

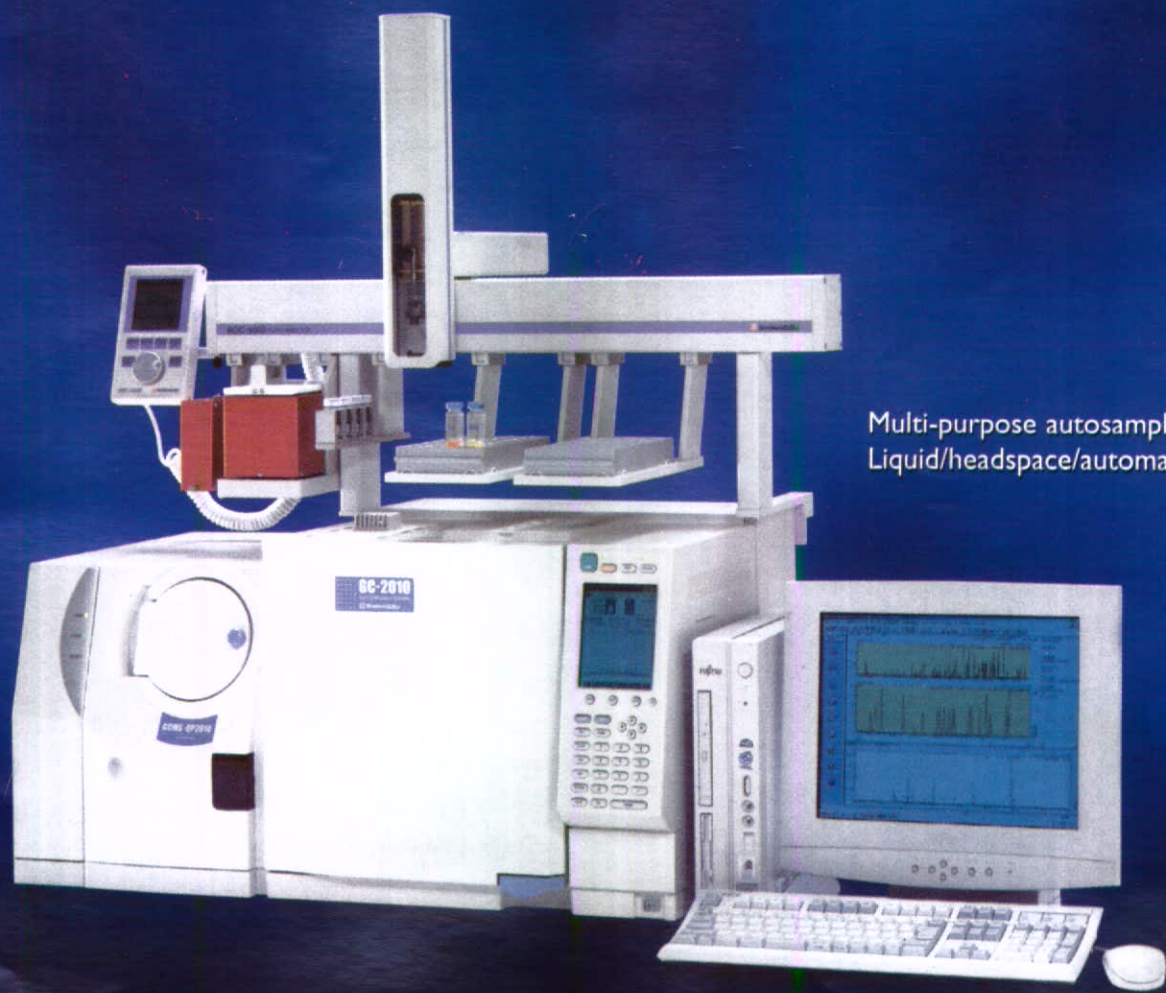


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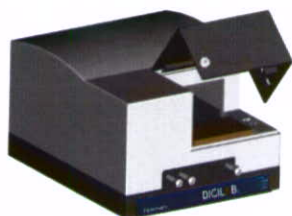
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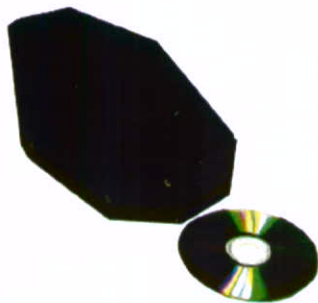
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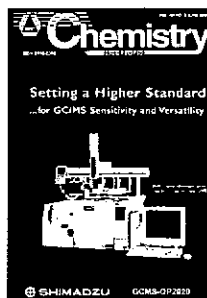
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UNIVERSITY AND INDUSTRY COLLABORATION TO EXPAND EXPORTS

New Zealand's light metals manufacturers are joining forces with the academic world to develop high-value light metal products for export markets.

The project, based at the Light Metals Research Centre (LMRC) at The University of Auckland's Faculty of Science has received \$1.4 million per year for four years from the Foundation for Research, Science and Technology.

Researchers in the Centre will work with academics from the University's faculties of science and engineering as well as Waikato University, AUT and industry partners, in an initiative offering significant benefits to the New Zealand economy.

Director of the Centre Dr Mark Taylor says the research will focus on transforming the value of light metals from the approximate \$3000 commodity value the raw metals fetch on the international market to components that can be worth \$50,000, or even \$100,000 per tonne. "We want to get the best out of these metals rather than selling them in their minimum value, semi-fabricated forms. That means turning metals such as aluminium, magnesium and titanium into high-end innovative components," says Dr Taylor.

"This not only enables us to get more value out of these materials, but keeps New Zealand one step-ahead of our competition in other countries. The market for mass produced articles is becoming increasingly difficult, and will become even more so, as the impact of China in the international scene increases."

The types of components include those found in the marine sector –

such as super yachts - and in the domestic architecture of bathrooms and kitchens, as well as high performance wheels and a multitude of other automotive parts.

"New Zealand manufacturers are making these components and finished products right now. What we aim to do is try to give them an edge over the competition by making these products even more sophisticated," he says.

Dr Taylor says the researchers and industry participants will work in partnership to develop new products, as well as look at ways to overcome specific problems, such as how to make aluminium as shiny as chrome. "It is about working together to solve problems that will give New Zealand a bigger slice of a competitive international market, and one which will increasingly look to recycle materials to produce energy and cost efficiency's through the economy.

"We believe that by working with industry and with the Government's New Zealand Trade and Enterprise, both the type of products and their speed to market can be improved," he says.

The University is part of an industry cluster, called the Light Alloys Manufacturing Group New Zealand (LAM-NZ), to help grow this manufacturing sector by increasing export value. Companies within the cluster include Ullrich Aluminium, ION Automotive, Diometrics, Titanbond, and HERA.

New Zealand Trade and Enterprise and Investment New Zealand have taken an interest in the group since its formation last year and are assisting the cluster to grow its membership and develop a comprehensive export strategy.

Dr Taylor says the research will be undertaken within the associated factories, using the companies' own equipment to ensure outcomes can be quickly adopted by industry.

"Factories in Hamilton, Auckland and Manukau are already being targeted for the research work. An underlying benefit of this strategy is the upskilling of the manufacturing businesses, and the researchers as well," he says.

Dr Taylor says the collaboration between different areas of the University, and from Waikato and AUT, is one of the strengths of the project.

"Many of the most innovative advances in light metals and other materials occur at the cross-disciplinary boundaries between surface science, dynamic thermal processing of materials and alloy or composite behaviour."

Dr Taylor and his team at LMRC consult internationally on the conversion of light metal ores to their metallic form. The Centre has collaborations with other research centres in North America, Europe and Australia.

GERMANY SET TO CHALLENGE NEW ZEALAND OLYMPIANS

While New Zealand's Olympics squad is training for the Athens Olympic Games, budding Olympians of a different sort are also in training mode - not for athletics but for the 2004 International Chemistry Olympiad that will be held in Kiel, Germany, in July.

Four Year 13 students have been chosen to compete at the Chemistry Olympiad after a rigorous selection process held at The University of Auckland recently. The process involved more than 100 students and was narrowed down to the final four at a week long chemistry camp, followed by a three-hour practical exam and a three hour theory exam. "The level of students competing this year has been outstanding.



Above: Budding chemists at the Chemistry camp at The University of Auckland

Participating in the Olympiad program demands achievement beyond a first year university level," says Dr Sheila Woodgate of the Faculty of Science at the University.

"The camp not only produced four exceptional students for the Olympiad, but provided a platform for many young New Zealanders from which to build a better appreciation of the study of chemistry."

The University of Auckland offers financial assistance, while its Department of Chemistry offers coaching and support for participants in the selection process and for the team once they have been chosen.

"It's a wonderful feeling to see the students get so excited and advance in such an intellectual environment. It's also a pleasure to read about their successes in the various national exams at the end of the year," says Dr Woodgate.

This year's team consists of Tony Chiu, Yun Huang and Aritra Ray from Auckland and Reed Roberts from Wellington. This is the second year that Aritra, a Mount Roskill Grammar School student and Yun, a Westlake Boys High School student have made it into the team.

The team head to Germany in July, where they will compete against 260 students from more than 60 other countries. Theoretical and practical questions will be posed from almost all sectors of chemistry, and are based on a set of preparatory problems supplied by the organizers.

A visitors' program will also allow the participants to get to know Germany in its scenic and cultural diversity and as a location for chemistry in research, teaching, industry and technology.

New Zealand has been sending teams to the Chemistry Olympiad competitions since 1992 and they have won many medals in that time. Dr Woodgate says the 2004 team intends to carry on the tradition.

HIGH CITATIONS FOR MARSDEN RESEARCH

The Marsden Fund aims to enhance New Zealand's knowledge base and contribute to the global advancement of knowledge. It has grown from a \$5.5 million fund in 1995 to \$33 million in 2003. Have its millions been well-spent?

A bibliometric analysis of publications arising from the Fund has just been completed. Articles funded by Marsden were compared to the total pool of New Zealand-authored articles for the period 1997-2001. Citation counts are a commonly used measure of publication impact, the rationale being that the more influential a piece of research is, the more often it is cited by other publications. Compared to all New Zealand-authored articles, the Marsden-funded articles were found to be cited, on average, 1.7 times more often. This elevated citation rate held true for almost all subject areas.

In other differences between Marsden-funded and total New Zealand-authored articles, Marsden articles

were weighted more towards fundamental areas of research, and while inter-sectoral collaborations within New Zealand (e.g. University-CRI) were less frequent on Marsden articles, international collaborations were more frequent, occurring on 48% of the articles.

Publication output from the Marsden Fund is on the rise: 13 articles were published in 2000 per million dollars of Marsden money spent in that year, and the Marsden-funded share of New Zealand-authored articles has risen from 2.6% in 1997 to 7.7% in 2001. In comparison, the Marsden budget has grown from 1.7% of New Zealand's government and higher education R&D spending in 1996, to 3.5% in 2002.

The report can be found at: <http://www.rsnz.org/funding/evaluation/impact.php>.

NEW APPOINTMENTS TO FOOD RESEARCH CENTRE

The Riddet Centre, established at Massey University last year, a national centre for research in food and biologicals have appointed three new principals. The Riddet Centre is a partnership between Massey University, The University of Auckland and the University of Otago.

The newly appointed principals are Professor David Mellor from Massey, a leading mammalian physiologist; Professor Dong Chen from The University of Auckland, an international leader in food engineering and Professor Jim Mann from the University of Otago, a pre-eminent human nutritionist.

NEW RESEARCH FACILITY AT THE UNIVERSITY OF AUCKLAND WILL HELP DEVELOPMENT OF NEW ZEALAND INDUSTRIES

A new research facility at The University of Auckland's Faculty of

Engineering will help New Zealand industries keep abreast with cutting edge technologies.

The Centre for Advanced Composite Materials (CACM) research facility was officially opened on Wednesday April 21, 2004, by the Minister for Research, Science and Technology, the Hon. Pete Hodgson.

The Centre has been established as a joint venture between The University of Auckland and Forest Research (FRNZ). It is also supported by a consortium of industries and the Foundation for Research, Science and Technology.

Last week the composites research group was also announced as a recipient of a Foundation for Research, Science and Technology (FRST) grant for the designing, developing and manufacturing of advanced composite structures. The group will receive more than \$10.2 million over a period of six years from this FRST grant, in addition to the support received from other New Zealand and overseas sources.

Faculty of Engineering Dean Professor Peter Brothers says he is delighted with the addition of the research facility to the Faculty's existing research and teaching programme.

"The new facility will take research in the area of composite products and manufacturing processes to a new level and it offers a wide range of research and learning opportunities to our academics and students. "In addition, we welcome the opportunity to work with Forest Research on this initiative, as well as other members of New Zealand industry who have a stake in the ongoing development of these research programmes," says Professor Brothers.

Research in advanced composite materials at the University first started in 1987, while the joint venture was formally established in 2002. It aims to pioneer innovative technologies in advanced composite products and manufacturing processes, to enhance the wealth of its members and to provide new business opportunities that will benefit New Zealand's economy.

Centre Director and Head of the Mechanical Engineering Department, Professor Debes Bhattacharyya, says increased interest in the research carried out by the Faculty meant that bigger custom-made premises were required.

"Since we first started research in this area, we have gone from strength to strength in terms of our research projects and opportunities and we have had growing support for our work from industry collaborators and overseas institutions.

"Interest is coming from a wide range of industries, varying from marine and forest product manufacturers, polymer and consumer products manufacturers, and aircraft maintenance and parts manufacturers," says Professor Bhattacharyya.

Forest Research Chief Executive Bryce Heard says the organisation is pleased to be so closely involved with an area of research that has the potential to drive real growth in the New Zealand economy. "The area of composites research opens up a whole new area of opportunities for New Zealand businesses and industry," says Mr Heard.

"New Zealand organisations are already world-leaders in this area of development and this new centre of research at the University will help all of us stay ahead of the competition. It's an exciting development for everyone involved."

The Centre is now located in an architectural award winning new building at the University's Tamaki Campus in Glen Innes, Auckland.

Research areas include innovative manufacturing processes like modified rotational moulding, development of novel biopolymers and polymer blends, modifications of synthetic and natural fibres like wood fibres, and the applications of nano- and micro-fibrillar polymers in composites manufacturing.

The Centre for Advanced Composite Materials is part of the Faculty of Engineering's Mechanical Engineering Department, but it also utilises the skills of researchers from

a variety of disciplines including Engineering Science, Chemical and Materials Engineering, Civil and Environmental Engineering and Chemistry. Forest Research staff will also contribute to research and are likely to be based at the Centre from time to time.

The CACM has been set up initially for six years, with a possible extension after an independent mid-term review.

BIBLIOMETRIC STUDY HIGHLIGHTS EFFICIENCY OF NEW ZEALAND RESEARCHERS

When publication quantity is compared to research dollars spent, New Zealand researchers are among the most efficient in the world. A report just released by MoRST, FRST, HRC and RSNZ, analyses New Zealand-authored articles, published in the 5 year period 1997-2001. It builds on MoRST's 2001 bibliometric study, and it compares New Zealand to other countries in terms of research publications' subject distributions, citation rankings and collaborations.

There is a worldwide trend towards increasing publication output, and New Zealand is no exception; our publication count has been increasing by around 4% a year since 1993. In productivity per capita, New Zealand ranks eleventh out of twenty comparison countries, but rises to first place per research dollar. All sectors increased their publication output from 1997-2000 except for the CRIs, whose output was 9% less in 2000 than in 1997.

The subject distribution of New Zealand-authored articles is similar to that of Australia; more than two thirds are published in the life science areas of medical and health sciences, biology, and agriculture-veterinary-environment.

As judged by citations, New Zealand articles have a reasonable impact, ranking us 17th out of 27 comparison countries. Three subject areas: chemistry, physics and agriculture-veterinary-environment, had citation impacts around 20% above the world mean; the remaining 7 subjects fell

below the world mean. Internationally co-authored articles had, on average, higher citations than other articles, and in line with other countries, New Zealand's rate of international collaboration is increasing, with 37% of articles internationally co-authored in 2001.

NEW ZEALAND - EUROPEAN SCIENCE AND TECHNOLOGY WEBSITE

Recently, a new web site opens its doors for business. Called "Co-Lab International", the site at <http://www.colab.rsnz.org> provides New Zealand researchers with up-to-the-minute information on developments on the European science scene, with particular emphasis on collaboration opportunities and associated funding. As the site develops, information will be assembled on countries outside Europe. Information on Europe will be supplemented by targeted emails to researchers interested in a particular country or topic. The seven topics listed at the top of the site are those currently emphasised in Europe's "Framework 6" programme. Watch the site for an opportunity to join one of the specialised lists.

The site is funded by New Zealand's Ministry of Research, Science and Technology and powered by the Royal Society of New Zealand. It is updated every day by dedicated staff at the Royal Society, whose job it is to research relevant European print, web, and email sources. Do you have information you want to add to the site? Just email Colab@rsnz.org with your brief text. Co-lab will also be pleased to receive information from European Union Embassies serving New Zealand.

ROYAL SOCIETY OF NEW ZEALAND TRAVEL GRANTS

Realising the importance to beginning scientists of the opportunity to travel overseas and present the results of their work at an international scientific conference, the Royal Society, in 1979, established a fund to enable it to assist students undertaking PhD

degrees at New Zealand universities to attend their first overseas scientific conference.

To be eligible students must be undertaking full-time PhD study in science and/or technology and must be New Zealand citizens or have permanent residency status. Due to limited funding, preference will be given to applicants who have received their secondary schooling and the majority of their tertiary qualifications in New Zealand. Preference will also be given to those students at an advanced stage of their PhD studies.

Funds are, however, limited and the pressure on them is likely to be appreciable; in consequence, grants to individual scientists are unlikely to exceed \$1,000. It is anticipated that students will seek other funding to assist with their conference attendance.

Electronic copies of the information and application forms are available from awards@rsnz.org; copies are also available on the Society's web site http://www.rsnz.org/awards/rsnz_awards/index.php. The closing date for the next round is 1 September 2004.

PLAN B: TURNING TERTIARY STUDENTS INTO ENTREPRENEURS

A new entrepreneurs club at New Zealand universities will soon be helping students turn their bright ideas into successful businesses. The club is being run by Realize Entrepreneurs, a business unit of Realize Technology Ltd. It will be piloted this year at the University of Canterbury, Massey University and Unitec with funding from New Zealand Trade and Enterprise (NZTE).

