



Chemistry

IN NEW ZEALAND

ISSN 0110-5566

Opportunities For Chemical Research In The Roding Industry

**New Zealand
Pharmaceuticals Ltd:
Thirty Years On**

Chemistry at the Interface

Recollections of 'Paradise'

**Content, Concept, Context
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 by Sean Bearsley and Richard Haverkamp

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NZ Science Scene

HAZARDOUS SUBSTANCES STRATEGY REDUCES COSTS BUT MAINTAINS SAFETY

The Minister for the Environment Marian Hobbs has released a plan to reduce the cost of complying with hazardous substances legislation without compromising safety and the environment.

The hazardous substances part of the Hazardous Substances and New Organisms Act 1996 came into force in July 2001, replacing a variety of laws regulating dangerous chemicals, pesticides and toxic substances.

"The Act represented a new approach to regulating hazardous substances," says Ministry Senior Operator Kay Baxter. "Experience in the first two years of the Act's operation highlighted some areas where it was not working as well as it should. The Hazardous Substances Strategy released by the Minister at the end of June is designed to iron out those problems."

The main change sees the streamlining of the processes the Environmental Risk Management Authority (ERMA) (the agency that decides on applications to import, develop, or manufacture hazardous substances in New Zealand) uses for assessing low risk applications. As a result, the costs of approvals for low-risk applications will be cheaper, encouraging the development of newer, safer chemicals for the market.

The strategy also outlines measures to simplify the transfer of hazardous substances from controls under the old legislation to the HSNO regime and proposals for improving compliance with HSNO and strengthening enforcement of the Act.

ERMA's enforcement role will be strengthened and other changes to the Act will clarify the part played by territorial authorities and regional councils, in monitoring compliance with the law and in enforcement where there have been breaches.

In developing the strategy, consideration was given to the recommendations of the Agrichemical Trespass Ministerial Advisory Committee, released last year. The Committee's recommendation to monitor national agrichemical use is also being implemented by a HortResearch project funded by the Ministry's Sustainable Management Fund. The project will look at how pesticides (including insecticides, fungicides and herbicides) are being used in New Zealand and the impact they are having.

"The strategy has been welcomed by the people in industry who'll be using the improved HSNO regime," Baxter says. "We're grateful for the help they, as well as local government, have given us in putting the strategy together."

Some of the changes outlined in the Hazardous Substances Strategy have already been implemented, but those involving changes to the hazardous substance approval process will be the subject of a public discussion document due to be released in November.

The proposals are quite separate from amendments, currently before Parliament, to the way HSNO operates on new organisms, including genetically modified organisms.

Copies of the Hazardous Substances Strategy can be viewed on: www.mfe.govt.nz

Contact: Kay Baxter,
Phone: (04) 916 7653
Email: kaybaxter@mfe.govt.nz

PLASTICS INDUSTRY WORKS WITH ERMA TO DECLARE POLYMERS NON HAZARDOUS

The Environmental Risk Management Authority has determined that seven commonly used groups of plastics are not hazardous. The seven applications to determine if these groups of plastics were hazardous were submitted by Plastics New Zealand (Inc). These decisions mark the first stage of an initiative by the industry group to formally confirm that the main groups of polymers, commonly used by the plastics industry in New Zealand, are not hazardous and therefore not subject to the Hazardous Substances and New Organisms Act.

The Authority decisions are the result of an initiative by Plastics New Zealand to work with ERMA New Zealand to identify which polymer groups could be determined non-hazardous. Joanna Wojnar, an organic chemist, was contracted by Plastics New Zealand to carry out the research. ERMA New Zealand in turn contributed by waiving the cost of processing the applications.

The polymer groups determined as non-hazardous include certain fluoropolymers, polyethers, polyamides, polyesters, polyolefins, polycarbonates and vinyl polymers, in their pure state without additives.

Plastics New Zealand, an association of plastics manufacturers and plastics raw materials suppliers, has a total of 166 members, representing more than three-quarters of the plastics industry in New Zealand. This technical work has benefited not only the Plastics New Zealand members but the plastics industry nationwide.

Carolyn Cox, Manager for Environmental Affairs with Plastics

New Zealand said "The great news is that we have formal confirmation by ERMA New Zealand that the polymers we work with are not hazardous in their pure state. It's a win-win situation. For ERMA New Zealand having these polymers determined non hazardous means they do not need to be transferred as part of Notified Toxic substances. For the Plastics Industry, it demonstrates that we are able to comply with new legislation and we are pleased to be able to confirm to the public that the substances we work with are not hazardous."

MALAGHAN INSTITUTE FORMS PARTNERSHIP WITH VICTORIA

The Malaghan Institute of Medical Research has formed a partnership with Victoria University of Wellington. The Institute will move from its rented premises at Wellington Hospital in Newtown early next year to Victoria's Kelburn campus, where it will be housed in a specially refurbished building.

The Malaghan Institute is the only independent biomedical research facility in New Zealand. Its scientists are investigating the nature, origin and causes of cancer, asthma, multiple sclerosis and infectious diseases.

Malaghan Director of Research, Professor Graham Le Gros, said, "The Malaghan has grown substantially in recent years. The breadth of our research has widened, we've taken on new staff and postgraduate students and we've bought a host of highly specialised equipment that is vital to our work. We have simply outgrown the space and we felt it was vital that we gained a new and permanent home."

Victoria University Vice-Chancellor Professor Stuart McCutcheon said the Malaghan's choice of Victoria as its new home reflected the University's growing strength in biomedical research.

"Three years ago, Victoria took the bold step of establishing unique degrees in biomedical science to

provide a link between learning in the fundamentals of modern molecular and cell biology and the clinical practices of health services. The Bachelor of Biomedical Science programme, which had its first graduates last year, provides majors in human genetics, molecular pathology, and molecular pharmacology and medicinal chemistry - all areas that are the focus of research by the Malaghan," he said.

OTAGO AWARDS RESEARCH MEDALS

The University of Otago's top research award has gone to geologist Professor Rick Sibson FRS FRSNZ and preventive medicine expert Professor David Skegg FRSNZ. Both will receive the University's Distinguished Research Medal, which comes with a \$10,000 grant for personal scholarly development.

A leading epidemiologist, Professor Skegg is the University's head of preventive and social medicine and has been prominent in expanding knowledge and raising awareness about breast and cervical cancer, HIV, and the safety of contraceptives. Leading Earth scientist, Professor Sibson, is at the forefront of earthquake science with his work on fault processes and earthquake mechanics.

UPDATE ON EUROPEAN INITIATIVES AND OPPORTUNITIES

The major focus of the following actions is to enhance New Zealand researcher engagement with the 6th Framework Programme (FP6) operated by the European Commission's Research Directorate-General (RDG). These are based on suggestions made by the delegation whose visit coincided with the Minister in early June 2003. Other initiatives were driven from the Minister's report to Cabinet, suggestions made by the NZ Embassy in Brussels and activities arising from

the Ministry of Research, Science and Technology's (MoRST) global links strategy.

FP6 Opportunities

Project Funding bid evaluator - RDG officials promoted this as the best mechanism for New Zealand researchers wishing to identify European strengths in their fields of expertise. So far MoRST, working with the Royal Society of New Zealand (RSNZ) and the Marsden Fund Council (MFC), has written to all Marsden Fund Principal Investigators inviting them to register, through the MFC, as evaluators. However, this is an opportunity for all New Zealand researchers.

Further information can be found at <https://emmfp6.cordis.lu/index.cfm?fuseaction=wel.welcome>

The most effective way of becoming involved with a FP6 project will be by working together with established collaborators in EU-member States, or with EU Candidate-country partners. Information on current and upcoming Calls for Proposals are available at <http://fp6.cordis.lu/fp6/home.cfm>

FP6 usually funds no more than 50% of a project's costs, so New Zealand researchers would be expected to contribute their own funding for the activity. As there is no New Zealand research funding dedicated to EU projects, this will have to be found from mainstream (PGS&T, Marsden Fund, University etc.) sources.

Marie Curie Actions

Marie Curie actions on mobility, training, knowledge transfer and excellence. Further information on Marie Curie fellowships can be found at <http://www.cordis.lu/fp6/mobility.htm> or <http://europa.eu.int/mariecurie-actions>

Erasmus World Programme

The Erasmus World Programme seeks to enhance the quality and reinforce the European dimension of higher education, by encouraging transnational cooperation between higher education institutions). This is another opportunity, particularly for New Zealand universities and polytechnics, to strengthen bilateral

relationships, principally through student exchanges, with European partners.

For more information on the Erasmus world programme visit: http://europa.eu.int/comm/education/world/index_en.html

MoRST-Driven Activities

MoRST intends to facilitate and financially support (through the International S&T Linkages [ISAT]) Fund, a delegation of leading New Zealand researchers to the Joint Research Centre facilities at ISPRA, in Northern Italy. This may be able to coincide with a visit by Ambassador Julie McKenzie from the Rome Post. This is most likely to take place sometime in the new year. Researchers interested in participating in this Delegation should be nominated by their Institution, no later than 30 September 2003.

Contact: Rick Petersen
Email: Rick.Petersen@morst.govt.nz

They will also arrange (via the Embassy and the RDG) for key researchers and/or research managers visiting Europe in the next six months to make calls on appropriate contacts in the RDG. Research providers should identify potential visitors to Rick Petersen.

Forum for European-Australian Science and Technology (FEAST) Cooperation

MoRST will ensure strong New Zealand participation in the upcoming Forum for European-Australian Science and Technology Cooperation (FEAST) meeting to be held on 13-14 November 2003 in Canberra. They aim to use the ISAT Fund to support participation by New Zealand researchers. Research providers should identify potential participants to Rick Petersen by 30 September. A New Zealand chapter of FEAST is being investigated.

European Organisation for Nuclear Research Agency

MoRST has recently agreed to have a Memorandum of Understanding with the European Organisation for Nuclear

Research Agency (CERN) through which New Zealand researchers will be able to participate in CERN projects. They expect the New Zealand Ambassador to Germany (who is accredited to Switzerland), to formally mark the signing of the MoU in a visit to Geneva in October.

Science and Technology Counsellor

The culmination of the campaign is the establishment of the position of Science and Technology Counsellor based in the New Zealand Embassy in Brussels. MoRST is working with the Ministry of Foreign Affairs & Trade (MFAT) towards finalising the scope, functional relationships, etc. They anticipate advertising the position by 30 September, selecting a preferred candidate before Christmas with the successful candidate taking up the role by 31 March 2004.

EU Member State Initiatives

MoRST-funded bilateral initiatives for Germany, France and the UK will also maintain a positive European profile for New Zealand RS&T. These initiatives include:

- the introduction of the von Haast German research fellowships which is a counterpart programme to the prestigious Alexander von Humboldt Fellowship programmes. Applications will be called for by September 30 and MoRST hopes that the first Von Haast Fellow will be announced in February 2004 at the Australasian von Humboldt Fellows' meeting).

- Dr Werner Friedrich, New Zealand Co-ordinator of the New Zealand-German Science & Technology Co-operation Agreement, will host in mid-September, a visit to New Zealand by Dr Matthias Hack (the German Science Ministry's Group manager of the International Bureau).

Further information on German links (including other upcoming visitors) can be obtained from Dr Friedrich at german.coordinator@morst.govt.nz

- Utilising the ISAT Distinguished Visitors' programme to bring key British science figures to New Zealand over the next nine months.

If you identify any opportunities for the UK distinguished visitor programme, contact: Felicity Merrington
Email: felicity.merrington@morst.govt.nz

UNIVERSITY OF MASSEY-LINCOLN ALIGNMENT TALKS AT CONCEPT STAGE ONLY

Massey and Lincoln Universities have moved to end "unnecessary public confusion" about an alignment between them recently, by jointly releasing a discussion paper outlining the rationale and benefits they see in collaborating in specific areas. Meetings last year led to a successful bid for Centre for Research Excellence funding. But, says Lincoln University Vice-Chancellor Dr Frank Wood, "nothing further has been formalised and merger is not part of the agenda." He says, however, that it makes considerable sense for the two organisations, with complementary skills and common client bases, to engage in dialogue aimed at enhancing each others' abilities and services to key sectors.

Meanwhile AUT has decided not to proceed with merger discussions with Waikato University.

\$300 MILLION ALLOCATED TO SUSTAIN NEW ZEALAND'S PRODUCTIVE FUTURE

New research projects that will ensure New Zealand's rural and urban areas prosper without damaging the environment have been allocated \$57 million per annum (more than \$300 million in total funding over the projects duration) from the Foundation for Research, Science and Technology.

The results of the 2002/03 sustainable development investment process were announced recently and the Foundation has now entered into the contracting process with the successful programmes.

The Foundation concentrated funding on its priority research areas, set after wide consultation with stakeholders such as researchers, local and central government, and industry. Priority research included water resource management, enhancing land production systems without compromising environmental health, understanding the human and social aspects of sustainability, and the development of sustainable cities.

This year there has also been a substantial increase in biosecurity research funded, from \$0.8 million per annum in 2001/02 to \$4.7 million per annum. In addition, a new initiative in the sustainable cities area saw \$1.5 million per annum allocated to programmes that will minimise the impacts of urban development by identifying low-impact designs. The focus will be on Auckland though the results will be applicable to other urban centres.

INTERNATIONAL METEOROLOGICAL ORGANISATION

Nominations for the forty-ninth awarding of the International Meteorological Organisation (IMO) Prize are now being called for. The prize is awarded annually to individuals for outstanding work in the field of meteorology or in any other field referred to in Article 2 of the World Meteorological Organisation (WMO) Convention. In choosing the recipient, the factors taken into consideration are the scientific value of the work accomplished and the services rendered at the international level.

Nominations must be received by 7 June 2004 to:

Secretary-General
World Meteorological Organization
P O Box 2300
1211 Geneva 2
Switzerland

For nomination forms contact:
Information and Public Affairs,
Office World Meteorological
Organisation
Email: ipa@gateway.wmo.ch

EXPLOSIVES START FOR HSNO

Explosives are now regulated by the Hazardous Substances and New Organisms (HSNO) Act 1996, as of the transfer date on the 28 August 2003.

Explosives are the first group of hazardous substances to be transferred to the HSNO regime since the hazardous substances part of the Act commenced in July 2001. The explosives group includes retail fireworks, display pyrotechnics, ammunition, flares and blasting explosives.

Chair of the Environmental Risk Management Authority, Mr Neil Walter said, "The implication of this transfer for explosives users will mean a continuation of effective risk management of these substances with a few minor changes. If you look at retail fireworks as an example, shops may display retail fireworks in the same way as they have done under previous law. Only now if you are handling a very large quantity of fireworks, that is more than 500 kg of retail fireworks, then you will need to ensure there is someone who is an Approved Handler to be present. If you are storing over 10,000 kg of fireworks, you need proper test certificates for location storage."

The new regulations giving effect to the transfer of explosives from the transitional parts of the HSNO Act (Part XV) to new controls under HSNO have been released by the Government. The transitional provisions of the HSNO Act for explosives ceased from 28 August 2003. The new and amended regulations for handling explosives and other hazardous substances that make the controls more workable are listed as follows:

They are:

- No. 2003/176 The Hazardous Substances (Fireworks, Safety Ammunition, and Other Explosives Transfer) Regulations 2003.
- No. 2003/177 Hazardous Substances (Classes 1 to 5 Controls) Amendment

Regulations 2003.

- No. 2003/178 Hazardous Substances (Classes 6, 8 and 9 Controls) Amendment Regulations 2003.
- No. 2003/179 Hazardous Substances (Fireworks) Amendment Regulations 2003.
- No. 2003/180 Hazardous Substances (Identification) Amendment Regulations 2003.
- No. 2003/181 Hazardous Substances (Packaging) Amendment Regulation 2003.
- No. 2003/182 Hazardous Substances (Disposal) Amendment Regulations 2003.
- No. 2003/183 Hazardous Substances (Emergency Management) Amendment Regulations 2003.
- No. 2003/184 Hazardous Substances (Tracking) Amendment Regulations 2003.
- No. 2003/185 Hazardous Substances and New Organisms (Personnel Qualifications) Amendment Regulations 2003.

Copies of these Regulations are available for sale from Bennetts Bookshops and will be available shortly at: www.legislation.govt.nz/

VICTORIA UNIVERSITY APPOINTS FOUR PERSONAL CHAIRS

Four distinguished scholars have demonstrated their high international esteem and have been appointed as Professors at Victoria University of Wellington. The appointments, which take place every two years, are a recognition of the international distinction of the Professors in their particular research fields and their meritorious performance in teaching, and other service to the University.

"Appointment to a Personal Chair is not part of the regular promotions process," said Vice-Chancellor Professor Stuart McCutcheon. "It is intended as a special recognition of outstanding scholarly achievement together with meritorious performance in teaching, research and other service to the University."

International referees make submission on the candidate's professional contribution to their respective discipline and comment on the regard with which they are held by their colleagues internationally.

"Distinguished service to the wider intellectual community or relevant profession is also taken into account. In each of 1999 and 2001, three appointments were made. This year four new Professors were appointed," said Professor McCutcheon.

Robert Easting

School of English, Film, & Theatre

A scholar in Medieval English Studies, Robert has been part of the Victoria University community since 1973. He has achieved international recognition for books published by Oxford University Press, Oxford, and by Brewer, Cambridge, including scholarly editions of texts in Middle English and Medieval Latin published for The Early English Text Society. In 1997 he received a Victoria University of Wellington Award for Excellence in Teaching and Research. Robert has taken on many administrative responsibilities at School, Faculty, and University level including his current role as Convenor of the Scholarships Committee.

Jim Johnston

School of Chemical & Physical Sciences

A graduate of Victoria University of Wellington, Jim is an internationally recognised research scientist in the areas of materials science, industrial chemistry and geochemistry. He is a Fellow of the Royal Society of New Zealand, a Fellow of the New Zealand Institute of Chemistry, and recipient of the RSNZ's Thomson Medal for Outstanding Contributions in the Fields of the Organisation, Administration or Application of Science and Technology. Jim has worked at Victoria University since 1975. During that time, he has carried out a range of activities with private sector agencies concerned with the development of new technology platforms and high performance products and is also a principal investigator with the MacDiarmid Institute for Advanced Materials and Nanotechnology. He has taken on significant administrative

responsibilities including as Head of School, Deputy Dean of Science, and Acting Pro Vice-Chancellor.

Stephen Levine

School of History, Philosophy, Political Science & International Relations

A specialist in comparative politics and international relations, Stephen's principal areas of research and publishing activity have been in the areas of human rights, constitutional change, electoral systems and voting behaviour. He has worked at Victoria University since 1972 and has been a Head of School from 1995-1998 and is currently Head of School. He is the author and editor of many publications and in 1997 was joint recipient of a Victoria University of Wellington Award for Special Academic Achievement in Research, and of a Wallace Award from the New Zealand Electoral Commission for 'the best academic paper, monograph or book on New Zealand electoral matters published within the previous year.' From 1995 to 2003 he served as Director of the publicly funded New Zealand Political Change Project, examining the impact of MMP on New Zealand's government and politics.

John Pratt

School of Social & Cultural Studies

A criminologist specialising in the history and sociology of punishment, and criminological and social theory, John has been with Victoria University's Institute of Criminology since 1988, where he was Acting Director for a 12-month period in 1999/2000. He has been editor of the *Australian and New Zealand Journal of Criminology* since 1997 and been a member of the editorial boards of other international journals. In 2000 and 2002 he received a Victoria University of Wellington Award for Excellence in Teaching and Research. He received a Canadian Studies Award in 1993 and a Marsden Award in 1997. He has regularly been invited to lecture on his work at prestigious overseas universities and to international conferences. His extensive publication record includes *Punishment in a Perfect Society* (1992), *Governing the Dangerous* (1997), and *Punishment and Civilization* (2002).

MARSDEN FUNDING ANNOUNCED

\$43.8 million dollars has been allocated to original and exciting research in this year's Marsden Fund round.

For the first time ever, funding for an iwi-based collaborative research project has been granted by the Fund. This proposal, which had to undergo rigorous evaluation, could provide a new model for the development of further such partnerships in other areas of the country. This project, initiated by Ngati Hine, will trace the history of pre-treaty Bay of Islands by synthesising European and Maori collective histories. "This exemplifies the ground-breaking work that the Marsden Fund is associated with," said Dr Diana Hill, Chair of the Marsden Fund Council.

"This year, \$43.8 million was granted to support 105 projects over three years, 19 more than last year. This represents 14.2% of all applications, an increase from 10.7% last year. This increase is due to an extra \$1.95 million from the 2003 budget and the remainder came from the Royal Society reserves," said Dr Hill. This is also the first time that funding for five years - long term support that will allow greater research continuity - has been offered. Three projects have been selected for this longer term funding.

"This year an unprecedented amount - \$2.7 million - has gone to emerging researchers of outstanding potential," added Professor Hill. The Fast-Start Marsden grants, first funded in 2001, give \$50,000 each year for up to two years.

The 28 Fast-Start projects for 2003 include Massey University's Dr Chris Wilkins' study of the role gangs play in the illicit markets for cannabis, amphetamine and ecstasy and Dr Christine Cheyne's work on New Zealander's interactions - or lack thereof - with local government.

A complete list of the 105 grants, including the name of the principal investigator, and the institution, is on the Royal Society website at <http://www.rsnz.org>

NEW WEBSITE TAKES AIM AT PROLIFERATION OF QUALIFICATIONS

A new website containing details of over 5000 qualifications makes a strong case for rationalising the number of courses available for study in New Zealand, says Associate Education (Tertiary Education) Minister Steve Maharey. <http://www.kiwiquals.govt.nz> has been launched at Parliament. It enables users to find and compare on the one site all quality assured qualifications available in this country. It currently covers more than 5000 qualifications offered by more than 1000 providers.

"I MET A TRAVELLER FROM AN ANTIQUE LAND": GENETICS AS HISTORY

Best-selling author Professor Bryan Sykes, from the University of Oxford, will be touring New Zealand giving public lectures in October and November.

Professor Sykes is The University of Auckland Sir Douglas Robb lecturer for 2003. The Royal Society of New Zealand, in partnership with the British High Commission and British Council New Zealand, is hosting additional lectures in Dunedin (with UNESCO), Christchurch, Nelson, Wellington and Palmerston North as part of the celebrations of the 50th anniversary of the discovery of the structure of DNA.

The new science of molecular genetics has transformed the way we view our past and has demolished any scientific basis for racism. The study of maternally inherited mitochondrial DNA has given us powerful new evidence about colonisation of the Pacific and the way in which *Homo sapiens* first settled Europe. It has solved issues that have perplexed scholars for centuries.

Professor Sykes is known around the world as the best-selling author of "The Seven Daughters of Eve" in which he traces the descent of Europeans to seven women who lived tens of thousands of years ago. He is the Founder and Chairman of Oxford Ancestors and is a Professor of Human Genetics at the University of Oxford. It is for his work in the field of mitochondrial DNA and Y chromosome analysis that he is most famous. His new book, "Adam's Curse", traces human descent through the paternal line looking at the Y chromosome and discovers that men are doomed to extinction.

His lectures dates are listed below.
Tickets from sykesdunedin@rsnz.org

Dunedin
UNESCO SCIENCE LECTURE
5.30 p.m. Thursday 23 October
St David Lecture Theatre
University of Otago
Cumberland Street

Christchurch
8.00 p.m. Thursday 6 November
A1 Lecture Theatre, University of
Canterbury
Entrance off Creyke Road

Nelson
7.30 p.m. Tuesday 11 November
Nelson School of Music
48 Nile Street

Wellington
7.00 p.m. Monday 17 November
Soundings Theatre, Te Papa

Palmerston North
Allan Wilson Centre Lecture Series
5.30 p.m., refreshments served from
5.00 p.m.
Tuesday 18 November
Japanese Lecture Theatre, Massey
University

2003 NEW ZEALAND SCIENCE & TECHNOLOGY MEDALLISTS

The Royal Society's New Zealand Science & Technology Medals Committee has awarded medals to the following recipients:

New Zealand Science & Technology Silver Medals

Dr Roger Cooper
Institute of Geological and Nuclear Sciences. For his exceptional contribution to the structure and origins of New Zealand's oldest rocks.

Professor Geoffrey Duffy
Department of Chemical and Materials Engineering, The University of Auckland. For his exceptional contribution to industry and the community over more than three decades in the field of fluid mechanics of fibre suspensions.

New Zealand Science & Technology Bronze Medals

Associate Professor John Ayers
Institute of Fundamental Sciences, Massey University. For his significant contribution to the development of novel cellulose-based ion exchangers that have led to the incorporation of new processes in the dairy industry, and innovative quality products being produced for the export market.

Professor Jeffery Hunter
Institute of Information and Mathematical Sciences, Massey University. For his significant contribution over an extended period to the public understanding of the role and importance that the mathematical and information sciences play in all spheres of the community including business and industry.

Dr Simon Nathan
Geological Society of New Zealand. For his significant contribution to geology in New Zealand.

Mr John Parkes
Landcare Research New Zealand Ltd. For his significant contribution to the application of research, particularly experimental research, to vertebrate pest management.

Dr John Quinn
National Institute of Water and Atmospheric Research Ltd. For his significant contribution to river ecosystem research.

These medals will be presented at relevant local functions around the country within the next 6 months.

Opportunities For Chemical Research In The Roding Industry

Sean Bearsley^a and Richard Haverkamp^b

^a Higgins Contractors Ltd, Palmerston North

^b Institute of Technology and Engineering, Massey University, Palmerston North

Introduction

The best roads are those you don't notice. A smooth driving surface is ideal for transit in terms of comfort, economy, and safety and it is the chemist that is helping the civil engineer achieve this. Although road construction has long been dominated by civil engineers the role of the chemist is becoming increasingly important. Through the design of improved paving materials, chemists are active in the construction of more durable, longer lasting bituminous pavements.

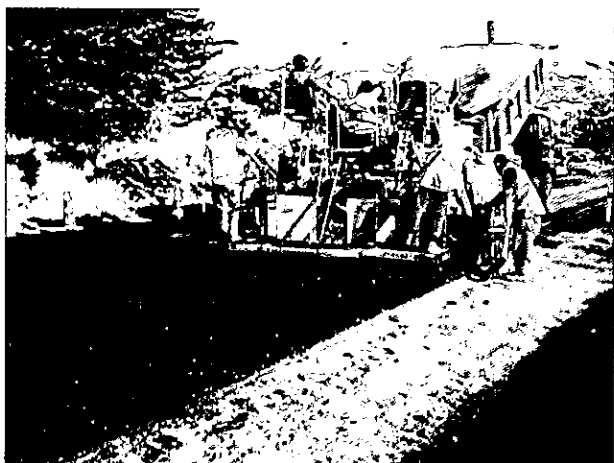


Figure 1: Construction of an asphalt surface on the Wellington Motorway near Porirua in 1999.

The vast majority of pavements in New Zealand use bitumen to bind mineral aggregates together to form a durable driving surface, either as asphalt or chipseal. Most bitumen is obtained as the residue from the vacuum distillation of crude oil although it also occurs naturally as mineral deposits in various forms. Perhaps the most well known deposit is the Trinidad Lakes on the island of Trinidad in the Caribbean.¹ Other commercially significant deposits are the Bermudez Lake in Venezuela and the tar sand deposits throughout Canada. Rock asphalt is mined throughout France, Switzerland, and Italy. Natural bitumen is also mined as the harder, friable minerals called Gilsonite (in Utah) and Manjak (in Barbados).

