results point to a mechanism of conformationally induced substrate activation by the biosynthetic enzyme. The required substrate preorganisation in the active site leads to a reactive twist-boat conformer in only one epimer of the cationic intermediate, which is poised to undergo rearrangement. More generally, the biosynthesis of sesterterpenes appears to sit between typical mono- and di-terpene biogenesis and that of triterpenes.
Facile hydrogermylation of unactivated alkenes

The 1,2-addition of element–hydrogen bonds across the unsaturated carbon–carbon bonds of alkenes is of immense importance to organic synthesis, and has been dominated by borane (HBR₂) reagents. With that said, alkene hydroelementations involving group 14 element(IV) hydrides (HER₃, where E = Si, Ge or Sn) are of considerable importance, but typically only proceed in the presence of transition metal catalysts and/or at elevated temperatures. The team of Professor Cameron Jones at Monash University has overcome these shortcomings by employing two-coordinate Ge II and Sn II hydride complexes, stabilised by bulky amides, in the facile catalyst-free hydrometallations of a series of unactivated terminal and internal alkenes (Hadlington T.J., Hermann M., Frenking G., Jones C. Chem. Sci. 2015, doi: 10.1039/C5SC03376D). These reactions are quantitative and are complete within a matter of seconds at ambient temperature, regiospecifically yielding anti-Markovnikov products. The unprecedented activity of the reagents stems from the empty p-orbital at their metal centre, which allows ‘pre-coordination’ of the substrate prior to its insertion into the E–H bond (cf. alkene hydroborations). In a number of cases, the hydrometallations have been shown to be cleanly reversible at room temperature and have been revealed by computational and kinetic studies to proceed via β-hydride elimination events.

Molecular beads on a string

Nature often uses similar building blocks such as proteins to undertake different roles in assembled biological structures. A collaboration between the Gyeongsang National University in South Korea and the Universities of Sydney and Queensland has demonstrated an unusual parallel in supramolecular chemistry in which a polyrotaxane chain has been spontaneously assembled in a stair-like configuration from near-rectangular ‘beads’ mechanically locked on a ‘string’ formed from the same two components (1 and 2) as the beads (Ju H., Clegg J.K., Park K.-M., Lindoy L.F., Lee S.S. J. Am. Chem. Soc., 2015, 137, 9535–8). Although examples of mechanically interlocked rotaxane molecular assemblies have now been known for several decades, the present assembly is the first reported in which the beads and string have the same empirical composition, each being composed of only two components. The assembly is driven by π–π stacking interactions between the beads and the string, with both these units precisely matched to satisfy the exacting steric and electronic conditions required for assembly of the highly complementary polyrotaxane arrangement that occurs in 3.
Light-controlled acid catalyst

Researchers at Monash University have made significant progress towards developing a novel acid catalyst. In industry, acid catalysts play a classic and important role in various organic synthesis processes. Liquid catalysts have the best performance but are difficult to separate from homogeneous mixtures, while solid catalysts are filtered easily but perform poorly. The researchers, led by Professor Doug MacFarlane, have discovered a light-activated, switchable acid catalyst material that consists of carbon quantum dots (CQDs) decorated with –SO\(_3\)H acidic groups. When exposed to light, the acidity of the modified CQDs increases (Li H., Sun C., Ali M., Zhou F., Zhang X., MacFarlane D.R. *Angew. Chem. Int. Ed.* 2015, 54, 8420–4). The new catalyst was tested in a ring-opening reaction of industrial relevance – the ring opening of epoxides by alcohols. The catalyst produced rates and selectivity in these reactions equivalent to those normally only achieved with much stronger, solution-phase acids. One of the advantages of the catalyst reported is that, as a solid material, it is easily removed from the reaction mixture.

Ancient indigo dye as new electron acceptor in organic photodiodes

Organic photodiodes (OPDs) have attracted increasing attention for applications in digital photography, medical sensing, artificial eyesight and optical communication. Typically, the active layer of an OPD consists of a blend of an electron donor and acceptor. At present, fullerenes have been the predominant acceptor in OPDs. However, solution-processable fullerene derivatives have a number of disadvantages, such as high synthesis and purification costs, low molar extinction coefficients in the visible region for broadband photodetectors and, conversely, a broad absorption wavelength range that makes them unsuitable for narrowband OPDs. On the other hand, indigo and its derivatives have been important dyes in industry for centuries, but the poor solubility of simple indigos in organic solvents has hindered their development and use in organic opto-electronic applications such as OPDs. Researchers at the University of Queensland have demonstrated a direct and simple solution to this problem by attaching an ethylhexyloxyphenyl solubilising group to 6,6′-dibromoindigo under copper-promoted Ullmann–Goldberg coupling conditions, which renders indigo solution processable and enables high-performance OPDs (Kim I.K., Li X., Ullah M., Shaw P.E., Wawrzinek R., Namdas E.B., Lo S.-C. *Adv. Mater.* 2015, 27, 6390–5). The fullerene-free OPD exhibits a spectrally flat response over the full visible spectrum (350–750 nm) with a high responsivity (0.4 A/W), detectivity (1×10\(^{12}\) Jones) and linear dynamic range (170 dB). These values are several orders of magnitude higher than those of the best solution-processed fullerene-free OPDs reported and comparable to those of state-of-the-art fullerene-based organic and silicon photodiodes.
A new approach to linking peptides

Although peptide ligation mediated by selenocysteine (Sec), the so-called 21st proteinogenic amino acid, was first reported in 2001, Sec ligation technologies are vastly underused for the preparation of peptides and proteins. Researchers at the University of Sydney led by Professor Richard Payne have recently reported a powerful new extension of Sec ligation chemistry for the synthesis of diverse (glyco)peptide and protein targets (Malins L.R., Mitchell N.J., McGowan S., Payne R.J. Angew. Chem. Int. Ed. 2015, 54, 12 716–21). The strategy employs Sec as a synthetic handle for peptide ligation chemistry and features an unprecedented post-ligation oxidative deselenisation protocol for the direct conversion of Sec into a native serine (Ser) residue. The reaction is mild and chemoselective, employing a water-soluble phosphine and the oxidant Oxone in aqueous media to provide native peptides in excellent yields. The utility of the ligation-oxidative deselenisation protocol is showcased through the construction of two highly glycosylated fragments of the mucin glycoproteins MUC4 and MUC5AC and the total chemical synthesis of the 70-amino acid, leech-derived serine protease inhibitor, Eglin C. This efficient and operationally simple method for the direct conversion of Sec to Ser expands the scope and flexibility of ligation chemistry at Sec, thus adding to the toolbox of ligation reactions for accessing proteins by chemical synthesis.

Breaking the rules (or not)

Bredt’s rule, now over 100 years old, states that the terminus of a double bond cannot exist at the bridgehead position of a caged bicyclic system. For a considerable period of time, natural products that contain a bridgehead double bond, i.e. anti-Bredt systems, have generated confusion in terms of their relationship to Bredt’s rule. Recently, Dr Elizabeth Krenske and Associate Professor Craig Williams at the University of Queensland re-examined Schleyer’s olefin strain (OS) energy, which has traditionally been used to classify parent bridgehead alkenes into ‘isolable’, ‘observable’ and ‘unstable’ classes, and used it as a predictor of natural product isolability (stability) (Krenske E.H., Williams C.M. Angew Chem. Int. Ed. 2015, 54, 10 608–12; see also inside cover 2015, 54, 10 378). This study strongly suggests that anti-Bredt natural products do not exist, i.e. natural products that do contain bridgehead alkenes should not be termed anti-Bredt, and that this method can assist with the future structural assignment of putative bridgehead alkenes natural products.
To celebrate the International Year of Light and Light-based Technologies (IYL 2015), the November issue includes a series of papers on photochemistry and related topics. The special issue has been put together by Drs Michael Oelgemöller and George Vamvounis, James Cook University, Townsville.

Titanium dioxide is an important agent in the conversion of solar energy to electricity. Norbert Hoffmann at the CNRS, Université de Reims Champagne-Ardenne, reports that it is also a versatile heterogeneous catalyst, which can be used to advantage in preparative photochemistry. Absorption of light by a TiO₂ particle leads to the formation of an electron–hole pair. Electron transfer from or to the particle of interest induces redox reactions. Such processes are often employed in the context of environmental chemistry, but they can also be utilised in the selective transformation of organic compounds, including oxidation and reduction reactions and the synthesis of heterocycles (e.g. quinolines, quinoxalines, pyridine, pyrrole and indole derivatives), often involving radical formation and cyclization. Many C–C bond-forming reactions have been performed this way. By adsorbing the substrates on surfaces, or by adding dyes or metal nanoparticles, visible (sun)light can be used to excite the catalytic system, resulting in conveniently mild reaction conditions.

Flow photochemistry is being researched intensely by the group of Michael Oelgemöller, who report photodecarboxylative benzylations of N-methoxycarbonylbenzimidazole under batch and continuous flow conditions. A series of photodecarboxylative benzylations of N-methoxycarbonylbenzimidazole was successfully realised using easily accessible starting materials. The reactions proceed smoothly, and the corresponding benzylated hydroxyphthalimidines are obtained in moderate to good yields of 52–73%. An advanced continuous-flow photoreactor is also described.

Shinichiro Fuse et al., Tokyo Institute of Technology, Japan, report an efficient, micro-flow, Arndt–Eistert synthesis of α-arylarboxylic acids. A sequence involving four separate transformations, namely acid chloride formation, nucleophilic acyl substitution, Wolff rearrangement and nucleophilic addition was performed in a continuous fashion in the micro-flow system without isolating any intermediates.