Realize Technology Director John Missen says 'Plan B' aims to help students turn technology ideas into business reality, by putting them in touch with experts in intellectual property, venture capital, design, marketing and other areas. Plan B is being funded through NZTE's Enterprise Culture and Skills Activities Fund - a contestable fund

used to support the development of a culture of enterprise and business success in New Zealand.

Plan B has an open membership on campus with no joining fee. Anyone (staff, students or alumni) are welcome to join if they have a technology business idea to develop and wish to contribute to a thriving and dynamic enterprise community. Please visit <http://www.planb.ac.nz> or <http://www.nzte.govt.nz/ecca> for more information.

2004 ACADEMY MEDALS AND AWARDS NOMINATIONS

The Academy suite of medals and awards available for 2004 are:

Hutton Medal - Earth sciences

Sir Charles Hercus Medal - Clinical sciences and technologies and public health.

T. K. Sidey Medal - Scientific research in electromagnetic radiation.

Cooper Medal - for the best account of research work carried out in New Zealand in physics or engineering.

Thomson Medal - in recognition of outstanding contributions in the fields of the organisation, administration or application of science and technology.

Hamilton Memorial Prize for beginners in scientific or technological research in New Zealand.

Hatherton Award for the best scientific paper by a PhD student at any New Zealand university in physical sciences, earth sciences and mathematical and information sciences.

Charles Fleming Award - for environmental achievement.

Electronic copies of the information and application forms are available from awards@rsnz.org or copies are also available on the Society's website http://www.rsnz.org/awards/academy_awards/forms.php. The closing date for applications and nominations is 2 August 2004.

The Water Chemistry – Public Health Decision-Making Interface

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presented in part at *Chemistry at the Interface* NZIC, Conference Nelson, December 2003

Introduction

Public policy and decision-making involves authorities such as Ministries and local Councils, setting directions or making choices on behalf of society or a community on issues in which there is a strong element of public good.¹ It may result in the development of legislation, the promulgation of Standards and Guidelines, or more generally in risk management decisions.

Science has a role in informing and supporting public policy and decision-making. This can be at a strategic level where, for example, science directly influences the formulation of strategies to deal with issues, or at a more technical level where scientific advice relates more specifically to the implementation of a policy or programme. International examples of science very directly informing policy and decision-making include climate change and, somewhat unsuccessfully, the handling of the BSE crisis in the United Kingdom.¹

In New Zealand, Crown Research Institutes (CRIs) have a key role in informing Government policy through the provision of scientific knowledge.² This is particularly true for the Institute of Environmental Science and Research Ltd (ESR) in its core area of public health. Public health is defined as the *science and art of preventing disease, prolonging life and promoting health through the organised efforts of society*.³ Consistent with this is a strong relationship between ESR's science and the decision-making of public authorities aimed at improving the health of the New Zealand population. ESR science and scientists inform at two levels: centrally, *e.g.* to the Ministry of Health in its public health programmes, and locally, *e.g.* to the 12 public health services around New Zealand.

One of the key areas involving ESR is environmental health, where a strong focus is on drinking water quality. In this article, three examples are presented of the application of chemistry and chemical knowledge to informing decision-making as it relates to drinking water quality and so the health of the New Zealand population. These examples span the need for chemistry to aid the response to public health emergency situations, through to chemical investigation to inform a specific public health strategy.

Water Chemistry Terms

The Ministry of Health has performed much work in New Zealand (with support from ESR) to provide for water

suppliers, regulators, and public guidelines to gauge the safety of drinking water. Some of this work is encapsulated in the *Drinking Water Standards for New Zealand 2000*.⁴ These Standards provide the maximum concentrations of chemical, radiological, and microbiological contaminants in drinking water acceptable to public health. Within the Standards, chemical contaminants that have health significance are assigned a *Maximum Acceptable Value (MAV)* where possible. The MAV is the maximum concentration of a constituent that is not considered to pose significant health risk to the consumer over a lifetime consumption of water. It is largely in the context of this work, and with the aid of the two terms defined above, that the examples in this article are discussed.

Example 1: Public Health Emergency – Mount Ruapehu

The Mount Ruapehu volcano at the west end of the Taupo volcanic province erupted spectacularly on 17 June 1996. The eruptions continued throughout the day; sonic booms, rocks jettisoned into the air, and a 12 km high ash plume that later deposited a 1.5 cm layer of ash in Taupo and other neighbouring cities were recorded.⁵ The eruption was immediately declared a civil defence emergency and a national Task Group was formed. This included ESR alongside the Ministry of Health to provide advice directly on public health considerations.

A key public health question was whether the volcanic eruption posed a threat to drinking water quality. In making an assessment ESR chemists had to consider possible routes of contamination to drinking water supplies, potential contaminants and their individual exposure assessments, and those supplies that might be affected. The drinking water supplies in the area around Mount Ruapehu are largely sourced from surface waters (rivers and lakes). ESR experts determined that the eruption could lead to contamination by ash fallout onto, or lava or lahar flow into the surface water, or leaching of ash, lava or lahar into the surface water. These options were considered by the Task Group and, following consultation with Council and health staff at Mount Ruapehu, it was concluded that ash fallout was the most likely mode for the contamination of drinking water supplies.

The next step was to consider the potential health impact of ash fallout. In this regard, ESR was fortunate to be provided with a sample of ash from the previous Mount Ruapehu eruption in 1995. While the actual concentrations of the constituents of the ash from the 1996 eruption would not necessarily be the same as those from 1995, analysis

of the sample identified the chemical constituents of potential health significance as shown in Table 1. By assuming the quantity of ash delivered through fallout an exposure assessment was performed by comparing the actual levels of chemical contaminants against acceptable health levels (the MAVs) as defined in the Drinking Water Standards.⁴ This is illustrated for arsenic, the most prevalent of the ash constituents with a potential direct public health risk as:

Determined: 0.05 mg As/kg ash.
 Assume: 1 kg ash falls into 1 m³ (1000 L) water.
 Hence: 0.00005 mg As/L water results from ash fallout.
 Whilst: 0.01 mg As/L is the MAV.

While the ash fallout presents an acute exposure and the MAV reflects lifetime exposure, this is the best available comparison. An analogous consideration of each constituent in turn showed that the chemical contaminants present did not present a direct health risk.

A further consideration for the water chemist was what impact ash might have on the chemical treatment of the water supply. Ash changes the physical parameters of pH, turbidity, and conductivity of water into which it falls and thus impacts markedly upon the water treatment processes and the water could then become susceptible to the microbiological contamination that it aims to protect against.

It was necessary then to determine those community supplies that might be affected by this secondary public health concern. The New Zealand national database, WINZ,⁶ captures and monitors information on all of the country's registered drinking water supplies and includes information on the specific treatment processes used. WINZ identified all of the water supplies in the Mount Ruapehu area that could be affected by ash fallout so that the potential effect of the changes in water chemistry (described above) to the known treatment processes could be assessed. While the chemical constituents delivered by ash fallout did not present a direct public health risk, the contamination of the supplies could change the physical parameters enough to disrupt the treatment processes and introduce microbiological risk. Approximately 20 water supplies were determined to be *at risk* from this threat.

Table 1. Chemical constituents of Mount Ruapehu ash and their associated potential health risk.	
Chemical Contaminants	Associated Potential Public Health Risk
SO ₄ ²⁻ , Cl ⁻	Indicators of contamination (most elevated)
As, Cr, Cu, Pb, Hg, Al, Br, F	Direct public health risk
Change in water pH, conductivity and turbidity	Secondary public health risk through treatment failure as a result of ash contamination

This concluded the chemist's job leaving the decision makers better informed for their response to the volcanic eruption and they deemed it unnecessary to close water supplies. Over subsequent days and weeks the local drinking water supplies were unaffected by the volcanic activity and the drinking water remained safe for public consumption. By September 1996, Mount Ruapehu was quiet.

Example 2: Public Health Emergency – Cyanide

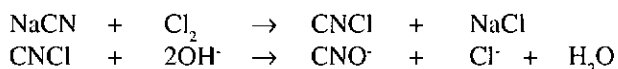
In March 2003, letters to the *New Zealand Herald* and embassies within New Zealand threatened to release cyanide into drinking water supplies if, and when, Iraq was invaded by allied forces. Moreover, there was a threat to provide a *demonstration of capability* that could include dumping cyanide into water supplies by using 25 kg of *weapons grade* cyanide purportedly held.⁷

Fortunately, New Zealand water suppliers were not entirely unprepared for such a threat as a risk management approach to drinking water quality is adopted with water supply security an explicit aspect, though sabotage is at the extreme of risk management! But no matter how well prepared water suppliers may be, cyanide is a threat that cannot be taken lightly since it is highly toxic, inhibiting terminal oxidase that results in cell death and, with no energy release, a person soon dies. Not surprisingly, cyanide is recognised in the Drinking Water Standards⁴ as a contaminant of health significance and has a MAV of 0.08 mg/L.

Auckland formed a local response team to the cyanide poisoning threat. The public health service was represented in the team, and ESR provided scientific advice to the local public health service representatives. The primary public health issue was whether 25 kg of cyanide presents a public health threat to Auckland's drinking water supplies. To assess this, ESR chemists considered the volume of water to which 25 kg of cyanide would need to be added to be of health significance, and then whether water treatment processes would protect against cyanide.

The answer to the first question, using the MAV and the lethal dose as the *health* benchmarks, calculations showed that the cyanide would have to be added to a small volume of water to be of health significance.

Auckland's water supplies are chlorinated, and ESR considered whether the chlorine present protected against potential introduction of cyanide to the supply. Cyanide reacts rapidly with chlorine to produce cyanogen chloride (CNCl), itself a highly toxic gas of limited solubility, but at pH >8 it is hydrolysed to cyanate ion (Scheme 1) that is only of limited toxicity; the rate increases as pH increases.⁸



Scheme 1. The breakdown of CNCl by hydroxide ion.

If the cyanide concentration in water is less than the MAV, there should be an adequate concentration of chlorine present from typical chlorination treatment to ensure that all of the CN⁻ is converted into CNCl. The concentration

of CNCl present in the water and the rate at which it decomposes will depend upon the pH of the water. Based on this chemistry, reassurances could be given to the public health service representatives that chlorination should provide some protection against cyanide contamination.

Although the primary public health issues had been addressed, the response team raised several secondary public health concerns that required input from ESR. Examples of these questions and the responses to them are given below:

What is the trigger level for cyanide contamination?

Through ongoing surveillance (and information in WINZ) it is known that cyanide is not normally detectable in drinking water supplies in New Zealand. Thus detection of any level of cyanide would imply its introduction to the water supply.

How could contamination by cyanide be detected?

There are several ways that cyanide contamination could be detected or suspected by the public health practitioner, not all of these involve chemistry and likely would be addressed in the following order:

- The most obvious way would be visually through any physical evidence of contamination, for example, damaged valves or pipes.
- Detection by the public through the smell or taste of cyanide in the water. Some 40-60% of the population can detect cyanide in this manner.
- The observation of increased chlorine demand in the treatment plant as the chlorine added for treatment is also consumed in the degradation of cyanide, as per Equation 1.
- The presence of cyanide could be confirmed by sampling and testing for it.
- In the very worst scenario, detection could be through morbidity or mortality of individuals.

In the event of cyanide contamination, what short-term usages of the water supply are likely to be harmful?

Based on WHO exposure data for short-term exposure (the levels are significantly higher than the MAV of 0.08 mg/L that protects against lifetime exposure) the following levels of cyanide in water should be safe for the activities indicated:

- Drinking, cooking, brushing teeth: 0.6 mg/L
- Toilet flushing (inhalation of volatile gases): 1.5 mg/L

How can cyanide be destroyed?

The chemistry of Scheme 1 shows that cyanide can be destroyed by chlorination at pH 8.5-9.

The information provided by ESR personnel to these and other questions aided the Auckland response to the cyanide threat. It underpinned critical questions including whether the threat was general to the water supply and whether it would need to be completely shut down. Clearly the information provided an insight into those activities still permissible were the supply contaminated with cyanide, and the way the supply could be remediated in the event of contamination. Thankfully, the chemists' advice was not put to the test, the threat was just that and was not realised.

Example 3: Public Health Strategy – Corrosion-derived Metals

ESR conducts an ongoing monitoring programme on behalf of the Ministry of Health to identify those chemical substances in New Zealand drinking water supplies that are present at potentially significant health levels. Put simply, the programme determines the most likely chemical contaminants and the chemical risks to a supply, and assesses the levels of chemicals present in the context of the Drinking Water Standards⁴ to determine if they are of potential health significance.

Over the first five years of the programme (1995–2000) heavy metals were found in a significant number of New Zealand's drinking water supplies. Figure 1 shows the concentration of heavy metals exceeding the MAV (and so at a concentration of health significance) and at 50% of the MAV (considered to be potentially health significant) against the population served by the supplies tested.

In terms of health effects, heavy metals have chronic rather than acute manifestations, and are most toxic to children and unborn babies. Lead is the most significant as it is a cumulative general poison acting on the central nervous system. Cadmium on the other hand, accumulates specifically in the kidneys, and is associated with renal dysfunction and kidney stones.⁹

The public health issue raised from the first five years monitoring was that the heavy metals Sb, Cd, Cr, Cu, Pb, and Ni are present in many New Zealand drinking water supplies at levels of potential health significance. It was suspected that the metals were not inherent to the source water, but rather associated with corrosion of plumbing fittings.

The Ministry of Health responded to these findings by considering i) a change the standards for plumbing materials, ii) treatment of the water so that it is less corrosive, and iii) flushing taps before use. The last option provides the best short-term response, is the least expensive and intrusive, is more readily instigated, and was preferred. Ideally, a combination of all three tactics should be adopted as the first two options provide the best long-term public

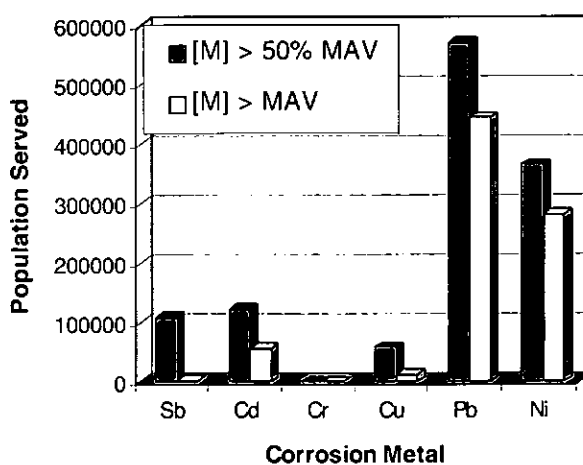


Figure 1. Detection of corrosion metals in all drinking water supplies 1995-2000.

health protection. Before the 'flushing' strategy could be promulgated, further information was required to assess its effectiveness and to provide guidelines as to how it was best achieved. ESR conducted a study to address these issues by considering the source of the corrosion metals, the volume of water required for an effective flush, and the required frequency of such flushing.¹⁰

School students were enlisted in three cities served by water supplies of different levels of corrosiveness. They collected samples and information on the water fittings so that 154 dwellings were tested.¹⁰ Three water samples were taken first thing in the morning at defined outflow volumes to represent water from the tap, from the house pipes/plumbing, and from beyond the property boundary (the distribution system) for each dwelling. The samples were analysed by Inductively Coupled Plasma-Mass Spectrometry (ICP-MS) for Sb, Cd, Cu, Pb, Ni, and Sn.

Figure 2 shows the analytical findings and, in particular, the effects of flushing the taps on the concentration of the corrosion metal. The study confirmed that plumbing fittings are the principal source of corrosion metal contamination. Accordingly, flushing will protect consumers against exposure to Sb, Pb, Ni, and Cd in 95% of cases. Flushing will also reduce Cu levels but to a lesser extent as it is also associated with water pipes. The study also determined that flushing a volume of <1 L would be adequate, and that a single flush first thing in the morning is the most effective way to achieve a reduction in heavy metal exposure.

These results gave direct information to the Ministry of Health for the most effective public health strategy on contamination of drinking waters by corrosion metals. This is reflected in the Drinking Water Standards⁴ which define both the requirements for compliance monitoring of corrosion metals and the advice water suppliers must give to consumers about the flushing of taps.

Conclusion

The examples detailed above provide a sense of the way chemistry and chemical knowledge can be applied to public

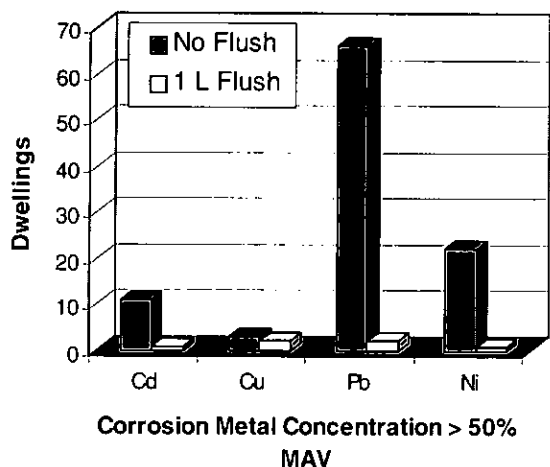


Figure 2. The effect of a 1 L flush on corrosion metals concentration.

health issues so as to inform decision-making. The selected examples span the range of applications of science in public health from the very acute, emergency situation, to a study carefully designed to inform and assess a specific public health strategy. They involve informing both local and central government public health authorities.

It will be appreciated that while the chemistry and/or chemical knowledge necessary to answer the questions is often straightforward, the public health implications are often very significant. At the same time, and particularly in emergency situations, answers are often required on a very short time scale and in the absence of all of the information desirable. The chemist then has to balance the tension between *scientific uncertainty* and the need to provide useful information to support the decisions that need to be made. Throughout the process, there is a need for the chemist to understand the *real life* context in which questions are being asked, and to communicate with decision makers in a way that informs through use of appropriate language, level, and conveying as necessary the limitations.