When considering its varied historical resumé, the use of bitumen for road construction is a relatively new field. The ancient Sumerians are believed to have used natural bitumen for caulking ships around 6000 BC. Bitumen was used as an adhesive and waterproofing agent around 3000 BC during the construction of a water tank at Mohenjo Daro in modern day Pakistan. The ancient Egyptians are known to have used bitumen (presumably from the Dead Sea) during the mummification process around 1200 BC (Figure 2). Natural bitumen was also used around 600

BC, as a grout for stone paving and as a waterproofing agent during the construction of King Nebuchadnezzar's palace at Babylon. In 1595, Sir Walter Raleigh used bitumen as a caulking agent for ships and during the 1800s it was also used as a pigment by artists and as part of a photographic process.¹



Figure 2: Egyptian mummy preserved using bitumen - see reference 1.

Bitumen Chemistry

Bitumen is a black or dark coloured semi-solid material that displays viscoelastic properties. It is resistant to chemical and biological degradation and has excellent waterproofing and adhesive properties. It is not a homogenous material as it contains colloidal-sized regions that are either structured or amorphous in character. It is not a polymer although it displays polymeric properties. It is not an oil although it is derived from crude petroleum oil and has attributes of an oil. It is not a resin, yet it possesses resinous properties.

No one has been able to definitively define bitumen chemically. Its composition can vary depending upon the crude oil source, the production route, and the location within the oil field. Bitumen is a complex mixture of aromatic and aliphatic, linear, branched and cyclic hydrocarbon molecules. The presence of nitrogen, oxygen,

and sulfur atoms in the bitumen molecules imparts polarity and has a substantial impact upon the visco-elastic properties. A typical elemental composition of bitumen is given in Table 1. However, an elemental analysis yields very little in the way of useful information about the expected performance properties of the bitumen. It is the arrangement of the elements and the molecular interactions between functional groups that determines performance. Knowledge of the fractional and chemical composition of bitumen can aid the bitumen chemist in understanding the performance of bitumen in terms of physical properties, ageing resistance, adhesive properties, compatibility with polymers, and suitability for emulsification.

Element	Typical Proportion
C	81 - 86 %
H	9 - 11 %
N	0.1 - 1.2 %
S	1.0 - 7.0 %
O	0.1 - 1.2 %
V	30 - 1500 ppm
Ni	10 - 200 ppm

Table 1: Typical elemental composition of bitumen taken from references 1 and 2.

Bitumen contains a wide array of functional groups (Chart 1). However, it is interesting to note that common functionality such as amino, ester, and alkene is not generally found in bitumen. Various metallic elements have been detected in bitumen, including vanadium and nickel. Metals may be present in colloidal form or as the salt of a carboxylic acid, a transition metal complex or a porphyrin array,¹ and are thought to be originally from the degradation of porphyrin-type molecules of biological origin, *e.g.* Mg from chlorophyll.

Bitumen can be fractionated into four types of compounds based upon molecular weight and polarity, namely asphaltenes, resins, aromatics, and saturates. The asphaltenes are highly polar and are composed of condensed aromatic ring structures. The individual molecules typically are less than 1000 g/mol in weight, but they can associate into micellar structures with a molecular weight in excess of 100,000 g/mol. The asphaltenes form the dispersed phase in the bitumen and are 'peptised' by the resin molecules. The majority of the nitrogen, oxygen and sulfur atoms are contained in the asphaltene and resin fractions, although sulfur is also found to a lesser extent in the aromatic and saturate fractions. Resins are polar, aromatic molecules that are thought to orient at the interface between the dispersed asphaltene fraction and the continuous aromatic and saturate fraction. The aromatic fraction may be slightly polar and is characterised by the presence of mono and fused aromatic

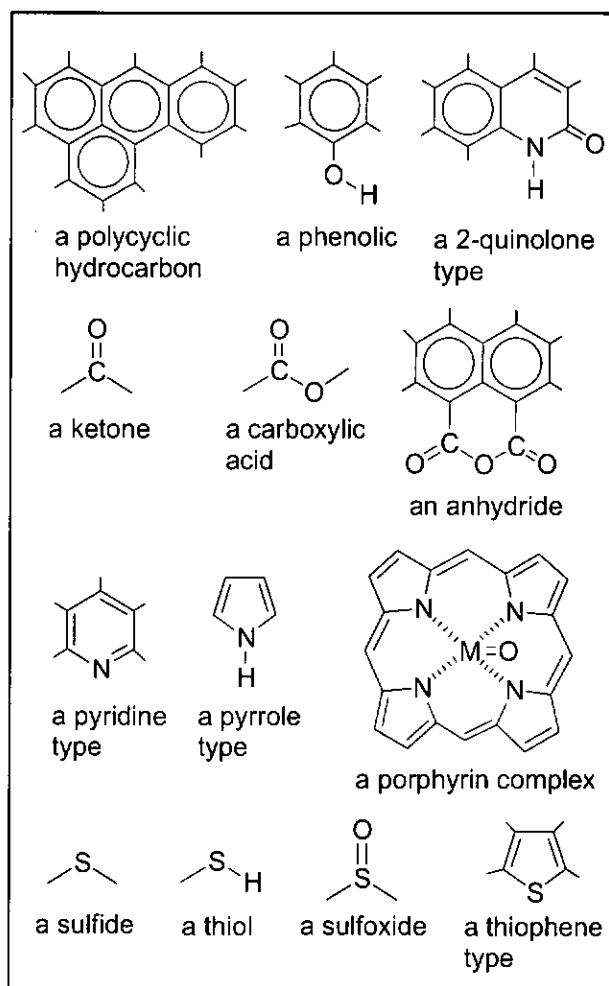


Chart 1: Functional groups found in bitumen - see references 2 and 3.

rings. It is a solvent for the asphaltene phase. Saturates are non-polar and are aliphatic in nature, are not miscible with the asphaltenes, and tend to flocculate the asphaltenes. They act as plasticisers in the bitumen and impart viscous flow properties.¹⁻³

Current challenges

The increased mass and volume of modern traffic has placed increased demands on the roading network. Consequently, various unique challenges have presented themselves for the chemist, most of which relate to the durability of bituminous pavements. Chemists can find employment in examining the following aspects of pavement construction using bituminous materials:

- Oxidation and durability of bitumen.
- Adhesive processes.
- Emulsification.
- Polymer modification.
- Recycling and environmental awareness.

Oxidation and Durability

Exposure of the bitumen to the effects of air, weather, and sunlight during its service life results in oxidation of the bitumen. Oxidation causes the bitumen to harden and eventually crack due to fatigue failure, which leads to a rapid deterioration in road quality. Research aimed at understanding the mechanism of oxidation and ways to

improve the durability of bituminous pavements has been undertaken in most developed countries including New Zealand.⁴

Atmospheric oxygen reacts with bitumen to form carbonyl and sulfoxide groups. The net effect is an increase in polarity and consequently an increase in interaction potential between molecules. Oxidation manifests itself as an increase in viscosity and modulus of the bitumen. Sulfoxides are formed by the oxidation of aliphatic and alicyclic sulfides. It is interesting to note that thiophenic and aryl sulfides appear resistant to oxidation. Carbonyl groups form by the reaction of molecular oxygen with saturated carbon atoms adjacent (or α) to benzylic structures.⁵ Oxidation also produces minor amounts of carboxylic acids and anhydrides. Despite an overwhelming body of literature, and although various theories have been postulated, the exact mechanism of oxidation is still speculative.

Adhesion

One of the major failure modes in bituminous pavements is lack of adhesion between the bitumen and mineral aggregate, which leads to a deterioration of the pavement surface. Adhesion agents are routinely added to bitumen in New Zealand to prevent adhesive failures in chipseals. The adhesion agents are based in alkylamine chemistry and have a surface-active role. In the presence of water the adhesion agent develops a slight positive charge while the mineral aggregate develops a negative charge. Consequently, an electrostatic attraction takes place that promotes wetting of the aggregate by the bitumen film in the presence of water (Figure 3). Previous research has shown that adhesion is enhanced by the presence of nitrogen-containing functional groups in the bitumen molecules.⁶ The nitrogen-based functional groups display tenacious adsorption to mineral aggregates and are resistant to displacement by water.

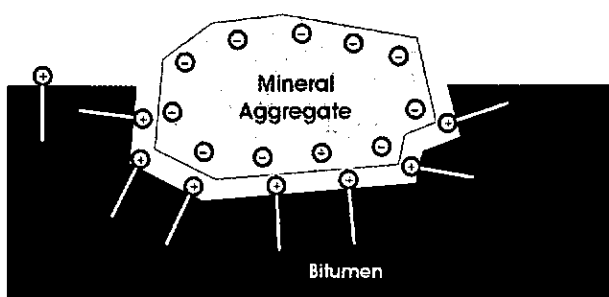


Figure 3: Orientation of adhesion agent molecules at interface between bitumen and mineral aggregate.

Polymer Modified Bitumen

Although bitumen displays excellent engineering properties at ambient temperature, it is at the extremes of its service temperature range that it tends to fail. Bituminous pavements can experience sub-zero temperatures in winter and temperatures approaching 60 °C in summer. At cold temperatures bitumen tends to become brittle and may crack, allowing the ingress of water and subsequent pothole

formation. High temperatures cause the bitumen to become too soft and may lead to the formation of flushed, bitumen rich surfaces that present a serious skid resistance hazard. Polymer modification of the bitumen can overcome these deficiencies by imparting both flexibility during cold weather and stiffness during hot weather. The end result is an extension of the service temperature range of the bitumen in much the same way that polymeric additives improve the flow properties of motor oils at temperature extremes. Obviously, the choice of polymer has a huge impact upon performance, but performance is also determined by the way in which the polymer interacts with the bitumen. A role of the chemist is to explore and improve the compatibility between the polymers and the bitumen.

Two classes of polymer are generally used for bitumen modification, plastomers and elastomers. Plastomeric types of modifiers include ethylene vinyl acetate (EVA), ethylene methacrylate (EMA), and polyethylene (PE). However, the most popular polymers for modifying bitumen in New Zealand are the group of thermoplastic elastomers known as styrene-butadiene-styrene (SBS) block co-polymers (Figure 4). These materials are blended with bitumen in a high shear process at 180–190 °C and the dispersion in bitumen is easily observed using fluorescent microscopy (Figure 5). The polymer does not completely dissolve in the bitumen but rather is dispersed to form a two-phase heterogeneous system.

Emulsions

The application of bitumen in an emulsified form is preferable in terms of safety and environmental considerations, and can be beneficial especially in the area of ensuring good adhesion to the aggregate. However, the formulation of quality bituminous emulsions is a rather complex process and it benefits from an understanding of the chemical processes involved. Bituminous emulsions are micron-sized dispersions of between 55 and 80% bitumen stabilised by emulsifying agents in an aqueous phase (Figure 6).



Figure 4: Spraying polymer modified bitumen on Carnegie Street in Napier.

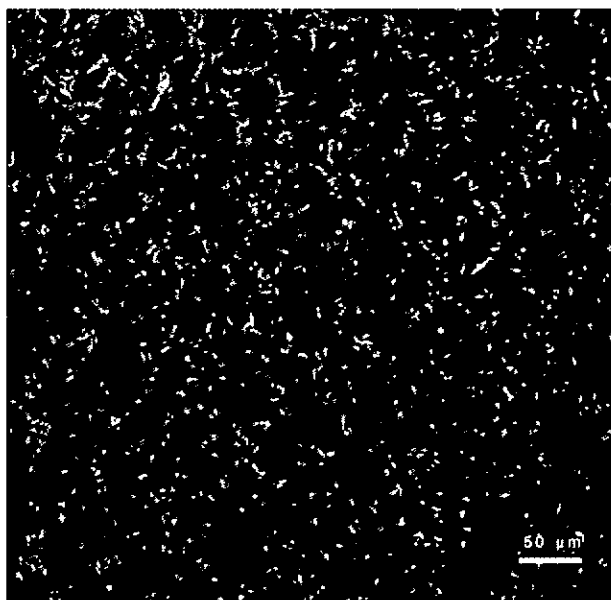


Figure 5: Fluorescence image of polymer-modified bitumen showing the light coloured fluorescing polymer dispersed throughout the bitumen matrix.

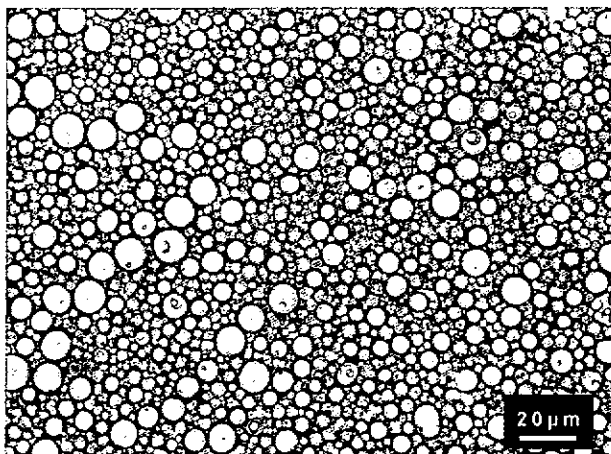


Figure 6: Optical microphotograph of a bituminous emulsion.

To be useful practically bitumen emulsions must remain stable for up to several weeks and even months during storage, transport, and pumping, but then quickly destabilise and coalesce as soon as they are applied during pavement construction. This *Jeckyl and Hyde* behaviour is achievable through the use of ionic emulsifiers. Cationic emulsifiers are the most popular in New Zealand because of their suitability for use with the types of aggregates that are available. They are based on alkylamine chemistry and are similar to the adhesion agents mentioned previously. The majority of aggregates used in New Zealand for road construction are greywacke, andesite, or basalt. Because of the presence of silica in these mineral aggregates a slight negative charge develops on the aggregate surface in the presence of water. Cationic emulsifiers confer a positive charge to the bitumen droplets. Consequently, when bituminous emulsion is brought into contact with mineral aggregate an electrostatic attraction takes place. This results in the separation of the bitumen and water phases and is referred to as 'breaking' of the emulsion.

Bitumen emulsions can be further classified according to their stability in the presence of mineral aggregate. The

choice and quantity of emulsifier and the pH of the system are prime determinants of how quickly the 'breaking' reaction takes place. The role of the chemist is to ensure that the emulsion remains sufficiently stable during storage, transport, and handling, but breaks quickly once in contact with the mineral aggregate. Since both bitumen and mineral aggregate are naturally occurring materials, their chemical properties are sometimes quite variable and consequently, the chemist is shooting at an ever-moving target!

Recycling and Environmental Awareness

Heightened awareness of environmental considerations is slowly forcing construction companies to consider the use of recycled materials in road construction. All manner of industrial waste-products and by-products have been used in pavement construction including the likes of waste plastics, crumb rubber from recycled vehicle tyres, recycled glass fibre, cellulose fibre, fly ash, slag, and waste oils. Research conducted in Europe and the USA has shown that the addition of waste polymers such as polythene, polypropylene, and crumb rubber can improve the performance properties of the bitumen. Unfortunately, the economic and political climate in New Zealand does not always provide the impetus for the use of such waste materials in road construction; it is generally less expensive to use virgin materials for the modification of bitumen.

Summary

Various challenges currently present themselves to those involved in the chemical aspects of civil engineering. These challenges are likely to increase in number and complexity as the availability of natural resources diminishes, and the industry comes under increased environmental and political pressures such as increasing traffic demands and ratification of the Kyoto Protocol. Consequently, it is highly likely that chemists will continue to play a vital role in the construction of roads and pavement surfaces as the demand for better-performing, value-added materials increases.

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INVESTIGATION INTO HOW RESEARCH RESULTS ARE COMMUNICATED

An investigation into the ways in which the results of scientific research are made public was launched this month by the Royal Society (London), the UK national academy of sciences. It has been prompted by a number of controversies surrounding how and when scientists communicate their research results to the public, and whether scientists should check each other's work before it is published.

A working group, chaired by Professor Sir Patrick Bateson, Vice-President of the Royal Society, and including members from the fields of consumer affairs, journalism, scientific publishing, and academic and industrial science, has issued a call for evidence to encourage submissions by the end of September about the strengths and weaknesses of current practices by researchers in communicating their results, and possible alternatives.

The working group will consider criticisms of the process of peer review and examine ways in which it might be improved. It will also investigate whether there are any alternatives to peer review for checking the quality of research results.

Sir Patrick said: "Peer review has been criticised for being too secretive, conducted behind closed doors and assessed by anonymous referees. It has also been suggested that it provides a way in which the establishment can prevent unorthodox ideas, methods and views, regardless of their merit, from being made public. We want to see if any evidence supports such a claim."

MILLENNIUM TECHNOLOGY PRIZE

A new technology prize has been launched under the patronage of the President of Finland, Tarja Halonen. It will be awarded in recognition of outstanding technological achievements aimed at promoting sustainable development in society and quality of life, as well as of extensive international cooperation to promote these objectives. The prize will be awarded for proposed achievements in four fields of technology— energy and the environment; communication and information; new materials and processes; and health care and life sciences.

The Millennium Technology Prize is worth one million euros and is awarded once every two years. The winner or

winners shall be an individual or a group of persons, or a research team, provided that the candidates have worked on the proposed technological innovation in the above-mentioned disciplines within the past ten years. Citizens of all nations are eligible. The winner or winners will be selected by an international award selection committee. The prize was set up by science associations, the Foundation for Finnish Inventions, the Walter Ahlström Foundation and the Confederation of Finnish Industry and Employers. The Academy of Finland and the National Technology Agency Tekes have also contributed.

RESEARCH FUNDING TO BE SPREAD MORE WIDELY IN UK

The UK Financial Times reports that plans to focus state research funding on only a few top universities have been changed, with the Higher Education Funding Council for England (HEFCE) now set to reward 200 departments from about 40 universities at the top rating level, rather than 100 departments from only 29 universities as originally planned. The Government has denied that the changes imposed by HEFCE represent a climb-down from their stated policy aims of focussing research funding.

PROFESSOR MARK WARNER WINS AGILENT PRIZE

Professor Mark Warner, an Honorary Fellow of the Royal Society of New Zealand, has won the 2003 European Physical Society's premier Hewlett Packard/Agilent prize. Professor of Theoretical Physics at the University of Cambridge and a Fellow of Corpus Christi College, Mark was born and educated in New Zealand and maintains strong scientific and personal links here. He is one of the world's leading physicists working in the field of soft condensed matter and has developed the definitive theories on liquid crystalline and other ordered, non-linear elastomers.

MULTIPLE AUTHORS, MULTIPLE PROBLEMS

Last week's editorial in Science magazine discusses how the average number of authors per scientific paper continues to increase, partially as a result of efforts to foster "team science". The article notes the problems this can cause in cases of misconduct and in assessing individual publication records. It suggests that one solution would be for articles to include an account of each author's contribution to the research described.

Famous/Fatuous Failures

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When Brian Halton requested that I write an article, I remembered that as a postdoctoral I had been requested to write a reasonably amusing and informative piece, so I thought, why not recycle that well-known article from the February, 1969 edition of *J. Southampton Chemical Society*? The title was never intended to be accurate, but rather it reflected a 1968 frustration-fed fixation on the letter F. Unfortunately it was self-fulfilling: in my absence a proofreader decided Berthollet and Berthelot were one person, and perhaps, as in the Greek tragedies, I had gone too far. In any case, a rewrite and update was required.

Failure comes in many forms, sometimes disguised as success, and *vice versa*. As a warning for what follows, it can be a fatuous failure not to recognise success, so keep track of where you chuckle! Also, the degree of failure depends on stature, for there is no shortage of dross. Barely had *Annual Reports* begun than reporters complained of the impossible number of papers being put forward, many of them incomplete and seemingly more designed to establish an author's priority than to establish a fact. In 1914 the organic reporter went further, and bewailed the number of papers issuing statements subsequently shown to be wrong, and the reluctance of certain authors to retract preliminary publications later found by the author's continuing research to be erroneous. What changes?

Science began in ancient Greece. The first recorded scientist was Thales who, in 1000 BC concluded that biogenesis occurred in water, and that water is fundamental. He studied water, developed hydraulics, and showed relevance through winning a battle by diverting a river. Unfortunately, the word 'fundamental' started something amongst lesser souls. What does it mean? When contemplating this early science, we must make allowances for the lack of vocabulary. Homer may have been poetic when referring to *a sunset of blood*, but there was probably no word for *red*. What was the need? Why describe grass as green? What other sort is there? Chemistry changed this when at about 500 BC the dyeing industry began, and indeed we fail to recognize how many empirical chemical facts the ancients collected. However, they did not use IUPAC nomenclature; so beware.

Searches for the fundamental diverted down several paths. There were three schools debating which of three elements were fundamental: air, fire and water. There were also those who believed atoms were fundamental, and Democritus concluded that heat was nothing more than atoms in motion. Such atoms were eternal, with some, such as those making iron rougher than others such as the smooth atoms of water. Otherwise all were supposed to be alike, except in shape, order, and position. We still fail to recognize Democritus as the origin of the kinetic theory of heat.

With several theories in vogue, a great mind was required to unify them. Empedocles did just that. He agreed with

the atomists, and added his suggestion that there were qualitatively different atoms. He stated that nothing comes into being or is destroyed, but is merely transferred to a different form, effectively the law of conservation of mass. However, it was with the schools of *elementists* that Empedocles made his mark: he agreed with all three prevalent schools of thought as to the basic elements and he added a fourth – earth! These elements were subjected to two moving forces, love and hate. There were experimental procedures, thus react fire upon its contrary (sea)water, whereupon the water passes away and air and earth come into being. Empedocles was also responsible for another theory: the velocity of light was fundamental, it was finite, and it had a precise value. Needless to say, all attempts at the time to measure it failed, but it is to the credit of the experimenters that they acknowledged the problem and most did not fill journals with spurious values.

Every good theory deserves someone to impose unnecessary mathematical irrelevancies. Plato took Empedocles' elements, and noted that there were five *perfect* shapes: tetrahedron, cube, octahedron, dodecahedron, and icosahedron. It was *obvious* that the sharp points of the tetrahedron represented fire, the solidity of the cube represented earth, the slipperiness of water arose from an icosahedron, while air had to be the octahedron. This logic predicts a fifth element!

Aristotle was not particularly interested in chemistry, which may have impeded its development, but he rejected Democritus' atoms in favour of a substratum. He described a reaction in terms of the components passing away, and a new form of compound coming into being. It is unclear whether he thought in terms of conservation. To complicate the situation, Aristotle then added the fifth element, ether, which he declared was first in rank and pervaded the universe.

Lesser minds had to make their additions, and if one cannot go forward, one can formalize! To these five elements were added four qualities: hot, cold, dry, and wet, and four principles: matter, form, cause, and purpose. Thus matter is a passive principle that becomes reality through form! Is this the first floccinaucinihilipilification in chemistry? Certainly it is not the last.

It would be a failure not to redress wrong opinions. Contrary to a recent BBC series on Alexander, Aristotle knew the earth was spherical, he knew its size, and he was the first to prove why it had to be spherical. Contrary to popular belief, he did believe in measurement and experiment, but like all Greeks of the time he was limited by the availability of equipment and he may have been a little unfortunate. Thus he proved that the Earth did not rotate. One of his proofs was along these lines. The Earth is a sphere of radius R . Throw a rock up vertically to a height h . If the Earth was spinning, then it should fall a

distance d behind the starting point. We observe the rock returns to the starting point; therefore the Earth is not spinning. One interesting point is that this implies he understood the law of conservation of angular momentum, and indeed on a liberal translation of other work, he came fairly close to the Principle of Least Action, at least for what he called natural motion. So, a problem for the reader: where did Aristotle go wrong? Note that $h/R \gg d^*/2\pi R$, where d^* is the smallest distance measurable.

Let's return to Empedocles. Perhaps we fail to allow for the vocabulary limitations. Consider his four elements as gas, liquid, plasma, solid. The procedure noted above is effectively *evaporate off the liquid and recover the solid*. Find me a real chemist who has not done that many times.

The Roman Lucretius appeared to come close to the truth about molecules. He considered that atoms formed immovable arrays, thus there was an array for *sparrow*, and that array was passed on to baby sparrows. Alter the array, accidentally through breeding, and the animal changes. Thus woolly sheep had been bred from the wild hairy ones with short wool. The concept of a genetic code and the possibility of genetic engineering are two thousand years older than you thought! The failure? Who has heard of Lucretius? Be honest, now!

While the Arabs made significant practical advances, their theoretical work failed to recognise atoms or molecules, and instead they introduced mysticism. They divided matter into two classes, spirits (mercury, ammonium chloride, and camphor) and souls (sulfur, oil, and arsenic sulfide) by classifying into degrees of oiliness. Thus souls are, by their very nature oily, while spirits have no oily properties. Oils catch hold of and unite with a body, so admixture is the property of souls. Yet there was an immediate flaw! Mercury behaved as a spirit with spirits and as a soul with souls. Unfortunately, this was compared with the planet Mercury, which when in conjunction with an auspicious star was auspicious, and with an inauspicious star

Thus Western chemistry became occult, and failed to discover the principle of the unreliability of the literature. The philosopher's stone, the elixir, and transmutation were firmly believed. In the 13th century, Lullus claimed to have transmuted 22 tons of assorted metal into gold. Much later, Van Helmont claimed to have transmuted 2,000 times its weight of mercury into gold by means of a quarter of a grain of philosopher's stone given to him by a stranger. He also produced full-grown mice in three weeks from wheat in a jar stoppered with dirty linen.

Van Helmont was not the most fortunate of experimenters. He did the famous schoolboy experiment of burning a candle in a bell jar over water, and noticed the contraction in volume. One wonders what the average teacher would reply to a pupil giving his explanation that the contraction is due to the pressing together of empty spaces in the air by smoke from the burning candle. Mention should also be made of the experiment that *proved* transmutation. In a vessel, with 200 lb. of earth, dried in a furnace but moistened with distilled water, was planted a small willow

tree, weighing 5 lb. 3 oz. This was watered with distilled water for 5 years, and a tree weighing 169 lb. was obtained. After washing the roots and drying in a furnace, the remaining earth weighed 2 oz. under the 200 lb. The wood, therefore, was created from water alone, as was the charcoal obtained from the wood. Furthermore, since charcoal is earth, earth is not an element, for water can be transmuted to earth. Poor Empedocles!

Sometimes the most spectacular failures are the failures to see the obvious, and the failure to follow Aristotle's principles of logic. Stahl strongly believed in phlogiston. He found that when metals burn they gain weight, which is really one of the key experiments in chemistry. He therefore deduced that phlogiston has negative mass! Then there was this logic. Wood is clearly phlogiston plus ash. Candle wax has no ash therefore it is pure phlogiston. Therefore you can make wood from candle wax and ash. Numerous failed attempts followed, but the theory persisted, so much so that Priestley, who strongly believed in phlogiston, failed to realise its significance when he discovered oxygen.

It was not until Lavoisier that chemistry started to find its way, but that was hardly in the most convincing fashion. To begin with, Lavoisier believed in transmutation because he found *earth* in the distillate after a distillation of water. Here was a further clear failure to comprehend the older literature. Subsequently, however, Lavoisier repeatedly distilled a sample of water, and finally convinced himself that earth was not being formed in the distillate.