Detection of trace amounts of explosives is, unfortunately, becoming ever more important. George Vamvounis and Nicholas Sandery report on a new colorimetric method, whereby photochromic compounds are explored as new, portable colorimetric sensors for nitroaromatics. A photochromic compound switches from colourless to pink upon exposure to ultraviolet light. In the presence of nitroaromatic explosives the photoswitching behaviour is suppressed, while a potential false positive (toluene) has little effect. The degree of photoswitching inhibition depends on the analyte’s absorption at the excitation wavelength.

Biradicals are usually very elusive species, except the oxygen molecule, which exists in a triplet ground state. Singlet biradicals are even more fleeting, because a bond should form easily between the two spin-paired centres. Manabu Abe (Hiroshima University, Japan) and co-workers have now achieved the simultaneous observation of both triplet and singlet cyclopentane-1,3-diyldiradicals (shown) during the intersystem crossing process. The intersystem crossing rate for the biradicals was unequivocally determined by the simultaneous observation of the decay of the triplet diradical (λobs = 320 nm) and the growth of the corresponding singlet biradical (λobs = 560 nm) on a picosecond timescale. The triplet biradicals were generated by triplet-sensitised laser flash photolysis of azoalkane precursors.
Researchers have been studying contrails since the world wars. What do we know about this very visible phenomenon of physical chemistry?

Look eastward just before dawn and you may see a jet aircraft leaving a trail of condensed ice and vapour – a contrail – in its wake.

Contrails are artificial cirrus clouds that form because water undergoes distinct phase transitions in the Earth’s cold troposphere. At approximately 25 000 feet (7620 metres) (cruising altitude for some commercial jetliners) the ambient air mixes with warm jet exhaust and the mixture then quickly cools to form a contrail.

Clouds (ice crystals) form from water vapour. A mixture of jet exhaust and water vapour skips the liquid phase at high altitude, changing directly to crystalline form, because of the very low pressures and temperatures.

The pressure and volume of contrail formation (or the amount of artificial cirrus cloud) are directly proportional to the temperature, which for most contrails is near –40ºC. The effective temperature of ice formation comes from the type of jet exhaust and the humidity surrounding the aircraft.

The physical explanation of contrails was formalised in the 1950s by H. Appleman and published in the Bulletin of the American Meteorological Society. Appleman’s contrail-forecasting chart (go.nasa.gov/1lhuiNG) has since been reviewed by NASA. A similar chart was used by the US Airforce Global Weather Center for many years to make contrail forecasts.

Clouds are formed as heterogeneous species of condensed water or ice crystals. Examination of contrails reveals that oxides of sulfur are the most likely to aid in the formation of ice crystals in the troposphere. Ice crystals form around microscopic droplets of sulfuric acid. The selective association of water and sulfuric acid adds stability – or makes the ice a likely species at the characteristic temperature.

Applying Langmuir’s work to contrail formation

In the early 20th century, chemist and physicist Irving Langmuir studied physicochemical dynamics of incandescent light filaments.

Although the study of incandescent bulbs seems far removed from that of cirrus clouds, it is how Langmuir came to understand the tungsten filament that interests atmospheric scientists.
tungsten metal + oxygen $\rightarrow$ tungsten oxide (brittle metallic solid)

Using a thermodynamic argument, we can compute how pressures, volumes and temperatures influence contrail/cirrus cloud formation, $P \propto T$ (at constant volume).

free nucleating surface + water vapour $\rightarrow$ [intermediate state] $\rightarrow$ water crystals (ice) + free nucleating surface

Langmuir’s educated guess illustrates how water vapour becomes ice (through an intermediate stage).

The equation governs how a designated temperature and pressure produce a given amount of ice. The constant (volume) can be regarded as the rate at which ice will form under atmospheric conditions. When discerning how water (both vapour and liquid) becomes crystalline from purely thermodynamic considerations, the type of ice (pure water and not heterogeneous mixtures of atmospheric constituents) is an important first approximation.
Contrail dynamics research for climatology

For two days after the World Trade Center tragedy on 11 September 2001, air traffic was at a near standstill, and the National Ocean Atmospheric Administration studied the effect of artificial cirrus clouds on temperatures. Climatologists determined that contrails raise effective global temperatures by approximately one degree.

According to NASA's Langley Research Center, there has been a 1% per decade increase in cirrus cloud cover over the US, likely due to air traffic (NASA).

... jet engines experience daily wear ... with resultant emissions including unspent fuel, aluminium, sulfur, manganese, chromium and barium.

\[
\text{H}_2\text{O} + \text{H}_2\text{SO}_4 \longrightarrow \left[\text{H}_2\text{O}---\text{H}_2\text{SO}_4\right] \quad \longrightarrow \quad \longrightarrow \quad \longrightarrow \quad \text{H}_2\text{SO}_4\cdot4\text{H}_2\text{O} \quad \text{and} \quad \text{H}_2\text{SO}_4\cdot8\text{H}_2\text{O}
\]

Forms of contrail ice and initial intermediate species, water and sulfuric acid.

Contrails from real-world exhaust mixtures

As with any combustible fuel, jet engines experience daily wear from routine to stressful flight conditions, with resultant emissions including unspent fuel, aluminium, sulfur, manganese, chromium and barium.

In research at the Queensland Institute of Technology (bit.ly/1RMqg9y) that cites studies performed by government agencies from the US, Australia and France, many metals and other inorganic species have been found in and around major airports.

The metallic species result from the corrosion of jet engines by the sulfuric acid in jet fuel.

Using a sulfurous/water vapour model, results point towards the equation shown in the diagram below (utilising Langmuir's theorem).

Gentle jet fuels

Research into ecologically conscious jet fuel is under way. Research groups from around the world are attempting to remove the soot (metal-containing species in exhaust) and sulfuric acid species found in the average jet liner exhaust.

The thrust of some groups is to manufacture synthetic fuel; plant oils or gasification of coal are under investigation.

John Jaksich holds a BA in chemistry from California State University East Bay. He writes for Decoded Science, Decoded Plants and Decoded Everything, covering various chemistry topics. This article adapted, with permission, from decodedscience.com.
NASA goes Down Under to tap high-altitude ice

Ice formation in engines while the plane is flying is a year-round concern. Researchers visited Darwin during its summer months to study the issue. They are part of an international team working to improve aviation safety by analysing high-altitude ice crystals with the help of a specially equipped French jet.

Engineers and scientists from three NASA facilities are supporting the European Airbus-led High Altitude Ice Crystals (HAIC)/High Ice Water Content (HIWC) flight campaign. The primary goal of the campaign is to fly into weather that produces specific icing conditions so researchers can study the characteristics present.

NASA’s Glenn Research Center in Cleveland supplied an isokinetic probe that was mounted under the wing of a French Falcon 20 aircraft. It measures the total water content in clouds that have high concentrations of ice crystals in the vicinity of oceanic and continental thunderstorms.

NASA’s Langley Research Center contributed sensors expertise. One team analysed data from the Falcon’s onboard weather radar. Another captured satellite imagery to help forecast where the jet might encounter the best icing conditions. Goddard Institute for Space Studies scientists provided their cloud expertise, using flight data to improve modelling algorithms to predict the high ice concentrations in these environments.

Over the last 20 years, the aviation industry has documented more than 200 incidents where turbofan jet engines have lost power during high-altitude flights. For many of these events, the aircraft were flying in the vicinity of heavy storm clouds, but with little activity showing on the weather radar at their flight altitude. Investigators developed a theory that the planes are actually flying through clouds with high concentrations of small ice crystals.

The crystals are drawn into the engines where they melt on the warm surfaces inside. Surfaces eventually become cold enough during flight that ice can begin to build up, which can affect the engine’s normal operation. This kind of ice crystal icing may be occurring more often because more planes are flying and at higher altitudes with more efficient bypass engines.

What the researchers learned will provide better information to the world’s aviation regulatory agencies. It should also help advance the development of technologies that may some day be able to detect the presence of ice crystals or lessen their effects in flight.

NASA
Chemists look forward to summer as much as anyone. The lab coats get shorter, we don our most fashionable safety specs, and the glassware gleams in the brighter light of day.

Academics rejoice in the weeks of research work, without all of the bothersome students cluttering up their universities, and students rejoice in their free time, thoroughly refreshed after dozing through months of lectures.

Yet the summer period doesn’t have to be quiet. All sorts of interesting and exciting opportunities arise for the most eager secondary and tertiary students to broaden their experience and flesh out their resumes.

Internships and summer work experience
The most obvious opportunity over summer is industrial/commercial work experience, either paid or unpaid. Some 20 years ago, I worked for a summer at a wax-blending factory, grateful to receive a nominal pay for my full-time work. At that time, it wasn’t even possible to graduate from industrial chemistry at the University of New South Wales without getting work experience.

A large minority of students will still get their first work experience this way. In the best cases, these will be transformative experiences, a revelation about the dynamic and complex world that blossoms outside the more structured academic boundaries.

Having said this, I place an important distinction between paid work experience and unpaid internships. The terms are sometimes used interchangeably, but as I discuss in the RACI ‘Understanding the Job Market’ video series (bit.ly/1Nou93Z), as an employer I actively avoid unpaid internships (see box).

