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Chemistry

IN NEW ZEALAND

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- 2002 Nobel Prize In Chemistry
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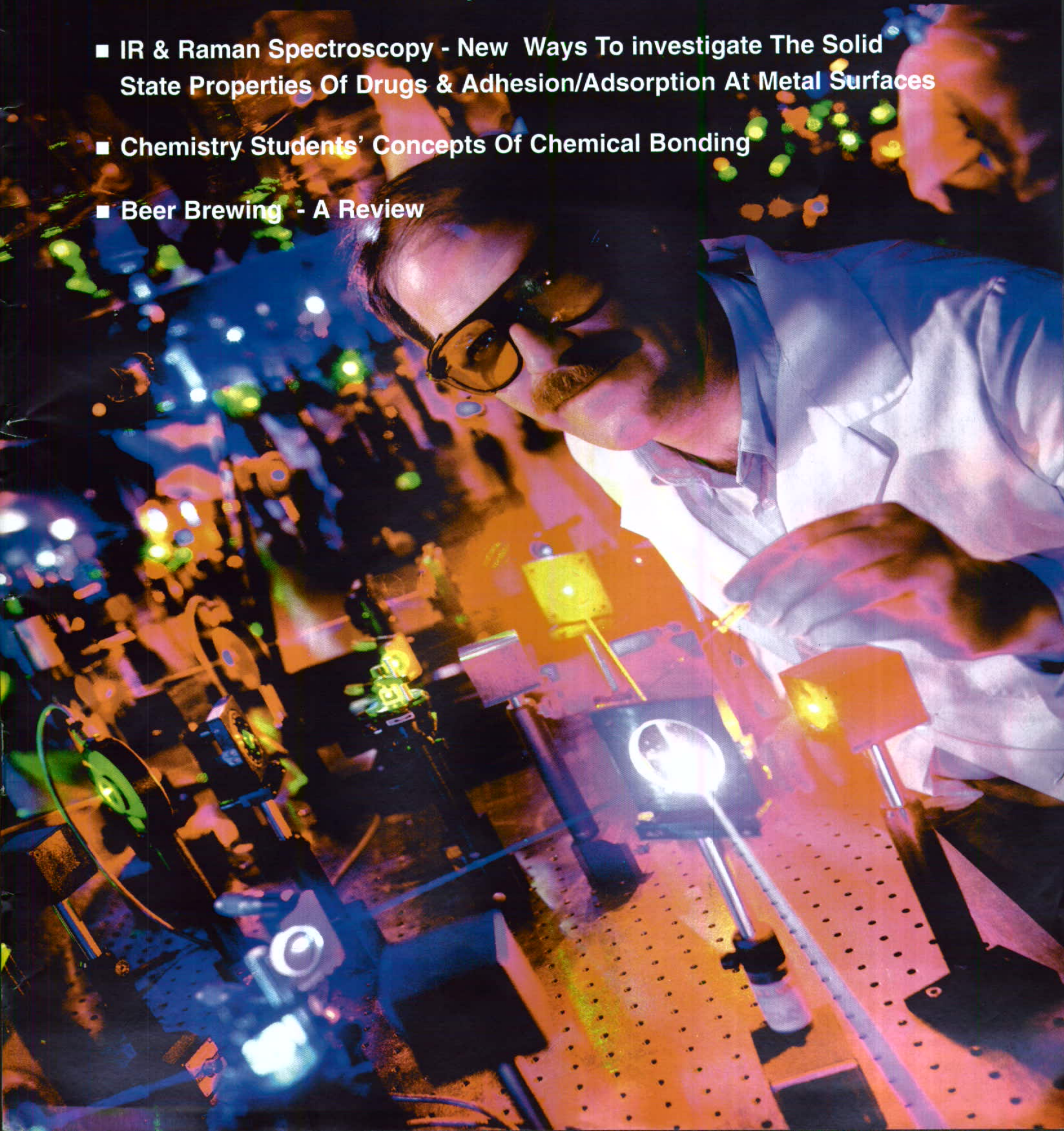

EDITORIAL

Wherefore art thou 'Journal'

Brian Halton

Journal (`jêr-`), n. **1.** (In bookkeeping by double entry) book in which each transaction is entered with statement of accounts to which it is to be debited. **2.** Daily record of events; (Parl.) *the J~s,* record of daily proceedings; daily newspaper, other periodical. **3.** Part of shaft or axel that rests on bearings (hist. unexpl); ...