Another failure worth mentioning is one by Isaac Newton. Newton devoted quite a lot of energy to alchemy, and spent some years searching for the philosopher's stone. To his credit, he failed! Newton also wrote, "Hypotheses are not to be regarded in experimental philosophy." Does this mean, no idle speculation for Newton? Perhaps only in public, and in advice to others, for his notebooks showed he considered that sulfurous bodies burnt strongly because of their interaction with light. Newton did not fail to be human. Freind, a disciple of Newton's, made the inevitable speculation that gravitation among particles of matter is the fundamental basis of chemical phenomena. Did he fail to appreciate the magnitude of G , or did he think that the gravity we feel is a second-order effect of something greater?

Newton opposed the occult, but it was Boyle who finally did away with it and the principles! He did not believe in elements, and he rejected the idea that air can take part in chemical reactions, even though he had carefully measured the gain in weight of a substance on combustion.

Forty years before Lavoisier disposed of phlogiston, Lomonosov had stated that atoms are fundamental particles which are in kinetic motion, and that this motion causes heat. Boyle's *fire particle* idea is incorrect, phlogiston does not exist, and matter is conserved. This is a fair recycling of Democritus, and, for that matter, of Newton. However, Lomonosov failed to make an impact, partly because he failed to go on the lecture/conference circuit of Europe – at that early date! Lavoisier disposed of phlogiston,

however, only to put his prestige behind the theory of caloric; the *subtle* fluid that poured out of a body as it cooled into the spaces of another body, causing the latter to swell. After the atomic theory, and the oxygen theory of acids, it was inevitable that the halogens should be thought of as oxides, but what is perhaps more surprising is that as late as 1865 chlorine was still held to be an oxide by at least one author! Davy, although a great discoverer of elements, “discovered” hydrogen in sulfur and phosphorus.

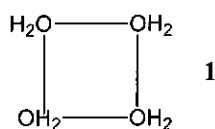
Berthollet visited Egypt and observed that the sodium carbonate/calcium chloride reaction could be made to go *the wrong way*, hence the mass of the reactants was important. This could have led him to deduce the law of mass action but unfortunately he did not believe in molecules, and he was certainly not alone in rejecting Avogadro’s hypothesis. Accordingly, he concluded that the masses would influence the composition of the compound; hence all gravimetric analyses are meaningless. Oops! Eventually, thanks to Cannizzaro, molecules became acceptable and Berthelot amended Berthollet’s hypothesis to the idea that reactions go in such a way as to give those compounds that liberate the most heat.

The biggest stumbling block to the acceptance of Avogadro’s hypothesis was the theory advanced by Berzelius that electrostatic forces held chemical compounds together. As a consequence the idea of H_2 was completely abhorrent to chemists of the time. As might be expected, organic chemistry provided a clue, but interpretation was difficult. Berzelius could not see that substituting a positive H by a negative Cl could occur, least of all yielding a compound of similar properties. At first he refused to accept that trichloroacetic acid was similar in nature to acetic acid, until it was proved by direct conversion.

Once the tetrahedral carbon atom was established, a quick publication was obtained proposing the impossibility of synthesizing small rings such as cyclopropane. Another failure! Less than one year later, cyclopropane was synthesized.

A failure of a slightly different kind is illustrated by the case of J. J. Waterston, who submitted a paper to the Royal Society in 1845. It was turned down, without reason, as “unsuitable for publication”, but was finally published in 1892, which may be a record for the longest editorial delay. The subject was the kinetic theory of gases, and the learned authorities, having learned nothing from Galileo, knew better than to let *obviously wrong* material into the literature.

The ionic theory did not make its way without opposition either. As late as 1908 a theory was postulated to explain solution phenomena. Water was postulated as a complex mixture of active molecules such as hydrone (H_2O) and hydrone hydronal (H_3O-OH) and inactive molecules that are polyhydrones such as the oxygen analogues of the cycloalkanes, e.g. **1**



where all the oxygens are tetravalent. These various forms would be in rapid equilibrium and when non-electrolyte was dissolved, it could give rise to active complexes or inactive hydrone complexes as well as polymers. With increasing dilution, more active molecules could be formed. This theory was supposed to account for the variation of product distributions with concentration on electrolysis, and for the value of ΔH on neutralization of acid/base better than the ionic theory. A further piece of evidence that was claimed to lend strong support to this theory was the isolation of two varieties of ice by Tammann.

On a different level, in 1868 an attempt was made to establish chemistry on the mathematics of operators. The paper starts with the observation “It is difficult to point to even one discovery in science for which we are indebted to symbolic operations” and then set out to rectify this. The author appeared to have strong objections to the atomic theory, thus “it is a fatal illusion to mistake the suggestions of fancy for the realities of nature and, under the baneful influence of such hypotheses the methods of positive science lose their hold upon the mind, until at length we are actually informed by the consistent advocates of these ideas that the science of chemistry has no other field for its activities than the obscure region of atomic speculations. However, a symbolic calculus affords the same indispensable aids as those given by the atomic theory, but in a more truthful and effective way.” To begin with, the mathematics were limited to equivalent weights thus “The symbol a is the symbol of the operation on unit space by which weight is generated – that is, of which the result is a weight”. One brief example of this calculus:

xy is the symbol of a single weight, which is composed of the same weights of the group $(x + y)$

In a chemical reaction

$$x + y = xy$$

1 is the operation of multiplying by 1

Let $y = 1$

$$x + 1 = x1$$

and since

$$x1 = x$$

$$0 = 1 \text{ (which can also be shown to equal } 2, 3, \dots, n \text{)}$$

Without explanation this looks suspicious, but even worse, the author was not in the habit of making concessions to his readers. Thus “There is considerable difficulty in the use of language for the expression of such abstract ideas, and these points would hardly become clearer by a fuller explanation. Let it be sufficient”. As for the truthfulness of his calculations, some of his relative weights were: hydrogen, 1; methane, 8; benzene, 39; carbon dioxide, 14; glycol, 31; lactic acid, 45; glycerine, 46.

The twentieth century had its share of the spectacular. In the early 1930s, there was much speculation as to the nature of the electron and universal constants, in some cases with ideas that do not seem to have caught on. One author noticed that the fraction $hc/2\pi e^2$ is approximately equal to 136. He decided that it should equal 136, because this is the number of degrees of freedom of two electrons in 16 space and reasoned that this deviation could be caused by the value of π being larger within the intense nuclear field

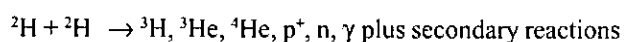
of the atom. Similarly, the ratio of the mass of the proton to the electron, which is approximately 1849, should be.

$$1849.6 = \frac{136^2}{10}$$

However, another author postulated that the real number was

$$1849 = 43^2 = (1^2 + 2^2 + 2^2 + 3^2 + 3^2 + 4^2)^2 = \left[\frac{1}{2} (2 + 8 + 8 + 18 + 18 + 32) \right]^2.$$

Then, of course, there were N-Rays, and even more impressively, *cold fusion*. Here, the electrolysis of D₂O was believed to give off anomalous heat, a *clear sign of fusion*. There are clearer signs, which refused to show themselves. Thus:



A number of chemists seemed to believe this reaction would work, and they protected themselves with standard laboratory safety glass. Most physicists who attempted to repeat these experiments were convinced it was nonsense, but carried out the work behind several feet of lead, or equivalent protection against neutrons. Several tens of millions of US dollars were spent/wasted on this.

We must not bypass polywater. This was made in trace amounts by sequential concentration, and had boiling points tens of degrees higher than ordinary water, and a density of up to 1.4. Lippincott recorded an infrared spectrum of polywater and calculated a hydrogen bond energy of 120-200 kJ/mole. A flurry of activity followed. Some may find sympathy for Bascombe, who, in mid-PhD, was required to continue with his thesis work *and* make large amounts of polywater. His continual failings to make anything other than water contaminated with silicic acid must have driven him quietly angry. Meanwhile Donahoe, in a letter published in *Nature*, cautioned that this might be the most dangerous substance on Earth: if it autocatalysed the formation of further polywater, the seas could polymerise and all life on Earth could end. Bascombe might have been feeling relieved to be continually failing.

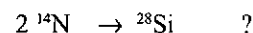
Now, if theory is going to be of any use whatsoever, it has to either deal with new circumstances, or admit it needs more development to be of any use. Well, there was not going to be much of the latter option with polywater. The first papers were a little speculative, thus polywater was an sp² H-bonded polymer, and another pointed out that a rhombic dodecahedron would be best to explain the reported density. Then molecular orbital theory hit its straps, finding that symmetric H-bonds are stable in highly condensed rings, a ring of six waters with symmetric H-bonds were the most stable, another that 5 waters formed a cyclic pentamer, but with asymmetric bonds. Another wrote "A very large number of reputable scientists have grave doubts as to the probable existence of polywater.... We have established its existence and characterised its properties by MO calculations." They concluded that polywater was an extended polymer, with a graphite-like structure. In the spirit of, "I have to get aboard!" one J. Pople calculated that cyclic H-bonded forms were the most stable, and that the cyclic hexamer was stabilised with respect to six water molecules by 302 kJ/mole.

The bubble had to burst, and it did when one worker noted that Lippincott's infrared spectrum bore a strange resemblance to sweat! Oops! But wait! Pople's calculations then produced: "There is evidence for the existence of a co-operative effect in hydrogen bonding associated with an O-H...OH...OH chain which enhances the stability of chain-like structures..." Then came: "molecular orbital theory indicates that Pople was wrong and water cannot form polymers because there would be deformation of bond angles." What exactly does that explanation mean? That the hydrogen bond is strong enough to be rigid? If so, the main finding fails. That molecular orbitals cannot turn corners? If so, the whole concept of molecular orbital theory tends to fall apart. What do you think?

The problem, of course, is that the very structure of molecular orbital theory lends itself to this type of error, as it is difficult to justify single discrete bonds, but how to fix it? Time for more reader participation! If electron motion follows a wave equation, given that Snell's law is nothing more than trigonometry imposed on a wave equation, should not electron motion follow wave mechanics? Specifically, should they not follow Fermat's principle or, given a change of refractive index be reflected or refracted? If so, then single bonds about carbon should be discrete, as the wave function does not refract without a change of refractive index. If they do bend, they bend reproducibly depending on the differences between potentials. Now, who agrees with that? Who fails? You or me?

Back to the subject of water, why not try something recent. Low velocity neutron scattering has shown that, at the attosecond level, water has the formula H_{1.5}O. This observation has been interpreted in terms of quantum entanglement. In the spirit of what the above authors had to face, *i.e.* an interpretation before the answer was known, interpret that!

What better way to conclude than to consider the end of the world? That is, after all, the ultimate conclusion. An hour or so before igniting the first nuclear detonation, one physicist raised the question, what if this triggers the reaction



Ooops! That would remove the atmosphere, and all life! Apparently this caused some fairly warm slide rules (remember them?) before they finally *convinced* themselves to press the button. There are, of course, rogue robots, rogue viruses, rogue organisms, black holes, but how about this that I heard recently on the BBC? A high-energy physics experiment might alter the structure of space, leading to all water going gooey, and ending life. Polywater! Oh dear!

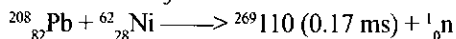
So we conclude our survey of some of those aspects that do not make it into the undergraduate courses. Why did such things go wrong? The simplest answer is that it is not quite so easy when you do not know the answer. Even Newton guessed wrongly at times. But look at it from the other side of the coin: these scientists at least made an attempt to address an important question. It might have been beyond them, but so what? Surely it is better to run the risk of failure than to never enter the field.

ELEMENT 110 IS NAMED DARMSTADIUM

At the 42nd General Assembly in Ottawa, Canada, the IUPAC Council officially approved the name for element of atomic number 110, to be known as darmstadtium, with symbol Ds.

In 2001, a joint IUPAC-IUPAP Working Party (JWP) confirmed the discovery of element number 110 and this by the collaboration of Hofmann *et al.* from the Gesellschaft für Schwerionenforschung mbH (GSI) in Darmstadt, Germany (*Pure Appl. Chem.* **2001**, *73*, 959-967). The most relevant experiment resulted from the fusion-evaporation using a ⁶²Ni beam on an isotopically enriched ²⁰⁸Pb target, which produced four chains of alpha-emitting nuclides following the presumed formation of ²⁶⁹110 + n. (S. Hofmann *et al.*, *Z. Phys.* **1995**, *A350*, 277-280).

bombardment of lead with nickel ions



In a soon-to-be-published second report, the JWP has re-endorsed the confirmed synthesis of element 110 by the team at GSI led by Sigurd Hofmann.

In accordance with IUPAC procedures, the discoverers at the GSI were invited to propose a name and symbol for element 110 to the IUPAC Inorganic Chemistry Division. Hofmann's team proposed the name darmstadtium, with the symbol Ds. This name continues the long-established tradition of naming an element after the place of its discovery.

IUPAC was formed in 1919 by chemists from industry and academia. For nearly 85 years, the Union has succeeded in fostering worldwide communications in the chemical sciences and in uniting academic, industrial and public sector chemistry in a common language. IUPAC is recognized as the world authority on chemical nomenclature, terminology, standardized methods for measurement, atomic weights and many other critically evaluated data.

More information about IUPAC and its activities is available at www.iupac.org.

For specific questions regarding the discovery and naming of element 110 contact:

Professor John Corish Email: jcorish@tcd.ie

Dr. Gerd Rosenblatt Email: grosenblatt@lbl.gov

For general questions about IUPAC contact:

Laura Abernathy, IUPAC Communications Specialist

Email: Laura@iupac.org

Website: <http://www.iupac.org/news/archives/2003/naming110.html>

VICTORIA AWARDS PERSONAL CHAIR TO DR. J. H. JOHNSTON



Jim Johnston, Head of the School of Chemical and Physical Sciences and Deputy Dean of Science, Victoria University of Wellington, has recently been appointed to a Personal Chair in Chemistry in the 2003 exercise. This is in recognition of his

significant contribution to research and teaching in materials science, industrial chemistry, and geochemistry.

For some two decades he has worked closely with industry in identifying and pursuing innovative and strategic research opportunities concerned with the development new technology platforms and high performance products. These include the production of titanium dioxide pigment for paint from New Zealand and USA beach sand ilmenite; the extraction of silica from waste geothermal water with specific characteristics and properties for use as a high performance filler in newsprint to enhance the optical properties and print quality of the paper; the design and development of nano-structured calcium silicates with specific functionalisation for use in high quality papers, anticorrosive paint, heat storage materials, humidity control and catalysis; novel composite materials utilising conducting polymers; and the development of wet air oxidation in the treatment of industrial organic waste and in the recovery of valuable filler minerals from waste de-inking sludge in the recycling of paper. He has published over 140 research papers and industry reports, and is an inventor on 10 patents. He has also supervised some 67 graduate student research projects and theses.

He is a Fellow of the Royal Society of New Zealand, a Fellow of the NZ Institute of Chemistry, and Recipient of the RSNZ's Thomson Medal for Outstanding Contributions in the Fields of the Organisation, Administration or Application of Science and Technology. Jim has worked at Victoria University since 1975. He has taken on significant administrative responsibilities including as Head of School, Deputy Dean of Science, and Acting Pro Vice-Chancellor.



NZIC BRANCH NEWS

Annual General Meeting

This 2003 Annual General Meeting of the New Zealand Institute of Chemistry will be held on Tuesday 2 December 2003 during the 2003 Conference — Chemistry at the Interface at Rutherford Hotel, Nelson. Further details about the meeting will be advised to branches closer to the date.

Nominations For Offices

Nominations are called for the offices of President, First Vice-President, Second Vice-President, Honorary General Secretary, and Honorary Treasurer.

Nominations can be made by Branches, or by any six members, and should reach the Honorary Secretary by 21 November 2003.

The address for nominations is:

Email: Secretary@nzic.org.nz

or
FREEPOST 96
New Zealand Institute of Chemistry
PO Box 39283
Howick
Auckland 1730
NEW ZEALAND

The First Vice-President is automatically nominated for the position of President.

The Second Vice-President is automatically nominated for the position of First Vice-President.

G Boston
Honorary General Secretary

AUCKLAND

Professor Margaret Brimble of The University of Auckland has been invited to take part in the first "Rosalind Franklin International Lecture Programme". This will involve a visit to the United Kingdom for a week (27 March to 3 April 2004) to present a series of lectures to universities and companies around the United Kingdom. At the end of the week there will be a half-day symposium sponsored by the Royal Society (UK) at Imperial College in London where Margaret will present a lecture on her research. The Rosalind Franklin International Lecture Programme has been initiated to expose young scientists in the United Kingdom to a greater number of internationally recognised and successful women scientists. Furthermore, at the International Congress of Heterocyclic Chemistry held in Fort Collins, Colorado in August, it was announced that **Professor Margaret Brimble** had won the election for **President of the International Society for Heterocyclic Chemistry**. A postal ballot of the entire membership of the Society was held prior to the meeting in Colorado. Margaret is the first President of the Society to have been elected from the Southern Hemisphere, and as President-elect, one of her first jobs will be finding a site in Asia/Australia/New Zealand for the 2007 International Congress of Heterocyclic Chemistry that over 1000 chemists will attend.

Congratulations to **Nicole van der Laak** who has been awarded a Gates Scholarship from Cambridge University together with an ORS award and has been accepted to reside at Clare Hall College. Nicole has been studying at the Department of Chemistry of The University of Auckland.

The **Chemistry Olympiad** competition was held this year in Athens, Greece. The team members included **Aritra Rae** (Mt Roskill College), **Graeme Mok** (Auckland Grammar), **William Shew** (Avondale College) and **Yun Huang** (Westlake Boys). William and Yun received bronze medals and Graeme received an Honourable Mention. Yun achieved the highest score of the group, completing all 2000 questions in the *BestChoice* website.

Congratulations to **Dongxiao Sun** (PhD student, Food Science) who has received a grant-in-aid totalling \$2,500 from the Maurice and Phyllis Paykel Trust. This will assist Dongxiao's travel costs to the 25th World Congress of the International Society for Fat Research in Bordeaux, France.

Rob Wallace has joined the Light Metals Research Centre of The University of Auckland. Rob has recently returned after 2½ years in Australia where he was involved in analysis and improvement of the coal transportation industry. He has joined the Light Metals Research Centre to undertake a Doctorate in Industrial Thermodynamics, in particular, increasing the heat flow through the side of aluminium reduction cells. Rob has over 7 years experience in the aluminium smelting industry in Development Engineer and Specialist Engineering roles at NZAS primarily focusing on carbon anode technologies.

Dr. Robert Kawczyk has joined the Department of Chemistry of The University of Auckland from the

Technical University of Munich. Robert takes up a postdoctoral Feodor-Lynen Alexander von Humboldt Fellowship. He will work on nano-structured gold compounds in the research group of **Peter Schwerdtfeger**.

Farewell to **David Callis** who is returning to the United Kingdom after having spent two years with NeuronZ. Farewell also to **Steven Taylor** (formerly Kennedy) who has left for New York City to take up a postdoctoral research position at Columbia University in the Department of Medicine. He will be working for Milan Stojanovic on a project that will investigate molecular machines.

Dr. Stéphane Verdier has joined the Department of Chemistry. Stéphane will be working in a joint project with the Research Centre for Surface and Materials Science on the interaction of organic coupling agents with aluminium surfaces. Stéphane comes to us from the Institut National Polytechnique de Grenoble, France.

Congratulations to **Anna Huang** and **Chi Zhang** who have both successfully completed their PhD degrees under the supervision of **Allan Eastaie**. They will graduate in the Spring Graduation ceremony in Auckland.

CANTERBURY

The Canterbury branch has had two changes of committee members in recent weeks. **Meryn Bowen** has left to start her PhD studies and **Chris Sumbly** completed his PhD and is currently a postdoctoral fellow with Michaela Harding in Leeds. We welcome **William Lewis** (Secretary) and **Jonathan Slater** to the committee.

At our June meeting **Christina McKerchar** (Ngati Kahungung, Ngati Porou) who has a background in nutrition and Maori health discussed some of the reasons why obesity rates are increasing, to epidemic proportions, in New Zealand. She also outlined current public health strategies to address this. Christina who has a Masters degree in Nutrition, drew on her considerable experience of having worked for four years for Te Hotu Manawa Maori, a Maori Health Provider who address nutrition issues in the Maori community. She currently works for Agencies for Nutrition Action (ANA), an incorporated society made up of member organisations with an interest in nutrition. ANA have worked to strengthen cooperative effort among nutrition agencies and with other sectors. Christina explained a number of initiatives that are addressing the obesity problem in New Zealand and in particular the effect of the Kai o te Hauora programme on Maori community nutrition. The 'Kai o te Hauora Programme' has run since 1995 and its aim is to 'empower Iwi and Maori communities with the skills, knowledge and resources to make informed status about their own nutritional status'. Her presentation was much appreciated and a lively discussion ensued.

The July meeting was entitled *Phenolic Fun* and was our annual wine tasting hosted by local wine maker **Kirsten Creasy**. Kirsten's evenings have been extremely popular and accordingly, there was little problem in filling the seats

(which had been limited to 40) with members from WRONZ, Canterbury Manufacturers Association, University of Canterbury Chemistry Department, ESR, Landcare Research and beyond.

Kirsten provided an outline of tannins in wines and then described the specific compounds, their function and effect on the wine. The phenolics of wine were then specifically addressed - how levels alter with time, the effect of maturation processes and so on. After the big build up we moved on to the (blind) tasting. Aided by a *mouth-feel-wheel*, eager tasters got together in groups of 3 to 4 and assessed the wines. At the end of each bracket Kirsten opened the floor to opinion on the wine type, country of origin and prevailing properties of the wines. It was clear the audience had some skill, and after a little jostling consensus and accuracy tended to be quite readily achieved.

In all, the tasting which lasted over 2 hours, involved 8 wines, from an unwooded chardonnay through to a fiesty zinfandel. Kirsten's excellent explanation of the chemistry, followed by the illustration of the characteristics in the wines tasted, once again provided an educational and fun evening.

Supporting Young Chemists: Canterbury and Westland Science and Technology Fair 2003

The NZIC Canterbury Branch was among the many local organisations supporting the Canterbury-Westland Science and Technology Fair. This very successful event, once again staged at the Christchurch Convention Centre, comprised over 350 exhibits from students from Years 7 to 13 with the younger years most highly represented.

This Branch provided a senior and junior prize for the *Exhibit Showing the Best Understanding of Chemistry* and with it two judges, **Cassandra Hinton** and **William Lewis**. Chemistry had quite a showing at the Fair, either as the main theme or as an essential aspect of the studies presented but as with last year's experience it was soon discovered that many of the eager exhibitors had a rather latent understanding of the chemistry involved.

At the senior level the prize went to **Leon Yu** (St Margarets) for her exhibit *Cu Sea You* for which she developed a spectrometric method of copper detection to monitor copper levels in contaminated seawater from Lyttelton Harbour. Year 9 students **Caitlin Williams** and **Michele Wilson** (Villa Maria) took the junior award for their *Burning Issues* display.

Canterbury University

The Chemistry Department has been host to a number of visitors in recent months. **Muna Al-Mandhary** returned for a month from Sultan Qaboos University, Oman. Muna who was here on sabbatical leave in 2001/2002 had to acclimatise to a 40 degree temperature drop! **Tom Morton** visited from University of California at Riverside. A physical organic chemist, Tom worked with **Murray McEwan** exploring issues related to conjugation and aromaticity in gaseous positive ions. **Professor Neil Connelly** from the University of Bristol also visited. silver

Professor Peter Gill, another Erskine visitor and originally a (North Island) Kiwi was a lecturer at Massey University (1993), and then at University of Cambridge. In 1996 he became Professor of Theoretical Chemistry at Nottingham in 1999. He was awarded the 1999 Dirac Medal of the World Association of Theoretically Oriented Chemists (WATOC). **Dr. Peter Duggan**, a Senior Lecturer at Monash University, also visited to work with **Richard Hartshorn**. Student **Allison O'Brien** returned to Colorado after several months working with **Greg Russell**.

Ben Perston has been awarded a **William Georgetti Scholarship**. These prestigious scholarships are administered by the NZVCC and are not restricted to science students. **Brett Davis** has been offered a three-year TIF (Technology for Industry) Fellowship to do a PhD involving a 3-way tie-up between the University of Canterbury, Syft Technologies Ltd., and the New Zealand Olive Oil Industry. **Daniel Milligan**, a former PhD student in this Department, has been awarded a FoRST postdoctoral fellowship and will join the SIFT group at the beginning of August. **Brett Davis** has had his enrolment as PhD approved and **Jenni Gadd** has recently begun a PhD supervised by **Andrew Abell** and **Louis Tremblay** (Landcare Research). Congratulations go to **Jared Panther** and **Kelly Anderson** who have been awarded Bright Futures Top Achiever Doctoral Scholarships.

Dr. Michael Lever of Canterbury Health Laboratories has had his adjunct appointment as a Senior Fellow extended for three years while **Professor Peter Steel** has just been appointed as an Adjunct Professor at James Cook University, Queensland.

Congratulations to **Chris Sumbly**, **Derek Martyn** and **Jeremy Harrison** who have all completed PhDs recently and moved on to Postdocs.

MANAWATU

In June, **Simon Fielder** (HortResearch) entertained the Branch on the topic of *Sex, Death and Synthesis*. His talk covered the work he and others are doing in HortResearch to develop a strategy for the control of the painted apple moth invasion in West Auckland. Simon's team is identifying the chemicals that occur in the natural pheromone that the female moth emits to attract the male and then they are attempting to synthesise it. In order to gain an appreciation of the extremely low levels of these chemicals that the male moth can detect we were asked, with mixed success – something to do with the wine and cheese? – to identify various chemicals by their smell. In July we held our annual *Careers in Chemistry* lunch function for students studying chemistry. This year's speakers were **Stephen van Eyk**, a research chemist at New Zealand Pharmaceuticals Ltd, **Tina Aomarere**, a teacher from Rangitikei College, **Amy Watson**, a research assistant in the Nanomaterials Research Centre at Massey University and **Dan Comeskey**, a research assistant at HortResearch working with Simon Fielder on the painted apple moth project. All spoke enthusiastically about their work and emphasised the need to keep on upgrading their skills after their first degrees. At this meeting the Manawatu

Branch Prize for the top chemistry student at UCOL was presented to **Leiza Turnbull**. The prizes to the top third year chemistry and biochemistry students at Massey had been presented earlier in the year to **Leila Chrystall** and **Carlene Starck**, respectively. In August, **Geoff Jameson**, Massey University, delivered his Royal Society of Chemistry, Australasian Lecture entitled *pHflexibility, pHunctionality and hydrophobicity of bovine β -lactoglobulin*. His talk, based on results from X-ray crystallography and NMR, gave a new insight into the critical structural role that flexible loops play in providing entropic stabilisation of for this important milk protein.