Acknowledgements

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References

1. Parliamentary Commissioner for the Environment, *Illuminated or Blinded by Science?*, Wellington, July 2003.
2. Ministry of Research, Science and Technology, *An Appraisal of Crown Research Institutes 1992-2002*, Wellington, 2002.
3. Acheson, D. *Public Health in England: A report of the Committee of Inquiry into the Future Development of the Public Health Function*, London, 1998.
4. Ministry of Health, *Drinking Water Standards for NZ 2000*, Wellington, 2002.
5. See: <www.url.co.nz/ruapehu/lahar_2003.html>.
6. See: <www.drinkingwater.org.nz>.
7. See: <www.nzherald.co.nz/storyprint.cfm?storyID=3300789>.
8. White, G.C. *The Handbook of Chlorination*, 2nd Edn., van Nostrand Reinhold: New York, 1986.
9. Ministry of Health, *Guidelines for Drinking-Water Quality Management in NZ*, Wellington, 1995.
10. Nokes, C. J. *Risk Factors Leading to the Appearance of Corrosion-Derived Metals in Drinking Waters*, ESR Report to the Ministry of Health, May 1999.

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Lanthanide Complexes: Luminescent Labels For Applications In Biochemistry And Immunology

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Introduction

Radioimmunoassay and fluorometry are very useful tools in many areas of the biosciences where the specific detection and quantification of biological material *in vitro* and *in vivo* is important. Current immunoassays use either dyes based upon fluorescent organic molecules or radiolabels. However, radiolabels have the inherent problems of cost, handling, lifetime, and disposal; the safe handling of radioisotopes is a major issue in many biological laboratories. "Fluorescent" labelling in contrast is relatively inexpensive, not dangerous, and luminescence (both fluorescence and phosphorescence¹) can be measured quickly and easily. However, fluorescent labels based on organic frameworks such as fluorescein also are not ideal as the half-life of their fluorescence is in the nano-to-micro-second range and long lived phosphorescence¹ is not usually observed due to quenching of the triplet by molecular oxygen.² Problems with these labels also arise from the background fluorescence of biomolecules, *e.g.* in the serum, whose half-life is of the same order of magnitude and often cannot be distinguished clearly; this affects the sensitivity. Lanthanide labels have some obvious advantages making them attractive as possible alternatives to radioisotope labels and organic dyes.^{3,4}

Designing a Lanthanide Probe

Lanthanide luminescence, more specifically phosphorescence, occurs in the millisecond range, and this enables the possible use of time-gated techniques. Fluorescence emanating from organic matter (such as proteins) that can interfere is allowed to fade away before the lanthanide luminescence is measured. Usually, a millisecond delay is needed between the initial irradiation of the sample and the measurement of the luminescence,³ so that only the label-based luminescence is recorded and the signal-to-noise ratio is greatly enhanced over a conventional fluorescence experiment. Lanthanide labels also have a large Stokes shift. For example, in the case of europium (Eu) the excitation and emission peaks are separated by >200 nm. This is advantageous as it allows the use of filter-based and multi-parameter instruments.

The optical transitions of lanthanide ions involve the 4*f* orbitals. These orbitals are shielded from their chemical environment by the outer 5*s*² and 5*p*⁶ electrons and are virtually unaffected by coordination environment. Hence, the energy levels of the lanthanide ion do not shift (± 20 cm⁻¹) or broaden significantly upon coordination and line-like absorption and emission spectra are observed. The *f*→*f* transitions are parity forbidden (Laporte rule) and, as a result, direct population of the excited state is

unfavourable.⁵ The observed extinction coefficients are low (~ 1 mol⁻¹ dm³ cm⁻¹) negating some of the advantages that might otherwise be associated with this technique.

The method commonly used to overcome this problem is the incorporation of an aromatic chromophore into the structure of the ligand that is bound to the metal centre. The chromophore provides the means to absorb the necessary energy involving ligand-centred or charge-transfer bands. The energy can then be transferred to the lanthanide centre populating the emissive excited state indirectly.⁵ This is called the antenna effect and is illustrated in Figure 1.⁶ An important measure of the effectiveness of this process is the quantum yield, Φ . In effect, this is the probability that a photon will be emitted by the lanthanide ion for each photon absorbed by the antenna ligand. To work efficiently, the relative energies of these various states are of great importance with that between the ligand triplet and the metal excited state especially so. Obviously, the excited triplet state of the ligand must be highest in energy and it is important that the difference in energy be significant to prevent back transfer from the metal centre to the ligand.

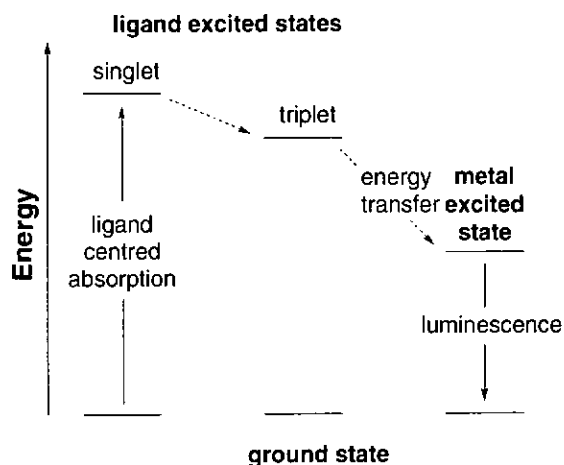


Figure 1. The antenna effect involving an absorbing ligand with emitting metal ion subunits.

The excited state of the metal can, of course, decay either by radiative (lanthanide luminescence) or non-radiative mechanisms. Non-radiative relaxation may occur by the interaction of electronic levels of the lanthanide ion with suitable vibrational modes in the nearby environment, *e.g.* coordinated solvent molecules, with lanthanide luminescence quenched very effectively by vibrational overtones of O-H, N-H and C-H bonds. In biological media the solvent is hydroxyl-containing water and so the use of a ligand that encapsulates the lanthanide ion can reduce significantly the impact of non-radiative deactivation

pathways by shielding the lanthanide ion and blocking direct co-ordination of solvent molecules.⁴ An appropriate lanthanide ion can be selected in order to obtain emission at the desired wavelength, viz. near infrared: Nd³⁺, Er³⁺; red: Eu³⁺, Pr³⁺, Sm³⁺; green: Er³⁺, Tb³⁺; blue: Tm³⁺, Ce³⁺.

There are still further considerations that have to be kept in mind when designing appropriate ligands for lanthanide ions. Free lanthanide ions are toxic and replace ions such as Ca²⁺ in biological systems. If they are to be used under physiological conditions then the complex must be chemically and thermodynamically stable in water and hence non-toxic.

Finally, the lanthanide label must be capable of linking to biological compounds such as DNA, RNA, antibodies, or proteins. Hence, appropriate linking groups need to be attached to the lanthanide complex. For DNA applications this group could be an intercalator that can slot between certain base pairs by virtue of π -stacking interactions.⁷ In contrast, protein probes need a chemically reactive linking group capable of forming a covalent bond (conjugate) under mild conditions with the targeted side-chains in the protein, e.g. lysine amino groups or cysteine thiol groups. The lanthanide-biomolecule conjugate also may be stable in the long term (years) thereby allowing repeated detection. This contrasts with radiolabels which have limited lifetime.

Figure 2 illustrates the constitution of a possible lanthanide probe for biolabelling purposes. The label is comprised of two parts, a reporting group consisting of the lanthanide shielded from the surrounding solvent and coordinated to an appropriate antenna ligand, and a linking group attached to the ligand, that can capture the biomolecules of interest as described earlier.

Ligand Design and Coordination Chemistry

Lanthanide(III) ions are hard metal centres (Pearson concept) with a general preference for hard donor atoms. Much of their coordination chemistry involves anionic oxygen donors like carboxylates and β -diketonate ligands while metal-ligand bonding is predominantly ionic in character. Therefore, coordination numbers vary (8 and 9 are most common but up to 12 have been reported) and geometries are controlled mostly by the spatial requirements of ligands.⁸

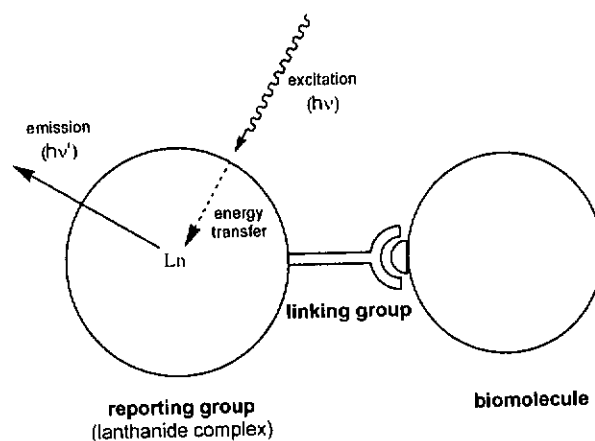


Figure 2. A lanthanide labelling system consisting of the emissive lanthanide complex and the linking group to biomolecules.

Various approaches have been taken to synthesise effective luminescent materials that carry a variety of large encapsulating antenna-containing ligands. These ligands can be divided into podands, calixarenes, macrocycles, and macrobicycles (cryptands) with examples presented in Chart 1.^{4a,c}

Podands - Podand-type ligands consist of a backbone and three chromophore-containing arms. Various architectures have been realized with carbon, nitrogen, and boron bridgehead atoms carrying different types of aromatic chromophores (see Chart 1) and their reactions with lanthanide ions usually result in nice crystalline complexes. While many of these products exhibit sensitized luminescence, they lack good stability and/or solubility in polar solvents such as water. In addition, in many cases the podand ligands do not shield the lanthanide centre sufficiently so that solvent molecules may coordinate to the metal causing a significant deactivation of the luminescence by the non-radiative pathways described earlier. For example, ligand [L]³⁻, a heptadentate ligand as shown by the structure of its lanthanide complex (Fig. 3),^{9,10} is made by Schiff-base condensation of a tris(aminoethyl)amine (tren) central unit with three equivalents of *ortho*-formylphenol. In solution, the lanthanide ion can increase its coordination number by binding solvent molecules.

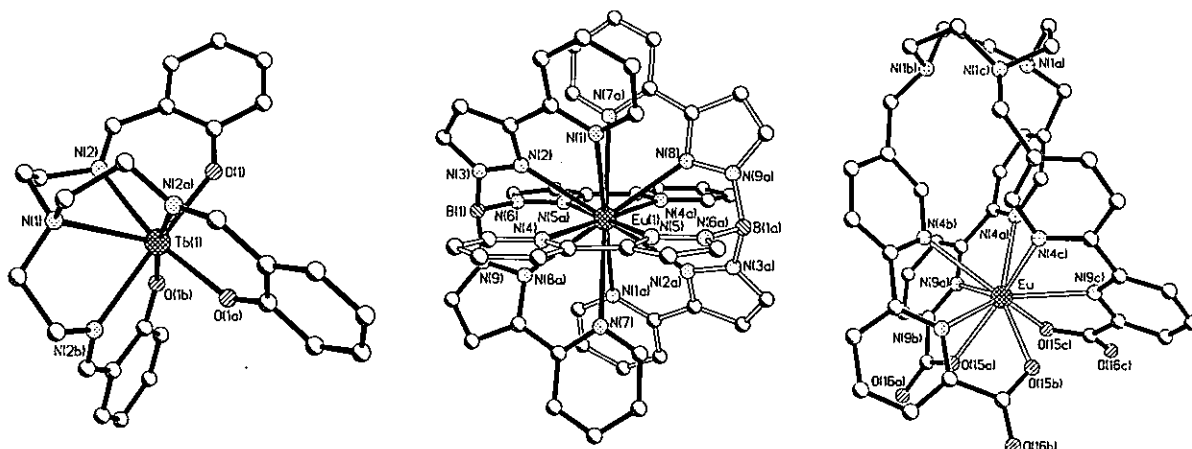


Figure 3. Examples of molecular structures of complexes with podand ligands, see refs. 9 and 10.

Parent tris(pyrazolyl)borate ligand [L^2] forms 1:1 and 1:2 metal:ligand complexes [$Ln(L^2)(NO_3)_2$] and [$Ln(L^2)_2$] $^+$. In solution, dissociation of the nitrate anions from the former complex leaves the lanthanide ion open to coordination by solvent molecules. Photophysical studies in water and methanol suggest the coordination of several solvent molecules. Luminescence lifetimes and quantum yields in aqueous solution are reasonable, but are greatly enhanced by use of CH_2Cl_2 as solvent as it lacks the deactivating O-H group. The [$Ln(L^2)_2$] $^+$ complex offers greater protection, because the metal center is encapsulated by two ligands in a 12-coordinate manner as shown in Figure 3 ($Ln = Eu$). However, solubility has prevented the photophysical study of this complex in solvents other than CH_2Cl_2 , in which high quantum yields and remarkably long lifetimes are observed.

The ligand [L^3] $^{3-}$ can also be viewed as a podand, although the apical group is a polyazamacrocycle, a ligand-type that is discussed below. The three carboxylate groups, each in the 6'-position of a bipyridyl chromophore, coordinate to the lanthanide(III) ion along with the bipyridyl nitrogen

atoms. This leaves the triazamacrocycle uncoordinated and gives 9-coordinate complexes. These successfully exclude water molecules from the lanthanide ion in aqueous solution, giving encouraging, long-lived luminescence ($M = Eu$: $\tau = 1.85$ ms, $\Phi = 0.12$; $M = Tb$: $\tau = 0.50$ ms, $\Phi = 0.10$).

Calixarenes - Photophysical studies have been conducted on a number of lanthanide complexes of calix[n]arenes, as discussed in a recent review.¹¹ Three examples of such ligands are depicted in Chart 1. The amidoether-functionalized calix[4]arene L^4 reacts with various lanthanide ions to form monometallic complexes and the macromolecular structure of its lutetium(III) complex^{9,12} is depicted in Figure 4. However, modest emission lifetimes (τ_{Eu} 0.73, τ_{Tb} 1.45 ms) and quantum yields (Φ_{Eu} 0.02, Φ_{Tb} 0.058) are recorded in acetonitrile solution. The emission spectra for both the Eu(III) and Tb(III) complexes show residual emission from the ligand triplet state, indicating incomplete energy transfer. In contrast, high quantum yields and long lifetimes have been reported for a series of calixcrowns with appended bipyridyl chromophores, such as L^5 (Chart 1). Photophysical studies in acetonitrile gave lifetimes of 0.95–1.38 and 1.83–1.93 ms, and quantum yields of 0.18–0.32 and 0.32–0.39 for the europium and terbium complexes, respectively.

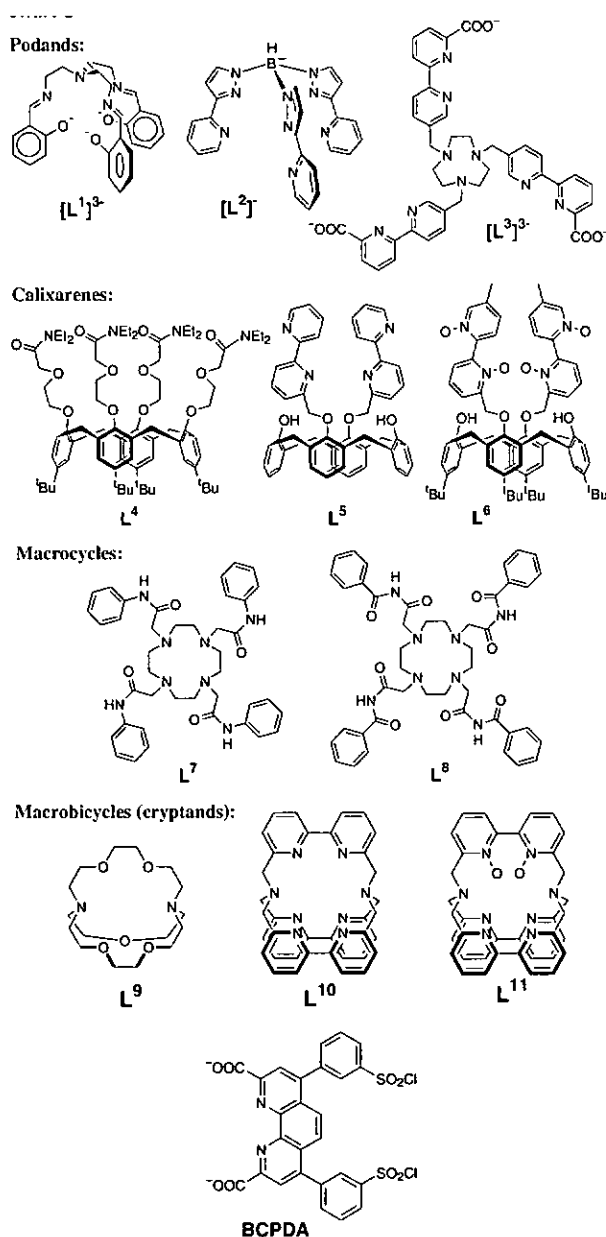


Chart 1. Ligand types.

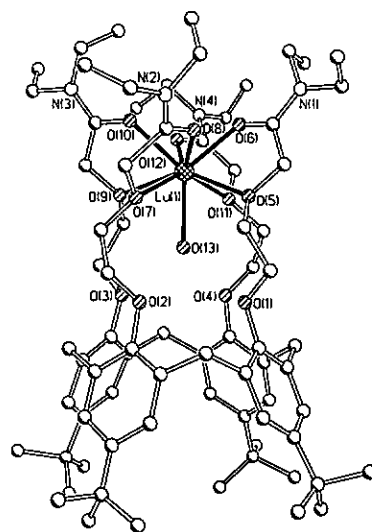


Figure 4. Molecular structure of a calixarene type complex, see refs. 9 and 12.

The bipyridyl- N,N' -dioxide chromophore has also been appended to a calix[4]arene, giving L^6 (Chart 1), which complexes with europium and terbium. The europium complexes are highly luminescent ($\Phi \leq 0.19$ in MeOH). Replacement of the bridging calixarene ring CH_2 groups with S, SO_2 , and/or substitution of the t -butyl group with sulfonate leads to greater water solubility as well as better complexing ability.

Macrocycles - Macrocycles are the most promising and best-understood ligand systems to date. Cyclen-derived macrocycles based on DOTA (1,4,7,10-tetraazacyclododecane-1,4,7,10-tetraacetic acid) form stable complexes with trivalent lanthanide ions, and the gadolinium complex is extensively used in magnetic resonance imaging (MRI) under the trade name

DOTAREM. Some of these complexes have also been developed to include linking groups that have been shown to bind to biological molecules.¹³ Another significant advantage of these compounds is that their syntheses are relatively simple and high yielding as required for commercial viability.