School’s in for summer

BY DAVE SAMMUT

Prefer a faster pace in the warmer months? There are plenty of ways to boost your CV or broaden your horizons.
Several Australian universities (such as ANU, University of Sydney and University of Queensland) offer paid and unpaid work experience, internships and research programs, in some cases with subsidised or fully paid on-campus accommodation. Generally, these are open to all Australian university students who have completed at least one year of study.

These opportunities can range from short experience programs to give an introduction and insight into what further research-based study is like, through to participating in fully blown research projects with some really interesting topics.

The University of Sydney and ANU, for example, offer 6–8-week programs for Australian and New Zealand students. On its website, the University of Sydney notes: ‘A summer scholarship in the School of Chemistry offers a unique opportunity for undergraduate students to obtain experience in chemical research and provide an insight into what it’s like working with well-established researchers in high quality research facilities’ (bit.ly/1ksxqGf).

These academic programs might be particularly worthwhile for students considering honours or postgraduate study, with a general view towards more academically oriented careers. For students with an eye on industry, there is no better preparation than direct commercial experience.

**Summer schools**

Summer school programs are another very interesting opportunity, run by a wide variety of institutions and organisations.

There are the direct summer school programs available through many universities, often taught in intensive blocks of classes. As noted by the Queensland University of Technology: ‘The summer program is a good time to complete any project work required

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**Unpaid internships: pros and cons**

Relevant work experience is of major benefit to any candidate. It is, of course, an opportunity to deepen the resumé and make the person more employable, but it is also much more than that. It is an opportunity to better understand the workplace and the industry, to learn the nuances that it is simply not possible to learn at university, and it is also an opportunity for a candidate to better understand their own interests. Quite simply, a great work experience (or even a bad one) can answer a lot of questions that you never knew to ask.

So it is completely understandable that work experience is a high priority for any candidate seeking to break into a new role, and that they might even offer their services for free in order to get that experience. This is particularly the case given that there is usually a productivity cost to the employer to train and mentor that candidate.

Over the years, I have very often been asked by candidates for unpaid work experience, but I refuse all requests unless I have the budget to instead offer paid work. This is for two key reasons. First, I have a philosophical objection to taking someone’s labour without paying, and regardless of the learning opportunity, people still have basic needs that only money can buy.

Second, an internship represents a pretty extreme version of a power imbalance. The intern has virtually no power, and it is a relationship that is fraught with the unpleasant possibility of unbalanced expectations. A solid case in point would be the recent news of the New Zealand United Nations intern sleeping rough in Geneva. In taking on an unpaid internship at the UN, he reportedly told the prospective employer that he had sufficient funds to cover his expenses in one of the most expensive cities on Earth. When he did not have enough funds, he resorted to sleeping in a tent, which is bad, and then went to the media with a story of how unfair it was that UN interns are unpaid. I can only imagine that his public slap in the face to the employer will hurt his career (I probably wouldn’t take the risk of hiring him, and I wouldn’t be alone in this), but ultimately both he and the employer came out of that with mud on their faces.

I would caution anyone looking at an internship (either employer or intern) to be very clear about: (1) your mutual expectations and obligations of the role; (2) what both parties will contribute and receive; (3) the (short and finite) time period; and (4) the arrangements at the conclusion of the period.

In the best case, an internship should be a mutually rewarding experience, and I would hope that this would be the case for the majority. However, I see plenty of potential for something to go wrong.
... opportunities can range from short experience programs to give an introduction and insight into what further research-based study is like, through to participating in fully blown research projects with some really interesting topics.

for your course. You can tailor this project to help your post-study career options’ (bit.ly/1LG3mxp).

For secondary students, the Australian Science Olympiad Summer School offers programs in biology, chemistry, earth and environmental sciences and physics (bit.ly/1hV3Xmi). Scholarships are available for public school students meeting key eligibility criteria for financial need.

Some TAFE’s offer short science courses over the summer. Both these and some of the university programs could be particularly interesting for people with a general interest in science. The key point is that you don’t have to be a scientist or already on a scientific career path to explore your interest in the field, to broaden your knowledge or generally learn more about hands-on practical science.

Study and work abroad
One option that would have very much appealed to me as a student is international study. Many well-respected institutions offer summer programs, although of course this generally refers to the northern summer, our winter.

As an example, Cambridge University offers a summer school program. ‘This program presents a great opportunity to undertake interdisciplinary study in the Sciences with some of Cambridge University’s finest teachers. The course has an interdisciplinary approach and includes a range of topic areas drawing from a wide range of experts. Sessions make use of some of the many splendid collections, museums and facilities within Cambridge.’ (bit.ly/1WeMgwrd)

The University of New South Wales offers global short course study opportunities through partner institutions such as Peking University (bit.ly/1PB9p2j). Queensland University of Technology offers internship opportunities with industry-leading companies (bit.ly/1XkZYzj). And there is a really cool opportunity to work and study at CERN in Geneva (bit.ly/1M9IR1C). These are just a few examples.

Some websites collate data and help organise overseas study opportunities. The Cambridge University example was taken from AIM Overseas (bit.ly/1PHCdzf), but there are others such as the Centre for International Studies (bit.ly/1RX5nK0) and Internnzoz (bit.ly/1LMLJzr). Having no direct experience with any of these, I can’t recommend any in particular.

Several of these sites also offer opportunities to gain international work experience.

Volunteerism
In a related fashion, several of the ‘meta’ sites have international volunteering opportunities available. As a concept, these could potentially offer incredibly rewarding international
There are many humanitarian, ecology and conservation, education and other projects seeking help. The UN [bit.ly/1jBHqwF] notes engineering professionals and laboratory technicians among its ‘professional backgrounds in demand’ [bit.ly/1NUXGFD].

More widely, science-based volunteer programs are less common, but international teaching is one area where science skills might be relevant. This might be one area that could appeal to a wide range of RACI’s membership, not only early-career scientists.

With any of the international opportunities, whether study, work or volunteering, a key factor is always going to be cost. For any of the programs, the participant is likely to be liable for their own travel, accommodation and living expenses, fees and insurances.

Taking AIM Overseas’ Cambridge University study program as just one example, it charged A$3990–5350 in 2015 for a four-week program, including tuition, accommodation, and AIM’s own fees. This did not include airfares, insurance or other personal expenses. It would be reasonable to budget something in the order of $10 000, which is a fair bit of money for an undergraduate.

More to explore

This is just a sample of a very large body of opportunities for education, growth and experience development over summer programs, both domestically and internationally. Much more information is available online.

So this summer, the message is ‘slip, slop, slap, study’.

Dave Sammut FRACI CChem is principal of DCS Technical, a boutique scientific consultancy, providing services to the Australian and international minerals, waste recycling and general scientific industries.
The Nobel Prize in Chemistry 2015 was awarded jointly to Tomas Lindahl, Paul Modrich and Aziz Sancar ‘for mechanistic studies of DNA repair’. See page 5 for news about this year’s Nobel Prizes in Physics and in Medicine. A full profile of the recipients for Chemistry will be published in our February issue.

Theoretical chemist Julian Gale and organic chemist San Thang, both RACI Fellows, were admitted this year as Fellows to the Australian Academy of Science.

Congratulations to all recipients of RACI awards in 2015. Winners were announced at an awards dinner in November and full details will be published in our February issue.

For his development of flotation technologies that have added billions of dollars to the value of Australia’s mineral and energy industries, Graeme Jameson FRACI CChem has received the inaugural $250 000 Prime Minister’s Prize for Innovation.

For his contributions to polymer science, nanotechnology and nanomedicine Cyrille Boyer MRACI received the 2015 Malcolm McIntosh Prize for Physical Scientist of the Year.
Chemical engineers from around the world gathered in Melbourne in October for the Asian Pacific Confederation of Chemical Engineering Congress. The conversation focused strongly on the impact of the profession on the world around us. APCChE is the largest gathering of chemical engineers in the region and was held in Australia for only the second time in 22 years. For the first time, the 2015 Congress incorporated the Institution of Chemical Engineers’ Chemeca conference. The Chemeca Medal was presented to Suresh Bhargava FRACI CChem. Greg Qiao FRACI CChem received the ExxonMobil Award. Ian Harrison FRACI CChem (pictured, left) was presented with the RACI Industrial Chemistry Division’s R.K. Murphy Medal by Division Chair Dr Gary Bowman FRACI CChem. (Courtesy IChemE; related news p. 10)

According to Thomson Reuters Web of Science, the most highly cited Australian research paper (in which an author’s affiliation and address is in Australia) within the subject of chemistry for 2015 was ‘Advancing the electrochemistry of the hydrogen-evolution reaction through combining experiment and theory’ by Yao Zheng and colleagues – cited 26 times (Angewandte Chemie – International Edition, doi: 10.1002/anie.201407031).

Assistant Minister for Health, Fiona Nash, announced in May that reforms to NICNAS ‘will streamline the assessment process for industrial chemicals to reduce the regulatory burden on the sector, while also ensuring Australia’s robust safety standards are maintained.’ An implementation plan was launched in September.

Chemistry – An Asian Journal celebrated 10 years with a special anniversary edition in January (see April issue, p. 9). The journal is a publication of the Asian Chemical Editorial Society, a group of chemical societies including RACI.
Colin Raston FRACI CChem has taken out an Ig Nobel Prize for ‘unboiling’ an egg, which happened in the context of research into applications of his vortex fluidic device (August issue, p. 6). The Ig Nobels ‘honor achievements that first make people laugh, and then make them think’.