Landcare Research

Harry Percival attended the *7th International Conference on the Biogeochemistry of Trace Elements* at the Swedish University of Agricultural Sciences, Uppsala, in June. The meeting attracted around 600 registrants from about 70 countries, presenting over 200 oral papers and about 500 posters. The programme comprised 5 keynote lectures, 10 symposia, and 14 scientific sessions. Harry presented a paper, *Change in soil solution chemistry after liming of a field-trial pasture soil amended with heavy-metal-spiked sewage sludge*. A welcome reception was held in the magnificent Uppsala Castle that stands on a promontory overlooking Uppsala and can be seen from some distance away. The keynote lectures were well worth attending and covered (1) the transfer of trace elements through the food chain, (2) trace elements and soil protection in Europe, (3) phytoremediation (4) bioavailability, and (5) trace element chemistry, contamination, and ecotoxicity. These topic areas and several others were covered in further detail in the symposia and scientific sessions. Some topics are "perennials" (or rather "biennials", as the ICOBTE conference series are held every 2 years at present), but this year arsenic in soils and groundwaters was one of the hotter topics because of severe arsenic contamination problems in countries such as Bangladesh. Harry also visited the Sala silver mine, about 1 hour west of Uppsala. This mine, Sweden's oldest and largest, is now a tourist attraction. The silver is associated with the lead mineral galena, with the ore bodies distributed throughout dolomite rock. The visiting group were underground for several hours in a temperature of about 5 °C so warm clothing was essential! After the conference, Harry was lucky to be invited to join a group of Belgian and Australian conferees celebrating Mid-Summer Eve festivities with a Swedish family at their holiday house on the coast east of Stockholm. The weather was cool but the Swedish schnapps decidedly warming!

Massey University

The *Massey University Chemistry Scholarship* has been awarded to first year student, **Ross Davidson**. The highly successful Year 12 Chemistry Field Trips to Massey University are again operating during the second semester. The students are able to perform a distillation of orange peel or synthesise a polypyrrole, and explore some of the associated chemistry. These Field Trips have already seen over 300 students from 16 schools get to sample the 'Massey Experience'. Over 900 year 12 Chemistry students will partake in the field trips spread over July through to October. Adrian Jull is coordinating the practical

exercise, with assistance from other staff and postgraduate students of the chemistry discipline in the Institute of Fundamental Sciences. Schools from as far afield as New Plymouth, Wellington, and Gisborne have enthusiastically taken up the offer of the field trip.



Above: New chemistry lecturer, **Mark Waterland**.

Mark Waterland has recently arrived from Industrial Research Ltd, Lower Hutt, to take up a lectureship in chemistry. Mark did his PhD with **Keith Gordon** at the University of Otago and then spent periods at the University of Rochester, New York, and Kansas State University on postdoctoral fellowships before a brief period as an assistant professor at the Southwest Missouri University. Mark describes his research interests as

being in physical inorganic chemistry and the spectroscopy of advanced optical materials.

There have been a number of new arrivals in **Carol Taylor's** group. **Li Hao** has started a postgraduate research degree. Hao has a Bachelor's Degree of Engineering from the Changchun College of Traditional Chinese Medicine and has done some postgraduate study at The University of Auckland. He will be investigating synthetic approaches to the modification of the side-chain of ginsenoside derivatives. **Karen Bang** is beginning as a PhD student on a new collaborative project with **Sharon Bisley** and **Ross Holland** at Fonterra. This FRST funded project is called *Biotransformations for Flavour Delivery in Advanced Foods*. Carol, Karen and a research technician yet to be appointed will be working on the synthesis of some potentially interesting flavour compounds. Karen has BSc and MSc degrees from The University of Auckland. Her MSc thesis involved investigations into the regio- and typo-selectivity of calf pregastric lipase, supervised by **Charmian O'Connor**, **Margaret Brimble** and **Carol Taylor**. **Kristin Bopp** joined the group from Germany in the first week of September. Kristin is an undergraduate at the University of Stuttgart and will be spending five months helping out in the general area of peptides containing hydroxylated and dihydroxylated prolines.

During July, PhD student, **Giovanna Moretto**, travelled to Newport, Rhode Island, to present her research at a Gordon Conference. As part of a collaboration involving her supervisors, **Simon Hall** and **David Officer** at Massey University, **Andreas Markwitz** at GNS, and **Tony Burrell** at Los Alamos National Laboratories, she has shown that Ion Beam Analysis is a promising technique for analysing conducting polymers. **Adrian Chaplin** has left for Switzerland to study for a PhD in organometallic chemistry under **Paul Dyson** at the Institut de Chimie Moléculaire et Biologique, Ecole Polytechnique Fédérale de Lausanne. He has been employed as a research assistant with **Eric Ainscough** and **Andrew Brodie** carrying some very challenging organic syntheses.

Massey News reports that the University Council has approved the purchase of a 700 MHz NMR spectrometer,

to be situated in the *Centre of Structural Biology*. It will be the only such instrument in New Zealand and the single biggest capital item of research equipment any New Zealand university has invested in. A new 400 MHz machine is also being purchased. The purchase of a high-field 700 MHz machine - a major piece of scientific equipment by any criterion - re-emphasises the University's commitment as New Zealand's premier research centre in protein science, says Head of the Institute of Fundamental Sciences, **Professor David Parry**. "It illustrates management's commitment to supporting high quality research and the necessary equipment to undertake that research. It is a wonderful start to the Vice-Chancellor's reign. That she is willing to take the plunge shows fantastic courage. It is something the whole University should take pleasure in." Massey has substantial expertise in the field but until now researchers have had to take their material offshore for analysis, says Professor Parry. "The new NMR machine will place Massey in a unique position as the only institution in New Zealand with the equipment and the staff with the expertise capable of tackling not just structure but analysis of protein-protein interactions." This is particularly important to New Zealand because of our reliance on the primary products. "Primary products are basically proteins - meat, wool, leather, all our main export industries." The new facility is also likely to attract further researchers, research funding and postgraduate students to the University, offering them opportunities not previously available in New Zealand, he says. "The new instrument will enable our researchers to pursue more projects involving high-field NMR techniques, gain more research contracts and strengthen Massey's already strong national and international reputation in the physical and biological sciences."



Above: Professors **Geoff Jameson**, **Pat Sullivan**, **David Parry** and **Robert Anderson** celebrating the go-ahead for Massey to purchase the 700 MHz NMR spectrometer.

The *Centre of Structural Biology* is led by **Professor Geoff Jameson**, recently awarded a Personal Chair in Structural Chemistry and Biology for his internationally-acclaimed research on proteins and small molecules. Along with Professor Jameson, the NMR spectrometer will be used by **Dr. Andrew Sutherland-Smith**, a structural biologist, **Dr. Patrick Edwards**, who is currently working on a jointly-funded project with the *Fonterra Research Centre* on milk proteins, **Dr. Steven Pascal**, an acknowledged expert in proteins and nucleic acids, and **Dr. Bill Williams**, an expert in oligosaccharides.

OTAGO

The big news from Dunedin is that we're losing Kate. Yes, **Kathryn McGrath** is leaving Otago for warmer, windier and more expensive climes in Wellington. She will be sorely missed in this part of the world, not least for her tireless efforts in inaugurating and organising staff-student social events within the Department, and also for starting the Otago alumni network. I, for one, will miss her invaluable fashion advice...



Above: Kathryn Magrath.

Henrik Kjaergaard gave an invited lecture *Vibrational overtone spectra of complexes in the atmosphere* at the joint 39th IUPAC congress and 86th Conference of the Canadian Society for Chemistry meeting in Ottawa in August. He also chaired an eventful afternoon session in the symposium *Theoretical chemistry in the environment* during which the second last talk was abruptly halted due to the North American power outage. Henrik's PhD student **Daniel Schofield** gave a talk entitled *Spectroscopy of atmospherically important radical water complexes* at the 58th International Symposium on Molecular Spectroscopy in Columbus, Ohio. On the way back from Ohio he attended the 4th RACI student conference on Physical Chemistry, in Albury, New South Wales and gave a talk entitled *Atmospheric applications of theoretical chemistry*.

Some news of current and former members of **Rob Smith's** research group has come to hand. **Andy Helm** (Hons 2001) worked as a Research Assistant on the mitochondria project in 2002 and left in February to take up a management training position at Interlock in Wellington. He has survived the transition and was recently promoted to a Team Coordinator position of responsibility. **Paul Garbutt** completed his MSc thesis and graduated in August. He has been working part-time for Chemsearch at the University of Otago this year. **Nicola Wales** (nee Daly) has also completed her MSc and is now resident in Christchurch working at Lincoln University. **Frances Blaikie** is in the final stages of writing her MSc thesis and will take up PhD study shortly after completion. **Daniel Webb** (Hons 2002) has returned from a short period on the skifields in the US to join **Ryan Hellyer** (MSc 2003) as a research assistant on the MitoQ project. **Linda Samuelsson**, a PhD student at Uppsala University, Sweden, is working in the lab as a visiting scientist for 2003 on a biological NMR project. She recently visited Sweden to

catch up with family and also dropped into the Carl Zeiss company labs of Jena, Germany, to study their fluorescence correlation spectroscopy techniques and hopes to apply some of the techniques to her research project. **Amanda Dixon** (MSc 2002) is now working as a university technical support person in the UK. **Vicki Adlam** (Hons 2002) is working as a HRC-funded research assistant on an animal-based project involving both the Chemistry and Pharmacology Departments at the University of Otago. She is extending the work she initiated in her undergraduate research project and expects to have a couple of months touring Europe in the summer before deciding on her next career move. Last November we welcomed back **Abdul Rahman bin Manas** who completed his PhD at Otago in 1983. Abdul worked for many years at Universiti Putra Malaysia rising to the rank of Associate Professor before taking up permanent residence in Dunedin. He is working on developing mitochondrial-targeted chemistry supported by FRST.

There are some new faces in **Keith Gordon's** research group. **Jarod Brain** from Massey is here for a year to do an MSc on "Spectroscopy of Porphyrins". His work is closely associated with the Advanced Materials for Energy Technology Development PGSF grant centred at the Nanomaterials Research Centre at Massey. **Natasha Lundin** started a PhD with **Allan Blackman** and **Keith Gordon** working on metal complexes with oxadiazole decorated ligands. These have some potential in electroluminescent devices. Natasha is a student of the MacDiarmid Institute for Advanced Materials and Nanotechnology. **Tracey Clarke** started her PhD in August, supervised by **Keith Gordon** and **David Officer**. Tracey is a recipient of one of the University of Otago's Prestige Scholarships. She is working on spectroscopy and computational chemistry of conducting polymers based on thiophenes.

On the teaching front, quantitative vibrational spectroscopy and multivariate analysis has been offered for the first time at 3rd year level within a chemistry course at Otago. The module focuses on quantitative analysis of pharmaceuticals using vibrational spectroscopy and involves Raman spectroscopy and principal component analysis. The course was devised by **Thomas Rades** (School of Pharmacy, University of Otago) and **Keith Gordon** with assistance from statisticians **Fred Lam** and **Austina Clarke** and graduate students **Clare Strachan**, **Destari Pratiwi** and **Sarah Howell**. The course has been very popular.

Keith Gordon and **Sarah Howell** attended the 11th International Conference on Time Resolved Vibrational Spectroscopy (TRVS 2003), Castiglione della Pescaia, Italy, in late May. The work presented was well received and we were able to start up collaboration with **Mike George** at the University of Nottingham. In fact, some of Sarah's compounds ended up at the ultra fast infrared laser facility at the Rutherford Appleton Labs in the UK. They showed some interesting transient mixed-valent behaviour. Sarah will be continuing the collaboration by visiting

Nottingham next year for a three-week stint doing time-resolved infrared spectroscopy.

Keith gave a short talk on *Raman Spectroscopy of Carbon Nanotubes* at the Symposium on Carbon Nanotubes (Intelligent Polymer Research Institute, University of Wollongong, Wollongong, Australia) on July 25. He has also been attending the organising committee meetings for next year's International Conference on the Science and Technology of Synthetic Metals (ICSM2004). You can check out the web site at: <<http://icsm2004.uow.edu.au>> The conference should be a blast!

Keith attended the Fourth International Conference on *Electroluminescence of Molecular Materials and Related Phenomena* (ICEL-4) in South Korea. He talked on *Light Emitting Devices from Blended Films of Ruthenium(II)bis(2,2'-bipyridine) (4,7-dimethyl-1,10-phenanthroline) complex with Poly(N-vinylcarbazole)*. PhDs **Clare Strachan** (co-supervised by **Thomas Rades**) and **Sarah Howell** attended the International Conference on Advanced Vibrational Spectroscopy (ICAVS-2) in Nottingham at the end of August. Clare presented a poster on *Quantum mechanical modelling of drug vibrational spectra* and Sarah presented a poster on *Structural changes of planar bridging ligands in MLCT excited states of metal complexes, probed by time-resolved resonance Raman spectroscopy and ab initio calculations*. Sarah was also chosen to give a student talk on her poster at the conference. **Tracey Clarke** attended a Photovoltaic Meeting at Wollongong in late August where the main contributors to plastic solar cell science and technology in New Zealand and Australia got together. She talked on some of our recent findings on electronic structure of terthiophene species elucidated through vibrational spectroscopy and computational chemistry.

Clare Strachan is currently in the UK at Teraview in Cambridge working on THz spectroscopy of polymorphic forms of drugs. The idea here is to use the THz region of the spectrum to probe the very low frequency absorptions that correspond to molecules flickering within the lattice; differing crystal forms (polymorphs) should show different features in this region of the spectrum. To get these frequencies requires the use of ultrafast femtosecond lasers. She will be there for almost three months getting data on a variety of systems and trying to get femtochemistry to meet pharmacy (*vide infra*).

Congratulations to **Thomas Rades** who has been offered the Chair in Pharmaceutical Sciences at the School of Pharmacy, University of Otago. Thomas has wide-ranging interests that span many areas of chemistry and last year gave a very interesting talk to the Otago Branch of the NZIC on Polymorphs in Drug Formulation and contributed to *Chemistry in New Zealand* as co-author of the paper *Spectroscopy and solid state properties of drugs: Will femtochemistry meet pharmacy?* (*Chemistry In New Zealand*, 2002, 66 No.4, 43-47).

WAIKATO

Hill Laboratories

Hill Laboratories is pleased to announce that it has purchased *BioTest Laboratories Ltd.*, a leading Waikato-based microbiology laboratory. The founders of BioTest Laboratories, **John Fam** and **Luke Rajan**, will operate BioTest Laboratories as a division of Hill Laboratories.

John and Luke are both recognized experts in their field of microbiological testing of foods, meat, and water. Together they have built an enviable reputation in the dairy and meat industries since the inception of BioTest Laboratories in 1992. The two companies share very similar philosophies towards high standards of customer service, scientific integrity and innovation and **Dr. Terry Cooney** (General Manager of Hill Laboratories) is delighted to have them join the team.

Hill Laboratories and BioTest Laboratories have had a long and amicable business relationship, as their respective chemistry and microbiological testing services have been very complementary. The amalgamation of BioTest Laboratories into Hill Laboratories means that BioTest now has the resources to develop innovative new microbiological services, while Hill Laboratories is able to offer its broad customer base a more complete range of high-quality, competitively priced testing services.

Hill Laboratories is one of New Zealand's quiet success stories. Founded by **Dr. Roger Hill** and **Anne Hill** in 1984 as a soil and plant-testing laboratory, it has steadily grown to become New Zealand's largest privately owned analytical laboratory. Based in Hamilton East, it provides a wide range of sophisticated testing services to customers throughout New Zealand, and overseas. With more than 140 staff, it is a leading employer of science graduates and will continue to operate as usual from its laboratory premises at Riverlea Road in Hamilton.

University of Waikato

Dr. Richard Coll won the most prestigious award provided by the World Association for Cooperative Education (WACE) named the **Donald MacLaren Award** in recognition of high achievement and continuing commitment to the enhancement of international cooperative education. This was presented to him at the biennial WACE conference held in Rotterdam last week.

A variety of biomedical, biomimetic and nanoparticle-based research is going on in **Michael Mucalo's** research group at Waikato. **Kavitha Babu** who recently completed her MSc thesis at Waikato on rhenium and gold colloids has begun a Chemistry and Materials PhD into drug delivery from gel matrices in collaboration with Interag, Hamilton. She joins **Grant Rennie** and **Stephen Gardyne** who are both doing an MSc in Chemistry also at Interag in the area of intravaginal drug delivery in cattle. All three students are TIF recipients from Technology New Zealand. To add to this biomimetic/biomedical theme of research in the Department, **Dougal Laird** is in the completion stages of his Masters research on hydroxyapatite growth on cholesterol and modified cholesterol surfaces. **Jacob Babu** is doing his Masters research in a completely different area, which is an in-depth chemical study of the commercial

colloid preparations being sold in various formulations which are often falsely hailed as so-called panaceas for all of society's ills. Many unscientific claims about the composition and mode of behaviour of these essentially electrolytic silver colloids has been made on unregulated media such as the Internet and it is Jacob's task to make sense of the colloids using some analytical techniques such as ICP-OES, TEM among others of silver colloids prepared using the various kits supplied to the general public for their generation.

The Department also had the pleasure of hosting **Dr. Katsuya Kato** from the Biofunctional Ceramics Group, Ceramic Research Institute, National Institute of Advanced Science and Technology, Nagoya, Japan as a visiting researcher in July and August. His research while in the Department centred on the development of *Smart Bone Implant Materials* in collaboration with **Dr. Michael Mucalo** and was supported by the Asia2000 Foundation. The research essentially involved the study of adsorption and desorption of bone morphogenetic protein mimics from amorphous calcium phosphate powders suspended in various media. Dr. Mucalo intends to continue this research in Japan later this year on a brief sabbatical and to have another member of the Biofunctional Ceramics Research group come out early next year to complete the research. Dr. Kato also gave a very interesting and well-presented seminar to the Department on the immobilisation of lipase enzymes in porous silica matrices. **Dr. Michael Mucalo** has also presented his bovine xenograft bone replacement material work (the clinical results) at recent Bioceramics (Sydney, December 2002) and Australian Society of Biomaterials conferences (Brisbane, March 2003).

A recent visitor to the Department was **Dr. Ragina Patel** (nee Singh) who completed an MSc in Chemistry at Waikato in 1980 with **Lyndsay Main** before attending The University of Auckland for PhD study. After a career in California in both academic chemistry and industrial biotechnology, Ragina now runs a tutoring services agency from her home across the Golden Gate Bridge, and also produces "Chem Play" educational board games <see: www.chemplay.com> which have apparently been very successful in the US where, as she points out, children study chemistry at a much earlier age than in New Zealand.

In July, **Dr. Michèle Prinsep** was an invited speaker at a symposium at the National University of Singapore organised to honour natural products chemist **Professor Sim Keng Yeow** on the occasion of his retirement from the Chemistry Department.

Ex-student **Scott McIndoe** has moved from Cambridge University to a lectureship at Victoria University, British Columbia where he will continue to develop new applications in mass spectrometry.

Wade Mace has submitted his PhD thesis and is awaiting his oral examination.

The Chemistry Department at Waikato is happy to congratulate **Dr. Richard Coll** on his recent marriage in Fiji to Sandhya Devi Appana, a science teacher in Suva. Sandhya will be coming out to Hamilton to join Richard permanently at the end of the year.



Above: Dr. Richard Coll recently married Sandhya Devi Appana in Fiji.

WELLINGTON

The June meeting of the Branch, under the title *Conservation at Te Papa*, was a site visit to the Conservation Unit of Te Papa - Museum of New Zealand, in Tory Street. The visit took the form of three informal presentations by conservators following an introduction to the housing and work of the unit by **Gillian Andreae**. The group of 30 or so who attended were treated to an exceptional evening with some of New Zealand's treasures currently under the skilful care of this country's leading conservators.

Each conservator specialises in very different materials. Their knowledge and skill is based on an understanding of the materials they work with, and also on knowledge of the manufacture processes and the social/aesthetic values behind the various collection treasures they work with. At Te Papa conservators are an essential part of caring for the collections and preparing them for exhibition at Te Papa and at other museums/galleries around New Zealand and internationally. No item appears in an exhibition without it having been assessed by a conservator.

Valerie Carson, the textile conservator gave a show-and-tell about her work with fabrics illustrated by her current activity of preparing dresses worn by Dame Kiri Te Kanawa that are to appear in an exhibition at about the time this will be read. One aspect of her work is the percentage dyeing process she uses for renovations and restorations.

Lesley Cobb and **Carolina Izzo** provided the group with examples of their paintings conservation and in particular assessments of solvent-based polyurethanes as glazes in modern works. Rapid yellowing (within 10 years) due to oxidation in light and dark has been identified and the impact that this must have on acquisition and collection policies pointed out. **Matthew O'Reilly** described some of his work as a framer of paintings and conservator of frames. He showed us some of his work with an early 19th century Italian chestnut frame to compliment the work of Carolina and Lesley on the painting involved. Issues associated with pigment analysis on historic frames were discussed.

It is hoped that a more detailed article about their work will appear in a later issue of *Chemistry In New Zealand*.

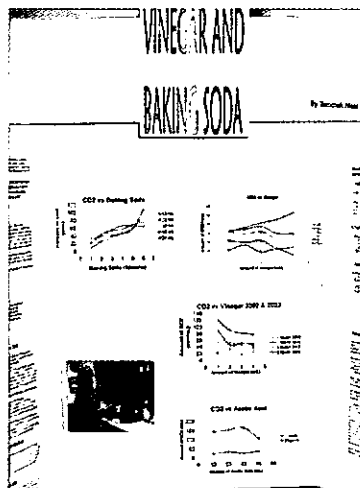
In July the topic of *Air pollution by airborne particles* was presented by **Perry Davy**, an Air Quality Scientist with the Greater Wellington Regional Council, responsible for the ambient air quality monitoring programme. He outlined the insidious health problems arising from 2–10 micron particles for which there is no known lower effect threshold, and some of which are carcinogenic. He described the Regional Council's monitoring programme, in which air is sampled and particles of various sizes collected on filters. These are weighed, to give total particulate matter, and the composition evaluated by elementary analysis using PLXIE (proton induced X-ray emission) at the IGNIS Gracefield laboratory. Recently Perry has also used neutron activation analysis at a reactor in South Korea. Elementary correlations, e.g. Al with Si and Na with Cl, indicate that the warm weather baseline particulate matter in Wellington is largely salt particles from the sea and soil-derived dust. In cold weather the particulate loading is greatly increased by sooty material and a correlation of carbon and potassium values indicates that this arises largely from the burning of plant material, in particular by wood burned in open fires and in inefficient wood-burning stoves. The development of inversion layers in valleys (Hutt and Wainuiomata) concentrates the pollutants and exacerbates the health problems. The contribution from traffic is localized to busy roads. He described air-flow modelling for the Wellington region which shows how local topography affects air movement.

The August meeting of the Branch, the **2003 Mellor Lecture** attracted the largest audience for many years, despite the day being cold, wet and wintry. **Professor Brian Halton** provided a survey of intermolecular attractions with *From electrostatic attraction to molecular machines* as his topic: Starting from the perception of electrostatic attraction between ions of opposite charge and the classical ionic lattice of sodium chloride he unravelled the chemistry that has revolutionised the modern discipline by way of charge transfer complexation and cation solvation that has seen the molecular machines evolve from concept to reality. Brian provided an excursion through the concepts of stabilization, molecular recognition and self-assembly, through to the molecular machines that have been reported in the very recent past. The lecture was very well received and its conclusion resulted in numerous plaudits.

The NIWA Wellington Regional Science and Technology Fair — 2003 took place at Victoria University during the last week of August using the facilities of the School of Chemical and Physical Sciences. Some 400 entries were set up for judging on Wednesday August 27 and public viewing for the remainder of the week. As seems to be unfortunately customary these days, few of the exhibits dealt with chemical issues. Nonetheless, those that did provided good insight and generally skilful measurements. The winning entries for the two Wellington Branch prizes are pictured and were:

Senior: *Hybrid Fuel Cells* by Arlo Armstrong-Kooy (Aeotea College)

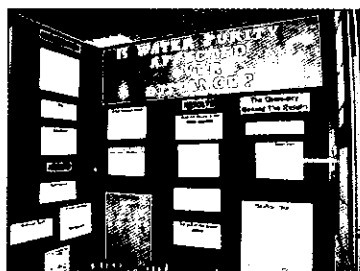
Junior: *Vinegar & Baking Soda* by Tamarah Neal (Paramate School)



Left: Tamarah Neal's NZIC Branch Prize winning entry, Junior Section - Wellington Science Fair.



Left: Arlo Armstrong-Kooy, NZIC Branch Prize winner, Senior Section - Wellington Science Fair.



Left: One of the many Wellington Science Fair entries.

The August/September period is a busy one for the Branch with the Wellington Science Fair and then the Branch Titration Competition and annual Chemistry Quiz Night. The titration competition was topical in that it involved standardising a solution of EDTA and then using that solution to determine the calcium carbonate content of a sample of the mud retrieved by NIWA from the ocean floor at a depth of 700 m. The winner was **Rachel Soja** (St. Orans College, Lower Hutt) and equal second were **Karl Dowland** (St. Patricks College, Wellington) and **Miriam Parwaiz** (Queen Margaret College, Wellington). The students had to weigh their sample, dissolve it, filter it, make up to 250 mL, and then titrate aliquots. Rachel not only got the expected answer, she was among the first to finish and calculated the results without assistance.

The Quiz Night featured some 128 students in teams of 4 from 14 colleges in the region including a team from Wairarapa College. The winners were a team called *Chemistry without Moro...nah!* from St. Patrick's College (Wellington) consisting of **Samer Hermiz**, **Kerry Cheung**, **Shane Swinerd** and **Adriaan Barnard**. In second place was *Captain McAwesome and His 23rd Armoured Funtime Chemistry Brigade* from Scot's College consisting of **Edward Chalmers**, **Reed Roberts**, **Richard Walker** and **Chris Westbury**. Third place getter was *Nigel the Return* from Heretaunga College consisting of **M. Rowney**, **Michelle Crosby**, **Angela Borowicz** and **William Laracy**. The Branch is indebted to staff, and particularly students, of Victoria University of Wellington, Chemistry for

organising what proved to be a highlight on the chemistry calendar. Sponsorship from Coca Cola, Hoyts Cinemas, McDonalds, Whitcoulls, and the Victoria University of Wellington Science Faculty is much appreciated.



Above: Wellington Chemistry Seniors Quiz Night.



Above: Economic No. 1.

Cawthron Institute

Registrations are filling fast for the *HABTech03 - Workshop on Marine Biotoxins (26-30 November 2003, Nelson)*. This APEC/MoRST sponsored event is being organised by Cawthron Institute immediately prior to the NZIC Conference. It is focussed on the latest technologies for detection and management of hazardous algal blooms and resulting contamination of water and seafood. Plenary lectures from a line-up of eminent international experts are combined with demonstration sessions on some of the latest techniques. This includes LC-MS, with Micromass/Waters loaning a Quattro-Micro TSQ to supplement the Cawthron Quattro-Ultima TSQ instrument.

Dr. Michael Quilliam (Institute for Marine Biosciences, NRC, Halifax) is taking a four month sabbatical at Cawthron. As well as assisting with HABTech03 he will be carrying out research on LC-MS of marine biotoxins. **Dr. Steve Kerr** (University of Otago) gave a lecture on the electrophysiology and neurotoxic effects of domoic acid and derivatives based on research using his innovative brain slice technique.