Ligand **L**⁷ (Chart 1) forms a complex with europium, where the lanthanide ion lies in the centre of the tetraazacyclododecane (cyclen) moiety. As the chromophore is not coordinated directly to the metal centre, energy transfer is inefficient and quantum yields are disappointingly low ($\Phi \sim 0.02$). In contrast, ligand **L**⁸ is a better sensitizer of europium ($\Phi \sim 0.247$ in H₂O) in the [EuL⁸]³⁺ complex that results (Fig. 5)^{9,14} and is among the best reported for any europium complex. Hence, this compound shows potential for biochemical applications and derived ligands that allow for coupling to biological molecules currently are being developed.

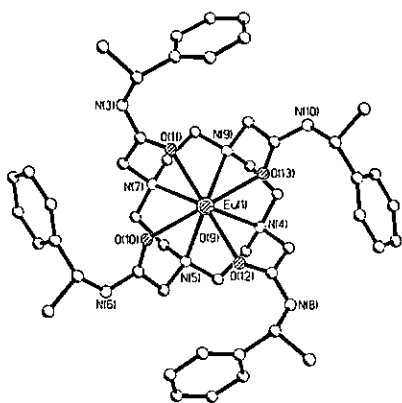


Figure 5. Molecular structure of a complex based on a macrocycle, see refs. 9 and 14.

Macrobicycles - By far the most elegant ligand systems are cage-like macrocycles. The first lanthanide complexes of this kind studied for their photophysics were the simple [2.2.1]cryptates, *e.g.* **L**⁹ (Chart 1). Due to the absence of a strongly absorbing chromophore and insufficient shielding of the metal centre from solvent molecules their luminescence properties are poor.

In order to improve the photophysical properties Lehn and coworkers incorporated strongly absorbing chromophores such as 2,2'-bipyridine (bpy) groups into the cage backbone, forming macrobicycles such as **L**¹⁰ and **L**¹¹. The photophysical properties of the europium and terbium complexes^{9,15} of **L**¹⁰ (Fig. 6) suggested the promise of this type of ligand. Subsequently, the derivative *N*-oxide ligand **L**¹¹ gave quantum yields of up to 0.20 in water for both europium and terbium complexes.

Biochemical Applications

Over the last few decades numerous methodologies have been developed for the analysis of biological molecules such as nucleic acids, proteins, carbohydrates and lipids, and new protocols are published almost daily. The original techniques utilized the sensitivity of radioactive labels in the detection and analysis of proteins by

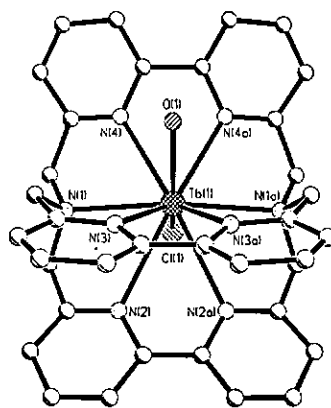


Figure 6. Molecular structure of a cage-like ligand, see refs. 9 and 15.

radioimmunoassay, and in the sequencing of DNA. Radioactive labels are still widely used despite the development of enzyme-linked colour reactions and fluorescent dyes as these newer methods often use several antibodies for detection and this makes them expensive.⁴ In addition, they are often less sensitive than radiolabelling. Although the ideal multi-applicable lanthanide label is still being sought for the detection and assay of biological molecules, there are growing numbers of examples where lanthanide labels are already being used. Two examples are discussed here.

The first effective lanthanide based immunoassay was developed in the 1980s.¹⁶ However, this Dissociation Enhanced Lanthanide Fluoroimmunoassay-type (DELFLIA) assay uses a different principle to the one illustrated in Figure 2. The lanthanide ion is actually removed from the biomolecule when the assay is developed and is then detected by the addition of an enhancing ligand (see Fig. 7).

A plate with multiple wells is coated with unlabelled antibody and reacted with antigen. After the immunoreaction another specific binding reagent labeled with a non-luminescent lanthanide chelate (such as isothiocyanatophenyl-EDTA-europium) is allowed to react with the immobilized analyte. After washing, the lanthanide ions are dissociated from the non-luminescent chelate by lowering the pH of the solution to 3-4 and the

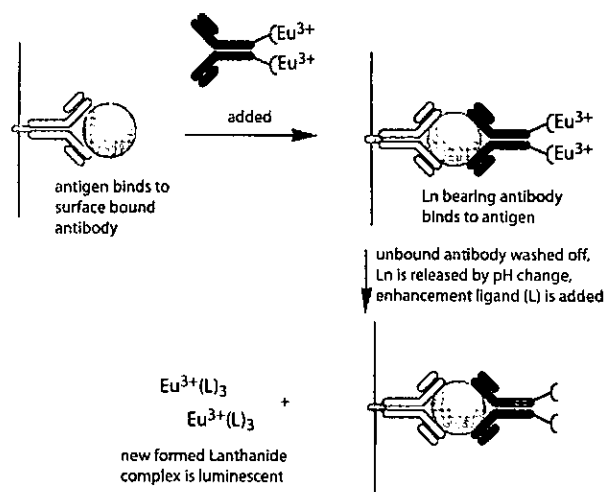


Figure 7. Dissociation Enhanced Lanthanide Fluoroimmunoassay (DELFLIA) illustrated.

enhancing ligand is added. This ligand usually contains antenna groups like aromatic β -diketones and a strongly luminescent complex is formed and detected.

The second common assay is the CyberFluor system¹⁷ that employs a luminescent lanthanide label as illustrated in Figure 2. Instead of the DELFIA approach that measures the luminescence from the released lanthanide ions in an enhancement solution, the luminescence of the label is detected directly from the surface of the solid support. As described above, ligands that fulfill all of the requirements for a stable, and hence non-toxic, water-soluble and highly fluorescent chelate are difficult to obtain. However, BCPDA - 4,7-bis(chlorosulfonyl)-1,10-phenanthroline-2,9-dicarboxylate] - satisfies the requirements for a good sensitizer and chelator. BCPDA also has a linking group and can react with the amino residues of proteins under mild conditions. It is used already in labeling a range of proteins like antibodies, avidin, or streptavidin.

Summary

Numerous possible lanthanide labeling systems are currently being developed, some with more potential than others. Many complexes fulfil one or two of the requirements of fluoroimmunoassay as described above but miss other important criteria. Currently, the best lanthanide complexes have millisecond excited state lifetimes in aqueous solution and quantum yields of approximately 0.3 (Eu^{3+}) and 0.6 (Tb^{3+}).^{4c} Much remains to be done in developing these as tools in time-resolved assays, particularly with regard to the development of a generally applicable sensor system.

References and Notes

1. For a more detailed explanation see: Sumbly, C.J. *Chem. in NZ*, **2002**, 86(1), 13.
2. Turro, N.J. *Modern Molecular Photochemistry*, University Science Books, 1991.
3. (a) Hemmilä, I.; Dakubu, S.; Mikkala, V.-M.; Siitari, H. and Lövgren T. *Anal. Biochem.*, **1984**, 137, 335; (b) Hemmilä, I. and Mikkala, V.-M. *Crit. Rev. Clin. Lab. Sci.*, **2001**, 38, 441; (c) Mathis, G. *Clin. Chem.*, **1993**, 39, 1953; (d) Hemmilä, I. *Applications of Fluorescence in Immunoassays*, Wiley: New York, 1991.
4. For reviews in this area see: (a) Sabbatini, N.; Guardigli, M. and Lehn, J.-M., *Coord. Chem. Rev.*, **1990**, 123, 201; (b) Faulkner, S. and Matthews, J. In *Comprehensive Coordination Chemistry II*, McCleverty, J.A. and Meyer, T.J. (Eds.), Elsevier: Oxford, 2004; (c) Motson, G.R.; Fleming, J.S. and Brooker, S. *Adv. Inorg. Chem.*, **2004**, 55, 361, and refs. cited.
5. de Sá, G.F.; Malta, O.L.; de Mello Donegá, C.; Simas, A.M.; Longo, R.L.; Santa-Cruz, P.A. and da Silva Jr., E.F. *Coord. Chem. Rev.*, **2000**, 196, 165.
6. Lehn, J.-M. *Angew. Chem., Int. Ed. Engl.*, **1990**, 29, 1304.
7. Hudson, B.P. and Barton, J.K. *J. Am. Chem. Soc.*, **1998**, 120, 6877.
8. Richardson, F.S. *Chem. Rev.*, **1982**, 82, 541.
9. Figs. 3-6 were generated from data downloaded from the Cambridge Crystallographic database as deposited by

the authors of refs. 10, 12, 14 and 15, respectively.

10. Left: Kanesato, M. and Yokoyama, T. *Chem. Lett.*, **1999**, 137; centre: Jones, P.L.; Amoroso, A.J.; Jeffery, J.C.; McCleverty, J.A.; Psillakis, E.; Rees, L.H. and Ward, M.D. *Inorg. Chem.*, **1997**, 36, 10; right: Charbonnière, L.; Ziessel, R.; Guardigli, M.; Roda, A.; Sabbatini, N. and Cesario, M. *J. Am. Chem. Soc.*, **2001**, 123, 2436.
11. Sabbatini, N.; Guardigli, M.; Manet, I. and Ziessel, R. In *Calixarenes 2001*, (Asfari, Z., Ed.), Kluwer: 2001.
12. Ramírez, F. de M.; Charbonnière, L.; Muller, G.; Scopelliti, R. and Bünzli, J.-C.G. *J. Chem. Soc., Dalton Trans.*, **2001**, 3205.
13. Bobba, G.; Frias, J.C. and Parker, D. *Chem. Comm.*, **2002**, 890.
14. Zucchi, G.; Scopelliti, R. and Bünzli, J.-C.G. *J. Chem. Soc., Dalton Trans.*, **2001**, 1975.
15. Bkouche-Waksman, I.; Guilhem, J.; Pascard, C.; Alpha, B.; Deschenaux, R. and Lehn, J.-M. *Helv. Chim. Acta*, **1991**, 74, 1163.
16. Yam, V.W.-W. and Lo, K.K.-W. *Coord. Chem. Rev.*, **1998**, 184, 157.
17. Evangelista, R.A.; Pollak, A.; Allore, B.; Templeton, A.F.; Morton, R.C. and Diamandis, E.P. *Clin. Biochem.*, **1988**, 21, 173.

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Otago's Input Into HAZMAT Risk Management In New Zealand

Brian H. Robinson and Wayne A. Temple

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Trained chemists use or deal with chemicals and hazardous substances as part of their normal occupation and are, by and large, comfortable with hazards posed by the use of chemicals in modern society. Despite the compliance costs (both money and time) associated with the implementation of the Hazardous Substances and New Organisms (HSNO) Act, they recognise the need for a national and international framework for the control of hazardous substances in the environment and workplace. But how many graduates and enforcement officers know how to classify chemicals, interpret toxicological data, and assess the risk rather than react to what is said in a Material Safety Data Sheet (MSDS)? How many graduates and workers are aware of the international system *Globally Harmonized System of Classification and Labelling of Chemicals* (GHS) introduced this year? From the middle of this year all Universities and three CRIs will work under a Code of Practice (Section 33, Exempt laboratories) - how many researchers and academics have seen this document and are aware of its implications? Do you know that Occupational Safety and Health (OSH) may audit your compliance of the Code every six months?

These are just some of the changes in the risk assessment and management of hazardous substances that impinge on the way in which we do chemistry in this country. In this article we focus on two aspects of our involvement at Otago in this area. The first is on the need to train both our graduates, and those in the workforce without a formal background in chemistry, and the second on risk management for the general public (*chemicovigilance*) and acts of deliberate chemical release.

Chemical Hazard Courses

In 2001, the University of Otago established a web-based postgraduate hazard management programme, administered by a Board of Studies within the Division of

Health Sciences, to meet an emerging need for professional training in risk and hazard management. This distance-taught multidisciplinary programme has proved popular with people in the workforce and students throughout New Zealand. To date, around three-quarters of the students are professionals who have an organizational role related to hazard management. Typically they are employed in central or local government although there are an increasing number from the private sector, and those who do the course as a way of establishing a career in hazard management.

Students can study towards a Certificate, Postgraduate Diploma, or Masters degree. Course work focuses on the scientific basis for the identification, assessment, prevention and remediation of physical, chemical and biological hazards, rather than operational issues. Teaching is mostly via Blackboard, the University's web-based teaching platform; there are no on-campus lectures. However, to fulfil practical requirements, students are sometimes asked to attend a workshop at one of the University's regional facilities. Courses run for 22 weeks and students join at any time.

Chemistry accounts for three of the core papers, the others being in biological hazards (2), public and occupational health, toxicology, and law; courses in radiation and physical hazards are also planned. Chemical Hazards (HAZX401), covers the New Zealand scene through the history of chemical management in New Zealand classification, introductory toxicology, HSNO legislation and chemical incident management, whereas HAZX411 has an international perspective and covers GHS, chemical weapons, disarmament protocols *etc.* This latter paper will be available to students in other countries. Environmental Risk Assessment and Management (HAZX404), looks at the procedures and role of the chemical consultant in environmental risk management, monitoring and statutory management of effluents and discharges.

Table 1. Total substance enquiries received: July 2002-June 2003

	Adults	Children	Animals	Other ^a	Unknown	TOTAL
Agricultural agents	676	421	287	588	4	1976
Bites/stings	291	94	7	154	2	548
Cosmetics	190	869	9	48	0	1116
Household agents	1767	4439	332	845	7	7390
Industrial agents	725	164	27	387	4	1307
Plants/fungi	299	1270	69	456	1	2095
Therapeutics	2909	4151	118	779	11	7968
Miscellaneous ^a	367	347	35	2894	2	3645
TOTAL	7224	11755	884	6151	31	26045

^a Includes Hazchem (spillages of hazardous chemicals, disposal methods, preventive procedures, MSDS requests, *etc.*), labelling and scheduling queries, plant identification, *etc.*

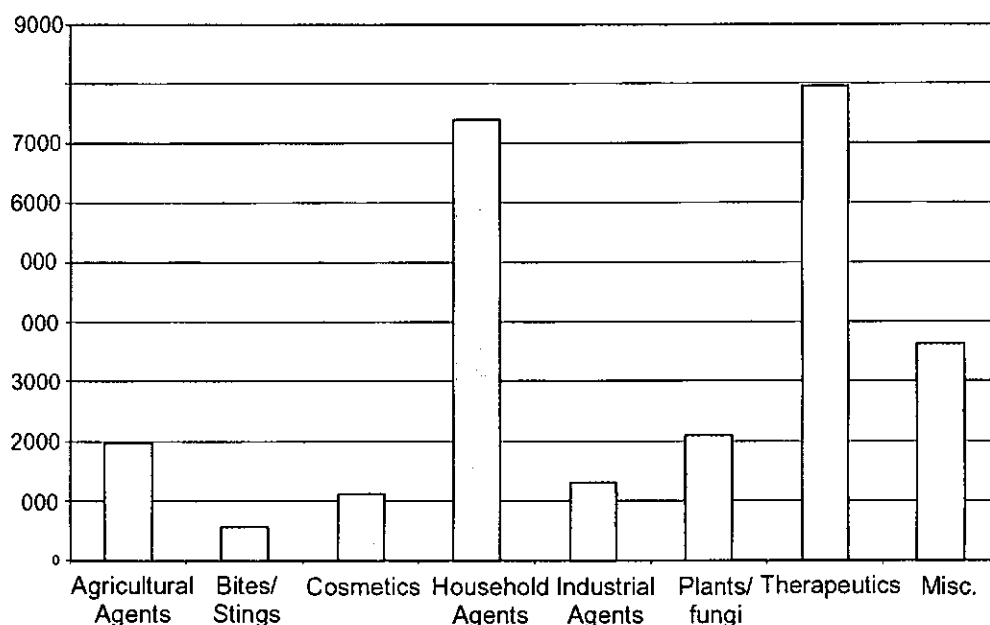


Figure 1. Distribution by agent for the period July 2002-June 2003 (total n = 26,045).

Chemicovigilance

Chemicovigilance is a function, which involves the active identification and evaluation of hazardous substance risks and phenomena in the community; an activity which should result in measures aimed at reducing the risks. Our involvement is at both the national and international level, and covers a range of operational and policy inputs. Perhaps the major operational input is via the National Poisons Centre.

The National Poisons Centre

The NPC is the only centre of its kind in the country and it plays an important role by providing appropriate information in the event of both major and minor incidents. It also takes an active part in the contingency planning, education, and training for chemical accidents. The Director (Dr. Wayne Temple) is supported by two Medical Toxicologists, ten information scientists, and three support

staff. The Centre is a service unit within the Department of Preventive and Social Medicine at the Dunedin School of Medicine, University of Otago. Currently, the Centre is funded predominantly by contracts with the Ministry of Health and the ACC, with support from the University and other agencies. The NPC answers enquiries both from health professionals and from the general public concerning acute poisoning and the toxic effects of chemicals, which may be encountered in emergencies of any sort. This service operates 24 hours per day, 365 days per year. The Centre receives approximately 24,000 enquiries per year (see Tables 1 and 2, and Fig. 1). This means that the information disseminated from the NPC may be rather complex, involving at the one extreme very simple information and advice for persons at the place of the accident, and at the other extreme a detailed discussion on toxicity data and treatment protocols when communicating with hospital staff. The mass media receive relevant information for transmission to the general public.

Table 2. Enquiries concerning household agents July 2002-June 2003

	Adults	Children	Animals	Others	Unknown	TOTAL
Air freshener	22	194	0	10	2	228
Animal remedy	2	7	1	1	0	11
Cleaner	469	788	43	101	0	1401
Detergent	98	885	9	29	1	1022
Disinfectant	75	274	5	22	0	376
Filler	13	10	3	1	0	27
Fumigant	0	1	0	1	0	2
Glue	64	93	4	20	0	181
Insect repellent	14	103	5	6	0	128
Insecticide	121	218	95	90	1	525
Laundry preparation	60	215	23	18	0	316
Paint	200	234	12	123	0	569
Petrol	147	142	3	25	0	317
Polish	12	51	2	5	0	70
Rodenticide	25	70	65	26	0	186
Spirit	177	66	1	40	1	285
Miscellaneous	268	1088	61	327	2	1746
TOTAL	1767	4439	332	845	7	7390

The Centre maintains a computerised database (TOXINZ; maintained by Jade Software Corporation - www.toxinz.com), currently listing more than 60,000 chemical and medicinal products, as well as hazardous plants and animals found in New Zealand. Medicines and pesticides information is furnished from Government agencies, and manufacturers and distributors provide this for other commercial products on a voluntary basis. The information available includes New Zealand trade and chemical names, physical properties, emergency action codes, toxicity data, signs and symptoms of poisoning, treatment, occupational safety, environmental data, management of fires and spills, and first aid procedures. The Centre has developed a computerised record of all enquiries regarding actual or potential toxic exposures, utilising a poisoning incident report format.