Larry Marshall joined CSIRO as Chief Executive Officer in January (see July issue, p. 18).

MinSik Cho (18 years old) of the CheongShim International Academy in Korea was awarded first prize in the 2015 IUPAC Physical Chemistry Division student cartoon competition for his cartoon describing the origins of colour in molecules. The theme of the competition this International Year of Light, was Light and Chemistry. His cartoon was selected both for the excellence of the artwork and the quality of the scientific message conveyed. The members of the Division board would like to wish him well in his further studies and thank him and the other entrants for participating in the competition.
Almost 84,000 students from 20 countries, including Vietnam (Nguyen Binh Khiem High School pictured) participated in RACI’s 2015 Australian National Chemistry Quiz.

NASA reported in September that dark, narrow streaks, called recurring slope lineae, on Martian slopes such as these at Hale Crater are inferred to be formed by seasonal flow of water on contemporary Mars. The blue colour seen upslope of the dark streaks are thought not to be related to their formation, but instead be from the presence of the mineral pyroxene. The imaging and topographical information in this processed, false-colour view come from the High Resolution Imaging Science Experiment (HiRISE) camera on NASA’s Mars Reconnaissance Orbiter. Planetary scientists using observations with the Compact Reconnaissance Imaging Spectrometer on the same orbiter detected hydrated salts on these slopes at Hale Crater, corroborating the hypothesis that the streaks are formed by briny liquid water.

Vale David Craig, theoretical chemist, and Carl Djerassi, organic chemist (see p. 32 and April issue, p. 30).

The importance of advanced physical and mathematical sciences to the Australian economy, commissioned by the Office of the Chief Scientist and the Australian Academy of Science, reported in March that advanced physical and mathematical sciences directly contribute around $145 billion to the Australian economy each year, or about 11% of GDP. Including the flow-on impacts of these sciences, the economic benefit expands to about 22% of the nation’s economic activity.

The figures only include the economic benefits of discoveries and innovations implemented in the past 20 years in physics, chemistry, earth sciences and the mathematical sciences. (Courtesy Office of the Chief Scientist)
New Fellows

Arthur Christopoulos is Professor of Pharmacology in Drug Discovery Biology, Monash Institute of Pharmaceutical Sciences and the Department of Pharmacology, Monash University, as well as a senior principal research fellow of the NHMRC. His research focuses on novel mechanisms of drug action at G protein-coupled receptors (GPCRs; the largest class of drug targets), in particular the study of GPCR allosteric modulators and biased agonists, and incorporates computational and mathematical modelling, medicinal chemistry, structural and chemical biology, and animal models of behaviour. He is an author of over 230 publications, including in leading journals such as Nature, Nature Chemical Biology, Nature Biotechnology, PNAS, Cancer Cell and Circulation, and has delivered over 160 invited international and national presentations across a broad range of disciplines, including pharmacology, medicinal chemistry, neuroscience, endocrinology, gastroenterology, cardiovascular and pharmaceutical sciences.

He serves/has served on the editorial board of eight international journals, including leading discipline journals such as Molecular Pharmacology, ACS Chemical Neuroscience, Journal of Pharmacology & Experimental Therapeutics and Pharmacological Reviews, is a consultant for numerous pharmaceutical and biotechnology companies, and Deputy Chair of the Nomenclature Committee of the International Union of Basic and Clinical Pharmacology (NC-IUPHAR). He has a strong track record of extensive and sustained competitive research funding from national (NHMRC; ARC) and international (NIH) agencies, in addition to pharmaceutical industry support, and is a scientific advisory board member to five companies. He regularly contributes to the broader discipline through senior roles for numerous national and international scientific societies, as well as a regular member of the NHMRC Assigner’s Academy and Grant Review Panels.

To date, Christopoulos has supervised 16 PhD and 16 Honours students, and has been the recipient of 16 national and international awards, including the John J. Abel Award from the American Society of Pharmacology and Experimental Therapeutics, the Rand Medal of the Australasian Society of Clinical and Experimental Pharmacologists and Toxicologists, and the James Black Analytical Pharmacology Lecturer for IUPHAR. In 2014, Thomson Reuters named him a Highly Cited Researcher in Pharmacology and Toxicology, and in 2015 he was the recipient of the Thomson Reuters Citation Award in Biology and Biochemistry.

Mark Mullett obtained an Associate Diploma of Applied Science from Central TAFE in 1990 while working at CSIRO. He was recognised with the RACI award for the Most Outstanding Chemistry Student at Diploma Level. He subsequently worked at Alcoa World Alumina as a research officer while he continued his studies on a part-time basis at Murdoch University. He received his BSc(Hons) in Extractive Metallurgy in 2001 and was promoted to experimental scientist, graduate research scientist and research scientist during this period of employment. Mullett then enrolled in a Master’s program at RMIT University, which he completed in 2006. Following his research, he was awarded the RMIT Surface Chemistry Award for 2006.

Mullett has worked for Hatch Pty Ltd for over six years as a process consultant and is a globally recognised consultant and technical manager who leads technology development and process engineering programs from concept development through to implementation. His key interests include the application of novel separation technologies into hydrometallurgical and wastewater circuits. These technologies bring about cost-saving measures and environmental compliance outcomes, providing the benefits of commodity recovery, impurity removal, water recovery, water discharge and reagent re-use. His interest in separation technologies led to his role on the Board of the Membrane Society of Australasia (MSA) and regular support of the MSA Early Career Researcher’s Symposium. During Mullett’s tenure on the MSA Board, he initiated and managed a mentoring program for young professionals and PhD students who were looking at academic or industrial career paths. He was also a member of the CHEMeca 2014 Technical Committee representing the RACI.

Prior to his current role with Hatch, he worked with BHP Billiton developing uranium resin in pulp technology for the Olympic Dam Expansion Project and spent 12 years with Alcoa World Alumina’s Technology Delivery Group, conducting industrial research on impurity removal from bauxite and liquor sources, mercury removal from gaseous and wastewater streams, VOC destruction from point and diffuse sources, and odour mitigation. He has over 20 publications and a patent.

His personal interests are fishing, camping and supporting the sporting and recreational activities of his four children. He has been actively involved in the Whitfords Junior Cricket Club and Whitfords Junior Football Club for a number of years, including coaching and committee roles.
John Melvin Swan  
25 April 1924 – 15 June 2015

John Swan was my colleague and mentor at Monash University where, between 1966 and 1984 he was, successively, Foundation Professor of Organic Chemistry, Pro-Vice-Chancellor and Dean of the Faculty of Science. JMS packed a lot into those Monash years, serving the university diligently but also making substantial contributions to public life. To those of us who knew John in one or other of his ‘lives’, the diversity of the crowd who gathered at Monash in July to celebrate his life was a revelation and a reminder of the esteem in which he was held.

Leaving school at age 16, John worked for ICIANZ as a junior laboratory assistant in the Albion explosives factory while studying part-time at Melbourne Tech (now RMIT University). He completed his Diploma of Applied Chemistry in 1944 and then studied at the University of Melbourne for the BSc that he completed in 1946. A CSIR scholarship took him to Imperial College, London, where he worked with Professor Arthur Cook on penicillin synthesis and was awarded the PhD degree.

Back in Australia, he took up an appointment with CSIR in the Wool Textile Research Group that would become the Division of Protein Chemistry. A period of leave in 1952–53, supported by a Fulbright Award, enabled him to work for a year with Vincent du Vigneaud at the Cornell University Medical School in New York City, where he contributed to the synthesis of the peptide hormone oxytocin. In the early 1950s, the semi-automated Merrifield peptide synthesis was yet to be developed so every intermediate had to be isolated and purified. Being a nonapeptide, oxytocin was well within the limits of this research methodology but compared to the modern methods, it would have been a lot more work. Earlier in 1952, he had married chemical engineering graduate Ailsa Lowen and she accompanied him to New York where she also worked in the Cornell laboratory. Ailsa had completed a PhD in physical organic chemistry at the Royal Holloway College of the University of London and was personal assistant to Dr Ian Wark at CSIRO.

The work on wool led John into research on sulfur compounds such as thiohydantoins (2-thioxo-4-imidazolidinones), but in 1960 he moved to the newly established Division of Organic Chemistry, led by Dr J.R. (Jerry) Price and began to concentrate on organophosphorus chemistry, an interest that continued for a time at Monash. Among the many things I recall from Monash are two that stand out: his research into the components of cigarette smoke and the foul-smelling smoking machine that was operated by a research assistant; and the Swan family holiday house at Phillip Island where young colleagues could earn a vacation by agreeing to mow the grass! It was no doubt the Phillip Island connection that got him involved in marine conservation issues, chairing inquiries into the threats to seagrass from the growing industrialisation of the Westernport shore, the health of Port Phillip, and the water supply in south Gippsland. I remember an RACI Organic Division symposium in Hobart at which John arrived by ship from Adelaide, having sailed on the Victorian Institute of Marine Science vessel.

John Swan was elected FRACI in 1955. He was editor of Proceedings of the Royal Australian Chemical Institute (precursor of Chemistry in Australia) 1959–1961 and H.G. Smith Medallist in 1965. In the learned academies he was FAA (1968) and FTSE (1994) and he was a Fellow of the Royal Society of Chemistry. Other awards included the David Syme prize of the University of Melbourne (1965) and the ANZAAS Medal (1994). He received the Australia Centenary Medal in 2001 and was made an Officer of the Order of Australia in 2002.