Olivier Laczka has returned to France after 4 months of Masters thesis project work with **Lesley Rhodes** on toxin production by the marine alga *Ostreopsis* and with **Doug Mountfort** on microbial biosensors. **Roel van Ginkel** and **Navreet Kaur** have joined the Biotoxin laboratory staff. Roel comes from Shell Research Centre, Netherlands and Navreet has a degree in Agricultural Chemistry from India.

Dr. Patrick Holland attended a workshop on the use of Receptor Binding Assay (RBA) in Trieste, Italy during

early September. The workshop was co-organized by the IAEA.

Industrial Research (Gracefield)

I have prompted locals to give some news. (My) only news here is that the inorganic chemists/materials scientist are beavering away writing FRST bids which are due in around September 15th. That's not much is it!

... but is better than nothing (*Editor*).

Victoria University

Recent visitors to the School have included the renowned crystallographer **Professor Roland Boese** (University of Essen) who has had a long-standing collaboration with **Professor Halton**. Apart from beneficial research discussion Roland spoke on the topic of *Crystal Engineering with Ethynyl Groups and Acetylene: From Molecular Complexes to Clathrates*. The elegant lecture provided an insight to 'whys and wherefores' of the deliberate construction of supramolecular motifs in the solid state, mostly using hydrogen bridges. Boese has successfully applied weak hydrogen bridges of the type $C-H \cdots X$ ($X=O, N$) with ethynyl groups and extended our experiences to the co-crystallisation of acetylene with various hydrogen acceptors. The excursion through crystal structures on such composites as acetylene-pyridine, the predictions, failures, and successes of crystal engineering culminated in a discussion of his latest results on gas hydrates - and here the commercial significance of natural gas pipeline blockages (methane-water crystallisation at temperatures of about 4 °C and 20 bar) becomes more than important!

Dr. John Hoberg has resigned his senior lectureship to take up an Associate Professorship at the University of Wyoming in Laramie. His five years at Victoria have seen the development of a strong group in biomedical research based upon sound organic synthesis.

It was announced on August 25 that the **Malaghan Institute** is to move to Victoria in early 2004. The Malaghan Institute is the only independent biomedical research facility in New Zealand with scientists involved in world-class research aimed to unravel the nature, origin and causes of cancer, asthma, multiple sclerosis and infectious diseases. The Memorandum of Understanding will see the Malaghan leave its rented premises at Wellington Hospital in Newtown early next year and move to Victoria's Kelburn campus.

Biotechnology is an area that the Government has placed great emphasis upon and Malaghan's work meshes neatly with Victoria's growing strength in biomedical research such that the association will strengthen and develop research collaborations between researchers in Victoria's science schools and those at the Malaghan and others working in biotechnology. It will also bolster Victoria's teaching in biomedical science, particularly the unique Bachelor of Biomedical Science programme.

Mr. Rob Keyzers (the student representative on the local Branch Committee for several years) has completed his PhD studies with **Dr. Peter Northcote** on marine natural products chemistry and is waiting to defend his thesis entitled *The Isolation of Biologically Active Secondary Metabolites from New Zealand Marine Organisms*.



Chemistry at the Interface

2003 Conference, Nelson
30 November – 4 December



NZIC Conference venue:
The Rutherford Hotel



Foyer Rutherford Hotel

Scope

This year's New Zealand Institute of Chemistry (NZIC) international conference focuses on 'Chemistry at the Interface'. It will explore a variety of the interfaces associated with chemistry, including:

- Synergy with materials science
- Commercial development
- Biology and drug discovery
- Interdisciplinary methodologies

On the following pages you will find a preliminary programme and the biographies of some of the key speakers

Venue

The Nelson region is an outstanding centre for recreation with beaches set in an area of native bush and sheltering mountain ranges, which give it a Mediterranean climate.

Registration

The conference registration fee for NZIC members and students are NZ\$450 and NZ\$190.

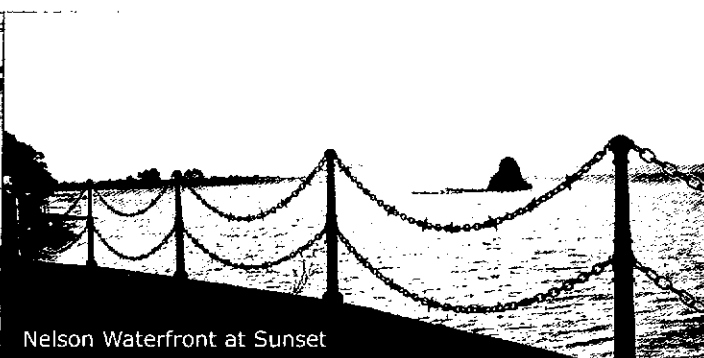
DEADLINE 15 SEPTEMBER 2003

Details for the conference are available from:

www.chem.canterbury.ac.nz/nzicconf03.htm

Invited Speakers

- Chris Abell (Cambridge)
Paul Clemons (Harvard)
Terry Collins (Carnegie Mellon University)
David Fairlie (Queensland)
Craig Hawker (IBM)
Cameron Kepert (Sydney)
Andy Phillips (Colorado)
Vickie McKee (Loughborough)
Dieter Seebach (ETH, Zürich)
John Tallarico (Harvard)
- Ted Baker (Auckland)
Mike Boland (Fonterra)
Margaret Brimble (Auckland)
Paul Callaghan (Victoria)
Bill Denny (Auckland)
Gary Evans (Industrial Research Ltd)
Shaun Hendy (Industrial Research Ltd)
Murray McEwan (Canterbury)
Kathryn McGrath (Otago)
Brian Nicholson (Waikato)
Warren Roper (Auckland)
Ian Shaw (ESR)
Rob Smith (Otago)
Peter Steel (Canterbury)
Carol Taylor (Massey)
Selwyn York (NZ Pharmaceuticals)



CONFERENCE PROGRAMME

TIME	SUNDAY 30 th Nov, 2003	MONDAY 1 st Dec, 2003	TUESDAY 2 nd Dec, 2003	WEDNESDAY 3 rd Dec, 2003	THURSDAY 4 th Dec, 2003
08.30		Plenary Lecture 2 SHAW	Plenary Lecture 5 BAKER	Plenary Lecture 8 KEPERT	Workshop
09.30		Plenary Lecture 3 COLLINS	Plenary Lecture 6 FAIRLIE	Plenary Lecture 9 CALLAGHAN	
10.00		Coffee Break	Coffee Break	Coffee Break	
10.30		Sympos A General	Sympos B Sympos C	Sympos D General Workshop	Coffee Break
11.00					
11.30					
12.00					
12.30					
13.00	Registration	LUNCH	LUNCH	LUNCH	LUNCH
13.30					
14.00			Plenary Lecture 7 PAUL CLEMONS JOHN TALLARICO	Plenary Lecture 10 HAWKER	
14.30					
15.00					
15.30					
16.00		Coffee Break	Coffee Break	Coffee Break	Coffee Break
16.30	WELCOME MIXER	Plenary Lecture 4 MCKEE		Plenary Lecture 11 C. ABELL	
17.00				Closing Ceremony	
17.30		POSTER SESSION I (Mixer)			
18.00	Opening Plenary Lecture 1 SEEBACH				
18.30					
19.00					
19.30					
20.00	Free for dinner		CONFERENCE BANQUET		
20.30					
21.00					
21.30					
22.00					

Symposium A – Interface of Chemistry and Biology; **Symposium B** – Techniques and Technologies of Chemistry at the Interface; **Symposium C** – Interface of Chemistry with the Commercial Sector; **Symposium D** – Interface of Chemistry with Materials and Nanotechnology.

The **Symposia** and **General Sessions** will run through the day and the **MacDiarmid Workshop** will run on the Wednesday and Thursday (details to be announced).

CHEMISTRY AT THE INTERFACE

The 2003 NZIC conference is to take place at the Rutherford Hotel in Nelson between November 30 and December 4 2003. There are **ten** conference plenary lecturers from overseas and **sixteen** New Zealand invited speakers. Time for contributed papers has been appropriately allocated. Conference information and a programme synopsis are produced separately for information. Here you will find details of the overseas plenary lecturers in the order that they are scheduled to speak as well as a pictorial appreciation of the venue and the Nelson environs.

Brian Halton
Editor

Professor Dieter Seebach

Dieter Seebach is Professor of Chemistry in the Laboratory of Organic Chemistry, the Chemistry Department of the Swiss Federal Institute of Technology (ETH) in Zürich, Switzerland. Born 1937 in Karlsruhe, Germany, as first child of Kurt Seebach, a teacher of ancient languages, and



his wife Erika, Dieter Seebach grew up and visited elementary schools in several small towns to which the family had been evacuated, in the turmoil of the last years of World War II. He then attended a classical-education secondary school in Karlsruhe, from which he graduated in 1956. Early on he developed an avid interest in

chemistry, converting the washhouse in his parent's home into a laboratory at the age of 14. Thus, it was with no hesitation that he chose to study chemistry at the Technische Hochschule and University of Karlsruhe, graduating in 1961, and receiving the doctoral degree in 1964 with a thesis on small-ring and peroxide chemistry, carried out under the supervision of **Rudolf Criegee**.

Dr. Seebach then moved to the United States (1965/66) for postdoctoral work with **Elias J. Corey** and then he joined the Harvard Chemistry Department in Cambridge, Massachusetts, as a lecturer. It was during this period that

a new synthetic method was developed, which is now referred to as the Corey-Seebach reaction.¹

After his return to Germany, Seebach started an independent university career in Karlsruhe, and he became a full professor of organic chemistry at the Justus-Liebig-University in Giessen in 1971 where he held the Liebig chair and was Director of the Institut für Organische Chemie, also chairing the department for one term, until 1977. In those years the principle of reactivity *umpolung* (now a chapter in organic-chemistry textbooks) was developed and demonstrated with numerous examples.² Research in the field of enantioselective synthesis started in Giessen (chiral solvents and additives, reductions with baker's yeast, tartaric acid as a chiral building block), and the term "chiral pool" was coined there. During this period Seebach held two half-year visiting professorships in the USA at the University of Wisconsin and the California Institute of Technology.

In 1977, Dr. Seebach was invited to ETH Zürich as successor to **Vlado Prelog**, who had won the Nobel prize two years before, in recognition of his contributions to stereochemistry. The team of strong colleagues (**Arigoni**, **Dunitz**, **Eschenmoser**, **Jeger**, **Oth**, and **Simon**) who researched and taught in the organic division, the superb spirit of the place, the equipment and research support, the excellent students of the institution, and the fruitful contacts with the pharmaceutical industry in Basel added up to an irresistible incentive for Seebach to move from Germany to Switzerland. Seebach has been at ETH ever since, also serving for two terms as head of the Laboratory for Organic Chemistry and for one term as Chairman of the Department of Chemistry.

During the first years in Zürich the interaction with the chemical crystallographer **Jack Dunitz** led to solid-state structure determinations of functionalized organolithium compounds (Li enolates, Li dithianes), and Seebach's group succeeded in identifying by NMR spectroscopy the species present in solutions of lithium derivatives (including so-called carbenoids) which are central to organic synthesis.³ Simultaneously, natural-product syntheses were performed (macrolides such as elaiophylidin, gloeosporon, myxovirescin), the work on oligo- and polyhydroxybutyrate (PHB) was started, the principle of self-regeneration of stereocentres (SRS)⁴ was recognized and executed with α - and β -amino- and -hydroxy-carboxylic acid derivatives, back-bone modifications of peptides were achieved, and a new class of chiral ligands, the TADDOLs, was invented which have turned out to be of general utility for syntheses of a variety of enantiomerically pure compounds.⁵

In recent years, the research interests of Dr. Seebach have been shifting towards bioorganic and supramolecular chemistry, as well as material science. Here the role of short-chain polyhydroxybutyrates in biology (ion-channels through planar or liposomal phospholipid bilayers) was demonstrated, establishing the existence of a fifth class of biomacromolecules (besides proteins, nucleic acids, polysaccharides, and polyisoprenoids).⁶ The structure of chiral dendrimers (molecules containing branches,

resembling those of trees) and their use for the synthesis of polymers with unusual properties, *c.f.* high-performance polymer-bound catalysts, are being studied.⁷ A most important new research area is the investigation of β -peptides, homologues and analogs of α -peptides and proteins, the functional molecules of life. Contrary to predictions and expectations of the community of peptide and protein specialists, it turns out that short-chain β -peptides form all the secondary structures (helices, sheets, turns) known to be formed by longer-chain α -peptides and proteins! Furthermore, β -peptides are totally stable to peptidases, and are therefore promising candidates for the development of new drugs.⁸

All these activities require a team of dedicated coworkers, as well as interdisciplinary collaborations, and they have led to numerous publications. The results obtained by the group have been described in *ca.* 750 papers and 145 PhD theses. In recognition of his achievements, Dr. Seebach was elected member of academies (*Deutsche Akademie der Naturforscher Leopoldina*, Halle; *Akademie der Wissenschaften und der Literatur*, Mainz, Germany; *Schweizerische Akademie der Technischen Wissenschaften*; *National Academy of Science*, Mexico), he received an honorary PhD degree from the *University of Montpellier*, France, and many awards were bestowed upon him, such as the *Karl-Ziegler-Preis* and *August-Wilhelm-von-Hofmann-Denkünze* (Gesellschaft Deutscher Chemiker), the *Centenary Lecture Award* (Royal Society of Chemistry, UK), the *Fluka Prize for the Reagent of the Year* and the *Marcel-Benoist-Preis* (Switzerland), the *King-Faisal International Prize in Science* (Saudi Arabia), the *Nagoya Gold Medal* (Japan), the *Award for Creative Work in Organic Synthesis* and the *Roger Adams Award in Organic Chemistry* (both of the American Chemical Society), and the *Tetrahedron Prize for Creativity in Organic Chemistry*.

Besides teaching, supervising research, writing papers, and serving the department, frequent travelling is a major task for Dr. Seebach, as for any scientist of our days; lectures on research results have to be given (over 850 so far), many of which involve whole series of presentations, such as the Japan Society for the Promotion of Science (JSPS) visit to Japan, the Korea Lectures (Seoul National University), the Andrews Lectures (University of New South Wales, Australia), the Rolf-Sammet Lectures (University of Frankfurt), and the Baker Lectures (Cornell University). In view of all the professional activities, there is little time left for the many hobbies Seebach has, but he is uncompromising about taking his daily swimming exercises, whenever and wherever possible.

Dr. Seebach lives in Zürich, within walking distance from his laboratories, with his wife Inge. They have two sons (Jörg and Lutz) and a daughter (Petra), ages 39, 32, and 35. The oldest son is a researcher at the University Hospital in Zürich, specializing in immune medicine, the youngest is also a medical doctor, and Petra owns a fashion company.

Selected publications

1. Gröbel, B.-T. and Seebach, D., *Umpolung of the Reactivity of Carbonyl Compounds Through Sulfur-*

- Containing Reagents, *Synthesis*, **1977**, 357-402.
2. Seebach, D., Methods of Reactivity Umpolung, *Angew. Chem., Int. Ed. Engl.*, **1979**, *18*, 239-258.
 3. Seebach, D., Structure, and Reactivity of Li-Enolates – From Pinacolone to Selective Alkylations of Peptides. Difficulties and Opportunities Offered by Complex Structures, *Angew. Chem., Int. Ed. Engl.*, **1988**, *27*, 1624-1654.
 4. Seebach, D.; Sting, A. R. and Hoffmann, M., Self-Regeneration of Stereocenters (SRS) – Applications, Limitations, and Abandonment of a Synthetic Principle, *Angew. Chem., Int. Ed. Engl.*, **1996**, *35*, 2708-2748.
 5. Seebach, D.; Beck, A. K. and Heckel, A., TADDOLs, Their Derivatives, and TADDOL Analogues: Versatile Chiral Auxiliaries, *Angew. Chem., Int. Ed.*, **2001**, *40*, 92-138.
 6. Seebach, D. and Fritz, M. G., Detection, synthesis, structure, and function of oligo(3-hydroxyalkanoates): contributions by synthetic organic chemists, *Int. J. Biol. Macromol.*, **1999**, *25*, 217-236.
 7. Seebach, D.; Rheiner, P. B.; Greiveldinger, G.; Butz, T. and Sellner, H., Chiral Dendrimers. In *Topics in Current Chemistry: Dendrimers*, F. Vögtle (Ed.), Springer Verlag: Berlin Heidelberg, Vol. 197, 125-164, 1998.
 8. Seebach, D.; Albert, M.; Arvidsson; Rueping, M. and Schreiber, J.V., From the Biopolymer PHB to Biological Investigations of Unnatural β - and γ -Peptides, *Chimia*, **2001**, *55*, 345-353; Seebach, D., Beck, A. K., Brenner, M., Gaul, C. and Heckel, A., From Synthetic Methods to γ -Peptides – From Chemistry to Biology, *Chimia*, **2001**, *55*, 831-838.

Professor Ian Shaw



Professor Ian Shaw is the National Food Safety Programme Manager at the Institute of Environmental Science & Research in Christchurch, an adjunct Professor in the Chemistry Department at the University of Canterbury, and a private consultant toxicologist. He obtained a 1st Class Honours

degree in Biochemistry from the University of Bath and gained his PhD in Biochemistry (Toxicology) at the University of Birmingham. He is a Fellow of the Royal Society of Chemistry, the Institute of Biology, and the New Zealand Institute of Chemistry and for two years served as a Justice of the Peace.

His various occupations have led him from the first UK lectureship in toxicology at University College London (1981–1985), to a short time in industry as Senior Clinical Scientist for Boehringer Ingelheim, a German Pharmaceuticals Company (1985–1987), to the Central Veterinary Laboratory where he became Head of the Biochemistry Department (1987–1992) and then to a Professorship in Toxicology at the University of Central Lancashire (1992–2000) before leaving the UK for a new life in New Zealand. He has been a member of many UK

committees and held a number of Honorary Positions, too many to list here, but these have included the Working Party on Natural Toxicants in Food, the Working Party on Veterinary Residues in Animal Products and the Advisory Committee on Pesticides. He was a Visiting Consultant Toxicologist to Preston Health Authority in the UK between 1995 and 2000. Until he moved to New Zealand he was a Member of the UK Government's Advisory Committee on Animal Feedstuffs and, despite his move, retained Chairmanship of the UK Government's Pesticide Residues Committee until December 2000.

He has been external examiner for the University of North London and the University of London, a member of the Royal Society of Chemistry's Applications and Examination Committee, and examined postgraduate theses for the Universities of Birmingham, East Anglia, North London and King's College London. He has written approximately 90 scientific articles, written for newspapers, and appeared on numerous TV and radio programmes. Latterly he has spent a significant amount of time (British Council funded) in Indonesia studying pesticides and their effects upon women and children. His principal research interest is human exposure principal to environmental estrogens and their potential pharmaceutical effects. He currently has seven postgraduate students in England, New Zealand, and Indonesia. He holds a patent for a test device for thiols in urine, co-authored the textbook, *Principles of Environmental Toxicology* (Taylor & Francis Ltd, London (1998)) which is soon to go into second edition, and his second book, *Is it Safe to Eat?* will be published in early 2004.

Professor Terry Collins

Professor Terry Collins is well known to the New Zealand scientific community as he was an invited lecturer at the last NZIC Conference and has published in this *Chemistry In New Zealand* (see *Chem. In NZ.*, **2001**, *65-3*, 15-17). He is the Thomas Lord Professor of Chemistry at Carnegie Mellon University where he directs the Institute for Green Oxidation Chemistry. He is also an Honorary Professor at The University of Auckland, New Zealand. He earned his BSc (1974), MSc (1975) and PhD (1978) degrees from The University of Auckland where his graduate advisor was **Professor Warren Roper**. After postdoctoral work at Stanford University with **Jim Collman**, he joined the faculty of Caltech in 1980 and the faculty of Carnegie Mellon University in 1987. Among his research awards are the 1998 Presidential Green Chemistry Challenge Award, the 1997 Award of the Japanese Society for Pure and Applied Coordination Chemistry, a Dreyfus Teacher-Scholar Award, and an Alfred P. Sloan Fellowship. Professor Collins has written and lectured widely on the possibilities before chemists to develop vibrant new economies to promote sustainability. His research program is focused on greening oxidation technologies by designing non-toxic catalysts for activating the natural oxidants hydrogen peroxide and oxygen for non-polluting oxidations. Professor Collins is currently the Associate Editor for the Americas of the journal *Green Chemistry*. He currently serves on the Editorial Advisory Board of *C&E News*. He is a Co-Chairperson of the annual Green

Chemistry and Engineering Conference held in Washington, DC at the time of the Presidential Awards Ceremony. He is the current Counsellor to the Gordon Conference Trustee Board for the Green Chemistry Gordon Conference. His catalyst design work has overlapped with the design of molecular magnetic compounds.

At the conference Professor Collins will present an overview of recent developments at Carnegie Mellon University's Institute for Green Oxidation Chemistry in catalyst design and technology development aimed at contributing to the development of sustainable chemical technologies. Eliminating the production of persistent bioaccumulative substances by industrial processes is a critical component of building a sustainable technology base. In oxidation chemistry, this requires green chemists to develop catalysts that usefully activate Nature's principal oxidizing agents, dioxygen and hydrogen peroxide, such that technologies relying on chlorine or metal-containing oxidants can be eliminated.

The address will describe a recent discovery that shows, for the first time, that Fe^{3+} ions can interact directly with dioxygen via coordination chemistry. The discovery has been made possible by the strong donor capacities and stabilities towards oxidative stress of certain TAMLs (patented activators developed by the Collins Group). The quantitative products are stable high valent m-oxodiiron(IV) complexes that have been isolated and structurally and electronically characterized. Substantial evidence from compound characterization further indicates that iron(IV) mono-oxoTAML radical cation complexes — two electron oxidation above the iron(III) state — are key intermediates in the formation and subsequent reactions of the iron(IV) dimers. The high valent species involved are also reactive oxidizing agents and several elementary catalytic oxidation processes employing dioxygen will be described.

The focus of the address will then move to catalytic disinfection processes. Integrating over all human suffering, by far the biggest component can be ascribed to ailments caused by water-borne pathogens. A new approach to water disinfection and to the decontamination of chemical and biological warfare and terrorism agents involving TAML activators will be described.

The broader sustainability context and central design lesson of the described work are as follows. As argued in New Zealand on a number of occasions, "sustainability" presents the most important field of ideas currently confronting universities. If we are going to achieve a sustainable civilization, chemists must undertake to solve the technological components of our present sustainability dilemma. The described work fits into a larger design context that has general significance to the development of other techniques and technologies within chemistry and more broadly at scientific interfaces that will promote sustainability. Simply put, by developing new technologies to move the elemental composition of the technology base closer to that of biochemistry, chemists can eliminate much of the pollution attributable to chemical technology.

Professor Vickie McKee

Professor Vickie McKee studied for her PhD with **Martin Nelson** at Queen's University, Belfast. After a postdoctoral position with **Professor Chris Reed** (a New Zealander) at the University of Southern California she accepted a lectureship at the University of Canterbury. This was followed by a Readership in Inorganic Chemistry at Queen's University, Belfast, and finally a move to Loughborough University where she is currently Professor of Inorganic Chemistry. Professor McKee has published widely and her work has resulted in a number of awards including the Richardson Medal for Chemistry (Queen's University, 1976), a Letts Studentship (Queen's University, 1976-9), and the NZIC Easterfield Medal in 1990.

Professor McKee's interests are focused primarily on synthetic and structural aspects of coordination chemistry, with particular emphasis on the use of geometric factors to control metal-metal interactions, and other properties in bi- or polymetallic systems. These find potential applications in fields ranging from bioinorganic chemistry to surface and solid state chemistry. Macrocyclic, cryptand, or related ligands provide frameworks inside which geometrically controlled arrays of metal ions can be constructed with predetermined properties. There are clear parallels between the constraints imposed on metal ions by synthetic ligands and those applied in protein metal binding sites and she has exploited this link to investigate bioinorganic model systems for manganese and copper metalloproteins. Control of redox potential is an essential feature of these systems and much of the fine tuning of redox properties appears to be achieved by the ability of the protein to impose particular geometric constraints on the metal centres. Recently, she has been investigating the subtle relationship between coordination geometry and redox level in complexes of manganese and other transition metals. The cooperative redox/geometry relationships seen in synthetic polynuclear manganese complexes have significant implications for the function of polymetallic biosites, such as the water-oxidising centre in Photosystem II. In related work with **Jane Nelson**, she has characterised a series of average valence $\text{Cu}(1.5)_2$ cryptates which are good spectroscopic models for the binuclear average-valence Cu_2 site in Cytochrome *c* Oxidase, and some other copper proteins.

Selected publications

1. McKee, V.; Nelson, J. and Town, R. M., Caged Oxoanions, *Chem. Soc. Rev.*, **2003**, 309-325.
2. Fontecha, J. B.; Goetz, S. and McKee, V., Di- Tri and Tetracopper(II) Complexes of a Pseudocalixarene Macrocyclic, *Angew. Chem., Int. Ed. Engl.*, **2002**, *41*, 4554-4556.
3. Cromie, S.; Launay, F. and McKee, V., Site-selectivity in a Heterotetranuclear Macrocyclic Complex, *Chem. Comm.*, **2001**, 1918-1919.
4. Dussart, Y.; Harding, C. J.; Dalgaard, P.; McKenzie, C.; Kadirvelraj, R.; McKee, V. and Nelson, J., Cascade Chemistry in Azacryptand Cages: Bridging Carbonates and Methylcarbonates, *J. Chem. Soc., Dalton Trans.*, **2002**, 1704-1713.

5. McCrea, J.; McKee, V.; Metcalfe, T.; Tandon, S. S. and Wikaira, J., Geometric Control of Redox Level in Tetranuclear Manganese and Cobalt Systems. *Inorg. Chim. Acta*, **2000**, *297*, 220-230.

Professor Ted Baker

Professor Ted Baker is a graduate of The University of Auckland Chemistry Department. After postdoctoral research at Oxford University, working with **Professor Dorothy Hodgkin** on the structure of insulin, he returned to establish New Zealand's first structural biology programme at Massey University. He is now Professor of Structural Biology at the University of Auckland, where he heads a lab of more than 30 researchers. Ted is a Fellow of the Royal Society of New Zealand, a winner of the Hector Medal as well as an International Research Scholar award from the Howard Hughes Medical Institute, and is currently Director of the Centres of Molecular Biodiscovery, one of the newly established Centres of Research Excellence (a CoRE). Current interests focus on experimental protein structure analysis and its applications to functional genomics and drug development, keeping a foot each in chemistry and biology.

Selected publications

1. Baker, H. M.; Anderson, B. F. and Baker, E. N., Dealing with iron: Common structural principles in proteins that transport iron and heme, *Proc. Natl. Acad. Sci. USA*, **2003**, *100*, 3579-3583.
2. McCarthy, A. A.; Baker, H. M.; Shewry, S. C.; Patchett, M. L. and Baker, E. N., Crystal structure of methylmalonyl-coenzyme A epimerase from *Propionibacterium shermanii*: a novel enzymatic function on an ancient metal-binding scaffold, *Structure*, **2001**, *9*, 637-646.
3. Kagawa, T. F.; Cooney, J. C.; Baker, H. M.; McSweeney, S.; Liu, M.; Gubba, S.; Musser, J. M. and Baker, E. N., Crystal structure of the zymogen form of the Group A streptococcus virulence factor SpeB: an integrin-binding cysteine protease, *Proc. Natl. Acad. Sci. USA*, **2000**, *97*, 2235-2240.
4. Paoli, M.; Anderson, B. F.; Baker, H. M.; Morgan, W. T.; Smith, A. and Baker, E. N., Crystal structure of haemopexin reveals a novel high-affinity haem site formed between two β -propeller domains, *Nature Struct. Biol.*, **1999**, *6*, 926-931.
5. Bewley, M. C.; Jeffrey, P. D.; Patchett, M. L.; Kanyo, Z. F. and Baker, E. N., Crystal structures of *Bacillus caldovelox* arginase in complex with substrate and inhibitors reveal new insights into activation, inhibition and catalysis in the arginase superfamily, *Structure*, **1999**, *7*, 435-448.