Both the NPC and the Department of Chemistry have input into other national and international activities. The NPC participates in the International Programme on Chemical Safety (WHO/ILO/UNEP), which has established a network of poison control centres throughout the world. The primary role in this group is to contribute relevant expertise and experience in the preparation and review of poisons information monographs (PIMs), the establishment of methodologies for recording case data and compiling files on local products, and the strengthening of poison information centres worldwide. The overall programme is known as the INTOX Project, with a primary objective of strengthening the capabilities of developing countries to prevent and respond to poisoning incidents by developing a multilingual interactive computerised poisons information package. The Canadian Centre for Occupational Health and Safety (CCOHS) is working with the IPCS and has recently released a CD-ROM product carrying approximately 1000 finalised PIMs and other global information components, which run under INTOX software. The NPC and other colleagues have, so far, completed or revised 122 PIMs for the Project. Locally, the Department of Chemistry and the NPC are represented on the Dunedin Hazardous Substances Technical Liaison Committee and the Emergency Services Executive Co-ordinating Committee. Both are heavily involved in giving chemicovigilant advice to, and providing the link between, Government Departments, the private sector, and United Nations agencies. Much of this is 'sensitive' but includes chemical risk assessment and management in the areas of health, international control, disarmament, terrorism, and chemical and biological weapons. They work closely with the enforcement agencies when dealing with the deliberate release of chemicals, both within New Zealand and overseas, and train people likely to be involved in such incidents.

Chemists have a vital role to play in chemicovigilance but it is one that is often overlooked. Demonstrable safe usage of chemicals is one way the general population can be convinced that chemicals and chemistry are important in a modern society. Equally, sensible risk assessment and management of hazardous substances is the prerogative of chemists.

FACS: PROJECT 2004-2005

Professional Ethics In Support of Chemical Disarmament

Project Director: Professor John Webb
Murdoch University, Australia
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At the FACS meetings in Brisbane, July 2001, Professor Webb outlined a project on the issue of professional ethics in support of chemical disarmament. The project developed from the Regional meetings held in Melbourne, May 2001 in support of the international treaty that prohibits the development, production, stockpiling and use of chemical weapons and on their destruction, known as the Chemical Weapons Convention (CWC). The Royal Australian Chemical Institute, the Australian Government, and the Organisation for the Prohibition of Chemical Weapons (OPCW), based in The Hague and responsible for implementation of the CWC, supported these meetings. Chemists and government officials from 14 countries in the Asia-Pacific region participated. A strong recommendation was for regional associations such as the Federation of Asian Chemical Societies to be actively involved in supporting the CWC.

In the intervening period, the need for professional awareness and support for the CWC has become even more urgent, particularly as the boundaries between biological and chemical agents becomes less distinct. IUPAC is also concerned, having hosted a workshop and later prepared and published a technical report on the Impact of Scientific Developments on the Chemical Weapons Convention.

The project would involve the creation of a regional network focused on the issue of professional ethics in support of chemical disarmament. The general objective is to develop a broader and stronger understanding and support for the CWC.

Specific activities could include:

- collection and comparison of Codes of Ethics and Codes of Conduct currently in place in Member Societies,
- identifying courses or professional development programs on CWC issues that are offered within national chemical communities,
- establish communication with the National Authorities in Government responsible for the CWC,
- develop proposals for funding to host national and regional Workshops on these issues, and
- support development of training materials, on-line and workshop-based, for professional awareness programs supporting the CWC.

NZIC is a member of the Federation of Asian Chemical Societies (FACS) and anyone interested in participating is asked to contact Professor Webb directly.

Ed.

CHEMICAL WEAPONS: PAST, PRESENT AND FUTURE*

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*Reproduced from Chemistry in Australia (*Chemistry in Australia*, 2003, 70(11), 6-9) with the permission of the author and the Journal. The article was submitted and published while Dr. Wheate was a Visiting Fellow at the School of Physical, Environmental and Mathematical Sciences, University of New South Wales, ADFA.

Chemical weapons have been used in warfare for over 1000 years, and even today continue to be developed. Future chemical weapons, which include dusty agents and binary nerve agents, are more persistent, more toxic and easier to use than conventional weapons.

History

Although World War I made the use of chemical weapons most famous, it can be dated back as far as 600 BC. It was at this time that Solon, Legislator of the Athenians, contaminated the Pheisthenes River with helleborus to give the defenders of Kirrha such violent diarrhea that they would flee the city. Over the next century chemical warfare was largely haphazard and solely employed the use of arsenic or other toxic fumes.

The first great leap forward arrived in 673 AD with the use of Greek fire, a mixture of sulfur, quicklime and liquid petroleum, which would burn both under and on water – making it perfect as a naval weapon – and release toxic fumes. The 15th and 16th centuries saw the introduction of more elaborate delivery systems, with poisons flung over city walls in chests or hollow mortar shells and the development of the first incendiary bombs, made from a mixture of turpentine and nitric acid.

Modern chemical agents were first used in Ypres in 1915, when chlorine gas was released from large cylinders. This surprise operation caused massive casualties and demoralisation, and demonstrated the need for protection from this kind of warfare. The first improvised mask was a cotton pad soaked in sodium thiosulfate, glycerine, and sodium carbonate. Consequently, in World War I, both sides used a great variety of chemical agents, the most damaging being the blister-producing agent sulfur mustard (see Chart 1). Military clothing, even with a respirator, gave little protection, and sulfur mustard inflicted thousands of casualties.

Since World War II, there have been several confirmed reports that chemical agents have been used in armed conflicts, including the Iran–Iraq conflict. Today, even with over 180 countries as signatories to the 1997 Chemical Warfare Convention¹ banning the development, production or stockpiling of chemical warfare agents, many other countries continue aggressive activities in this area.

Chemical agents were not used in World War II, but at the end of the war stockpiles of newer agents, called nerve gases, were discovered. These were found to be effective in much lower concentrations than those agents known up to that time. The standard of training, preparedness of the services and the fear of retaliation were possible reasons why chemical agents were not used.

Modern chemical warfare agents

Modern chemical warfare agents are divided into five classes based on their effects on the human body:

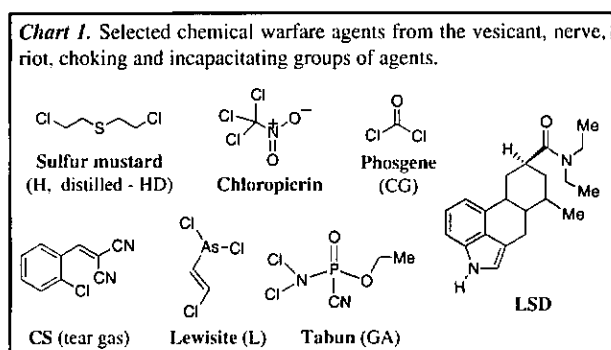
- pulmonary oedemagens (choking agents including chlorine gas, phosgene, chloropicrin)
- sternutators, lacrimators, and psychochemical agents (incapacitants including vomiting and tearing agents)
- blood agents (cyanide-containing or cyanide-releasing agents)
- vesicants (blistering agents)
- nerve agents.

The two agents most likely to be used in modern warfare are vesicant and nerve agents.

Vesicants

Vesicants (blister agents)² are intended to cause injury by blistering. Rather than causing death, they place an enormous logistical burden on an opposing force (as well as lowering morale). Vesicants attack and burn the eyes, mucous membranes, respiratory tract, and skin, causing blisters that can take many months to heal.

There are three categories of blister agents: mustards, arsenicals, and urticants (Chart 1). Mustards include sulfur mustard (H, distilled mustard - HD), sesqui mustards and nitrogen mustards (HN1, HN2, HN3). The mustards



penetrate well into skin and other materials, such as wood, clothing, rubber, and paints, and are very persistent in cold and temperate climates. Because mustards have delayed effects (4-6 hours or more), unprotected individuals can be exposed to large doses without immediate response.

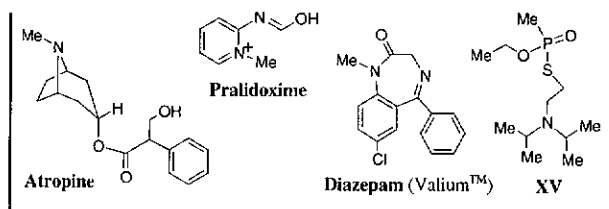
Arsenical vesicants also have delayed blistering action, but, unlike mustards, they tend to produce immediate pain. The principal arsenical of military interest is lewisite (L - Chart 1). Other arsenicals are the mustard-lewisite mixture (HL) and the substituted double chlorinated arsines [dichloro(phenyl)arsine, dichloro(ethyl)arsine and dichloro(methyl)arsine].

Urticants are vesicants with disagreeable and penetrating odours that cause an immediate and severe burning sensation, as well as intense pain, numbness and swelling. The most common urticant is phosgene oxime ($\text{Cl}_2\text{C}=\text{NOH} - \text{CX}$).

Nerve agents

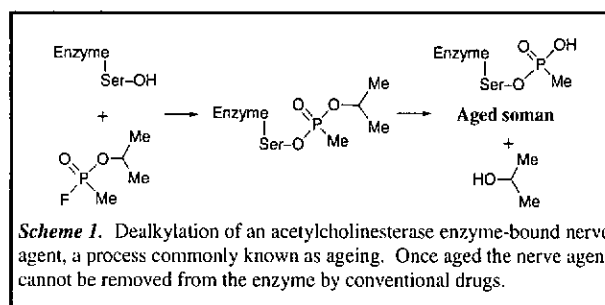
Nerve agents³ were first discovered in Germany during the 1930s and are chemicals that disrupt the mechanism by which nerves transfer messages to organs (see Chart 2). Blocking the activity of acetylcholinesterase, an enzyme that normally destroys and stops the activity of the chemical neurotransmitter acetylcholine, causes the disruption. The primary military nerve agents are tabun (GA), sarin (GB), soman (GD), GF and *O*-ethyl-S-[2(diisopropylamino)ethyl]methylphosphonothioate (VX, Chart 2).

Chart 2. The chemical structures of the nerve agent VX and the antidotes used to treat nerve agent poisoning. Atropine is used to relieve the symptoms of nerve agent poisoning, diazepam (Valium™) is used to control convulsions, and oximes (HI-6, obidoxime and pralidoxime) are used to reverse the binding of nerve agents to the acetylcholinesterase enzyme.



The physiological symptoms associated with nerve agents begin within seconds or minutes (depending on the dose) after skin contact or exposure to the vapours or aerosols of these compounds. At low levels of exposure, symptoms range from dripping nose, tightness in the chest and pinpoint pupils to excessive salivation, sweating, and nausea. At higher levels, symptoms range from vomiting, cramps, twitching/jerking, staggering, headache, confusion, and loss of muscle control to coma, convulsions, and death. When liquid agents are applied to the skin, the onset time is longer (up to 18 hours) than with inhalation (10 minutes).

Nerve agent treatment is effective when given immediately after exposure and requires the administration of an oxime enzyme reactivator and atropine.³ However, if the enzyme has hydrolysed (the action of enzyme hydrolysis is called ageing - Scheme 1), it cannot be reactivated.



Future chemical warfare agents

Dusty agents

Dusty agents are a new way to disseminate mustard and nerve agents. Dusty mustard and dusty nerve agents are made by combining standard agents with a particle carrier like talc or diatomaceous earth. These agents are similar to conventional insect powders such as Ortho® Ant-Stop, which uses the organophosphate insecticide Chorpyrifos, combined with a suitable inert carrier.

Because dusty agents are very fine particles they are able to travel great distances, and release the toxic agents much more slowly than conventional mustard and nerve agents. In addition, the fine particles are thought to be able to penetrate gaps in standard protective clothing. As such, during the Persian Gulf War many soldiers wore ponchos in addition to protective clothing, to help keep dusty agents out. While no dusty agent was used during the Gulf War nor found during subsequent UNSCOM weapon inspections, there are reports that dusty agents were used by Iraq during the Iran-Iraq war in the 1980s.⁴

Binary nerve agents

As early as the 1950s the US military was looking at making nerve agents that were safer and easier to handle on the ground by personnel. This led to the development of novel binary nerve agents - agents made from two non-toxic precursors, a 'common' organophosphate and another industrial chemical. These are mixed together in the weapon (in-flight) to produce the nerve agent. The first binary nerve agent, Big Eye (BLU-80/B), a 500 pound bomb containing a VX-like nerve agent, is thought to have been developed in the 1980s.⁵

Typical binary nerve agent bombs contain two separate, hermetically sealed, plastic-lined containers. For binary sarin (GB2, Scheme 2) the first container holds methylphosphonic difluoride (DF) and the second isopropyl alcohol and isopropyl amine, the latter chemical to act as a binding agent to soak up the hydrofluoric acid produced in the reaction.

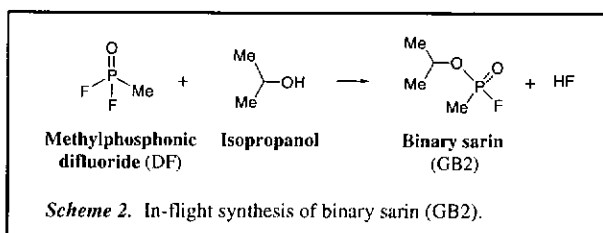


Table 1. Physical properties of some modern chemical warfare agents.

Agent	Common name (abbrev.)	Chemical group	Effect on the body	Vapour pressure (mm Hg)	Appearance	Smell	LC ₅₀ (mg.min/m ³)	Antidote	Solubility
Bis-(2-chloroethyl)sulfide	Sulfur mustard (H, HD)	Vesicant	Slow to form, painful blisters	0.11	Yellow to colourless oil	Mustard or rotting onions	1500	Nil	Fats, organic solvents
Dichloro(2-chlorovinyl)arsine	Lewisite (L)	Vesicant	Intense pain on contact with skin then blistering	0.395	Brown liquid	Geraniums	1200	Anti-lewisite (dimer-captopropanol)	Ether, alcohols, organic solvents
Isopropyl methylphosphonofluoridate	Sarin (GB)	Nerve	Convulsions, respiratory failure	2.9	Colourless oil	Sweatish	100	Atropine, oxime, diazepam	Alcohols and other organic solvents
(O-ethyl-S-(2-(diisopropylamino) ethyl)methylphosphonothioate	VX	Nerve	Convulsions, respiratory failure	0.0007	Colourless oil	Nil	10	Atropine, oxime, diazepam	Alcohols and other organic solvents
Carbonyl chloride	Phosgene (CG)	Choking	Pulmonary oedema	1180	Colourless gas	Newly mown grass	3200	Nil	Benzene, toluene, acetic acid, liquid hydrocarbons
Trichloronitromethane	Chloropicrin (PS)	Choking	Pulmonary oedema	16.96	Yellow to colourless, slightly oily liquid	Pepper-like, chlorine	200	Nil	Acetone, alcohols, organic solvents
Diphenylaminearsine chloride	Adamsite (DM)	Incapacitant	Vomiting	Negligible	Light green to yellow solid	Coal fire	15 000	Nil	Soluble in furfural and acetone; slightly soluble in common organic solvents; insoluble in water
3-Quinuclidinyl benzoate	BZ	Incapacitant	Delirium lasting several days	–	White solid	Nil	200 000	Physostigmine	Organic solvents
Hydrogen cyanide	AC	Blood	Prevent the utilisation of oxygen	Negligible	White crystals or powder	Almonds	300	Sodium thiosulfate, dicobalt edetate, amylnitrite	Water, alcohols, glycerin

LC₅₀ is defined as the concentration of agent required per minute to kill 50% of a population.

In the mid-1990s Russian scientist Vil Mirzayanov (who was jailed between 1992 and 1994 for publishing information about Russia's secret binary nerve agent research) expressed his concerns in the *Wall Street Journal* (24 May 1994). According to reports, Russia was able to secretly produce binary agents because they had inserted loopholes into the 1997 Chemical Warfare Convention to permit their production.⁶ Two such agents – Substance 33 (thought to be 10 times more lethal than VX) and another code-named Novichok (Russian for 'newcomer') – are able to be disguised from weapons inspectors because the chemicals used for the binary agents are common agricultural chemicals. Worryingly, it is also thought that some binary nerve agents are not blocked by conventional chemical protective masks.

Agents of opportunity (including toxic industrial chemicals)

In addition to conventional warfare agents, a large and growing number of potentially harmful chemical compounds can be found in, or introduced into, the environments of deployed forces. For example, troops could be exposed to propellants, explosives and pyrotechnic (PEP) hazards, and a growing number of toxic industrial chemicals (TICs). As military operations become more urbanised, the range of industrial chemicals readily available to a retreating or occupying force number in the hundreds of thousands. Almost any chemical that is toxic to humans can be used to contaminate ground or produce injuries. Chemicals that could be used include the volatile halogenated hydrocarbons (carbon tetrachloride, chloroform, hexachlorobutadiene), simple aromatic hydrocarbons (benzene, styrene, toluene), acids, nitrogen- and sulfur-containing compounds (acrylonitrile, ethylene thiourea), ethers, ketones, phthalate esters, metals (arsenic, cadmium), and industrial stores of pesticides (chlordan, dichlorvos).⁷

Soporifics

Finally, specific pharmaceutical chemicals and bio-regulators could also be used. While expensive to produce, they derive their benefit, compared with more conventional incapacitating agents, from not being covered by the 1997 Chemical Warfare Convention. Soporifics are pharmaceuticals that put people to sleep, and include barbiturates and opium derivatives. In addition, the effects of soporifics are more predictable than psychochemical agents like BZ (Table 1) and LSD (which, instead of incapacitating, may cause feelings of invincibility and aggression).

The best example of the effectiveness of soporifics was the alleged use of an opium-based drug to incapacitate Chechen rebels holding 800 people hostage at a Moscow theatre. Popular opinion puts the death of 120 of the hostages down to the use of Fentanyl by the Russian elite Spoznaz special military forces to subdue the terrorists.⁸

Conclusion

More toxic and useful chemical agents continue to be developed around the world, despite the large number of signatory countries to the 1997 Chemical Warfare Convention. As a result all countries need to continue to develop new means to detect and protect against these agents.