Never one to be inactive, in later life John bought a folding bicycle and he could be encountered exploring the Melbourne area when he was not on the bowling green. Kneeling down to deliver the bowl was a struggle for many of his older colleagues, so John and some friends invented a metal ‘bowler’s arm’ that enabled the bowler to deliver from a more upright position. As a prototype, it wouldn’t be allowed in competition bowls but it certainly met a need and the solving of design problems in good company gave considerable pleasure.

We watched John’s slow decline in the last year of his life and were aware that he passed away peacefully at home. He is survived by his four children, eight grandchildren and a great-grandchild.

A full biographical memoir will be published by the Australian Academy of Science in 2016.

Ian D. Rae FRACI CChem

JMS packed a lot into those Monash years, serving the university diligently but also making substantial contributions to public life.
Professor David Craig
Theoretical chemist at ANU

Professor David Parker Craig A0 FAA FRS was born 23 December 1919 in Sydney. Craig appreciatively recalled having excellent mathematics, physics and chemistry teachers as part of his early education, an experience which sparked his lifelong interest in the intersection of physics and chemistry.

Craig enrolled at the University of Sydney in 1937, receiving a bachelor's degree in 1940 and a Master of Science the following year. In 1941, his scientific career was interrupted by war service; Craig served in Australia for three years before being assigned to return to the University of Sydney as a lecturer and researcher in physical chemistry. It was during this time that he met his future wife Veronica (Ronia) on a train between Sydney and Nowra; Craig would later say that meeting her was the best thing that ever happened to him.

In 1946, Craig was awarded a Turner and Newall Research Fellowship and he departed Australia for University College, London. After receiving his PhD in 1949, Craig was appointed lecturer at University College, where he remained until 1952. He returned to Australia as a professor of physical chemistry at the University of Sydney, and then in 1956 moved back to England as professor of theoretical chemistry at University College, a position he held for the next 11 years. By this point Craig was thoroughly immersed in his pioneering research regarding excitons in molecular crystals.

Craig returned to Australia for good in 1967, taking up the role of Foundation Professor of physical and theoretical chemistry at the Australian National University. There he remained until his retirement in 1984, a distinguished career that included holding the position of Dean of the Research School of Chemistry from 1970 to 1973. Following retirement, Craig continued at ANU as a Visiting Fellow in the Department of Chemistry, researching and authoring papers with a focus on molecular quantum electrodynamics.

Craig was elected as a Fellow of the Australian Academy of Science in 1969, and later became Treasurer in 1985 before serving as President from 1990 to 1994. He also served on the Prime Minister’s Science and Engineering Council, was Chairman of the Queen Elizabeth II Fellowships Committee, and was appointed a member of CSIRO Executive from 1980 to 1985.

Craig was the recipient of numerous awards, including the H.G. Smith Memorial Medal (1972) and the Leighton Memorial Medal (1991), as well as being made an Officer of the Order of Australia in 1985. He was further honoured with an eponymous wing at the Research School of Chemistry in 1995, as well as the Australian Academy of Science’s David Craig Medal, which recognises outstanding contributions to chemical research. Craig was elected a Fellow of the Royal Society In 1968 and named a Distinguished Fellow of the Royal Society of New South Wales in 2009.

Professor David Parker Craig passed away at the age of 95 on 1 July 2015. He is survived by his wife Ronia and children Andrew, Hugh, Mary Lou and Douglas, as well as nine grandchildren and four great-grandchildren.

AUSTRALIAN ACADEMY OF SCIENCE

Liversidge lecture series now online
Professor Archibald Liversidge was the first Australian chemist to gain an international reputation, and to be elected to Fellowship of the Royal Society (London). In his will he made bequests to the Royal Society of New South Wales, the Australasian Association for the Advancement of Science, and the University of Sydney, Department (now School) of Chemistry, for the funding of three series of Research Lectures on chemistry, by Australian chemists. His will also provided for the establishment of a series of Research Lectures under the auspices of what was then the Chemical Society (London), now the Royal Society of Chemistry, and another through Christ’s College, Cambridge University.

The Royal Society of New South Wales series of Liversidge Research lectures is unique, in that the Society has consistently published the Lectures in the Journal and Proceedings of the Royal Society of New South Wales, from 1931 to the present.

During the period 1931–2000 there were 32 Liversidge Research Lecturers.

Craig was elected as a Fellow of the Royal Society in 1968 and named a Distinguished Fellow of the Royal Society of New South Wales in 2009.

As one of my retirement projects, I scanned the 32 lectures from the Journal, re-organised them into an A4 format, and wrote a brief biographical sketch (with portrait) about each of the 32 lecturers. The compilation has an introductive biographical sketch of Liversidge, and contains the details (lecture title/author) of each of the other Liversidge lecture series.

This series of Liversidge lectures has now been made electronically available by Sydney University Press (through the Fisher Library), and with permission of the Royal Society of New South Wales. Each of the 32 lectures, together with the biographical sketch of the lecturer, may be downloaded individually.

I hope that this facility will be a useful vehicle for introducing graduate students to our chemical heritage.

Online access to this compilation is now available at http://openjournals.library.usyd.edu.au/index.php/LIV/index.

David J. Collins FRACI CChem
Plastics and environmental sustainability

Plastics and environmental sustainability is a fine book, packed with informative data and well worth reading. Author Anthony Andrady comprehensively surveys the issues typically raised in discussions of sustainability and plastics, presenting a balanced account, supported by extensive referencing of original source material. Andrady’s approach is to present you with the nature of the problem and facts of the matter. Then he discusses some ameliorating solutions and comments on their efficacy. You are now in a position to make up your own mind. There is no attempt at barrow pushing for either side. The analysis of plastics-related issues is lucid, with references to the research base supporting and contradicting popularly held notions.

Plastics materials seem to evoke deep emotions in people, ranging from ardent enthusiasm for something even better than sliced bread, through to an apparent belief they are the invention of the devil incarnate. I’m pretty confident if you read this book, then you will have a balanced view of the role of plastics materials in a world which probably ought to be husbanding increasing demand and diminishing resources rather more judiciously than it does. Yes, plastics are pretty amazing materials, but there are plenty of things we could be doing to minimise their global impacts, particularly post-use. Andrady uses a womb-to-tomb life-cycle model to follow plastics materials from creation to ultimate disposal. He discusses the synthesis and properties of polymeric materials, through their compounding and fabrication, towards their ultimate disposal. Frequently, post-consumer plastics find their way to landfill or into the oceans. Post-consumer plastics notwithstanding (and there are many materials that are either too hard or too expensive, or too low in demand to recycle), as a society we have a long way to go in minimising our plastic waste streams. At the very least, they represent a source of embodied energy (the combustion of which creates carbon dioxide, of course!), even if alternative fates of pyrolysis or other monomer recovery strategies are economically unattractive. And then there are the various nasties, such as carcinogens (vinyl chloride monomer, for example) and endocrine disruptors (like bisphenol A), which can leach from plastics materials into streams, waterways and ultimately the food chain. Andrady points some ways forward here as well.

Overall, I enjoyed this book a great deal. It is highly readable, with the sole exception being the author uses a lot of abbreviations, not just for polymer names but for less familiar concepts like GWP – global warming potential – for example. However, this is a minor annoyance in an otherwise very good book. I commend it to those with an interest in plastics and/or the environment as a useful and thought provoking work. Even if you disagree, there is still a huge mine of information and a towering list of references within its covers! Well worth reading, indeed!

R. John Casey FRACI CChem

Soil chemistry
Strawn D.G., Bohn H.L., O’Connor G.A., Wiley Blackwell, 2015, hardcover, ISBN 9781118629253 (also available in softcover and as an ebook) 375 pp., $266.95

Soil chemistry is the fourth edition of a comprehensive book about the chemistry of soil. And soil is pretty important stuff! We are absolutely reliant on the soil as a source medium to grow the food necessary for our very existence. Indeed, the UN declared 2015 the International Year of Soils, to emphasise how critical soils are in counteracting climate change, while the Australian Government appointed former governor general Michael Jeffery ‘Advocate for soil health’ (2014 extended for 2015). Furthermore, World Soil Day will occur on 5 December 2015. The ancient philosophers were right. Earth (soil), Air, Fire (sunshine) and Water are basic elements of all food production. Soil intersects with the atmosphere, hydrosphere, biosphere and lithosphere, so, if you are looking for an area of applied chemistry of utterly fundamental importance, then soil chemistry is probably it!

This book first appeared in 1976 as a text for soil science students. Subsequent editions have maintained the goal of providing an undergraduate text, but additionally broadened the scope and coverage so it now provides a useful resource for professionals with an interest in soils to understand and review concepts. There are lots of good tables throughout, providing ready information on chemical properties of soils. Coverage appears comprehensive, ranging from fairly fundamental ideas, across redox reactions in soils, the chemistry of clay soils, and organic matter in soils, to discussion of soil colloids, adsorption processes in soils, soil acidity and salinity of soils. The development of ideas seems logical. Each chapter is accompanied by revision questions. There is no detailed referencing throughout the book (deliberately, according to the foreword), which may limit use for the professional. However, there is a bibliography at the end. There are interesting Special Topic boxes throughout to pique interest.
My biggest gripe is one of style rather than substance. The font size, line spacing and fairly uniform black-and-white presentation meant that, for me anyhow, the book was a bit of a slog. The writing is fine (the message is there), but a bit more colour and glitz would make the entire package more appealing, to both students and other readers.