Professor David P. Fairlie

Since his PhD with **Greg Jackson** at the University of New South Wales, Professor David Fairlie has held research and teaching positions at nine Australian and North American Universities (Adelaide, ANU, NSW, Stanford, Toronto, WA, Bond, Griffith, Queensland). He is currently an ARC Australian Professorial Fellow at the University

of Queensland and in December 1999 he co-founded a startup company *Promics Pty. Ltd. (Brisbane)* based on discoveries in his laboratories. During the last five years he has attracted considerable industry funding and he has presented 90 conference papers, published 80 scientific papers in 5 branches of chemistry (organic, medicinal, biological, inorganic, theoretical) and 6 branches of biology (pharmacology, immunology, virology, parasitology, cancer biology, neurobiology), and filed 8 patents on chemical synthesis and anti-inflammatory, antitumour and antiviral drugs.

Professor Fairlie's research mainly addresses molecular mechanisms of chemical reactions, biological processes, disease development and drug action. Much of this work is strategic chemistry, focused currently on creating small molecules that structurally and functionally mimic bioactive surfaces of proteins. His group is also heavily involved in rational drug discovery using state-of-the-art methods and development of novel generic technologies towards new compounds that regulate enzymes, cellular receptors, RNA or DNA. Techniques used include computer-assisted molecular design, solution and solid phase organic synthesis, parallel synthesis methodologies, 2-D NMR spectroscopy and protein crystallography. The work is multidisciplinary and involves close association with pharmacologists, virologists, cancer biologists, and neurobiologists who study functional responses to compounds in models of human disease (inflammation, viral and parasitic infections, cancer, Alzheimer's disease). Some members of the group are also involved in enzyme and cellular assays, protein expression, target validation, and more basic chemical research in organic and coordination/organometallic chemistry.

Selected recent publications

1. Glenn M. P. *et al.*, Conformationally Homogeneous Cyclic Tetrapeptides : Useful Three-Dimensional Scaffolds, *J. Am. Chem. Soc.*, **2003**, *125*, 640-1.
2. Kelso, M. J. *et al.*, A Cyclic Metallopeptide That Induces Alpha Helicity In Short Peptide Fragments of Thermolysin, *Angew Chem., Int. Edn.* **2003**, *42*, 421-4.
3. Hansford, K. A. *et al.*, D-Tyrosine As A Chiral Precursor To Potent Inhibitors Of Human Non-Pancreatic Secretory Phospholipase A2 (IIa) With Anti-Inflammatory Activity, *ChemBioChem.*, **2003**, *4*, 181-5.
4. Reid, R. C. *et al.*, Conformationally Constrained Macrocycles That Mimic Tripeptide β -Strands In Water and Aprotic Solvents, *J. Am. Chem. Soc.*, **2002**, *124*, 5673-5683.
5. Singh, Y. *et al.*, Novel Conical, Cylindrical, and Macrocyclic Peptides From The Cyclooligomerization Of Thiazole Amino Acids, *J. Am. Chem. Soc.*, **2001**, *123*, 333-4.
6. Kelso, M. J. *et al.*, The First Solution Structure Of A Single Alpha Helical Turn. A Pentapeptide α -Helix Stabilised By A Metal Clip. *J. Am. Chem. Soc.*, **2000**, *122*, 10488-9.
7. Tyndall, J. D. A., *et al.*, Synthesis, Stability, Antiviral Activity, and Protease-Bound Structures of Substrate-Mimicking Constrained Macrocyclic Inhibitors of HIV-1 Protease. *J. Med. Chem.*, **2000**, *43*, 3495-3504.

Dr. Paul A. Clemons

Dr. Paul Clemons is an Institute Fellow at the Institute of Chemistry and Cell Biology at Harvard Medical School, and Head of Systematic Chemical Genetics in the Initiative for Chemical Genetics, a National Cancer Institute-sponsored program in the application of chemical genetics to basic research in cancer biology <see: <http://iccb.med.harvard.edu/systematics/index.htm>>. He received his BS in Biochemical and Biophysical Sciences at the University of Houston in 1995, and his MA and PhD in Molecular and Cellular Biology at Harvard University in 1997 and 2001, respectively. Dr. Clemons trained with **Professor Stuart L. Schreiber** as his PhD thesis advisor.

His research interests include the intrinsic chemical diversity of large collections of small molecules, the use of such small molecules to modulate biological processes in a cellular context, and multidimensional analysis of large datasets resulting from high-throughput and/or high-content screening of such small molecules. Of particular biological interest are signal transduction events along growth factor receptor signaling pathways, as well as differences in metabolic state between healthy cells and diseased cells. His one-bead, one-stock solution approach to chemical genetics (*Chem. Biol.*, 8, 1167-1195) is a technology platform capable of delivering thousands of novel small molecules, prepared by diversity-oriented organic synthesis (DOS), to hundreds of diverse biological assays. Applying principles of multidimensional data analysis reminiscent of genomics, he has begun systematically to explore the relationships between chemical structure and perturbations of intact biological networks. He has undertaken an experimental strategy, termed *library annotation*, designed to generate phenotypic "fingerprints" for novel small molecules using cell-based assays and he has also exposed several pilot "diversity sets" of small molecules to multiple, independent biological assays, and has devised an error-modelling strategy to render the results from different assays formally comparable. Of particular conceptual importance to his approach is the notion of the chemical genetic *modifier screen*, in which library compounds suppress or enhance the effects of small molecules with known mechanisms of action. Analysis of such experiments represents the chemical genetic equivalent of *epistasis analysis*, a powerful analytical technique in genetics. Combining the experimental approach of modifier screens with the analytical power of epistasis analysis underscores the strong theoretical relationship between genetics and chemical genetics. Present focus is on representing our experimental data in ways that can reveal properties of the underlying biological networks, and in representing *chemical diversity* in ways that allow feedback, in the form of global biological outcomes, to inform DOS at the library design stage.

Selected publications

1. Clemons, P. A.; Koehler, A. N.; Wagner, B. K.; Sprigings, T. G.; Spring, D. R.; King, R. W.; Schreiber, S. L. and Foley, M. A., A one-bead, one-stock solution approach to chemical genetics, Pt.2., *Chem. Biol.*, 2001, 8, 1183-1195.

2. Wagner, B. K. and Clemons, P. A., An even-handed approach, *Trends Biotech.*, 2001, 20, 53.
3. Clemons, P. A.; Gladstone, B. G.; Seth, A.; Chao, E. D.; Foley, M. A. and Schreiber, S. L., Synthesis of calcineurin-resistant derivatives of FK506 and selection of compensatory receptors, *Chem. Biol.*, 2002, 9, 49-61.
4. Wagner, B. K. and Clemons, P. A., Dual-purpose drug discovery, *Trends Biotech.*, 2002, 20, 492-493.
5. Wang, B.; Nguyen, M.; Breckenridge, D. G.; Stojanovic, M.; Clemons, P. A.; Kuppig, S. and Shore, G. C., Uncleaved BAP31 in association with A4 protein at the endoplasmic reticulum is an inhibitor of Fas-initiated release of cytochrome C from mitochondria, *J. Biol. Chem.*, 2003, web version: 15 Jan 2003.

Dr. John Tallarico

Dr. John Tallarico is currently Head of Chemical Technology and an Institute Fellow at the Harvard Institute of Chemistry and Cell Biology (ICCB) which is a joint initiative of Harvard Medical School and Harvard University where research is focused on developing the nascent field of chemical genetics.

Prior to this position, John received his BA in 1993 in chemistry from Miami University, Oxford, Ohio and PhD from Boston College (Massachusetts, USA) in organic chemistry in 1999. His postdoctoral studies were at Harvard Medical School and Harvard University as a Fellow of the Cancer Research Fund of the Damon Runyon-Walter Winchell Foundation under the guidance of **Professor Stuart L. Schreiber**. It was at this time that Dr. Tallarico began his work in the field of chemical genetics where he worked with a team of researchers to build the chemical technology platform central to the ICCB discovery efforts. His laboratory is specifically interested in the areas of diversity-oriented synthesis (DOS), solid support/linker chemistries and cheminformatics. His group is generally interested in using chemistry-based approaches to solve any problems faced by the field of chemical genetics.

Dr. Cameron J. Kepert



Dr. Cameron Kepert took up an academic position at the University of Sydney following a Junior Research Fellowship at the University of Oxford and degrees from the University of London (PhD) and the University of Western Australia (BSc(Hons)). His research is broadly centred on Materials

Chemistry, and focuses on a range of interests that include porosity on both the nano- and meso-scales, spin crossover, magnetism, electronic conductivity, negative thermal expansion and *in situ* diffraction techniques. He has co-authored two book sections, two international patents and more than 40 journal publications, and has recently been awarded the RACI Rennie Medal.

Dr. Kepert's research interests centre around molecular framework materials that are crystalline solids containing extended networks constructed by the linkage of metal atoms by multiply-coordinating ligands. Considerable interest has arisen in this area with the realisation that metal-organic framework synthesis offers considerable flexibility and control over structure and properties, thereby offering rare pathways to rational materials design. Dr Kepert's research has seen the discovery and characterisation of a wide range of unique and interesting framework materials:

- **Nanoporous phases:**¹⁻⁵

Molecular materials displaying reversible sorption and desorption of guest molecules. A particular highlight in this area has been the discovery of the first chiral nanoporous phases⁵ that have been shown to display chiral selectivity in their host-guest chemistry leading to potential application in enantioseparations. Other work has provided the first demonstrations that desorbed framework lattices may be robust enough to support large regions of complete void, thereby drawing a direct link with more conventional nanoporous materials such as zeolites.

- **Electronic and magnetic phases:**¹

The incorporation of atomic or molecular constituents with electronic or magnetic function, e.g. localised electrons, delocalised systems, redox-active species, etc., into molecular frameworks is being investigated with an aim towards constructing materials with novel electronic and magnetic properties. A highlight in this area has been the generation of nanoporous materials that switch between different electronic states in response to variation in the host-guest chemistry.¹ These materials have opened a new window into the investigation of the spin-crossover phenomenon and have possible application in a range of areas including molecular sensing.

- Molecular solids that display the rare phenomenon of negative thermal expansion (NTE), i.e. contraction upon warming.

Dr Kepert has also embarked on a major collaboration with Australian industry in the generation of nanomaterial-based technologies for the environmentally-friendly dispersion of agrochemicals.

Selected publications:

1. Halder, G. J.; Kepert, C. J.; Moubaraki, B.; Murray, K. S. and Cashion, J. D., Guest-Dependent Spin Crossover in a Nanoporous Molecular Framework Material, *Science*, **2002**, *298*, 1762-1765. {Perspective: Turnbull, M. M. and Landee, C. P., Porous Materials with a Difference, *Science*, **2002**, *298*, 1723-1724}.
2. Cussen, E. J.; Claridge, J. B.; Rosseinsky, M. J. and Kepert, C. J., Flexible Sorption and Transformation Behavior in a Microporous Metal-Organic Framework, *J. Am. Chem. Soc.*, **2002**, *124*, 9574-9581.
3. Fletcher, A. J.; Cussen, E. J.; Prior, T. J.; Rosseinsky, M. J.; Kepert, C. J. and Thomas, K. M., Adsorption Dynamics of Gases and Vapours on Ni₂(4,4'-bipyridine)₃(NO₃)₄: a Nanoporous Metal Organic Framework Material, *J. Am.*

Chem. Soc., **2001**, *123*, 10001-10011.

4. Rujiwatra, A.; Kepert, C. J.; Claridge, J. B.; Rosseinsky, M. J.; Kumagai, H. and Kurmoo, M., Layered Cobalt Hydroxysulfates with both Rigid and Flexible Organic Pillars: Synthesis, Structure, Porosity, and Cooperative Magnetism, *J. Am. Chem. Soc.*, **2001**, *123*, 10584-10594.
5. Kepert, C. J.; Prior, T. J. and Rosseinsky, M. J., A Versatile Family of Interconvertible Microporous Chiral Molecular Frameworks: The First Example of Ligand Control of Network Chirality, *J. Am. Chem. Soc.*, **2000**, *122*, 5158-5168.

Dr. Craig Jon Hawker



Dr. Craig Hawker carried out his PhD studies with **Professor Sir Alan Battersby** at the University of Cambridge (1985-1988) and followed that with a postdoctoral fellowship at Cornell University (**Professor J. M. J. Fréchet**; 1988-1990).

Dr. Hawker has received a number of awards and honours including: a Queen Elizabeth II Research Fellowship (University of Queensland), an Adjunct Professorship of Chemistry at the University of Queensland, the Bayer-Stein Lecturer (University of Massachusetts, Amherst, 2003), a Co-operative Research Award (American Chemical Society, 2003), a Whitby Memorial Lecturer (University of Akron, 2002), the Cornforth Lecturer (University of Sydney, 2002), the Melville Lecturer (University of Cambridge, 2002), an IBM Corporate Technical Recognition Award (2002), an S. Marvel Award in Creative Polymer Science (American Chemical Society, 2001), and the Young Scientists Award (IUPAC, 2000). Dr. Hawker is also the editor of a number of international journals and publications including the *Journal of Polymer Science*, *Polymer Bulletin*, *International Journal of Polymeric Materials*, *Chemistry of Materials*, *Macromolecules*, *Progress in Polymer Science* and *Polymer*. He also serves on a number of technical and advisory boards worldwide.

A primary focus of Dr. Hawker's research is the development of new synthetic techniques that address issues such as versatility and synthetic ease and the application of these techniques for the preparation of functionalized macromolecules with controlled architecture. Recent developments in the area of dendritic or 3-dimensional macromolecules has relied on novel 'Click' chemistry while the development of new living free radical polymerization methods utilizes the concept of reversible termination by stable free radicals such as nitroxides. These functionalized materials are then exploited in the general nanotechnology-materials science arena for the fabrication of surface-active structures for a variety of applications. Recent work has integrated fundamental studies with the development of nanostructured materials with advanced properties and functions in microelectronics and biotechnology.

Selected publications

1. von Werne, T. A.; Germack, D. S.; Hagberg, E. C.; Sheares, V. V.; Hawker, C. J. and Carter, K. R., A Versatile Method for Tuning the Chemistry and Size of Nanoscopic Features by Living Free Radical Polymerization, *J. Am. Chem. Soc.*, **2003**, *125*, 3831-3838.
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Professor Chris Abell



Professor Chris Abell studied for his PhD with **Jim Staunton**, working on the biosynthesis of aromatic polyketides. Together they introduced the use of the β -shift in ^{13}C NMR spectroscopy as a method for following the intact incorporation of a C-C-D unit in biosynthesis. Professor Abell then moved to Brown University as an SERC Nato Postdoctoral

Fellow to work with **Professor David Cane** on terpene cyclase enzymes. In 1984 he was appointed to a University Demonstratorship in Cambridge. At the same time he took up a Research Fellowship at King's College, Cambridge.

Professor Abell introduced molecular biology to the Chemistry Department, initially cloning porphyrin biosynthetic enzymes in collaboration with **Professor Alan Battersby**. His interest then turned to the shikimate pathway, where he exploited isotopically labelled, and fluorinated substrate analogues in studies on dehydroquinase and chorismate synthase. The Abell group was among the first to use electrospray mass spectrometry to detect intermediates in enzyme reactions. Since the mid 1990s he has collaborated with **Dr. Alison Smith** (Plant

Sciences) and **Professor Tom Blundell** on the study of the pantothenate (vitamin B5) pathway. Recently they completed the structural characterisation of all the enzymes on the pathway.

Through the 1990s part of the Abell group focused on developments in combinatorial chemistry in association with Zeneca Pharmaceuticals. Their efforts were focused on the development of linkers and a novel encoding strategy. This research led to an interest in nanotechnology and collaboration with **Dr Trevor Rayment**. Together they have shown how the Atomic Force Microscope can be used to detect chirality at a surface, to study enzyme-ligand interactions, and to create novel surface topographies. A recent collaboration with **Dr. David Klenerman** has exploited a nanopipet for creating submicron arrays of proteins and DNA.

Professor Abell's passion for enzyme structure and inhibition and his longstanding interest in drug discovery were key factors that led to him co-founding Astex Technology (1999) together with **Tom Blundell** and **Dr. Harren Jhoti**. In 2002, he co-founded Akubio (2002), a biosensor company exploiting rupture event scanning, a technique developed in Cambridge in collaboration with **Dr. David Klenerman**, **Dr. Victor Ostanin** and **Dr. Matt Cooper**.

Professor Abell has received the RSC Hickinbottom Award and the ICI Research Award in Organic Chemistry. He has held visiting professorships in Christchurch, Santiago de Compostela, and the Australian National University. He is the Professor of Biological Chemistry in the University of Cambridge, and the Todd Hameid Fellow at Christ's College. His current research is focused on novel approaches for the design of enzyme inhibitors, and exploiting biological systems in nanotechnology.

Selected publications

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CONTENT, CONCEPT, CONTEXT

Which Order In A Chemistry Course?

Kath Fletcher ^a

^a Kath Fletcher is a self-employed consultant and course facilitator. She retired from her position as HoD Science at Central Hawke's Bay College, Waipukurau in 2001.

Introduction

This article describes the use of an investigative, integrated, flexible, and real-world approach to the teaching of Chemistry and Science in a New Zealand secondary school. It also looks briefly at some research in the field of inquiry learning and constructivism. The writer learned Chemistry, as most readers of this journal will also have done, from teachers and lecturers who told the facts, expounded the laws and principles, and expected their students to show by a written examination only, that they had been learned. There was no opportunity at either school or in the BSc degree structure for independent student investigation unless an honours programme was undertaken. Has this really changed?

Teaching in everyday contexts

In the early 1980s I became inspired to teach Chemistry in the context of the student's everyday world. How boring for students at the start of their first real chemistry course to begin with "The Structure of the Atom" I thought, yet that is how most courses began. Why did students choose Chemistry as a subject? Certainly not to be exposed to the intricacies of sub-atomic particles before they had any experiences of how substances behaved.

Most traditional textbooks began with this topic and many still do. I found one¹ with chapters entitled, *The Air We Breathe – Even If It Chokes Us*, *The Water We Drink - And Dump Our Wastes In*, and *Chemistry Toxicology – From Hemlock To Heroin*, etc.

The hardness of local water supplies, newspaper reports of high nitrate levels in local streams, and the hot February weather with options for swimming at the local beaches, town and home swimming pools or the rivers led straight into the study of water and solutions. Simple volumetric analysis and conductivity experiments to compare water samples brought in by students from villages and farms made Chemistry relevant to their own lives. They soon learned about compounds, ions, atoms, solubility and precipitation, etc., on a "need to know" basis.

Therefore I set out along the contextual, investigative science route without knowledge of any research in this area. Over the next 20 years of my teaching career I used this approach for many but not all topics in Chemistry and Science classes at all levels in the secondary school system.

Half a century ago, high school courses in the separate sciences were centred on the *discipline* — a structure of great power and beauty — and they brought in as examples only those that could be simply explained by using conventional scientific arguments. Textbooks focused on

presenting scientific principles and concepts in a linear fashion. Applications, if they were included at all, were generally placed near the end of each chapter.

In the mid-1960s, when I started teaching, projects supported by the Nuffield Foundation in Britain and the National Science Foundation in the USA attempted to reform the teaching of science. Very soon after these projects got under way, but too late to influence them, David Ausubel presented² an alternative perspective of learning — the distinction between *meaningful* and *rote* learning:

"To learn meaningfully, individuals must choose to relate new knowledge to relevant concepts and propositions they already know. In rote learning new knowledge may be acquired simply by verbatim memorisation and arbitrarily incorporated into a person's knowledge structure without interacting with what is already there."

He also states:

"If I had to reduce all of educational psychology to just one principle I would say this: The most important single factor influencing learning is what the learner already knows."

In the late 1980s a review of curricula in many countries identified an approach to teaching the sciences through the everyday experiences of the students. Two of these were the *ChemCom* project in the USA and the work of the Salter's Group³ at the University of York. The latter groups' contextual philosophy stated:

"Students should approach their studies through work related to familiar everyday situations, materials or issues. Considerable care is taken to encourage a wide variety of teaching and learning activities. These should encourage not only the learning of facts and principles but also investigational skills, general study skills and the personal and social skills required for exchange of scientific ideas with others."

More recent research into preferred contexts and reasons for choosing them showed that students selected *Everyday Life*, *Living Things*, and *Sports* contexts as the most preferred ones and the *laboratory context* as very clearly the least favoured one.⁴ The most important factors affecting students' selections of contexts were their relevance to their real-life activities (positive effect) and their similarity to school text-books (negative effect). They selected preferred contexts for affective reasons such as being enjoyable rather than for cognitive reasons such as being easy to understand. However, students should learn not only concepts with such examples but also they should

be given some opportunity to practise their formal thinking in abstract situations. Before I had read any research on this topic I had already written in my Department Scheme that contexts should:

- Not be limited to the direct daily environment of the student but should increase the range of scope for the student.
- Provide opportunities for challenging lessons.
- Indicate the role of science in everyday life.
- Be equally distributed over areas of reality in everyday life, e.g. living, energy, food and nutrition, health, work, leisure, and recreation.
- Stimulate the cognitive development of the student.

The real advantage, I believe, in using contexts in the real world of the student is that it encourages teachers to become facilitators of learning. There is a shift from teaching by imposition to teaching by negotiation. However, I agree with Coll and Taylor⁵ that there is no point in trying to teach by negotiation something that is so well agreed upon by teachers and scientists that it may as well be a fact.

Inquiry Learning and Constructivism

Inquiry learning in its purest form is one in which the student is the centre of attention and where the teacher does not review the need for additional information or demonstrate an alternative method to gain needed information.⁶ Constructivism broadly supposes that knowledge is actively constructed by learners through their interaction with physical phenomena and interpersonal exchanges.⁷ It is claimed that constructivist ideas have had a major influence on science educators over the last decade.⁸ Classroom teachers have to cover the curriculum but:

There are times when teachers must perforce be didactic and say what pupils should do in order to achieve certain aims. However, it is a matter of balance and the range of teaching strategies and techniques must vary across a wide spectrum, from overt classroom control to covert conceptual change and back again. While there must be room for input, exposition, explanation, demonstration, description, direction, reference, showing, modelling, and so on, the overall balance must be towards teaching-as-managing, not teaching-as-telling.

The National Curriculum of New Zealand- *A Discussion Document* made the following claim:⁹

The National Curriculum will provide for flexibility, enabling teachers to design appropriate programmes to meet the learning objectives and to adapt their programmes to changing social and economic needs and to the needs of their students.

Chemistry in some schools and tertiary institutions is still taught solely by using a three-step process:¹⁰

1. The teacher or lecturer introduces the content verbally.
2. A 'cookbook' activity is used to illustrate and verify the new content.
3. Students practice the new content by working through relevant problems, questions, or an activity structured by the teacher.

By changing the order of this traditional approach teachers in secondary schools can gradually change to a new inquiry-based learning approach for some curriculum topics. The plan might be:

1. The exploratory phase — where students have relevant and concrete experiences in the laboratory. Students then plan an investigation to answer the question posed. In this they also plan how they are going to communicate their results.
2. The content phase — where students are introduced more explicitly to the science concepts.
3. The application phase — where students apply what they have learned to a new situation.

Is this not "Scientific Method" as used by researchers, viz. **OBSERVE** ⇒ **GENERALISE** ⇒ **THEORISE** ⇒ **TEST** ⇒ **RETEST** ⇒ **REPORT**? So rather than losing the scientific method, I believe that inquiry learning, which starts with observation, is reinforcing it by teaching science in the way that science is "done". The activities chosen should force the students to ask "Why?".

Various methods can be used to make observations and to collect data:

- Trial and error — "Let's do some experiments and see what happens".
- A demonstration of a "discrepant event" may be used to start the thinking.
- Planned research.
- Accident or luck.

The simplified scientific method, which can be followed even in Primary School Science is:

- What is the question I want to answer?
- What do I think the answer is?
- What will I have to measure to find out?
- What other things will I have to keep constant?
- Should I repeat the investigation to be sure of my results?
- How can I explain my results?
- How will I tell people about it?
- Is there a different explanation?
- Have I found ideas for further investigation?

The National Science Education Standards for the USA¹¹ has an inquiry standard as the first of the content standards and a list of fundamental student abilities for inquiry learning at grades 9-12.

Keeping it all in perspective

In the last decade at least, some students moving on to tertiary institutions from a number of New Zealand secondary schools have become used to carrying out their own extended investigations at the different levels of the school system. Now, with the introduction of the NCEA and standards based assessment of student practical investigations in all of the science disciplines, *most* science students from *all* secondary schools will take with them a grade which describes their level of achievement in the important field of investigative science. Those students who achieve with excellence in the Level 3 Achievement

Standards, and especially those who gain the Scholarship Standard in the future, will have demonstrated a high level of critical thinking and application of ideas.

The challenge I believe is for the tertiary sector to build on the skills the students have acquired. Many would deem this to be impossible in the huge classes in first year Chemistry. That may well be so. However, the occasional unexplained demonstration in a lecture, a problem-solving laboratory exercise or two where the right answer is not as important as the process used, may well keep these skills alive in students. An assignment requiring analysis of given information or one which requires the student to find research information and summarise it, may take more time to mark than the traditional laboratory recipe-type experiments but more information about what the student understands will be gained.

I have heard many a supervisor of honours students complain that the fourth-year students cannot plan their research projects, they cannot write coherent reports or present seminars. In the past, science students may not have arrived with any experience or expertise in these areas. That will very soon be no excuse! Will these important skills be ignored until the fourth year of a degree or will they be nurtured and improved upon in the undergraduate courses?

To all teachers at all levels I would say—be flexible in the sequence of teaching, flexible in the activities you choose, vary your teaching strategies, challenge your students to higher level thinking, and do it all with enthusiasm.

Edward B. Butler, an American scientist said: "One man has enthusiasm for 30 minutes, another for 30 days, but it is the man who has it for 30 years who makes a success of his life".

References

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MINUTES OF THE 18TH NEW ZEALAND GEOCHEMICAL GROUP BIENNIAL GENERAL MEETING

8 July 2003, Edward Percival Station, Kaikoura

Meeting started at 2:00 pm

President: Ed Mroczek

Secretary: Catherine Chague-Goff

Attendees

Ed Mroczek, Catherine Chague-Goff, Doug Sheppard, Graeme Lyon, Jonathan Kim, Dick Glover, Nigel Newman, Kevin Brown, Jenny Webster-Brown, Chris Hendy, Donna Falconer, Rebecca Bibby, Andrew Cook, Kenichi Fukuda

Apologies

Kerry Webster

Minutes of the previous meeting were read but it was agreed that they would be accepted only after correction. We wish to apologise to Dr R. M. Carr for the error reported in the minutes of the 2001 BGM. The discussion on the Whakatane conference travel expenses should not have mentioned Mel Carr and did not relate in any way to his

attendance. Subject to this correction, the minutes were accepted (Doug Sheppard/Graeme Lyon).