References

1. Available at the Office for the Prohibition of Chemical Weapons website: <www.opcw.org>.
2. Marrs, T.C.; Maynard, R.L., and Sidell, F.R. *Chemical Warfare Agents: Toxicology and Treatment*, John Wiley and Sons: New York 1996.
3. Kassa, J. *Review of oximes in the antidotal treatment of poisoning by organophosphate nerve agents*, *J. Toxicology Clin. Toxicology*, **2002**, *40*, 803–16.
4. Tucker, J.B. *Evidence Iraq used chemical weapons during the 1991 Persian Gulf War*, *Nonproliferation Rev.*, **1997**, *No. 3*, 120.

5. Department of the Army: Binary chemical munitions program. *Programmatic Environmental Impact Statement ARCSL-EIS-8101, 1981, 1-7.*

6. American Foreign Policy Alert No. 23, *Moscow placed loopholes in Chemical Weapon Convention: Treaty won't ban two classes of binary nerve agent*: <www.afpc.org/fpa/fpa23.htm>.

7. Strategies to Protect the Health of Deployed U.S. Forces: *Detecting, Characterizing, and Documenting Exposures*;

Appendix B: Harmful Properties of Chemical Agents. Division of Military Science and Technology and Board on Environmental Studies and Toxicology, McKone, T.E.; Huey, B.M.; Downing, E. and Duffy, L.M. (Eds.). National Research Council, 2000, 161-83 (available online at: <www.nap.edu>).

8. Wax, P.M.; Becker, C.E. and Curry, S.C. *Unexpected 'gas' casualties in Moscow: a medical toxicology perspective, Annals Emerg. Med., 2003, 41, 700-5.*



CHEMISTS

(polymers, biopolymers, bio/organic chemists, natural products)

Vacancy Number 03/04 - 13

We are seeking applicants for a number of positions as Research Chemists at various levels of knowledge or research experience with one or more of polymers, biopolymers, bio/organic chemistry, natural products, and/or chemical extraction processes and/or the use of biobased resources (agricultural crops, forestry resources, other biomasses) in specialty chemical/polymer markets. Applications from recently qualified graduates or for post-doctoral research positions for fixed terms are also possible. The positions are due to expansion of our Biomaterials Engineering Unit and may also contribute to work undertaken in other Forest Research Units, such as PAPRO (Paper Pulp and Packaging), Cellwall Biotechnology Centre, Wood & Fibre Quality and EcoSmart Technologies/Bioconversion, and will involve significant interactions with other research organisations in New Zealand and internationally.

The appointees will be expected to contribute at a science level to projects aiming to further our understanding in the characterisation, isolation, transformation, production and industrial application of biobased chemicals and polymers. The development of processes and chemistries for biopolymer materials or specialty chemicals as entities themselves is one aspect but the work may also include further development of formulated products utilising the extracts from renewable plant resources (such as adhesives, coatings, polymer additives, cosmetics, ...).

The successful candidates will be expected to conduct research within the Biomaterials Engineering Unit as part of a number of multi-disciplinary research projects. The overriding theme of the Unit is the wider utilisation of biobased, renewable materials. Although particular prior experience in such materials is not essential, a bachelors degree or higher and/or relevant experience in one or more of the following areas is desirable:

- Polymer chemistry.
- Chemistry of biopolymers or natural products.
- Manufacturing or extraction processes for chemicals and polymers.
- Organic chemistry with experience/emphasis in polymers or natural products or biochemistry.
- Biochemistry with experience/emphasis in polymers and organic chemical intermediates/derivatisations/characterisations.

The appointees would be expected to actively participate in an interactive, multi-disciplinary team and be able to communicate (written/oral) effectively. Some positions will include research programme planning and implementation and, depending on qualifications and experience, will involve the supervision of other staff.

Position description and application forms are available on request.

Applications to be made on the Forest Research application form. Please include a curriculum vitae and quote the Vacancy Number above. Please forward to the address below.

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Payroll and Personnel Services
Forest Research
Private Bag 3020
Rotorua
Phone (07) 343 5899
Email: kirsty.mitchell@forestresearch.co.nz

Further information and inquiries on the technical contents of the roles is also available from alan.fernyhough@forestresearch.co.nz

Forest Research is an Equal Opportunities Employer

Patent Proze

By John Landells and Helen Palmer

INVENTORS' OWNERSHIP AND REMUNERATION

The large majority of workers throughout New Zealand are not employed to create inventions during the normal course of their work. The opposite can be said for chemists, who, as scientific researchers, are almost entirely focused on the technological application of their science. This applies even within the traditionally non-commercial sector where many academics' work now involves the creation of useful inventions because of the increasing commercial focus by universities. But are there situations where a chemist could claim ownership to his/her inventions? And if not, could chemists claim remuneration if their inventions were to succeed commercially?

Ownership of Inventions

In the absence of specific terms in an employment contract governing ownership of intellectual property, the general rule in New Zealand is that an invention created by an employee during the normal course of work belongs to the employer. A written contract containing express intellectual property ownership provisions is clearly the best way to resolve any uncertainty over the ownership of inventions.

Situations can become complicated when the employee creates an invention outside the normal course of his/her work and no contractual terms exist to provide any clarity. Employment law imparts quite high obligations on all employees to act in 'good faith' and even higher fiduciary obligations can arise by being employed in a trusted senior position. Essentially, the entire relationship between the parties can be examined to determine ownership over an invention. For a chemist who is employed to invent, it can become very difficult to determine what is outside the "normal course of work".

The advantage of an express contract can therefore flow both ways and assist the employer and the employee by providing clarity on what type of independent work by the employee could give rise to ownership in inventions without breaching any obligations.

In a recent Australian decision, in *Victoria University of Technology v Wilson & Ors* [2004] VSC 33 (18 February

2004), a professor and senior lecturer developed an internet based e-commerce system. The invention was developed mostly in their own time but with considerable use of the University's resources. They also attracted funding by holding themselves out as representing the University. All intellectual property was eventually transferred to an independent company owned by them. After the University discovered these activities, an acrimonious train of events finally led to court proceedings. Their employment contracts did not contain any intellectual property ownership provisions, apart from generally incorporating university policy, which did not help because the University had yet to formalise an intellectual property policy.

The scope of the professor's and senior lecturer's employment duties did not involve any expectation to create patentable inventions. However, the professor, as head of the department, was held to have control in determining any new employment expectations in the department. The court found that until the ownership of the IP was transferred to his company the professor had unwittingly extended the employment expectation in the department to cover their e-commerce invention. Furthermore, it was held that the trusted senior positions of the two academics carried a fiduciary obligation of full disclosure. This meant that in transferring IP to their company they had deprived the University of a business opportunity and without full disclosure and consent had breached their obligations to the University. It effectively meant that the invention, or at least the benefits of the invention, belonged to the University.

This case provides a lesson for persons employed to invent that it is essential before undertaking any independent work that full disclosure occurs and a formal agreement is reached with an employer.

Inventor Remuneration

New Zealand does not currently have any law requiring extra remuneration of an employee for delivering a successful invention. However, many countries, including France, Spain, Germany and Japan, do require employers to remunerate employees who create a commercially successful invention. Absence of such law in New Zealand can be countered by the inclusion of appropriate remuneration clauses in employment contracts.



John Landells

Helen Palmer and John Landells of Baldwins specialise in chemistry and biotechnology patents. Helen joined Baldwins in 2000. She has a PhD in chemistry from The University of Auckland and postdoctoral research experience. John joined Baldwins in 2003. He has a PhD in chemistry from the University of Otago and is in the final stages of completing an LLB at Victoria University of Wellington.



Helen Palmer

Japan's patent law, requiring "adequate remuneration" to employees who create inventions, has recently been interpreted in a very favourable light towards employees. In *Yonezawa v Hitachi Co. Ltd*, the Tokyo High Court awarded ¥163 million (about NZ \$2.4 million), which was about 14% of the estimated global profits, to an inventor employed to develop more precise laser beams for compact disc players. A day later the Tokyo District Court in *Nakamura v Nichia Chemical Co. Ltd* took the previous day's record to a new high by ordering an ex-employer pay ¥20 billion (about NZ \$290 million) for a revolutionary blue light emitting semiconductor. This award was about half of the estimated global profits and included patent related profits from estimated future sales.

These two decisions represent to us a backlash in Japan against the previous oppressive treatment of employees by the corporate sector. It will be interesting to see if foreign investment in R & D will suffer in Japan as a result of the

current trend whereby large multinationals will seek to develop technology in alternative employer safer environments.

It is unknown whether legislative changes will ever occur in New Zealand to allow remuneration of employees for the creation of commercially successful inventions. We recommend that employees wanting to obtain reasonable remuneration for commercially successful inventions that they have been employed to create, negotiate for inclusion of appropriate clauses in their employment contracts.

A reminder: if you have any queries regarding patents, or indeed any form of intellectual property, please direct them to:

Patent Proze
Baldwins
P O Box 852, Wellington.
Email: email@baldwins.com

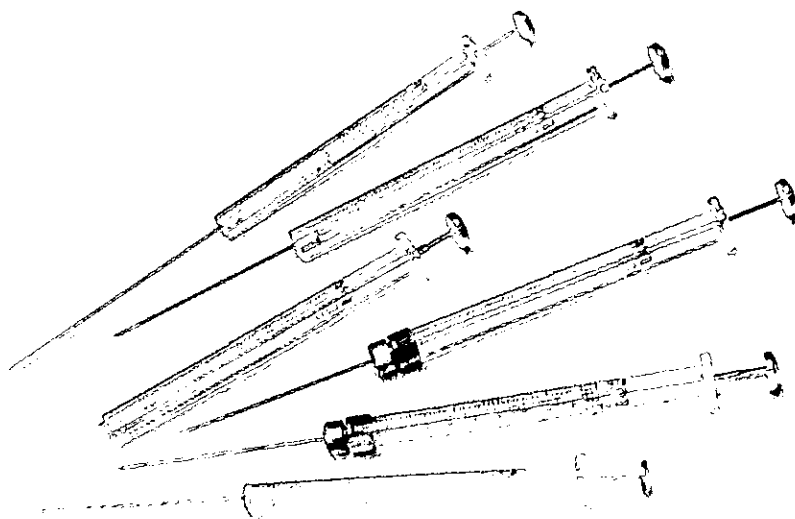
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Conferences & Seminars

1-4 August 2004

5th Australasian Workshop On Mutation Detection Methods, Cancer Gene Analysis And Diagnostic Applications

Mercure Resort, Queenstown, New Zealand
<http://www.genomic.unimelb.edu.au/nz.html>

1-6 August 2004

The SPARC 3rd General Assembly

Victoria, British Columbia, Canada
Email: norm.mcfarlane@ec.gc.ca
<http://sparc.seos.uvic.ca/>

10-11 August 2004

BioFestival 2004, Agbio And You

Melbourne, Australia
<http://www.biofestival.com>

10-11 August 2004

MDN (Medical Device Network) Showcase 2004

Melbourne, Australia
<http://www.mdnshowcase.com>

10-13 August 2004

Forest Entomology And Biosecurity Under The Auspices Of The International Union Of Forestry Research Organisations

Heritage Hotel, Hanmer Springs, New Zealand
Contact: Eckehard Brockerhoff
Phone: (03) 364 2812
<http://www.forestresearch.co.nz/iufro2004>

15-29 August 2004

XVIIIth International Symposium On Medicinal Chemistry

Copenhagen, Denmark and Malmo, Sweden
<http://www.ismc2004.dk/>

24-28 August 2004

New Zealand Institute of Medical Laboratory Science Annual Scientific Meeting & Conference and Immunology Special Interest Group Meeting

Kingsgate Hotel, Hamilton, New Zealand
Contact: Robin Allen
Email: allenr@waikatohb.govt.nz
http://www.eenz.com/waikato_info.htm

1-3 September 2004

Asia Pacific Horticulture Conference

Hyatt Coolum, Sunshine Coast, Queensland, Australia
Contact: Richard Williams
Email: richard.williams@uq.edu.au
<http://www.aushs.org.au/comference>

4-9 September 2004

8th International Global Atmospheric Chemistry (IGAC) Conference

Christchurch Convention Centre, Christchurch
Contact: Kim Gerard

Email: kim@conference.co.nz

<http://www.IGAConference2004.co.nz>

5-6 September 2004

Canterbury Health Science Research Conference

Christchurch School of Medicine and Health Sciences
Christchurch
<http://www.cmrf.org.nz/index.php?page=conference>

5-8 September 2004

2004 International Conference On Bioinformatics (InCoB)

Aotea Centre, Auckland
<http://www.incob.org>

9 September 2004

Royal Society Council Meeting

Auckland

12-15 September 2004

Horizons In Livestock Conference

Gold Coast International Hotel, Queensland, Australia
<http://www.livestockhorizons.com>

23-24 September 2004

Laboratory Automation And New Technologies In Process Research And Development

The Boston Marriott Long Wharf, Boston, USA
<http://www.scientificupdate.co.uk/confs/automation/auto.htm>

26-30 September 2004

ComBio 200. The Annual Conference Of The Australian Society For Biochemistry & Molecular Biology, The Australia And New Zealand Society For Cell And Developmental Biology And The Australian Society Of Plant Scientists

Burswood Resort Convention Centre, Perth, Australia
<http://www.asbmb.org.au/combio2004/>

26 September - 1 October 2004

4th International Crop Science Congress

Brisbane, Australia
<http://www.regional.org.au/>

27 - 28 September 2004

World Pharma IT

London, England, United Kingdom
<http://www.oxfordint.co.uk/pharmait/index.htm>

4-5 October 2004

Chiral USA 2004

The Boston Marriott Long Wharf, Boston, USA
<http://www.scientificupdate.co.uk/confs/chiralus/chiralus.htm>

18-19 October 2004

RNAi Europe

London, England, United Kingdom
<http://www.RNAiEurope.com>

1-4 November 2004

The Scale-Up Of Chemical Processes

The Burlington Hotel, Dublin, Ireland

<http://www.scientificupdate.co.uk/confs/scaleup/scaleup.htm>

4 November 2004

Functional Foods Symposium

Auckland

Contact: l.ferguson@auckland.ac.nz

7-10 November 2004

AUSBIOTECH 2004 - Going Global

Brisbane, Queensland, Australia

<http://www.ausbiotech2004.com>

22-26 November 2004

19th Annual DNA Technology Workshop

An introduction to the theory and practice of DNA technology. Early enrolment advised to secure a place in this popular course.

Massey University (Palmerston North Turitea Campus)

Contact Email: R.E.Bradshaw@massey.ac.nz

<http://imbs.massey.ac.nz/workshop.htm>

28 November 2004 - 1 December 2004

The 14th Annual Queenstown Molecular Biology Meeting

In conjunction with the New Zealand Society for Biochemistry and Molecular Biology

"Molecular Mechanisms in Cell Biology"

Rydges Hotel, Queenstown

Contact: Billie Masters, Conference Organiser

Email: billie@jsmasters.co.nz

<http://www.qmb.org.nz/>

9 December 2004

Royal Society Council Meeting

Wellington

17-19 January 2005

Protein Crystallography in Drug Discovery

South San Francisco, California, USA

<http://www.ProtCrystConf.com>

14-16 February 2005

Screening Europe

Geneva, Switzerland

<http://www.ScreeningEurope.com>

10-14 July 2005

7th World Congress Of Chemical Engineering

Glasgow, Scotland, United Kingdom

<http://www.chemengcongress2005.com>

CANTERBURY AWARDS PERSONAL CHAIR

On the last day of the NZIC Nelson Conference it was announced that Conference Chairman, **Andrew Abell**, had been appointed to a personal chair in Chemistry at the University of Canterbury. Andrew studied for his PhD with Dr. Ralph Massey-Westropp at the University of Adelaide, working on the mechanistic, stereochemical, and structural problems of terpenes isolated from *Eremophila rotundifolia*. 1984 saw him in Cambridge as a postdoctoral fellow with Professor Sir Alan Battersby working on the biosynthesis of vitamin B12 and related compounds. In 1987 he accepted a lectureship at Canterbury where he has been ever since.

Professor Abell currently works in a number of areas at the interface of chemistry and biology. One such area is the design, synthesis and biological properties of non-steroidal inhibitors of steroid 5 α -reductase, an enzyme that catalyses the bio-transformation of the male sex hormone (testosterone) into dihydrotestosterone (DHT). High levels of DHT lead to cancerous and non-cancerous enlargement of the prostate as well as skin conditions such as acne and hirsutism. These new inhibitors lack many of the side effects of traditional steroid-based compounds. His work involves close collaboration with the international pharmaceutical industry where he has been



employed as a consultant. Andrew has recently extended this *rational* approach to enzyme inhibitors to the design of new potential herbicides and pharmaceuticals for the potential treatment of tuberculosis. X-ray crystallographic studies of the enzyme allows for the design of compounds that inhibit dehydroquinase, an enzyme specific to the shikimate pathway found in plants and simple microorganisms, but not animals.

Other areas of interest include the design and synthesis of new classes of peptidomimetics (analogues of important natural peptides) that inhibit proteases associated with important diseases and pathological infections, including AIDS, emphysema, and arthritis. This work also involves close collaboration with the pharmaceutical industry. Most recently, his group has developed ring-closing metathesis chemistry to give important derivatives for use as structural motifs and enzyme inhibitors.

Professor Abell has received a number of awards including the NZIC Easterfield Medal, the C.S.R. Chemicals Prize, a George Murray Scholarship, and a Senior Fulbright Scholarship. He has trained and supervised in excess of seventy postgraduate students and postdoctoral fellows and he has published widely.



NEWS

From The President

The well-known quotation by Dickens: *Annual income twenty pounds, annual expenditure nineteen pounds nineteen shillings and six pence - result happiness. Annual income twenty pounds, annual expenditure twenty pounds ought shillings and six pence - result misery* summarises the present financial situation of the New Zealand Institute of Chemistry. The aim must be to manage our core operations (Branches, the Journal *Chemistry in New Zealand*, and administration) from the subscription income but we don't. To put it simply, the Institute only survives because additional income from conference, the educational publication (CHEM NZ), and the Chem13 exam props it up. This is not a fiscally responsible way to operate since none of these other income streams are guaranteed as secure. Personally, I feel that income from these latter two activities should be put back into chemical education in New Zealand and profits from conferences should be used for activities such as promoting the chemical sciences in the community. In this respect Council has agreed to a donation of \$2000 for this year's SCICON meeting that caters for science teachers.