Overall, *Soil chemistry is a tour de force* of ... well, soil chemistry. If you read it, then you will learn a great deal and richly enhance your understanding about the dirt beneath your feet, why it behaves the way it does and how you might go about modifying its properties. Probably, like me, you will be struck by just how important this stuff we call soil is to our existence and how globally important it is in the ongoing cycling of the 'environment'. Really, and possibly mildly astonishingly, it is all applied physical chemistry! At the risk of trivialising a very good book, you might even be able to apply your new knowledge on the local level to answer the question of why the kale in your veggie patch is not thriving (although the book, alas, makes no mention of the role of pesky possums!)

At last. A ‘dirty book’ worth reading!

R. John Casey FRACI CChem

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**One hundred years of the Bohr atom**


For a long time I had the impression the Bohr atom was only important as a stop on the road to proper quantum mechanics, something that had caught the public imagination but was not really of great scientific importance – the conventional symbol for atomic energy, a fun semi-classical derivation of the radius of the 1s orbital in hydrogen which can’t readily be extended to more interesting atoms and some Fantastic Four comics where atoms are tiny planetary systems. These were what I thought of as the legacies of the Bohr atom. My impression of Niels Bohr himself was heavily influenced by the portrait in Robert Junck's *Brighter than a thousand suns* – a grand old man of science, given to obscure and impenetrable pronouncements, whose 'Copenhagen interpretation' would enable generations of psychedelic misinterpretations quantum mechanics.

After reading *One hundred years of the Bohr atom*, I am happy to report I was wrong on both counts. The Bohr atom had a longer innings as a fruitful and active theory than I thought, as the cornerstone of the ‘Old Quantum Mechanics’ through the decade 1914–24. More significantly, it introduced most of the counter-intuitive concepts of quantum mechanics that are most important for chemists, concepts we are now so familiar with that we no longer think of them as counter-intuitive. Here is Rutherford, for example, commenting on a draft of Bohr’s first revolutionary paper:

> There appears to me one grave difficulty in your hypothesis ... How does an electron decide what frequency it is going to vibrate at when it passes from stationary state to another? It would seem to me that the electron knows beforehand where it is going to stop.

As for Niels Bohr, I found it a pleasure to meet him when he was young and audacious, to learn more about what a multi-faceted scientist and person he was, and gain a greater appreciation of his constructive contributions to science and society far beyond the Bohr atom.

The 26 individual essays in this book are divided into four parts. I found the more historical and biographical ones – gathered in ‘Part 1. The quantum atom: origins and popularisation’ and ‘Part 4. National and institutional aspects’ – to be most valuable. As well as discussing aspects of Bohr’s life and career before, during and after the publication of his atomic model, these cover such topics as the treatment of quantum theory in early books of popular science; early ‘models’ of atoms in every sense of the word; and a discussion of how the ‘plum pudding’ model as we have it in our textbooks today is a very different beast from the theory as it was actually understood by J.J. Thomson, since we see it from a modern viewpoint saturated with the Bohr model. ‘Part 2. Early atomic theory: principles and techniques’ was very interesting, showing how the Bohr atom was applied and extended before being subsumed in the new quantum mechanics. However, it was frequently hard going; the more fluently you can read equations and the more you already know about Arnold Sommerfeld’s extension of the Bohr model, then the more you will enjoy this section. In both Part 2 and ‘Part 3. Philosophical and contemporary aspects’ I occasionally got the feeling the connection to the theme ‘One hundred years of the Bohr atom’ was becoming tenuous and authors were writing about whatever they felt like. But only occasionally.

This book is highly suitable for anyone with more than a passing interest in the history and philosophy of science who is already familiar with the big picture of the development of quantum mechanics. I will find it most useful as a source of anecdotes and quotes to enliven first year physical chemistry lectures.

*One hundred years of the Bohr atom* is an impressive demonstration of how a single idea can have an impact that is huge and unpredictable, causing ripples long after and far away from its origin. Ideas are like wandering stock – you never know where they will end up or what trouble they will cause!

Chris Fellows FRACI CChem
In Vino Analytica Scientia, 2015

The 9th In Vino Analytica Scientia (IVAS) conference was held in Trento, Italy, from 14 to 17 July this year. The actual venue was Mezzocorona in Trentino, a 30-minute trip from the city of Trento where many of the participants were accommodated. This meant that we travelled each day by bus between the towering cliffs of the Dolomites, a UNESCO world heritage site. Those of us who were able to keep our eyes open at 7:45 am, the bus departure time, could contemplate the sheer majesty of the region on our way to the meeting.

The IVAS meetings have always had a considerable emphasis on the chemistry and measurement of phenolic compounds and this was continued at this meeting. The opening plenary lecture by Victor de Freitas from the University of Porto addressed the ABC of polyphenols in wine in relation to sensory aspects. Victor identified the complex mechanisms that are involved in A(stringency), B(itterness) and C(olour), stressing that there is now increasing evidence for the role played by specific compounds in each of these sensory aspects. For example, the presence of the catechol group as in (−)-epicatechin and the galloyl group as in pentagalloylgucose seem to be important in stimulating the taste receptors for bitterness (TAS2Rs). The stability of anthocyanins, responsible for colour, may well be modulated by polysaccharides and the binding constant for the interaction between malvidin-3-glucoside and salivary proteins has been measured.

Regarding astringency, Susana Soares, also from the University of Porto, described a series of in vivo experiments that examined the interaction of salivary proteins and wine tannins in a model system. While there is a general theory that wine tannins interact with and precipitate salivary proteins, especially proline-rich proteins (PRPs), this work showed that the tannins interact first with acidic PRPs and statherin, followed by glycosylated PRPs and then basic PRPs. Statherin and related peptides are now receiving more attention in discussions on wine astringency. It is clear from the work of the research group in Porto that a greater understanding of specific chemical composition of salivary proteins and tannin molecular structure is needed to formulate a detailed mechanism of astringency. There is obviously a lot here to contemplate next time you partake of a glass of red wine!

A different perspective on phenolic compounds was presented in the keynote lecture by Begoña Bartolomé from the Institute of Food Science Research in Madrid. Here the emphasis was on the interaction between phenolic compounds in wine and gut microbiota. The concept behind this research is that the two-way interaction may lead to the growth of beneficial bacteria while inhibiting pathogenic ones. Perhaps I can suggest somewhat tongue-in-cheek that this concept is not new as one finds in the Bible an exhortation from St Paul to Timothy to ‘use a little wine for thy stomach’s sake’. But maybe that is more a comment about the quality of the water in those days.

The researcher in this wine health field now has access to techniques for monitoring bacterial communities as well as tracking the fate of the phenolic compounds and their metabolites. The research is complex and requires a large number of participants, which in turn suggests the need for a well-funded research budget.

The other main conference theme was metabolomics and I will need a follow-up column to address this in the depth that it deserves. One paper, however, deserves mention here as it relates to the wine of the region. Fulvio Mattivi and colleagues from the Research and Innovation Centre of the Fondazione Edmund Mach in San Michele all’Adige presented the results of a study on the sparkling wines of the Trento (Trento DOC) and Franciacorta regions. The analytical approach used solid phase micro-extraction with two-dimensional GC and time-of-flight mass spectrometric analysis. Some 1600 compounds were found by this untargeted metabolomic approach, with the Trento DOC wines showing good concentrations of terpenes including linalool and rose oxide as well as hexanol and hexenols.

The meeting was a great success, both scientifically and socially. There were 250 registered participants from 30 countries with a significant number being young researchers. There were three contributed papers by Australians: Joanna Gambetta (University of Adelaide), Andrew Clark (Charles Sturt University) and Sigfredo Fuentes (University of Melbourne). The poster prizes were restricted to researchers under 32 and this required the Scientific Committee to evaluate 83 posters for the three prizes – a rather difficult challenge. Much to my surprise, my poster was classified as ‘under 32’ and when I raised this little problem, I was asked to wear a cap back-to-front, so then ‘no-one would realise’!

One of the pleasures of a conference in Europe is lunch: good food and the opportunity to taste a range of wines from, in this case, the Trento region. Fortunately, we were not tested on the wines to see how our aroma perception matched the metabolomic study described above. As I mentioned in my November column, the first day concluded with opera and a wine tasting. Day 2 finished with a visit to a winery and the gala dinner ended the third day. This banquet was held in Castel Katzenzungen in the Sud Tyrol region. A beautiful venue with a four-course meal with matching wines.

If you are keen to try something different this festive season, track down some of the sparkling Trento DOC wines. Made from Chardonnay and Pinot Noir, they challenge the best wines from Champagne in quality. I was fortunate to be presented with a magnum of 2006 Ferrari and a 2009 Rotari Alpe-Regis, both absolutely amazing wines.

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

We live in a world where the prices of many products required for everyday life are influenced by the prevailing price of crude oil. Crude oil is the basic building material for the production of transport fuels and chemicals. In urbanised economies such as ours, transport fuel prices significantly influence the cost of food by impacting on farming, fertilisers, harvesting and transport to markets. Crude oil produces the basic materials for the production of commodity plastics (for rigid consumable items as well as packaging) and synthetic fibres (polyester, nylon, spandex (Lycra™) and Kevlar™) to produce clothing that cannot be produced from natural fibres.