It should also be noted that Graeme's name was misspelt (as Graham) in the previous minutes (in the minutes book only), but he didn't make a big fuss about it. However, it should be corrected.

Matters arising from previous minutes

1. Mineralogical Society: to be discussed under general business.
2. No other matters arising.

President's report (by Ed Mroczek)

The job of the President is very much a sleeping one till approximately 6 months out from the next conference when the job of organising the next biennial conference begins. This job is however made easier by help from colleagues, which spreads the load. However, for the day to day operation of the society I would like to thank Graeme Lyon for regularly producing our newsletter, Richard Glover for diligently looking after the financial aspects and Liz Kennedy for maintaining our website.

There is always one issue to consider, the need for all of us to be more proactive and support the Editor in his thankless task of producing the newsletter. Perhaps we could discuss a system for sharing the responsibility across a wider circle for writing the odd article or news on topical geochemical issues relevant to New Zealand and the wider world as was suggested by Jenny Webster-Brown in her report in 2001.

When reviewing the beginnings of the society it is clear that the reason for our "success" is an interest in each other's work and of course always choosing interesting places to hold our conference. In this time of decreasing interest but increasing suspicion of science we can show the relevance of our discipline to New Zealand (and increase our funding!). However we have to spread the word and how we do this is up to us. Another issue in this regard is our very small subscription fee. I would like this to be increased so that we can do more for the membership and in turn attract more members, who then see the benefit of being part of the Group.

(Comment from the floor to the effect that people choose to go to more prestigious conferences. Hint for the next conference: to have it at the Millbrook Resort, Queenstown, then we'll definitely have to increase the conference fees).

There was some suggestion about changing the time to October-November, as July is not a good time. Uproar from the floor, as this would mean no students would be able to attend. July is perfect for a field trip, since there is no teaching. After all that, it was decided that we couldn't decide on the date now and that it was left to the next President to sort that out.

President's report accepted (Graeme Lyon/Chris Hendy).

Treasurer's report

Dick Glover presented the accounts (see attached). There was a loss at the last conference in Leigh. The Past President indicated that she would have liked to get the balance a bit sooner (instead of finding out at this conference). Dick Glover noted that the financial statement is dated to the 28 February - this keeps this year's conference out of the balance sheet. Four newsletters were sent and it costs less because a number of them are now sent by email. Dick was thanked for his hard work.

The adoption of the financial statement was moved by Doug Sheppard, and agreed to.

Dick will organise a monthly automatic transfer to the Serious Saver account, as we can obtain higher interest rates. There were some discussions about conference subscriptions, but it will be reported later under general business, so as not to disrupt the order of the reporting and confuse the Secretary.

Elections

President	Chris Hendy (nominated by Ed Mroczek, since Chris had suggested that he would organise the next conference) carried with tumultuous applause and relief from the audience.
Secretary	Catherine Chague-Goff (nominated by Ed Mroczek, seconded by Doug Sheppard).
Treasurer	Richard Glover (nominated by Ed Mroczek, seconded by Catherine Chague-Goff).
Editor in chief	Graeme Lyon (nominated by Jenny Webster Brown, seconded by Kevin Brown).

Assistant Editor Doug Sheppard (volunteer) seconded by Graeme Lyon. Nigel Newman suggested there should be corresponding members to contribute to the newsletter.

Auditor Mike Stewart (nominated by Dick Glover, seconded by all).

Committee members Nigel Newman (Christchurch), Jonathan Kim (Dunedin), Doug Sheppard and Graeme Lyon (Wellington), Ed Mroczek (Wairakei), Kevin Brown (Auckland South), Kerry Webster (Auckland North).

Signatories for the NZGG accounts: Dick Glover, Ed Mroczek, Kerry Webster, Mike Crump.

General business

Subscription rates

There was quite a long and heated discussion about whether to increase the rates or leave them as they are (I think I have heard that story before), so I will spare you the details of the debate. The motion that the incoming committee could consider revising the subscription rates was passed despite considerable uproar from the floor (well, only three members, but they made as much noise as the rest).

Royal Society

There has been no response from the notice put in the Royal Society of New Zealand email about the conference. It was also advertised in the Globe (published by GNS). Chris Hendy will write a report about the conference and send it to the Royal Society. Catherine Chague-Goff proposed to write a short report for Water & Atmosphere (published by NIWA).

Amalgamation with the Mineralogical Society

Graeme Lyon read the letter from Warren Dickinson (on behalf of the Mineralogical Society), as Rodney Grapes left New Zealand some time ago. The Mineralogical Society has a very small membership (47) and very little money.

Moved: That Graeme Lyon should send an email to Warren Dickinson and suggest that the New Zealand Geochemical Group incorporates the members of the Mineralogical Society (instead of having both societies merging).

Moved by Kevin Brown, seconded by Doug Sheppard. It was considered that a name change could be made in the future, but in the meantime the newsletter would have a subtitle referring to any inclusion of the Mineralogical Society.

The members of the Mineralogical Society could join the NZGG (and of course pay subscriptions - Dick Glover who had remained quiet for a while suddenly showed great interest and got his calculator out).

The motion was agreed to by the meeting.

Graeme will send a copy of the next two newsletters to all members of the Mineralogical Society.

Next conference

To be held in about two years time, probably in Orakei Korako, to be organised by Chris Hendy (who will determine the exact details of the conference).

Meeting closed at 3:05 pm

Conferences & Seminars

2-3 October 2003

Scitech03, Conference For Laboratory Technicians
Eastern Institute of Technology, Taradale, Hawke's Bay
Convenor: Kay Memmott: Kay@hnhs.school.nz

9-10 October 2003

Rotorua Lakes Public Symposium
Centra Hotel, Rotorua
Contact: Rotorua Lakes 2003
P O Box 2008, Rotorua
Fax: (07) 362 4701
Website: <http://www.rotorua.rsnz.org>

13-15 October 2003

5th Annual Conference Of The Australasian Research Management Society
Sheraton Hotel, Auckland
Contact: Greg Pringle: gpringle@unitec.ac.nz

13-16 October 2003

Lifting R&D Performance - Australasian Best Practice
Website: <http://www.cmsl.co.nz/arms03/>

14-15 October 2003

Large Scale Chromatography
Marriott Long Wharf, Boston, USA
To register visit: http://www.scientificupdate.co.uk/confs/chroma/chroma_reg.html

16 October 2003

Commonwealth Study Conference In Australia And New Zealand
www.csc2003.org

20-23 October 2003

Tenth Asian Chemical Congress (10 ACC 2003)
Joint Conference With Eighth Eurasia Conference On Chemical Sciences (EuAsC₂S-8)
Hanoi, Vietnam
Contact: Professor Dr Huynh Van Trung

21-22 October 2003

CHIRAL USA 2003 Conference And Exhibition
InterContinental Hotel, Chicago, USA

21-23 October 2003

NZ Institute Of Hazardous Substances Management Annual Conference
Theme: "Globally Harmonised and Ready for Business"
Pacific Park Hotel and Conference Centre, Dunedin
Email: ralexand@dcc.govt.nz

23 October 2003

"I Met A Traveller From An Antique Land" Genetics As History By Professor Bryan Sykes
5.30 p.m. St David Lecture Theatre, University of Otago
Cumberland Street, Dunedin
Tickets: sykesdunedin@rsnz.org

22-24 October 2003

Greening The City: Bringing Biodiversity Back Into The Urban Environment
Conference Of The Royal New Zealand Institute Of Horticulture (In Association With the CCC, ECan, Landcare Research and PGG)
Chateau on the Park, Christchurch
Email: d&amoyle@xtra.co.nz
Web: <http://www.mzih.org.nz/pages/conference2003.htm>

3-4 November 2003

Integrated Catchment Management National Workshop
WEL Energy Trust Academy of Performing Arts, University of Waikato, Hamilton
Contact: Nick Edgar
Phone: (04) 977 2524
Email: nick@landcare.org.nz

5-6 November 2003

Preparation, Management And Exploitation Of Biotech And Life Science Patents
Wellington
Download conference brochure at
http://www.lifesciencesnetwork.com/repository/sem_brochure.pdf
Conferenz website: www.conferenz.co.nz

6 November 2003

"I Met A Traveller From An Antique Land" Genetics As History By Professor Bryan Sykes
8.00 p.m. A1 Lecture Theatre, University of Canterbury
Entrance off Creyke Road, Christchurch.
Tickets: sykeschristchurch@rsnz.org

6-7 November 2003

Nutrition Society Of New Zealand Annual Conference "Too Little, Too Much"
Dunedin Public Art Gallery, Dunedin
Contact: tim.green@stonebow.otago.ac.nz

11 November 2003

"I Met A Traveller From An Antique Land" Genetics As History By Professor Bryan Sykes
7.30 p.m. School of Music, 48 Nile Street, Nelson
Tickets: sykesnelson@rsnz.org

13 & 14 November 2003

Preperation, Management And Exploration Of Biotech And Life Science Patents
Auckland
Download conference brochure at:
http://www.lifesciencesnetwork.com/repository/sem_brochure.pdf
Conferenz website: www.conferenz.co.nz

12 November 2003

Royal Society Of New Zealand Fellows' Annual General Meeting, New Fellows' Seminar, and Fellows' Dinner

Auckland
gill.sutherland@rsnz.org

13-14 November 2003

"Fresh Water New Zealand: Problems, Processes And Priorities."

Royal Society of New Zealand Conference
AUT, Auckland
gill.sutherland@rsnz.org

13-15 November 2003

Conference In Honour Of Keith Pavitt "What Do We Know About Innovation"

University of Sussex, United Kingdom
http://www.sussex.ac.uk/spru/events/KP_Conf_03/

17 November 2003

"I Met A Traveller From An Antique Land" Genetics As History By Professor Bryan Sykes

7.00 p.m. Soundings Theatre, Te Papa, Wellington
Tickets: sykeswellington@rsnz.org

18 November 2003

"I Met A Traveller From An Antique Land" Genetics As History By Professor Bryan Sykes

5.30 p.m. refreshments served from 5.00 p.m.
Japanese Lecture Theatre, Massey University, Palmerston North
Tickets: sykespalmerston@rsnz.org

17-19 November 2003

Sustainable Business Network Conference

Aotea Centre, Auckland
See <http://www.sustainable.org.nz/conference2003>

18-21 November 2003

New Zealand Hydrological Society Annual Conference

Taupo, New Zealand

23-27 November 2003

Fourth Southern Hemisphere Symposium On Undergraduate Mathematics Teaching, Delta '03

Rydgcs, Queenstown
igoodwin@maths.otago.ac.nz
<http://www.maths.otago.ac.nz>

24-28 November 2003

DNA Technology Workshop: An Introduction To The Theory And Practice Of DNA Technology

Massey University, Palmerston North
Information and enrolment: <http://imbs.massey.ac.nz/workshop.htm>

26-28 November 2003

The Meteorological Society Of New Zealand Inc. 24th Annual Conference

Christchurch
Contact: r.turner@niwa.co.nz
Website: <http://www.metsoc.rsnz.org>

27-29 November 2003

Deep-Sea Chondrichthyan Fish Conservation And Management Meeting

University of Otago, Dunedin
Website: <http://www.deepsea.govt.nz/legal/pre-conference.asp>

30 November - 4 December

NZIC Chemistry At The Interface

Rutherford Hotel, Nelson
Website: www.chem.canterbury.ac.nz/nzicconf03.htm

1-4 December 2003

Geological Society Conference

Website: <http://www.gsnz.org.nz>

1-5 December 2003

3rd International Wildlife Management Congress

Christchurch, New Zealand
www.conference.canterbury.nz/wildlife2003

1-5 December 2003

Deep Sea Conference

Queenstown
Website: <http://www.deepsea.govt.nz>

1-5 December 2003

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Website: <http://limsoc.rsnz.org/Limsoc%20conference2002.htm>

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Royal Society Council Meeting

Wellington

19-23 January 2004

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Cape Town, South Africa
Contact: Mrs Elizabeth Danckwerts (Secretariat)
SC2004@botzoo.uct.ac.za
<http://www.uct.ac.za/conferences/sc2004>

26-30 January 2004

Mathematics In Industry Workshop

The University of Auckland (City campus), Auckland
g.c.wake@massey.ac.nz

5 - 8 April 2004

2004 Entomological Society Of New Zealand Conference

Contact: Richard Harris
Email: harrisr@landcareresearch.co.nz
<http://www.ento.org.nz>

19-23 April 2004

The 4th International Conference On "Applications Of Stable Isotope Techniques To Ecological Studies"

Museum of New Zealand Te Papa Tongarewa, Wellington
See <http://207.195.94.13/isoecol/>

Recollections of 'Paradise'*

K. R. Webb¹

The following article came to the attention of the Editor as an alumnus of Southampton University. The charming and delightful prose that so elegantly describes the undergraduate laboratory of ca. 1940 is reproduced here for the senior members of the Institute to reminisce, and for the younger generation to gain insight to 'how it was done' in the dark ages!

Brian Halton
Editor

*Reproduced (with minor editorial revisions and the addition of a few notes) from the *Journal of the Southampton University Chemical Society*, 1964, 21 (with permission).

In the early 1940s Chemistry at the University College, Southampton (as it then was) consisted of two so-called semi-permanent single-storey brick structures, two extremely rickety and dilapidated wooden army huts which stood 'out in the fields', and two lecture rooms plus a small preparation room, in the main University building. In 1964, at the time that this was written, the two brick buildings remained and Engineering used the westernmost one. Formerly it accommodated the Physical Chemistry teaching laboratory, two small research laboratories, a dark room and the Departmental library which, during one terrible night in World War II, was invaded by hungry rats who gnawed several volumes of *Trans. Faraday Soc.* and badly savaged a little monograph on the cyclotron – but all that is another story!

The other brick hut was the main chemistry laboratory (Inorganic and Organic), and also contained two stores, a tiny fume room, a balance room, Professor Adam's private sanctum² (also used as a staff tea room!) and two small, more or less private rooms in which Organic members of staff carried out their researches, using also one or two benches at the back of the main laboratory, as space allowed, for similar purposes. This building still stands, and has now been divided, after redecoration and some modernisation, between Physiology and Bio-chemistry, and Zoology.³ Beneath it was a small, mysterious, gloomy crypt, used for storing acids and solvents.

The two wooden huts now claim our attention. One, which was by this time used only as a store for glassware etc., was still grandly called 'the Research Hut'. It had earlier been used for just that purpose by physical chemists. The other was the junior laboratory – more often called 'the Inter. Hut', and it is of its delights and horrors that we must now speak. Perhaps a point should first be made that in those days a one-year course (the so-called Intermediate BSc course) was provided in most departments of the old University College for students who had left school after taking the equivalent of 'O' level, and were, therefore, really doing an 'A' level course in one year. At that time, the sixth forms of many schools were much smaller, or less well developed, than now, so this Intermediate course was definitely useful. It also served as a revision course

for people who had failed the Higher Certificate examination, i.e. 'A' level. In addition to pure scientists, the Chemistry Inter. group often included students doing First MB, or the Intermediate examination of the Pharmaceutical Society and, in later years, some Engineers who had to qualify in Intermediate Chemistry.

Let us now take down in imagination the rusty old key of the Inter. Hut and in Mr. Balson's well-remembered phrase 'open up them Pearly Gates'.

The hut consisted of a fair sized laboratory fitted with very ancient but solid benches that had been brought up from the old Hartley College in High Street. These benches were fitted with curious round sinks, each having a massive porcelain plug stopper so that the sink could be used as a pneumatic trough. There were also two small rooms for stores and a primitive balance room, with matching balances. On account of a gradual settling and near collapse of the floor of this hut, some of the benches sloped at drunken angles making it necessary, when allocating laboratory working places, to put a tall man at that end of a bench which rose several inches above floor level and a little chap at the other end which had sunk with the floor. Keeping a burette absolutely vertical on these benches was a counsel of perfection rather than a strictly practical proposition; nor was the matter made easier by the fine collection of very warped and rather tottery wooden burette stands then available. A further remarkable feature of the floor was that one could find, near the demonstrator's table, a kind of epicentre, and when one stood thereon and shook a bottle vigorously, the whole laboratory rocked up and down and a general creaking and swilling could be heard rising and falling in the frowsty air.

One long bench, running along one side of the hut, was usually assigned to most of the lady members of the class. Naturally this arrangement allowed them some gossiping freedom but, at the same time, being all in one place they could easily be called to order by the demonstrator if cackling reached nuisance level. It should be mentioned, too, that the hut roof leaked fairly freely, and a pool of water sometimes collected near this long bench. Ladies were recommended to wear Wellingtons in wet weather. One summer, an attempt was made to remedy these leaks by retarring the roof. It then merely leaked tar dribbles for a week or so, and when the cold November rains returned, it leaked water rather more freely than before, the whole roof structure having evidently been strained by workmen walking on it to put on the tar.

Again, the lighting was a bit troublesome; it consisted of very ancient pendant sockets and bulbs fitted with corroded enamelled reflectors hanging mainly over the benches. Now and again corrosion and age caused 'shorts', and a whole fitting would then burn quietly from the shade

upwards to the boss in the roof and would finally crash on the bench below. A warning shout from colleagues or demonstrator usually prevented damage to workers or apparatus. Power was brought to the hut from a neighbouring building by two rather amateurlly slung cables, and when the wind blew at all strongly these cables swayed and the laboratory lights flickered on and off in a quite remarkable manner.

Heating also merits a word. There were three or four ancient, rather toothless gas fires, but after a bomb on Southampton gas works had made gas a bit uncertain, two sombre, round, solid-fuel stoves were set up in the hut on brick and cement hearths – so-called tortoise stoves – presumably because they were slow to warm up, slow to cool down when really hot, and, first thing in the morning, slow to stop smoking when they had just been lit with damp wood and reluctant burning solid fuel. The atmosphere was thus, at 9 a.m. before a Saturday morning lab class, rather like that of an unsuccessful papal ballot – black smoke everywhere; however, by noon this had been replaced by thick white clouds of ammonium chloride which billowed out from the opened end doors of the hut like incense rising round the Ark of the Covenant. This was because evaporation to dryness and ignition in group VI – we did old style ‘bucket and spade’ type qualitative analysis in those days – had to be done in the open or in the only fume cupboard which had any extraction device, and *that* was by means of a lighted gas jet which, if turned up nearly full, tended to set the roof on fire! The present writer well remembers one Saturday about 12.45 p.m. when he helped Professor Adam to swab roof woodwork around this fume cupboard with ammonium and sodium phosphate solutions to prevent some charred portions from smouldering during the weekend.

Finally, there was the water supply. A main cock in one of the store rooms was always shut off after classes, and the whole water system carefully drained by Mr. Buxey, head steward, lecture assistant and storekeeper, and a pillar of the Department since early in the century, who knew all the vagaries and leaking tricks of ancient water pipes, sink pipes, etc. Nevertheless, on really cold winter mornings – in spite of an early lighting of the tortoise stoves – we would arrive to find the main water pipe frozen solid between main cock and hut floor, where it entered.

Operation ‘Firebucket’ was then set in train. The one and only junior technician would carry two or three fire buckets across the frozen wastes outside over to the Main laboratory, and having emptied them out and thoroughly washed them, bring them back filled with clean tap water. The buckets were then stood in front of the stoves and any washing up water was ladled out of them. A separate supply of distilled water was brought over for actual experimental work. Meantime, the demonstrator who, of course, in early days coped single-handed (but classes were not so large as now) abandoned all teaching functions for an hour or so and, having arranged a long rubber tube and Bunsen, retired into the stores and played a flame full blast up and down the frozen iron water main, praying meantime to the patron saints of cast iron, plumbers *et al.* that no split or burst would appear when thawing began. Fortunately his prayers were always answered, and about 10.30-11 a.m. a sepulchral gurgling sound, a throbbing of the pipes and soon a great cheer from the occupants of the laboratory indicated that mains supply had been successfully restored.

In addition to all these delights there were, of course, minor exasperations such as drawers jamming and sinks and gas taps leaking – but these were merely little pinpricks sent to try us, as was, too, the formidable elderly lady – a retired medical auxiliary and almost old enough to have been the demonstrator’s grandma – who had to be shepherded safely through practical First MB.

Yes, we all had happy times in the old Paradise, and believe it or not, when an enthusiastic demonstrator offered to open the hut for a couple of days extra practical in the first week of a vacation, his long-suffering charges not only turned up in numbers, but some even asked for more!

Notes

1. Dr. K. R. Webb was a lecturer in chemistry (inorganic) at Southampton University from about 1940 until his retirement.
2. Professor N. K. Adam was the foundation Professor of Chemistry who retired in 1957.
3. This was in the 1960s, the building is no longer evident.

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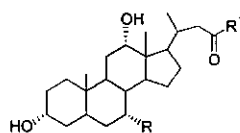
PO Box 1869,

Palmerston North,
New Zealand

Email: selwyny@nzp.co.nz

Website: <http://www.nzp.co.nz/>

(1) and cholic acid (2) from bovine and ovine bile, respectively. By late 1974 a factory was under construction on a green field site at Linton, a rural area ten minutes drive from the Massey campus.



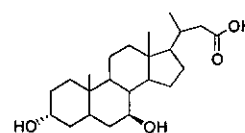
1a. R = H, R' = OH; deoxycholic acid

1b. R = H, R' = NHCH₂CH₂SO₃H; taurodeoxycholic acid

2a. R = OH, R' = OH; cholic acid

2b. R = OH, R' = NHCHCOOH; glycocholic acid

2c. R = OH, R' = NHCH₂CH₂SO₃H; taurocholic acid



3, ursodeoxycholic acid

The original customer for the bile acids, Roussel UCLAF, used a 26-step process to convert the bile acids into corticosteroids. Eventually, fermentation technology surpassed this method but fortunately, before Roussel ceased using bile acids, another bile acid, ursodeoxycholic acid (urso) (3), started to gain increasing use as a gall stone dissolution drug and then even greater use as a liver protection drug. Companies in Italy and Japan now convert cholic acid to urso in a 6-step synthesis.

This growth has meant that even though NZP has grown its product list from two in 1975 to about fifty today, cholic acid still accounts for about 50% of the company business. It has also meant that NZP has long outgrown the New Zealand bile supply and now imports about 85% of the bile it needs from several countries, mainly the Americas.

The heritage from the New Zealand meat industry meant that the initial focus was on adding value to animal byproducts resulting in products such as:

- ferritin - extracted from the spleen,
- peptides - extracted from the thymus gland and elsewhere,
- peptones - extracted from various tissues for use in the microbiological media industry,
- taurine - for use in infant formula and other food applications,
- chondroitin sulfate - from trachea,
- heparin - from intestinal mucosa.

Problems with animal tissue

Thirty years ago, a shopper in a health food store would have been able to find many products of animal origin. Today there are almost none. The main driver for this change has been the fear about bovine spongiform encephalopathy (BSE) infecting humans as a variant of Creutzfeldt-Jacob Disease (vCJD). The precautions taken by governments around the world have been extreme while research to understand the disease has been carried out. This fear has translated into huge consumer resistance to animal-based products and has severely hampered NZP's business over the years — the statisticians who initially predicted vCJD deaths in the tens of thousands have now reduced their predictions to “between 40 and 500 over the next 80 years!!!”

Many companies making animal-based products have lost huge amounts of business since the BSE crisis began. For

Introduction

From the outside, New Zealand Pharmaceuticals Ltd (NZP) looks like a thirty-two year old company steeped in the traditions of extraction and purification of bile acids. On closer inspection one will find that a twenty-five year struggle to diversify has been going on, and only in the last few years are there signs of this struggle starting to bear fruit. However, without the strength of the base business, the many investigations into non-bile and more recently, non animal-based natural biochemicals, would not have been possible.

The purchase of the business from Orica (formerly ICI) by the management almost six years ago certainly has made it possible for the company to explore opportunities that would have not been a fit with the previous owners. In this article I shall recap on the history of the company, describe a few of the pitfalls of our career, and describe a couple of the exciting new directions that we are taking.

A brief history of NZP

NZP was established 32 years ago as a joint venture between Tasman Vaccine Laboratories Ltd (40%) and the meat industry (60%). However, it was the collaboration between Massey University and TVL that gave the joint venture a “technical home”. It was on the University campus that Brian Service, a chemical engineer with a couple of years experience and Richard Garland, a new PhD graduate chemist (currently NZP's Managing Director), formed the nucleus of a small team that developed and scaled up the process to extract deoxycholic

NZP, the biggest impact was the loss of a \$3M ferritin business in Italy.

New directions

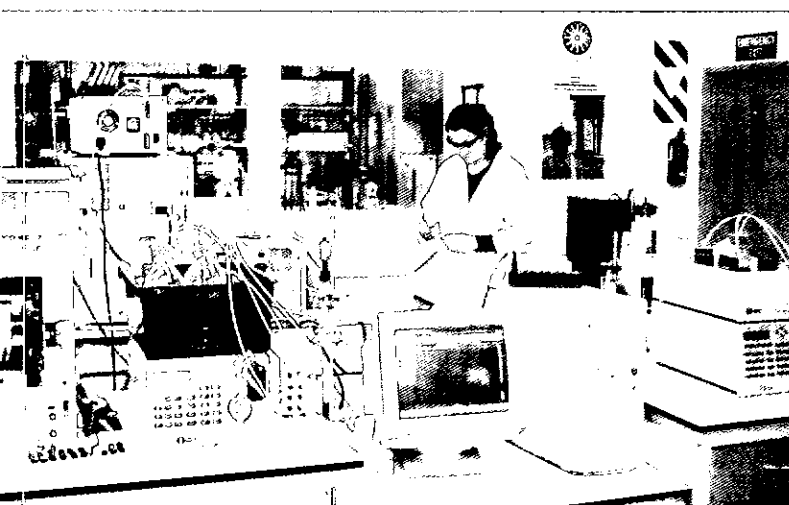
Although the BSE crisis forced NZP to look beyond the animal area for new products, commercial success was not easy to achieve. In examining how to implement a strategic move away from animal-based products, NZP had to carefully examine its collective skills including:

- many years of manufacturing experience with biochemicals,
- purification expertise,
- Good Manufacturing Practices (cGMP),
- a skilled team of scientists recruited from several scientific disciplines,
- a customer base that includes 'big Pharma', diagnostic companies, supplements companies, and modern biotechnology companies,
- strong relationships with several Crown Research Institutes and universities.

This led to the formulation of new criteria for evaluating development opportunities. Thus our ideal product needs to:

- have some novel features yet be acceptable to regulatory authorities,
- have some exclusive intellectual property involved,
- have a measurable (useful) biological activity or use, and
- have a strong, identifiable market opportunity.

Adding NZP's skills and international market network to the intellectual property and international connections of the CRIs has been the key to identifying several promising new opportunities. These involve some chemical synthesis and some plant extracts.



Chemical derivatisation – chemical synthesis

The survey of capabilities within New Zealand, coupled to inquiries from our customers and new inquiries from overseas, has led us to explore opportunities based around simple chemical synthesis. In this area, several opportunities gained momentum through collaboration with Industrial Research Limited <IRL; see: www.irl.cri.nz/carbo>.