The choice is straightforward. Either we scale down what we do in order to reduce our expenditure or we increase our membership. Council spent time at its April 16 2004 meeting to discuss a paper that I had prepared for the meeting. If we were to scale down our activities where would the savings come from? Those of you who say cut back on administration should try and deal with the complications of for example GST; Conference organisers have found that they can easily get into difficulties over this! Would you get rid of *Chemistry in New Zealand*? Would you abandon the branches and run everything at a national level? These are the sorts of questions we are grappling with. Once Council has agreed to the final form of the paper it will go to the Branches and be put on the NZIC web site (see below) for feedback from you members of the Institute. I have already had some very thoughtful comments from members as a result of my Editorial in the last issue of *Chemistry in New Zealand*.

Council has done more than just discuss possible future directions. We have acted on things that cannot wait. One of the most important of these is getting an increased use of the NZIC web site. Manawatu Branch members, Grant Boston and Stephen van Eyk, formerly put a lot of work into the site. Now, the Canterbury Branch has taken responsibility for updating the site and Rebecca Hurrell is working on this. I am optimistic that by the time you read this issue of *Chemistry in New Zealand*, the pages will be

CHEMICAL EDUCATION TRUST 2004 DISTRIBUTION

Applications are invited from secondary school chemistry teachers (senior chemistry teacher via Head of Science) for grants from the NZIC Chemical Education Trust to promote the teaching of chemistry in their school. For the 2004 distribution grants of about \$400 are envisaged but greater or lesser amounts can be applied for.

Applications should be received no later than 14 August 2004 and addressed to:

Dr. P. T. Holland,
NZIC Chemical Education Trust,
Cawthron Institute,
Private Bag 2,
Nelson
Email: patrick.holland@cawthron.org.nz

a useful source of information. Did you know that Branch Secretaries could put Branch news up on the web pages? If your Branch is not using this facility then chase your committee up and get them onto it. My hope is that the NZIC web site will be the first place members and potential members will go to read about the NZIC and what its activities.

All Branches have been asked to think about members that can be elected to the Fellowship of the NZIC. We all need to think about this and you can either apply individually or be nominated by your Branch or other Fellows. The criteria for FNZIC are quite wide ranging and provided under Rule 9 (see: <http://www.nzic.org.nz>). If you are interested in becoming a Fellow contact your Branch or apply yourself; If you prefer I am happy to discuss this with you.

We have been seeking new sponsors for our two of our prizes to replace SGS and FERNZ, and I am hopeful that we will have agreements with new sponsors soon. Council has decided to change the closing date for all prize applications to August 30. Details about these and our other prizes can be found on the web page.

One of the roles of Council is to nominate Institute members to serve on various national or international bodies. For example I was nominated for the Royal Society of New Zealand Council and was duly elected. Brian Halton (Wellington) has been actively involved with Pacifichem organisation on the Institute's behalf for many years; he is to be replaced by Rob Smith (Otago) for the 2010 conference. Kip Powell (Canterbury) is our representative on the IUPAC Union Advisory Committee and Hicham Idriss (Auckland) has just been nominated for the committee of the Asia-Pacific Association of Catalysts Societies (APACS). It is important that we are seen to be an active organisation and be represented on such international bodies.

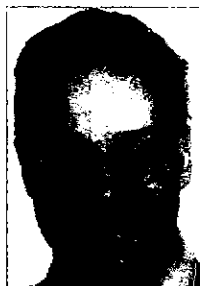
Finally, I would like to say thank you all for your ongoing support of the Institute while we work towards a more

viable organisation. Members who are passionate about the chemical sciences and are willing to support their professional organisation are much appreciated. I always welcome your feedback on anything concerning the Institute - just email me <A.Brodie@massey.ac.nz>.

NZIC Prizes

The closing date for the receipt of applications/nominations for the 2005 NZIC prizes, the HortResearch Prize for Excellence in Research, the Nufarm Prize for Excellence in Industrial and Applied Chemistry, and the Chemical Education Prize has been extended and now closes on 30 August 2005, <see: <http://www.nzic.com.nz>>.

New Fellow: *Dr. Owen J Curnow*



Dr. Owen Curnow was elected a Fellow of the Institute last November and a profile follows. Owen obtained his MSc from the University of Waikato under the tutelage of Professor Brian Nicholson. He then went to the University of Michigan where he worked for his PhD with Professor

David Curtis on the chemistry of Mo-Co-S clusters towards gaining an understanding of the industrial hydrodesulfurization (HDS) process. This was partially supported by a Fulbright Travel Grant. He then undertook postdoctoral study; firstly, in 1992 at Dartmouth College with Professor Russell P. Hughes where he made the first perfluorocyclopentadienide complex $[\text{Ru}(\text{C}_5\text{Me}_5)(\text{C}_5\text{F}_5)]$, and subsequently, on an Alexander von Humboldt Fellowship at the University of Heidelberg with Professor Gottfried Huttner, where he made the first group 13 indenide complex $[\text{InBr}(\text{Cr}(\text{CO})_5)_2]^{2-}$. Here he began his work on phosphinocyclopentadienide ligands.

In December of 1993, Owen took up an academic position at the University of Canterbury where he is now a Senior Lecturer. His research has focused on functionalised or conformationally-constrained cyclopentadienyl ligands, particularly with phosphine substituents. This class of compounds is very important in organic synthesis now due to the extensive use of organometallic homogeneous phosphine ligand-containing catalysts. Recently, he has studied a ferrocene with phosphinoindenide ligands that flip over to the other face of the ring at room temperature in THF; this process was unknown for ferrocenes, despite over 50 years of intensive international research.

Dr. Curnow's NZIC work has involved him at the local level serving as Canterbury Branch Treasurer and nationally as organiser of the New Zealand contribution to the International Chemistry Celebration in 1999. This latter included National Short Story Competitions, the National High School Chemistry Challenge with finals at Parliament Buildings, and the National Flag Competition which culminated in an exhibition at the Te Papa National Museum. Most recently, he was the Secretary of the 2003 NZIC Conference in Nelson.



BRANCH NEWS

Comments contained in the Branch reports on the outcomes of the performance based research funding (PBRF) exercise in the tertiary sector have been excluded in the hope that a balanced article on the outcomes will be forthcoming.

Ed.

AUCKLAND



Above:
Peter Schwerdtfeger
(photo credit: Massey
News)

Peter Schwerdtfeger has taken up the new position of Professor of Theoretical Chemistry, at Massey University, Auckland. He was previously at the University of Auckland, where he had a personal chair. Professor Schwerdtfeger says the reputation of the Institute of Fundamental Sciences and the opportunity to be part of it attracted him to Massey. He comes with an outstanding research record and has attracted research funding of \$5.4 million. Some of the highlights in his academic career include: the Alexander von Humboldt Feodor Lynen Award, the SGS prize, Fellowship of the Royal Society of New Zealand, Fellowship of the New Zealand Institute of Chemistry, Hector Medal, James Cook Fellowship, and three Marsden Awards. Professor Schwerdtfeger will lead the *Physical Sciences Research Centre* that is being established at Massey's Auckland campus.

The University of Auckland

Congratulations are offered to the following staff and students from the Department of Chemistry of The University of Auckland!

Brent Copp has been awarded a grant totalling \$14,750 from the Maurice & Phyllis Paykel Trust. Good news Brent and our best wishes. **Shane Lal** has received the *Edible Applications Division Student Excellence Award* from the American Oil Chemists' Society. The award recognises an outstanding graduate student working toward an advanced research degree related to the Division's area of

interest. **Geoff Waterhouse** has been awarded the L.H. Briggs Memorial Prize for the Best Chemistry Doctoral Thesis. **Margaret Brimble** and **Caryn Burgess** have been awarded a grant of \$81,300 from Genesis Oncology Trust for their project *Synthesis of telomerase inhibitors based on the rubromycins*.

University Research Grants for New Staff Research Fund have been received by **Dr. Laura Nicolau** for the application of micro-oxygenation to improve the aroma profiles of New Zealand red wines; **Associate Professor Hicham Idriss** for the mineral origin of life - a surface science investigation; **Associate Professor Jim Metson** for pumping and gas handling manifold for online gas analysis; **Dr. Gordon Miskelly** for *Beyond RGB – improved detection using multispectral imaging*; **Dr. Brent Copp** for forward chemical genetic studies of marine natural products; **Dr. Paul Kilmartin** for electrochemical micro-oxygenation of wine; **Professor George Clark** for DNA/drug crystal structures using synchrotron data; **Associate Professor Bob Anderson** for pulse radiolysis studies of electron transfer in redox proteins and DNA; **David Barker** for his project entitled *An enantioselective approach to epiquinamide – a nicotinic acetylcholine receptor selective agonist*. **Professor John Arnold** (UC Berkeley, USA) is visiting the Department of Chemistry and is hosted by **Penny Brothers**.

CANTERBURY

The Canterbury Branch began the year with its annual Student BBQ with the University Staff Club providing a picturesque, though rather windy setting for the evening, which provided a great opportunity for chemistry students to meet, mingle and have a drink with their colleagues, academic staff, and the local NZIC community. Two of the student prizes were awarded and Branch Chair **Jan Wikaira** gave an outline to prospective members of the benefits of membership. The Branch also held a Baking Competition in the University of Canterbury Chemistry Department in March; there was fierce competition and many of the onlookers enjoyed the spoils. The Baking Competition raised additional funds for Branch sponsorship during the year; recipes for a Chemistry Cookbook are being compiled for the same purpose.

Our April meeting was a seminar presented by **Dr. Pauline Rudd**, a senior Research Fellow visiting from the Glycobiology Institute at Oxford University. In her talk entitled *Oligosaccharides and Disease*, Pauline disabused the audience of the somewhat over-simplified, textbook perception many have of proteins and their structures. Many important proteins are processed to coat their surface with specific oligosaccharides rather than being mere appendages; these oligosaccharides are often of comparable size to the host protein and essential to the biological function of it. Pauline described the pioneering work done at the Glycobiology Institute that has provided detailed insight into the nature of these molecules and she highlighted significant roles for surface oligosaccharides in important diseases.

ESR

Dr. Jeff Fowles, a toxicologist specializing in chemical constituents of tobacco products, sat on the Ethics of Tobacco Product Harm Reduction expert advisory panel to Health Canada in February. He discussed *Should we be regulating tobacco one chemical at a time?* in an invited presentation at Health Canada and talked of *A cancer potency approach to characterizing the carcinogens in cigarette smoke* in an invited presentation at the US National Cancer Institute.

Dr. Brent Gilpin presented work on faecal source identification using chemical indicators at the Environmental Source Tracking Workshop in Guildford (UK). Brent described his research, which investigates the application of fluorescent whitening agents and faecal sterols, both indicative of human activities, to determine sources of environmental pollution in New Zealand.

ESR congratulates **Dr. Jan Gregor** for her recent re-election to the National Science and Technology Roadshow Board of Trustees and the Christchurch Science Technology Trust Board (Science Alive!).

Christchurch Polytechnic Institute of Technology

Dr. David Hawke attended the *Measurement Uncertainty* seminar organised as part of the CITAC/IRL Workshop on Traceability & Uncertainty in Wellington in May. Laboratory quality issues are an important, and growing part of the courses on analytical chemistry taught at CPIT.

University of Canterbury

Once more **Syft Technologies Ltd.**, the company established to develop SIFT commercially, has been successful in securing a total of \$4.84 million (over four years) in the recent FRST awards of Research for Industry grants. At the same time, **Dr. Randall Allardyce's** appointment as an Adjunct Senior Fellow has been renewed and he will continue to collaborate with **Professor Murray McEwan**, including work on the commercialisation of the SIFT-MS technique.

The Department recently farewelled **Dr. Jonathan Morris** who has taken up a position at the University of Adelaide. Jonathan, a Chairperson of the Canterbury Branch of the NZIC for several years, has been an active and important part of the Department for seven years and he will be missed both in professional and social capacities. **Professor Lew Mander** (Research School of Chemistry, ANU) is visiting the Department as an Erskine Fellow for the second term.

The Department has welcomed **Dr. Gerhard Lang** as a Postdoctoral Fellow in the Marine Group. Gerhard completed his PhD thesis at Wurzburg (Bringmann) where he investigated secondary metabolites from sponge-associated microorganisms. Another international addition to the department is **Dr. Axel Neffe** who is working on the cataract project for two years as a University Postdoctoral Fellow. Axel has recently finished his PhD (Design, Synthesis and Analysis of CD4 Binding Peptidomimetics,

University of Hamburg - Bernd Meyer). **Jenny Malmström** (Chalmers University of Technology - Sweden) departed earlier in the year after a six-month stay working with **Dr. Alison Downard**. Jenny promises to be back and doing the Coast-to-Coast!

Seven students have commenced PhD studies in the Department this year. Honours graduates **David Pearson**, **Neroli Eggeling**, **Blair Stuart**, **Jennifer Zampese**, and **Sam Yu** are returning, and **David Bones** is back from a year off. **Jennifer Zampese** has started her project with **Peter Steel** and has received a Todd Foundation Award for Excellence. **Cherry Chen** and **Tim Simpson** have been awarded 1st Class Honours for their MSc theses.

MANAWATU

Landcare Research

Dr. Benny Theng is travelling to the USA shortly to receive the Bailey Distinguished Member award, and to give the Bailey Lecture *Of Clays, Colloids, and Composites* at the Clay Minerals Society meeting.

Massey University

A new research centre at the Palmerston North campus signals a new era of partnership between academia and the corporate world. The *Anzode Research Centre* has come a joint venture between the University and a group of United States-based investors, headed by **Chris Officer**; its aim is to commercialise a new zinc battery technology developed by chemists **Drs. Simon Hall** and **Michael Liu**. The two have discovered a chemical answer to the problems that have plagued developers of rechargeable zinc batteries. Their resulting battery survives 1200 recharging cycles, where other zinc-based anodes have failed at as few as 30 cycles. Deputy VC (Palmerston North) **Professor Ian Warrington**, says the centre demonstrates the willingness of the University to form partnerships with global entities to take research discoveries to the commercial stage - "We should look back on this as being the first of many such successful partnerships".



Above: Opening of the Anzode Research Centre, left to right: **Professor Ian Warrington**, **Chris Officer**, **Dr. Simon Hall** and **Dr. Michael Liu**.

Bill Williams, a new lecturer, has been awarded the Royal Society of Chemistry Food Group Junior Medal. **Simon Hall**, **Emily Parker** and **Carol Taylor** were recently awarded Institute of Fundamental Sciences Distinguished Teaching Awards for their outstanding efforts in third-year chemistry classes. **Joyce Sewry** is a sabbatical visitor from the Department of Chemistry, Rhodes University, South Africa. Her interests are in the fields of chemometrics and first year foundation courses for science students.

Assistant lecturer, **Adrian Jull** organised another successful high school chemistry teachers meeting in May based on the theme *Making Light of Chemistry*. **Dr. Mark Waterland** presented some ideas about how to use Grätzel Cells (dye sensitized liquid junction cells based on mesoporous TiO₂) in a high school science and chemistry programme. **Dr. Lola Berber-Jimenz** (a visitor from California) then outlined the differences and similarities between education here and there. Afterwards the teachers went into the laboratory to build the Grätzel cell using blueberry dye extract as one of the components. Judging by the success of the practical session the evening was enjoyed by all.

Year 12 chemistry field trips to Massey are starting again in June, thanks to **Adrian Jull**. Schools are booked in from as far a field as Gisborne and Taranaki. Currently, three experiments are planned, *extraction of orange oil*, *making a conducting polymer*, and *healthy plant pigments*. About 900 students attended last year and a similar number are expected from June and October this year.

HortResearch

A new gas chromatography mass spectrometer has recently been installed for use on projects that involve synthetic chemistry such as biosecurity work with moth pheromones, flavour compounds in fruit, and work in conjunction with AgResearch, developing a metabolomics platform for discovery and identification of new plant compounds.

OTAGO

The local branch kicked off the year with dinner at the Joseph Mellor restaurant, followed by a talk from **Associate Professor Dave Crow** from the Geology Department at the University of Otago. Amongst other things, Dave spoke about his fieldwork in some of the more exotic regions of the Himalayas.

We were very fortunate in having **Professor Brian Johnson** (Cambridge University) present a lecture to the local branch in early April titled *Nanoparticles in Catalysis and Devices*. Brian is well known to several of the more venerable staff members here, having spent a brief period of sabbatical leave at Otago in the early 70s.

This year **Dr. Jason Price** (ex-Len Lindoy's group, Sydney) and **Dr. Robyn Handel** (ex-Ed Constable's group, Birmingham/Basel) have joined **Associate Professor Sally Brooker**'s research group. Sally will be on sabbatical leave from July 3 until the end of November. She will present a lecture, and **Rongqing Li**, **Yanhua Lan**, **Dr. Jason Price**,

and **Dr. Markus Weitzer** (ex-Schindler's group, Erlangen) will present Brooker Bunch posters, at the ISMC conference in Cairns. Sally will briefly visit Sydney University and UNSW before taking up a three-month visiting Professorship at the Centre for Nanostructures in Karlsruhe, Germany. She will then visit a number of collaborators in Universities in Ireland and the United Kingdom before returning to New Zealand.

Dr. Henrik Kjaergaard, Daniel Schofield, and Daryl Howard attended the RACI/NZIC Physical Chemistry Conference in Hobart in February and presented a paper entitled *Atmospheric applications of Vibrational Overtones* and the posters *Electronic spectroscopy of the H₂O-HO complex* and *Highly vibrationally excited formic acid: Resonance coupling between OH and CH stretching vibrations*. Henrik is continuing as the New Zealand representative on the RACI physical chemistry section and is in the process of compiling an e-mail list of all physical chemists in New Zealand. Please send your details to <henrik@alkali.otago.ac.nz>. Henrik attended the Theory and Applications of Computational Chemistry Conference, TACC2004 in Gyeongju (South Korea) in February 2004 and gave a lecture *Vibrational Overtones in Complexes*. His student, **Timothy Robinson**, successfully completed his PhD on *Near infrared spectroscopy of aromatic molecules* in May.

There have been several changes in **Rob Smith's** lab of late. Visiting scientist **Linda Samuelsson** has returned to Sweden in order to complete her PhD. Much of the work she undertook at Otago, using various NMR techniques to probe counteracting osmolyte activity, will be incorporated into her PhD thesis submission to Uppsala University. Two new research associates, **James Cambridge** (PhD with Jim Coxon, Canterbury), working on a joint project with **Mike Berridge** (Malaghan Institute), and **Debra Gauntlett** (ex-Waikato University; MSc degree with Meryllyn Manley-Harris), working on research and development aspects of the mitochondria chemistry project, have joined the Department.