The cost of fuels and chemicals is very dependent on the prevailing price of crude oil. The major portion of crude oil is traded on the spot market. For transport fuels, the cost is direct and almost instantaneous in that changes in the price of crude oil results in changes to fuels within a few days and sometimes within hours. For example, the cost of petrol shows a strong correlation with the price of crude oil.

![Graph: Correlation of the price of gasoline (petrol) and Tapis Blend crude oil on the Singapore spot market]

The graph shows a very strong correlation for gasoline (petrol) with Tapis crude oil traded on the Singapore market. A rise and fall in the price of Tapis produces a commensurate effect in Australia about a week later due to the material hold-up in the delivery chain.

For chemicals, the cost of production is determined by the cost of the feedstock (oil price related) and other factors that influence the final production cost. These factors are the cost of the capital for the production facility and the operating cost of the plant (labour, maintenance, other chemicals and catalysts that may be required, insurance etc.). Although chemical processes are capital intensive, for most chemicals the dominant cost is that of the feedstock and hence production cost is related to the price of oil.

However, other factors also affect the price paid for chemicals that are used in the economy at large. These encompass the general state of business (the business cycle), the relative availability of the product (shortages and gluts), which may have location specific factors, for instance the presence in a locality of a dominant supplier. Thus as the price of crude oil rises and falls, so does the level of the price of chemicals, but the correlation is far lower than that observed for crude oil derivatives such as transport fuels – gasoline (petrol) and diesel fuel.

Although there are regional differences in price that can be exploited by traders and suppliers, transport logistics are now very efficient so that there is little persistent difference in the cost of chemical products across the world, especially solid goods that can be shipped in containers (e.g. commodity polymers) or large bulk carriers (e.g. fertiliser).

Starting from crude oil, producing a final product selling into the economy at large can involve several intermediates. The chain of materials from oil to product involves increasing added value. This value chain is illustrated for polyester in the flowchart on page 37.

Crude oil is first distilled to produce the naphtha fraction, which is used to produce ethylene (by steam cracking) and aromatics (BTX, by reforming). The aromatics intermediate (BTX) is used to produce p-xylene, which is then oxidised to p-teraphthalic acid (PTA). The ethylene fraction is oxidised to ethylene oxide, which is then hydrated to produce mono ethylene glycol (MEG). The PTA and MEG are then reacted to produce the polyester polyethylene terephthalate (PET). This is then sold to the final users to produce yarn, sheets or bottles.

Large integrated petrochemical complexes perform all this chemistry from crude oil to PET, which is sold to downstream customers. However, all of the intermediates are bought and sold on the chemicals market so there are opportunities to enter this value chain at any stage from suppliers with excess material or specialising in producing any one of the intermediates.

This is the case for biochemical producers, who can enter the value chain for PET by producing MEG from bio-ethylene produced by dehydrating ethanol that has been produced from renewable sources. Entirely bio-PET is still a problem because renewable routes to aromatics or PTA are not well defined and well away from commercialisation. There has been an enormous surge in research into the production of bio-PET, thanks mainly to announcements by The Coca-Cola Company that they would like their products to be available in renewable containers.

There are several approaches to produce bio-aromatics, none of which is very well defined at the present. One is to use bio-ethylene as the feedstock for producing aromatics by oligomerising the ethylene followed by conversion over a zeolite catalyst to an aromatic. Another is to use a C₂ species such as succinic acid produced by glucose fermentation, which is used to produce a bio-butadiene, which is subsequently coupled to produced p-xylene. Another proposal is to produce carbon monoxide and hydrogen by gasification of biomass, which is then converted via methanol to aromatics.

There is a large and growing trade in recycled PET (R-PET), especially in the larger economies. R-PET enters the value chain at the very end but interestingly most R-PET is used to produce
fibre or sheeting rather than being recycled into bottles.

Since the beginning of 2015, we have witnessed a major fall in the value of crude oil and this is leading to price falls in the chemicals sector. This price fall is making it more difficult for producers of renewable and recycled materials to enter the value chain because their feedstocks have generally not fallen in value as much as that of crude oil. We may witness a marked slowing of entrants into the renewable and recyclable chemicals sectors as their price premiums relative to conventional fossil fuel derived products are squeezed.

Although chemical processes are capital intensive, for most chemicals the dominant cost is that of the feedstock and hence production cost is related to the price of oil.
Global Innovation Index 2015 – we rank 17th again!

Our global rankings are all over the place. Our national men’s soccer team ranks 94th in the world, our national women’s soccer team is 9th, the Australian men’s cricket team is ranked 2nd for Tests, we are the 6th largest country with the 56th largest population and with the lowest number of children under five who are underweight.

So is being 17th in the Global Innovation Index (GII) something to worry about?

The Prime Minister thinks so. He convened an Innovation Roundtable at Western Sydney University on 16 October to assist Minister for Industry, Innovation and Science Christopher Pyne in developing a new innovation policy agenda. The meeting was also attended by three other Ministers and a selection of business and research leaders. They discussed a wide range of ideas to boost our innovation output, including tax incentives and other high-level policy initiatives.

Paul Keating once said that policy is determined by those who show up, but a more evidence-based approach may produce better outcomes.

The Global Innovation Index (GII) is an annual survey of innovation in 143 countries developed by Cornell University, INSEAD and the World Intellectual Property Organisation. It is based upon five measures of Innovation Inputs and two measures of Innovation Outputs. In other words, it measures and compares national systems of innovation.

The Index was launched in 2007 with the 2015 edition just published. On both occasions, Australia ranked 17th.

Does Australia’s steady ranking reflect the fact that changing national systems of innovation is a bit like turning around the Queen Mary? Well, not really. In 2007, the top five countries (in order) were the United States, Germany, the United Kingdom, Japan and France. In 2015, the top five countries are Switzerland, the United Kingdom, Sweden, the Netherlands and the United States. Sweden is the biggest improver here, moving from 12th to 3rd. Japan is the biggest loser, down from 4th to 19th.

Australia’s ranking is heavily grounded in its Innovation Inputs. Here it ranks 10th in the world. The top five countries in the world for Innovation Inputs are Singapore, Switzerland, Finland, Hong Kong and the USA, reflecting their substantial investment in education, research and development.

By implication, Australia’s ranking is heavily compromised by its Innovation Outputs. Here it ranks 24th. The top five countries for Innovation Outputs are Switzerland, Luxembourg, the Netherlands, Sweden and the UK, reflecting their capacity to translate their inputs into high-quality goods and services.

The GII also compares inputs to outputs, thereby producing an efficiency ratio. Remarkably, the country with the highest efficiency ratio in the world is Angola, but its inputs are so small that this is not saying much. On the other hand, Switzerland comes second, which says a lot. Australia ranks 72nd in its efficiency ratio, which also says a lot about our capacity to leverage on our investments.

Our Innovation Input Index would be much higher if not for five major weaknesses: specifically, our Government expenditure per secondary pupil as a percentage of GDP (ranked 69th), the percentage of our graduates in science and engineering (77th), GDP per unit of energy (69th), the percentage of our gross expenditure on R&D that is financed from abroad (84th), and the percentage of our total imports that is in ICT and services (78th).

The GII also identifies five major weaknesses in our Innovation Output Index: specifically, our spending on computer software as a percentage of GDP (46th), our exports of ICT and services as a percentage of total trade (79th), our FDI net outflows (114th), our cultural and creative services exports as a percentage of total trade (61st), and related to this our output of feature films (64th). It is our view that addressing our main input weaknesses would go a long way in addressing our output weaknesses.

In terms of inputs, we are clearly underspending on secondary education and this may have an impact on the quality of our science and mathematics education since those areas of education are typically more expensive. Innovation needs many inputs but the input of science and engineering graduates is very important and in this measure we are falling behind other countries in our region, notably Singapore, China and Korea. These two weaknesses are interrelated. Poorly resourced secondary science and mathematics education translates into students losing interest and not pursuing these areas at the tertiary level.

We need to do more to encourage overseas companies to invest more of their R&D budgets in their own laboratories in Australia, and also in our universities and publicly funded research institutes (PFRIs). This enhances our research connections to the major wealth generators of the world and has the potential to open up connections to global supply chains.

Universities and the PFRIs can also play an important role by systematically ‘marketing’ their skills and capabilities to the
major companies of the world. The long-term success of the Boeing–CSIRO collaboration makes for a useful case study. Boeing and CSIRO have been collaborating successfully on research and development for 25 years. This collaboration commenced as a result of CSIRO systematically exposing Boeing executives to its skills and capabilities. Boeing’s presence in Australia is the company’s largest footprint outside the US.

The fact that Ford, GMH and Toyota will no longer manufacture automobiles in Australia does not have to mean that these companies will be cut off from Australia’s research and innovation capabilities. Indeed, it may open up opportunities for our SMEs to be drawn closer to the global supply chain.

Our GDP per unit of energy use is ranked 69th. Innovation in both energy use and production is highly dependent on government policy. Putting a price on carbon is one way of driving more efficient energy use as well as reducing the use of fossil fuels in energy production. This is an area in which our new Prime Minister could show leadership.

In terms of outputs, our low rankings on software expenditure and on ICT and services exports indicate that many of our business enterprises have not fully embraced the digitisation of manufacturing and services. This will require the completion of the NBN and a concerted effort by industry departments and industry associations to inform and educate our companies of the opportunities in this area.

Rankings are not important in and of themselves. But our ranking in the Global Innovation Index is a wake-up call. Above all, the efficiency ratio highlights what anecdotal evidence has been saying for a very long time. We are good at invention but poor in translating our inventiveness into products and services.