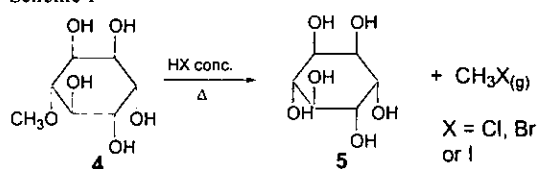
D-Pinitol (4)

Through a co-operative venture with IRL we developed a technology to extract the cyclitol 3-O-methyl-D-chiro-inositol (D-pinitol or pinitol) (4) from the heartwood of a pine species. Sales of pinitol were slow for several years but continued interest by international research laboratories has stimulated strong niche market interest. Pinitol is unusual in that it shows a reasonably strong insulin modifying activity in rodents, but it is only weakly active in humans. However, recent tests using pinitol gained the interest of sports nutrition companies and several "combination" products are now on the market.

D-chiro-Inositol (5)

A derivative of pinitol called D-chiro-inositol possesses a different and more active biological activity compared to pinitol. Although D-chiro-inositol is found widely in edible plants, e.g. soya beans, it is formally prepared from demethylation of pinitol by a halo acid (Scheme 1). This product has shown some interesting activity helping women with Polycystic Ovary Syndrome and it may also find its way into the sports nutrition market.

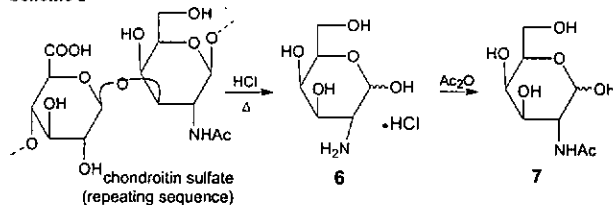
Scheme 1



Galactosamine hydrochloride (6)

Galactosamine hydrochloride is produced by the acid hydrolysis of Chondroitin sulfate, a polymer of the disaccharides, N-acetyl-D-galactosamine and D-glucuronic acid. Galactosamine hydrochloride and its close relative N-acetyl-D-galactosamine (7) (Scheme 2) have become popular chemical building blocks in research related to cancer vaccines and other biologically active oligosaccharides.

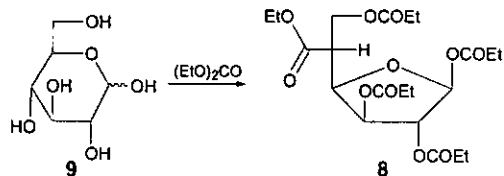
Scheme 2



Pentapropanoyl-β-D-glucofuranose (8)

Pentapropanoyl-β-D-glucofuranose is a stable, crystalline form of glucofuranose prepared from glucopyranose (9), the conventional and stable form of glucose (Scheme 3). This compound is rare in nature and is not easy to prepare in a crystalline form, which is not a problem in research laboratories but a technical challenge at an industrial scale. The crystalline form of this chemical makes it a very useful raw material for chemical syntheses.

Scheme 3

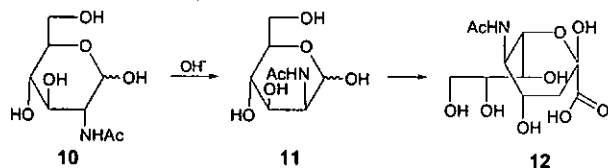


N-Acetyl- β -D-mannosamine (11)

The technology behind the synthesis of *N*-acetyl- β -D-mannosamine (11) (Scheme 4) was licensed from IRL. This product is produced by a base catalysed epimerisation of the C2 carbon of *N*-acetyl-D-glucosamine (10). The synthesis, like most syntheses we are investigating, is very simple on paper but there is a very fine line between epimerisation and base catalysed degradation. When reactions are undertaken on the 100 kg scale there is a very narrow window between success and an expensive failure!

N-Acetylmannosamine is in strong demand in the biotechnology sector as it is a precursor to the important monosaccharide, sialic acid (12). Sialic acid is present in a wide range of biologically active oligosaccharides. For instance, it occurs in epithelial tissue, the first line of defence for many organisms. It is the basis of the anti-influenza pharmaceutical Relenza and it is the key monosaccharide in the bioactive sialyloligosaccharides found in egg white and colostrum.

Scheme 4



Conjugated bile acids: glycocholic acid (2b) and taurocholic acid (2c)

There are also opportunities for synthetic derivatives of the bile acids. We have received several small grants from Technology New Zealand to support the isolation and purification of conjugated bile acids. The conjugated bile acids act as natural detergents and are finding application in drug delivery systems.

Cholic acid is normally found in nature conjugated to the amino acids, glycine, or taurine. Glycocholic acid and taurocholic acid are extremely difficult to separate from raw bile and should be much easier to synthesise from the amino acids and cholic acid in a peptide coupling-type reaction.

Although there are many articles in the scientific literature which suggest that it is easy to synthesise the conjugated bile acids, in practical terms the yield is quite low and is not practical on our desired commercial scale. We recently completed a synthesis project funded by Technology New Zealand and subcontracted to IRL, which showed us many

ways of how not to prepare taurodeoxycholic acid. The results led us to abandon the research literature and to address the synthesis from a different perspective.

NZP has recently committed to the development of a GMP standard synthesis capability that will complement IRL's GlycoSyn facility. The facility will not be as sophisticated as that at IRL but it will add to the New Zealand resource in this area.

Plant-based projects

NZP recently became a part of two technology-based joint ventures involving marine polysaccharides and further plant extracts.

Marine polysaccharides – Marinova and IRL

NZP is working with IRL and the Australian company, Marinova, to create a trans-Tasman venture to produce galactofucan sulfate polysaccharides for the anti-viral market (see: *Australasian Biotechnology*, 2003, 13(3), 39). It is NZP's role to extract the galactofucan sulfates from the seaweed, *Undaria pinnatifida*. Marinova has surveyed and developed a sustainable harvesting technology and is developing markets. NZP will undertake the extraction and IRL is involved in ongoing research on identifying biologically active products in *Undaria* and from other seaweeds.

More plant extracts – Just the Berries

NZP has also become a joint venture partner in Just the Berries Limited (JTB). JTB is the outcome of the mutual interest in developing a range of products initially based on the blackcurrant anthocyanins. A number of clinical studies around the world have demonstrated that anthocyanins are beneficial to the cardiovascular system and for reducing degeneration of macular tissue. Anthocyanins have also delayed age related cognitive degeneration in rodents.

The oil of the blackcurrant seed is also very interesting as it is one of the few seed oils to contain both the w-3 and the w-6 fatty acids. The w-3 fatty acids have different biological activities to the normal plant seed fatty acids that are based around the w-6 family.

The future

NZP's relationship with IRL in the carbohydrate area is proving very fruitful and we have seen a number of potential new products emerge over the last few years. We are embarking also on research programmes with HortResearch, Crop & Food Research, and Massey University to support clinical efficacy. We have also been working closely with several multinational biotechnology and pharmaceutical companies and developing a modest synthesis capability. Altogether, these opportunities will ensure an exciting future for New Zealand Pharmaceuticals Limited.

Patent Proze

By Jane Calvert and Helen Palmer

REVIEW OF THE PATENTS ACT 1953

Last month, the Associate Minister of Commerce released a ministerial paper announcing the Government's recommendations for the amendment of the Patents Act 1953. These recommendations form the final part of a much-awaited review of the Patents Act 1953. The Act is 50 years old and in need of an overhaul so that it reflects developments in New Zealand's social and technological climate.

The implementation of the ministerial recommendations will mean that it will be harder to obtain patent protection in New Zealand. The threshold for showing that an invention is patentable will be harder to reach. In the past, it has been possible to get a patent application through to grant on the basis that the subject matter of the application is novel, but not necessarily inventive. The 1953 Act does not specify that patent examiners should consider whether or not an invention is obvious or lacking inventiveness. The recommendations made in the ministerial paper mean that examiners at the Intellectual Property Office of New Zealand (IPONZ) will now be able to assess inventiveness before the grant of a patent. This will mean that some patents for dubious or lower threshold inventions will not be granted.

To add to this, the threshold is also being lifted because the Government is now recommending the adoption of a "balance of probabilities" standard. This means that a patent will only be granted if, on the balance of probabilities, the requirements for patentability are met. In the past, the applicant has always been given the benefit of the doubt for any issue that was in contention between the applicant and IPONZ. The implementation of the

Government's recommendations may result in some increase in costs for patentees, possibly due to prolonged negotiations with examiners at the time of examination of a patent application.

The Government has also included a recommendation to establish a Maori Consultative Committee. IPONZ does not currently have a formal system of consultation with Maori about patent applications. The Government has recommended the establishment of a committee which IPONZ is able to consult when it believes that a patent application may impact on Maori rights or interests. The establishment of a consultative committee is consistent with the Trade Marks Act 2002 and with the recommendations of the Royal Commission on Genetic Modification.

The committee would provide advice to the Commissioner of Patents about whether an invention claimed in a particular patent application may be derived from traditional knowledge or indigenous plants or animals, and whether the commercial exploitation of the invention might be contrary to Maori values.

The patent attorney profession is welcoming these changes, which will bring New Zealand more into line with the rest of the world. We understand that the legislation to amend the Patents Act 1953 will be introduced into Parliament early next year.

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

Patent Proze
Baldwin Shelston Waters
P O Box 852, Wellington.
Email: email@bsw.com

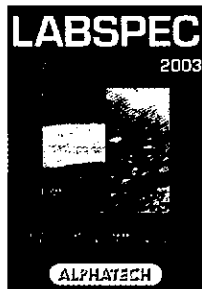


Jane Calvert

Jane Calvert and Helen Palmer of Baldwin Shelston Waters specialise in chemistry and biotechnology patents. Jane is a patent attorney and solicitor. She joined BSW after completing a PhD in chemistry at the University of Canterbury in 1994. Helen joined BSW in 2000. She has a PhD in chemistry from The University of Auckland, and has had postdoctoral research experience in the USA and New Zealand.



Helen Palmer



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Estimating Organic Complexation Of Heavy Metals In Soil Solutions: Influence of the Organic Carbon-To-Metal Ratio

Harry Percival

Landcare Research, Private Bag 11 052, Palmerston North

Introduction

Knowledge of trace metal speciation in the aqueous solution between solid soil particles (the soil solution) is important for predicting the behaviour of trace metals in soils. The uptake by plants of many metals, their toxicity, and their leachability to groundwater, can show a marked dependence on the aqueous speciation of the metals.

Organically complexed forms of a trace metal in solution are intrinsically less toxic than weakly complexed or free ionic forms, but also can increase metal mobility. Knowing when organic complexation is likely to be significant without resorting to the use of detailed models is a problem. Another problem is that solutions containing dissolved organic carbon (DOC) often contain organic complexants that are either unidentified or of undetermined concentrations. A simple method is needed to estimate when organic complexation of a heavy metal is going to be significant. This can be done using the molar ratio of DOC and the concentration of the metal in the solution.

Estimation of organic complexation

Molar ratios of DOC to metal in solution (carbon-to-metal) are related to degrees of organic complexation as a percentage of total concentration of soluble metal. Carbon-to-metal values are calculated from the two readily obtained measurements of solution concentrations of metal and DOC. The carbon-to-metal values at which the degree of organic complexation is likely to be significant, say 10% and greater, differ from metal to metal and with solution pH.

Estimation of the degree of organic complexation has been made using a "mixture model" of fulvic acid, which involves transforming DOC concentrations into an equivalent set of nine organic acids whose reactions are well characterised and used to simulate the organic, metal-complexing portion of the soil solution.¹ The model comprises the simple carboxylic acids citric, maleic, phthalic and salicylic, the amino acids arginine, lysine, ornithine and valine, and benzenesulfonic acid. These are well-defined compounds with known thermodynamic equilibrium constants.

Although "mixture models" can be difficult to validate directly, they are useful over a wide range of pH values and ionic strengths, and can easily be incorporated into computer models of trace metal complexation. Trends can then be established for environmental conditions under different scenarios. Therefore, this model was incorporated

into the computer model GEOCHEM-PC² and applied as described by Percival *et al.*³ As an example of this approach, organic complexation for the metals copper (Cu), nickel (Ni), and zinc (Zn) was estimated for the conditions that are specified in Table 1. DOC concentrations vary over the likely range that could be encountered in soil solutions. The 0.02 M CaCl₂ background was provided to simulate typical ionic strengths in soil solutions. The values for pH vary over the range typically found in soil systems.

Table 1. Conditions for the estimation of organic complexation of Cu, Ni, and Zn for a total soluble metal concentration of 10 µM for each metal in an ionic background of 0.02 M CaCl₂.

DOC concentration (µM)	Carbon-to-metal molar ratio	pH
0.1	10	3, 4, 5, 6, 7, 8, 9
1	100	3, 4, 5, 6, 7, 8, 9
10	1000	3, 4, 5, 6, 7, 8, 9
100	10 000	3, 4, 5, 6, 7, 8, 9

Results

For each of the metals, and at all carbon-to-metal ratios, the percentage of organic complexation generally increases with pH (see Figure 1). For each metal at each pH value an increasing carbon-to-metal ratio produces an increase in organic complexation. At higher pH values of 7–9, metal solubility greatly decreases and precipitation of Cu, Ni, or Zn can occur depending upon the carbon-to-metal ratio.

If we take 10% organic complexation to be the threshold at which it becomes significant, then Table 2 shows those combinations of carbon-to-metal ratio and pH that provide a degree of complexation of 10% or greater. As noted in Table 2, this excludes those conditions where precipitation of the metal is likely to take place. The onset of precipitation will vary with the total concentration of soluble metal. The 10 µM metal concentration falls within the range normally observed in soil solutions, but substantially higher concentrations could encounter precipitation conditions at lower pH values and higher carbon-to-metal ratios. Competition between the metals for ligands in the soil solutions is not taken into account in this illustrative example but it would only have a secondary effect on the broader picture that is drawn here.

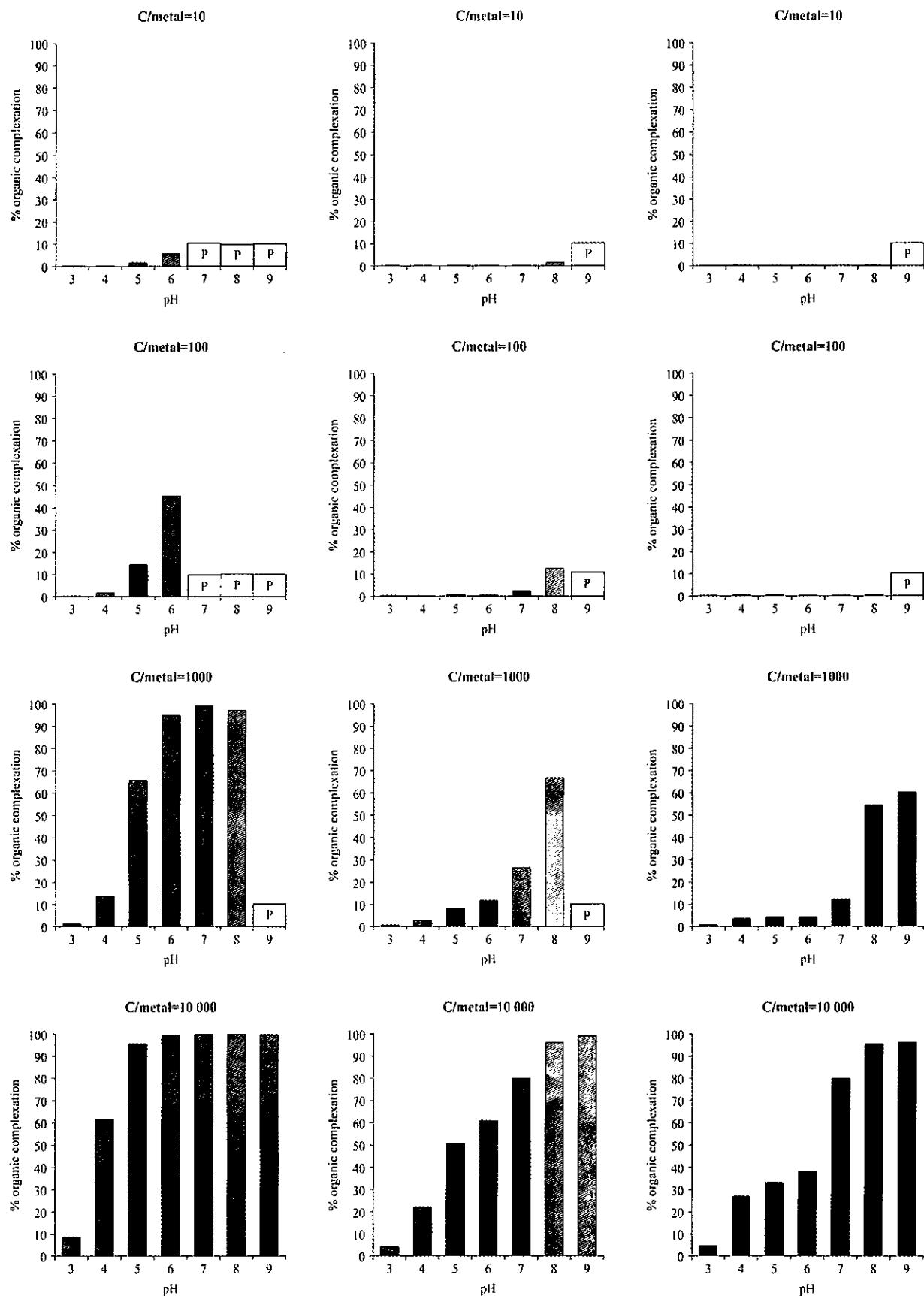


Figure 1: Percent (%) organic complexation as a function of pH and carbon-to-metal molar ratio for (l to r) copper, nickel, and zinc. The total soluble metal concentration is 10 μ M for each metal; symbol P indicates that metal precipitation is likely to occur.

Table 2. Carbon-to-metal molar ratio and pH at which significant (>10%) organic complexation occurs for each of the metals Cu, Ni, or Zn.^a

C:Cu	pH 3	pH 4	pH 5	pH 6	pH 7	pH 8	pH 9
10					<i>P</i> ^b	<i>P</i>	<i>P</i>
100			Cu	Cu	<i>P</i>	<i>P</i>	<i>P</i>
1000		Cu	Cu	Cu	Cu	Cu	<i>P</i>
10 000		Cu	Cu	Cu	Cu	Cu	Cu

C:Ni	pH 3	pH 4	pH 5	pH 6	pH 7	pH 8	pH 9
10							<i>P</i>
100						Ni	<i>P</i>
1000				Ni	Ni	Ni	<i>P</i>
10 000		Ni	Ni	Ni	Ni	Ni	Ni

C:Zn	pH 3	pH 4	pH 5	pH 6	pH 7	pH 8	pH 9
10							<i>P</i>
100							<i>P</i>
1000					Zn	Zn	<i>P</i>
10 000		Zn	Zn	Zn	Zn	Zn	Zn

^a Each solution contains a total metal concentration of 10 μ M.

^b the symbol *P* indicates that metal precipitation is likely to occur.

Conclusions

For a given pH and carbon-to-metal ratio, Cu-organic complexation is likely to be substantially greater than for Ni or Zn at the same molar concentration of soluble metal, and Ni tends to be more complexed than Zn. The higher the pH and the carbon-to-metal ratio, the more likely organic complexation will be significant. High levels of organic complexation inhibit the onset of metal precipitation at the high end of the pH range.

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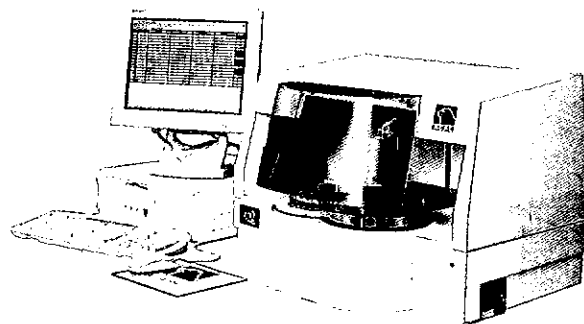
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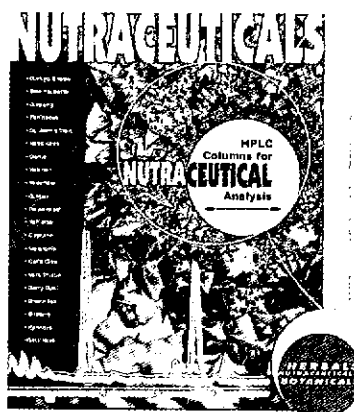
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patented ion mirror system enables the increased sensitivity of the new ICP-MS, effectively focusing all ions, regardless of their mass, into the entrance of the quadrupole, resulting in a transfer efficiency up to 20 times better than that of conventional ICP-MS theory. This innovative design redirects the ion beam through 90 degrees via a parabolic electrostatic field.

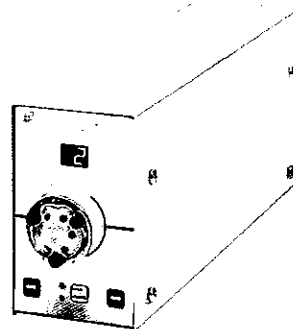
Photons and neutrals are a major source of background noise in ICP-MS but because they don't react with the electrostatic field of Varian's ion mirror, they pass immediately through to a turbo molecular vacuum pump. By filtering photons and neutrals away from the mass analyzer, background signal is greatly reduced. The new ICP-MS includes software that allows more direct linking to the Internet for fast access to technical support and customer service and also has features to enhance usability, productivity, and performance. The new ICP-MS features another world first - the only all-digital detector with up to nine orders of linear dynamic range. Users will be able to determine low and high concentration analytes without the need for time-consuming dilution and without the need for cumbersome analogue-to-digital conversion. The Varian ICP-MS also includes a Telediagnosics® service which further enhances the ease-of-use of the system by allowing Varian, Inc. engineers to perform remote fault diagnosis over a modem line.

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- Maximizes instrument utilization



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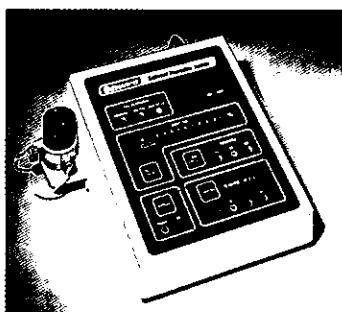
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MASS FLOW CONTROL OF SPLIT FLOW ENHANCES THE PERFORMANCE AND REPEATABILITY OF THERMAL DESORPTION METHODS

Ai Scientific now offers a range of thermal desorption (TD) systems for sorbent tubes, canisters or on-line gas/air streams from Markes International Limited. 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.

Incorporation of the MFC accessory also allows split flows to be entered and re-called as part of each stored thermal desorption method. This means that a sequence of up to 100 tube samples entered on an Ultra-UNITY automated thermal desorber may comprise several 'sets' of samples; some at high (industrial) concentrations requiring high split and some at trace (ambient) concentrations requiring low split. The appropriate TD method, including split flow settings, will be automatically re-called and implemented for each set as required. The MFC Accessory also works in concert with Markes' unique SecureTD facility for quantitative re-collection of split sample for repeat analysis. For example, using the MFC Accessory on an AutoSecureTD system (for automated desorption and re-collection of up to 100 sorbent tubes) allows split ratios to be set relatively high whenever unknowns are being analysed. This prevents risk of system contamination from unexpected high concentration samples. However, if subsequent primary analysis, shows the initial split settings were too high, compromising method sensitivity, the re-collected samples can simply be re-analysed using lower split flows programmed using the MFC.

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The syringe only concept of Combi PAL, combines the exact manual sample injection procedure of an experienced GC chromatographer, with the precision and throughput of an automated sampling system.

The SPME mode allows you to select a preconditioning step and agitate or heat the samples during the extraction itself.

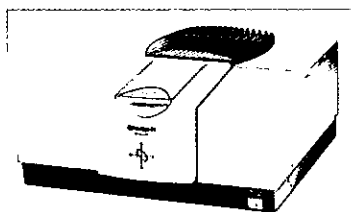
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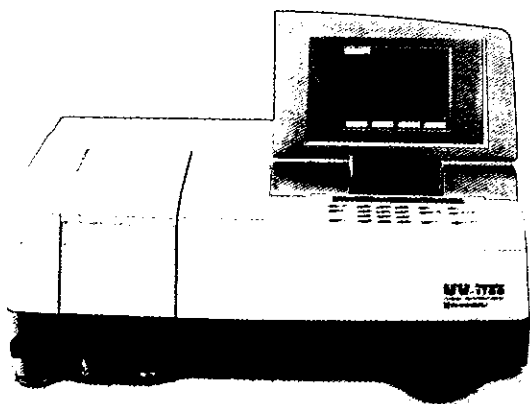
Dynamic auto-alignment is offered as a standard feature. With state-of-the-art technology, the Shimadzu dynamic alignment system continuously maintains optimal alignment during data acquisition, ensuring consistently reproducible spectra without the need for tedious mechanical adjustments. The IRPrestige gives unprecedented signal-to-noise for an FTIR in its price-class; peak-to-peak S/N is 40,000:1 or better, guaranteed!

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OMEGA OPTICAL LAUNCHES NEW WEB-BASED BUILD-A-FILTER FOR CUSTOM FILTER SPECIFICATION & QUOTING

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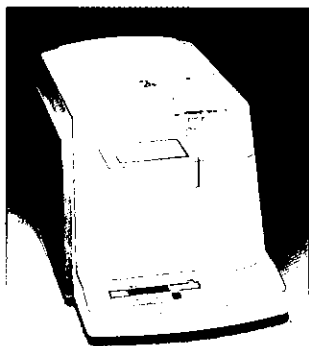
Rapid Custom filters are available from 190 nm in the UV to 2500 nm in the IR in a variety of filter types including: bandpass, narrowband, wideband, longpass, shortpass, edge, rejection band, beamsplitters, mirrors, and absorption glass. An extensive selection of off-the-shelf components results in a wide range of transmission and blocking specifications. Pricing is competitive with standard catalogue filters.

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SHIMADZU HIGH THROUGHPUT AUTOSAMPLER



The Shimadzu SIL-HT is a high performing autosampler in terms of sample injection speed, sample capacity, and minimizing sample carryover of highly adsorbent sample components. These features are in increasingly high demand and essential for high throughput analysis.

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SHIMADZU CLASS-VP 7 CLIENT/SERVER CHROMATOGRAPHY DATA SYSTEM

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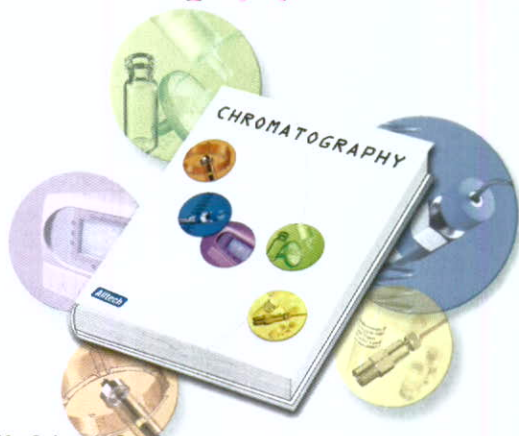
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