Somewhat belated news from the Marine and Freshwater group is that **Dr. Doug Mackie** has arrived back in the Department after spending a post-doctoral period with Dr. Stan van den Berg (Liverpool, United Kingdom) where he was researching iron-binding natural organic matter ligands in seawater. Doug is now employed on a new Marsden grant awarded to **Keith Hunter** and **Philip Boyd** (NIWA; Hon. Lecturer in Chemistry). This research is concerned with tracking the transport of Australian dust to the Southern Ocean around New Zealand and its subsequent influence on phytoplankton growth in these iron-limited waters. **Dr. Jonathan Kim** is also working on this research programme. **Dr. Sylvia Sander**, who joined Marine and Freshwater in late 2001, took time out for the birth of her first child, Isabella, but is now back in the lab working on a new PGSF grant, sub-contracted from NIWA, concerned mainly with the behaviour of colloid particles in estuaries. Sylvia, originally from Germany, has considerable expertise in electrochemical methods of analysis having spent a period as a researcher at EcoChimie BV, an instrument manufacturer in the Netherlands. Another

recent arrival is **Mr. Barry Anderson** (research technician) who arrived in December last year. Barry has had a varied career, including many years as a baker! He completed his technician training at the Christchurch Polytechnic at the end of 2002.

The group played a major role in a recent oceanographic cruise called FeCycle. This involved labeling a 7 km x 7 km patch of ocean west of Otago with SF₆ followed by a 2-week intensive investigation of chemistry, physics and biology of the patch. The primary focus was on determining the budget for iron cycling through the water and biota. Group members involved were **Russell Frew, Robert Strezpyk, Phil Boyd, Keith Hunter** and **Sylvia Sander**. The group also hosted **Professor Dave Hutchins** from the University of Delaware for a visit both before and after the cruise.

Keith Hunter has been appointed to the Editorial Board of the new journal, *Environmental Chemistry*, under CSIRO Publishing, partly as an offshoot of the *Australian Journal of Chemistry*. Keith was also involved as a Working Group chair at the OCEANS conference in Paris, a meeting devoted to developing a new international research programme in biogeochemistry of the oceans. The new programme, now titled IMBER (International Marine Biogeochemical and Ecological Research) has now been formulated as a draft proposal for IGBP (International Geosphere-Biosphere Program).

WAIKATO

The Waikato Branch *National Crystal Growing Competition* is on again this year. Please contact: **Associate Professor Bill Henderson**, Chairperson, Chemistry Department, Waikato University, Private Bag 3105, Hamilton, Phone Direct: 07 8384656; Fax: 07 8384219; Email: <hende@waikato.ac.nz> for details.

At the May meeting, **Dr. Carrick Devine** (HortResearch, Hamilton) gave a very interesting and well-attended talk entitled *Myths of Diets*, which covered discoveries made while looking at certain diets for animals and sportspersons through to popular diets such as the Atkins Diet. After hearing the talk, **Sir Don Llewellyn** commented that given all the things one shouldn't eat, it was a wonder that he was still alive! Also at the meeting, current third year chemistry students, **Jolene Brown** and **Simon Thwaite** were presented with their joint award of the J.E. Allan prize for the best all round performance in second year chemistry.

University of Waikato

The Chemistry Department put on a number of displays for the University Information Day on April 30. These included liquid nitrogen and pyrotechnics, and **Bill Henderson** gave a well-attended talk. The School of Science and Technology also ran a *Whodunnit* murder mystery scenario in which participants had to visit each Department in the School to collect evidence. In Chemistry they had to develop a fingerprint found on a note on the victim's body and match it to that of one of the suspects.

Michael Mucalo attended the 4-yearly 7th World Biomaterials Congress held in Sydney from 17-21 May. It was a large conference with upward of 1400 participants and a reasonable sized Exhibition. He presented his latest clinical research on implantation of bovine-derived bone replacement materials and had a poster presentation on some fundamental biomimetic work performed by his MSc student **Dougal Laird** that tries to gain an insight into pathological calcifications arising in atherosclerosis.

A major refurbishment of the Inorganic and Organic Chemistry research laboratory has now been completed and the research students have moved back. The lab was officially *christened* and there was an appropriate supply of drinks and nibbles; the event revealed a number of excellent bakers and cooks amongst our graduate students!

Bill Henderson has four new MSc students this year, **Jessica Zhu** (phosphonate-based anticorrosive pigments), **Kelly Kilpin** (synthesis and biological activity of new gold(III) complexes), **Sunita Jeram** (also with **Merilyn Manley-Harris** on phosphine functionalised supports for materials separations), and **Kristina Pham** (chemistry of platinum sulfide complexes). They join **Brad White** (chemistry of the $\text{Pt}_2\text{S}_2(\text{PPh}_3)_4$ system) and **Lucia Ying** (ionic liquids) who are completing their MSc studies. Brad recently spent two weeks at the National University of Singapore (funded by the Asia 2000 Foundation) working with Professor Andy Hor. We also congratulate him on his recent marriage to Vicky.

WELLINGTON

The March Branch meeting was a membership drive and student poster competition for students of chemistry in the region. Prizes (sponsored by the School of Chemical & Physical Sciences and Faculty of Science) were awarded to John Moraes, Liu Xianming, and Andy McFarlane. The evening included a sausage sizzle and refreshments were kindly sponsored by the Wellington Brewing Company from its micro brewery on the waterfront; NZIC membership numbers were boosted.

In April **Bryce Williamson** gave the 2005 Mellor Lecture entitled *The Jahn-Teller in the Ferricenium Radical* that included a synopsis of ferrocene $[\text{Fe}(\text{cp})_2]$ and the recognition that its bonding was one of the most significant events in the development of organometallic chemistry. The very stable radical cation ferricenium, $[\text{Fe}(\text{cp})_2]^+$, was soon discovered and much work was initiated, mainly intended to elucidate the nature of the bonding in such systems. Bryce described the Canterbury work on the vibronic interactions that occur in orbitally degenerate species with axial symmetry and how they can be investigated by magneto-optical methods. By using argon matrices fields are typically one or two orders of magnitude weaker and this has led to a fuller understanding of crystal field, Jahn-Teller and spin-orbit interactions with the surprising result that the vibronic mechanism (through the Ham effect) has the greater responsibility for the observed quenching of orbital angular momentum.

May saw VUW biochemist **Alan Clark** discuss *Glutathione transferases - enzymes for almost everyone*. Glutathione S-transferase (GST) is a member of an enzyme class that is found almost universally in aerobic organisms, animals, plants and bacteria with detoxification of a vast range of chemically reactive toxins that can damage cellular constituents as the main role. Recently, it became apparent that they may play a more subtle role in protecting us from chemical damage, *e.g.* in mammals, some appear to signal the onset of a potentially dangerous state and initiate a complex series of defensive responses. Alan's discourse considered the wide-ranging roles of these enzymes and presented some of the VUW studies involved.

BRANZ

Dr. John Duncan, BRANZ Manager, Building Industry Research, was awarded honorary membership of CIB – the International Council for Research and Innovation in Building and Construction – at the CIB Congress in Toronto in early May. He was awarded it for his outstanding contribution in leading CIB as Programme Committee Chairman 1995-1998 and President 1998-2001, during his 12 years on the Board of the Council from 1992-2004. **Dr. Gareth Kear**, until recently a Research Fellow at University of Queensland, joined BRANZ in June as a materials scientist.

Responsibilities for **Wayne Sharman** and **Adrian Bennett** will be changing slightly, as they and John Duncan form a small team focussed on ensuring that the building and construction sector is getting the best outputs it can from investment by the Association of the Building Research Levy.

Victoria University

The School of Chemical & Physical Sciences farewelled **Professor Brian Halton** at the end of March.

Brian Halton was born in Lancashire, United Kingdom. He gained BSc(Hons.) (1963) and PhD (1966) degrees in chemistry at the University of Southampton (UK) and then spent a year at the University of Florida as a Postdoctoral Fellow (Battiste) and a second as an Assistant Professor.



Above: Professor Brian Halton.

He then joined the Chemistry Department, Victoria University of Wellington as a Lecturer in Chemistry in 1968 and progressed through the ranks of Senior Lecturer and Reader to a Personal Chair in Chemistry in 1991. He was awarded a DSc by Victoria University in

1987 and was elected to Fellowship of the Royal Society of New Zealand in 1992.

Professor Halton is an internationally recognized scientist of the highest calibre who has dedicated some 36 years of his professional life to providing excellence in research and teaching in organic chemistry, and in the wider promotion and service to chemistry. During this time Brian set and maintained the highest possible standards and level of excellence in all his activities. His hallmark is that of quality, rigour and integrity, which he successfully communicated to students of organic chemistry at all levels through well-structured informative lectures, tutorials, laboratory exercises and research leadership and supervision. The many hundreds of students, who have been educated under his expert tutelage at both the undergraduate and graduate levels, have enjoyed an international chemistry education comparable to the best in the world. This is evidenced by the senior and leadership positions his past students now hold in internationally prestigious institutions. His high international standing provided a valuable pathway for his graduate students to work with similarly internationally recognized scientists in quality international research institutions. He supervised 41 graduate research students of which 11 were PhD and 26 BSc(Hons) students.

He is an established international leader in his research field of fundamental and highly strained small ring organic molecules and maintains a consistent output of excellent research papers in high quality peer reviewed international journals. In 1984 he published what has become the classic

paper on the synthesis of the first aromatic structure fused with a three-membered ring that allowed for further conjugation within the molecule; this provided the basis for a new group of highly strained molecules with exceptional thermal stability. Since then, Professor Halton has lead the field in these cycloproparene-based supranatural compounds where he has made a substantial contribution to the synthesis of these unique materials and to their characterization and understanding through spectroscopic, X-ray structural and theoretical studies. He collaborates widely with fellow international scientists and has received numerous invitations to present guest lectures at prestigious research institutions and plenary lectures at international conferences.

He has published extensively with some 116 research papers, 12 review articles and 5 book chapters, edited 10 books, and co-authored two classic organic photochemistry texts. His work is of the highest quality and is cited extensively by co-workers and followers in the field.

Professor Halton has actively promoted the discipline and profession of chemistry. He has held the office of President of the New Zealand Institute of Chemistry, been a Council Member, and also served in most other positions of responsibility in the Institute at Branch and National level over many years. He continues as Editor of the Institute's journal *Chemistry in New Zealand* (from 2001) and is responsible for the improved quality of this publication. Also, he has been the Institute's representative on the organizing committee for the Pacific Basin Chemical Congress *Pacificchem* for the 1989, 1995, 2000, and 2005

events where he has contributed substantially to the organization and smooth running of these very large international congresses. He has also been instrumental in facilitating financial support to enable postgraduate students to attend the congress. That Australasia is formally involved in this major event is due entirely to his efforts.

Professor Halton has also served the wider university and student community as the Victoria University-nominated Newman Trustee and a member of the Trinity-Newman Board during which time he has provided input into facilitating improved student accommodation.

Brian Halton retired on 31 March, 2004 after some 36 years of continuous service in chemistry.

The School of Chemical & Physical Sciences welcomed in May, **Dr. Joanne Harvey** as a lecturer in Organic Chemistry. Joanne, a VUW graduate, gained her PhD at ANU (Banwell) and carried out postdoctoral work at York (**Professor Richard Taylor**); she will be lecturing at all levels of the degree programme and has commenced research in the arena of synthetic organic chemistry with the total synthesis of bioactive natural products and their analogues as specific aims.

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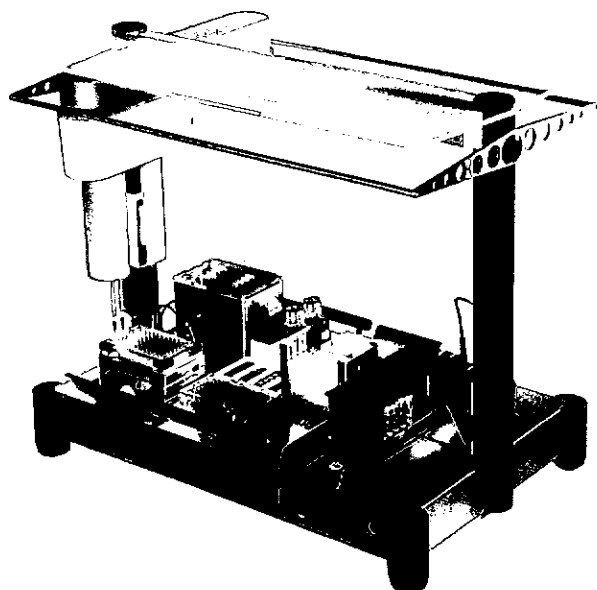
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Ai Scientific announces the release of the Markes range of manual and automated thermal desorption (TD) systems for pumped/diffusive sorbent tubes and canisters or on-line gas/air streams. This innovative range of products has recently been enhanced by the introduction of an electronic mass flow control (MFC) accessory for the split vent. In compliance with key standard methods such as US EPA TO-17 and ISO 16017, Markes thermal desorbers incorporate the option to split the sample both before and/or after the focusing trap such that samples ranging in concentration from high ppm to low ppt may all be quantitatively analysed. The split may also be used while the system is in standby (to minimise air/water background) and during pre-tube desorption purge stages (to enhance the purge flow.) The new MFC Accessory allows independent selection and electronic control of the split flow at each stage of the TD process. This enhances the performance of TD methods by allowing the split flow to be independently optimised at each stage, for example, minimised during standby and increased during tube purge.

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SpotCheck Near-IR Portable Spectrometer

Ai Scientific announces the introduction of the Digilab SpotCheck NIR, a novel portable near-IR AOTF spectrometer for material identification and quality control applications.

The Spotcheck NIR is a compact, versatile, and rapid molecular detection and analysis system which supports customer needs for bringing molecular spectroscopy to the sample vs. the sample to a laboratory. This instrument, based on an acousto-optic tunable filter (AOTF), is about the size and weight of a video camera and is operated via a PC through a USB connection. This unique, patented device is all solid-state with no moving parts. It has been engineered for a wide variety of applications such as liquid fuel analysis, pharmaceutical analysis, and gas monitoring.

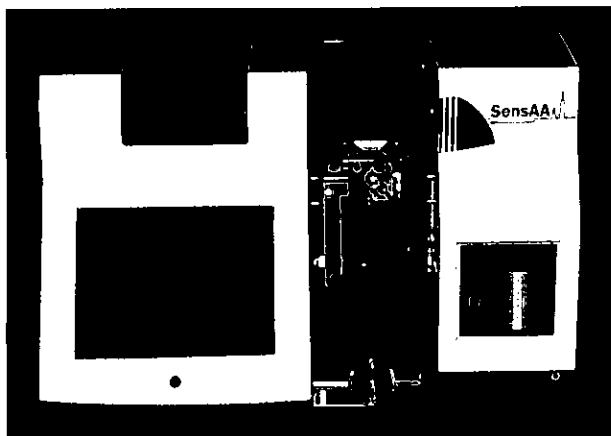
The Spotcheck NIR portable spectrometer will initially be focused on the unmet needs for cost effective, rapid analysis in plastics recycling. During the second half of 2004, the product capabilities will be extended to the identification and quantitative analysis of many other materials through integration with Digilab's Resolutions Pro Software Package.

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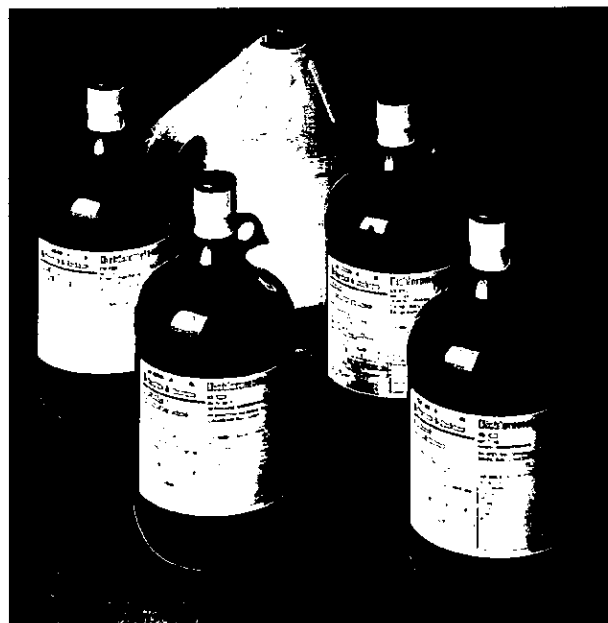


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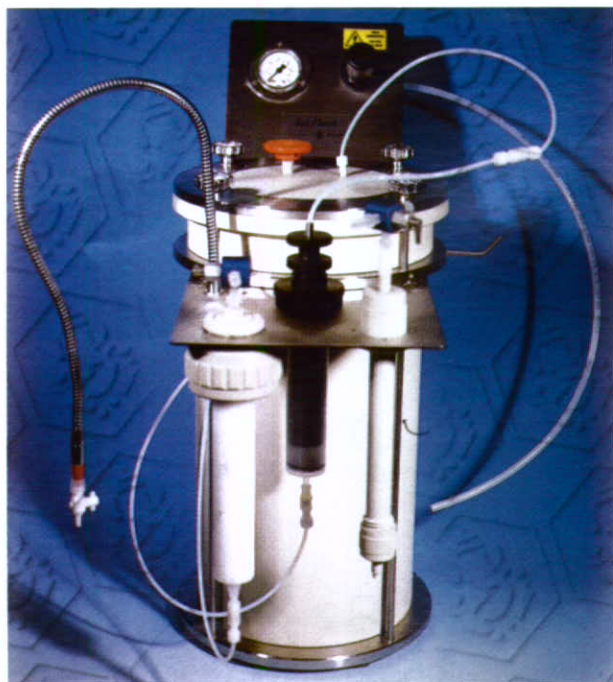
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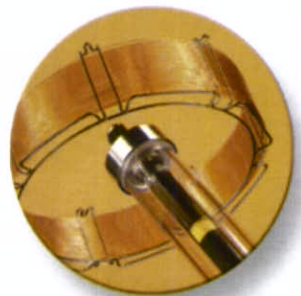


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For More Information on Chromatography Solutions

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