The current policy zeitgeist, led by the Prime Minister, offers an important opportunity to obtain more benefit from our inventiveness, and to lift our overall innovation performance through evidence-based policy.

Professor Tom Spurling AM FTSE FRACI Chem is at the Centre for Transformative Innovation, Faculty of Business and Law at Swinburne University of Technology. Professor Michael Gilding is the Executive Dean of Swinburne’s Faculty of Business and Law.
Tilting the scales of environmental justice

In September, Melbourne hosted Clean Up 2015, an international gathering of 700 researchers, regulators and practitioners in the field of contaminated land. The opening session was also the venue for the Brian Robinson Memorial Lecture, which commemorates the contribution to environmental protection of the late Dr Brian Robinson AM, Chairman of EPA Victoria from 1986 to 2001. Dr Robinson, a chemist, was also a key early backer of the CRC for Contamination Assessment and Remediation of the Environment, the conference organiser.

Brian Robinson’s vision of environmental justice also went beyond engaging with the community. Reflecting his background as an analytical chemist, he was adamant that the EPA’s decisions should be based on sound science.

In delivering this lecture to the 2015 conference, the current Chairperson of EPA Victoria, Ms Cheryl Batagol, reflected on Dr Robinson’s commitment to environmental justice – the concept that all citizens have a right to reliable information about how environmental conditions might affect their lives. Brian Robinson is regarded as an early exponent of this concept, not just in his pronouncements and regular media appearances, but also in his determination that the EPA must consult widely with the community as part of environmental regulation in Victoria. EPA staff, at all levels, were well aware that they needed to engage with stakeholders in any decision or action involving the Authority. Long-running community engagement groups were established in areas of high environmental concern such as near oil refineries and other major chemical facilities. Robinson’s vision in this area also extended to community engagement in the collection of environmental data, and a scheme of Community Access to Air Monitoring was trialled.

Brian Robinson’s vision of environmental justice also went beyond engaging with the community. Reflecting his background as an analytical chemist, he was adamant that the EPA’s decisions should be based on sound science. This was in keeping with the second leg of the environmental justice principles, that the information upon which the community relies is based on sound scientific data, and is thoroughly reliable. Ms Batagol cited some recent examples of where these twin principles were relevant, and how the communications landscape of 2015 can make achievement of environmental justice a bigger challenge.

In another paper delivered to the conference, Ms Danielle-Marie Torresan from the South Australian EPA described how environmental justice can be compromised by other needs of society. She discussed a situation where vapour intrusion from groundwater contamination beneath residential properties was indicated to cause a potential health risk for occupants, and investigations concluded that evacuation of residents would be required. Plans to communicate this information, as well as for the evacuation, were developed across government agencies at high levels.

The plans envisaged that all affected residents would be informed on the same day, and at close to the same time. Even the state environment minister was planning to be part of the door-knocking exercise. However, the plans went awry after unscheduled release of information to the media on the day before the communications were due to start. As a result, a large media contingent descended on the affected neighbourhood, and this distressed many of the residents and hindered the communications plan. Much community anger was expressed, with residents feeling that the government agencies had either let them down or were deliberately trying to keep them in the dark.

When further investigations were started, to identify the extent of contamination, drillers installing groundwater wells were followed by camera crews and journalists who watched their every move. Media reporting was sensationalist, and residents were given anecdotal, and often low-quality, information second-hand. Efforts of government agencies to assist the community, especially those who had to relocate, were impeded by the need to respond to media requests to provide instant answers. The situation illustrated how media requirements for drama and controversy can easily work against the principles of environmental justice. It also indicated that that information should be provided to the public as early as possible, even if it is not fully precise or complete.

Both Batagol and Torrsesan used the term ‘Dr Google’ to describe the tendency of citizens and media to seek their own information from the internet, rather than rely on expert information from their actual circumstances. Also, there was a tendency to doubt first-hand information if it didn’t reinforce their findings from the internet.

This all suggests that, despite the promise of the information age and the ability of digital media to give citizens fast access to information, the outcome can be a market for ideas and opinions that aren’t necessarily well founded, and this is, of course, an impediment to environmental justice.
Two people who had helped in my career passed away this year. I'll have more to say about John Swan in another place, but here I want to write about Brian Johnson who was one of my chemistry teachers at Footscray Tech.

Brian was a Mildura boy who graduated from the University of Melbourne and entered the teaching profession at Footscray. As well as his scientific and educational credentials, his ability as a footballer made him a significant figure in any company. He was a meticulous teacher with a gift for explaining concepts that helped students to see where specific examples fitted into the broader scheme of chemistry. An example I remember from those days was his concentration on colligative properties – not a term you hear much these days. I struggled a bit to recall exactly what they were, and so I checked with J.W. Mellor (Modern inorganic chemistry 1922) ‘in contradistinction to additive properties, colligative properties depend on the relative number of molecules present and not on the kind of molecules – for example, the freezing and boiling points of solutions’. So there you have it, osmotic pressure, Raoult’s law and all that. Brian was always a stickler for the right word and I understand that he later taught chemists how to use their language.

Brian’s career as a teacher was cut short by a football injury that cost him the sight of one eye. Leaving the profession, he returned to the university as a postgraduate student studying natural products chemistry with R.G. Cooke. We met again when I joined the same research group for my MSc research. Brian was the most senior member of the group and we all learned a lot from him. For his MSc degree, he worked on the structure of an Australian plant pigment, haemodorin, and its aglycone haemocorin. These compounds had unusual perinaphthenone (phenalenone) structures and had been isolated from Haemodrin corymbosum. For his PhD, he worked on the beautifully coloured quinone pigments of another Australian plant, Ventilago viminalis.

Cooke and his students worked on haemocorin for years until the final structure was finally completed by Ian Rainbow. Along the way, a number of model compounds were synthesised and since the structure seemed to involve a phenyl(naphthalene) ring system, Cooke assigned syntheses of a number of these to his other students so they had something to do while the slow extraction of plant material and equally slow chromatography was proceeding. Mine was 1-methoxy-4-methyl-6-phenyl-naphthalene.

In 1960, Brian ran out of plant material and so a small party drove to Baradine in central New South Wales, where Ventilago viminalis had been reported to grow. After a Q&A session in a pub, a knowledgeable local led them to a specimen of Ventilago and was astonished when Brian produced a small extraction kit and checked that the root bark extract gave the characteristic colour with alkali before they collected enough material to sustain the research.

At the conclusion of his time at Melbourne, Brian was guided by Lloyd Jackman to postdoctoral studies in University of California, Los Angeles, with Saul Winstein, where he was close to the non-classical carbonium ion controversy that stimulated such a lot of good chemistry in the 1960s and 1970s. After he returned to Australia in 1966 to take up an appointment at the University of Western Australia, Brian’s research at first featured quite a bit of norbornane chemistry but later he returned to his love of Australian natural products, albeit with alicyclics rather than the aromatics of his Melbourne days.

Over the years, we met from time to time, notably at RACI Organic Division conferences, and we once shared a trip to America as members of a small group who went shopping for NMR spectrometers. Staying fit was always part of Brian’s life even if it meant going through his exercise routine down the back of the Boeing 747 as we yawned and stretched after our trans-Pacific sleep. Passengers were unsure what to make of a bloke doing handstands but that was just Brian the fitness fanatic.

In the late 1980s I stayed with Brian when I was in Perth to deliver the Bayliss Youth Lectures. Lunch with Sir Noel was another highlight of that visit, and a third one was gazing on the America’s Cup that was for a short time domiciled in Perth.

Brian’s career was marked by commitment to whatever he was doing. And it was not just to research and teaching, although he ran the third year laboratory for 30 years. Younger members of staff remember him fostering a sense of belonging, for example by organising (with Don Watts) end-of-term (later semester) squash tournaments, and also the wine bottling events. Football continued as part of his life: he coached junior teams for the Floreat club and also a University team. Retirement in 1997 was only a sort-of-retirement because he continued for a while with first-year tutorials and, together with his wife, Doris, undertook consulting work for local chemical companies.

Our last meeting was in May 2014 when I was in Perth to help with archiving the papers of University of Western Australia’s Jack Cannon. Doris brought us together for dinner and although it was clear that at age 81 Brian was fading, we enjoyed a long chat about old times. Something I didn’t know about until then was Brian’s interest in gardening. He had some years before won a prize for it and even in the evening darkness I could see that what he and Doris had done was something very special.

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

Arows
Tin and iron, perhaps, found in slate mining comeback. (6)
9Element against loss of electron from bread? (8)
10First unit rated equipment analysing carbamide. (4)
11Used 10 Across on a t^3 device which reduces the amplitude of a signal. (10)
12Lucubrating dusty gin cocktail. (8)
15Copper 17 Across made up point of supply. (6)
17Parent rocks over rough elementary school beginnings. (4)
19Expands gravity lines. (5)
21 Constructed over cheese. (4)
22Amuses funny suspect. (6)
24Pour cold water on Spooner regarding royal figure. (8)
26New 29 Across nice as the ratio of voltage to current. (10)
29Wind down the balance. (4)
31Needs to slam radical queries. (8)
32Nothing remiss over iodine and carbon acid. (6)

Graham Mulroney FRACI CChem is Emeritus Professor of Industry Education at RMIT University. Solution available online at Other resources.
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Best wishes for the festive season and for 2016