Magazine (-zen), n. **1.** Store for armour, ammunition, and provisions; store for gunpowder or other explosives. **2.** Periodical publication (now usu. illustrated) containing articles by various authors.

... or so my trusty dictionary tells me! Pragmatically this Journal is a magazine with its purpose to serve the needs of the Institute membership without preference to any one sector. My term as editor has now run its course through six issues and eighteen months of "b, s & t" (though the occasional G&T has helped!) and comments, such as we have received, have been positively encouraging and, surprisingly, only rarely critical. Some feel that the magazine is too academic. It is not intentional, but is it surprising? By far the majority of articles for general consumption through these pages come from the academic sector. Unfortunately, few articles come from industrial or other sources. Current concerns with intellectual property protection have facilitated far more meaningful discussion from that sector of NZIC in recent times and this is very much for the benefit of the majority of us. As a 'volunteer' editor I do not have the ability to spend more hours soliciting and writing copy. So come on industrialists and those of you who feel under-represented, tell us about your organization and what you do!

Each issue has its distinct New Zealand flavour but it is the Branch News that informs us (and our members and subscribers overseas) of the large numbers of activities taking place throughout the country. But what of our industrial happenings, member movements, *etc.*? Unless the information is provided we cannot print it! In this regard providing a small news item is at least one order of magnitude easier than going for a blood test - it takes but a few minutes, engenders a feeling of well being, and doesn't need to be done too often!

To provide some more general content, this final issue for 2002 contains an article on the DuPont empire that is now in its third century of operation—and here I am grateful to Rick Stevenson of *Chemistry in Britain* for the text and the DuPont media guide for the pictorial illustrations—and one on wing from David Meads of Speight'sin Dunedin. I hope that other industrial enterprises in this country feel left out! The provision of an article relevant to, and beneficial for, the NZIC membership can come from any source, and I am only too happy to receive them.

Each Branch is now providing much of the issue content on a rotating basis so that there is opportunity to provide an article when your Branch has that responsibility - at any other time please feel free to contact me. After all if providing news is better than a blood test, then writing an article cannot be any more painful than, and just as advantageous as, donating blood!

The schedule for copy the next 18 month is:

March 2003
Vol. 67(1): Copy Date January 26, 2003
WAIKATO BRANCH

June 2003
Vol. 67(2): Copy Date April 26, 2003
CANTERBURY BRANCH

September 2003
Vol 67(3): Copy Date August 26, 2003
MANAWATU BRANCH

November 2003
Vol. 67(4): Copy Date October 26, 2003
WELLINGTON BRANCH

March 2004
Vol. 68(1): Copy Date January 26, 2004
AUCKLAND BRANCH

June 2004
Vol. 68(2): Copy Date April 26, 2004
OTAGO BRANCH

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The New Zealand Institute of Chemistry Incorporated
P O Box 39-283, Howick
Auckland, New Zealand
Phone: +64-9-5356495
Fax: +64-9-5353476
Email: NZICOffice@nzic.org.nz
WWW: http://www.nzic.org.nz

Managing Editor & Publisher:
Robert B Lyon
Ancat Holdings Limited
32 Murvale Drive
Bucklands Beach, Auckland
P O Box 38-546
Howick, Auckland, New Zealand
Phone: +64-9-5353475
Fax: 64-9-5353476
Email: chemistry@ancat.co.nz

Advertising Sales:
Ancat Holdings Limited
32 Murvale Drive
Bucklands Beach, Auckland, New Zealand
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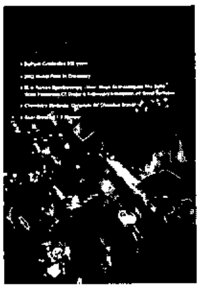
Howick, Auckland, New Zealand
Phone: +64-9-5353475
Fax: +64-9-5353476
Email: chemistry@ancat.co.nz



On the cover ...

DuPont 200 Years - Holographic Technology Research Engineer Mark Armstrong was part of a 1990s thrust into holographic technology for brighter electronic display screens.
Photo courtesy of DuPont.

NZ SCIENCE SCENE

NEW STAFF AT NZ SCIENTIFIC LTD

NZ Scientific Ltd is pleased to announce that it has employed a new sales and support representative for the Perkin Elmer Instruments product range.

Narender Sharma has joined us from Labindia; the PerkinElmer agents for India. Narender had been selling PerkinElmer Instruments for 6 years with Labindia. Before that he lectured in Chemistry at an Engineering college for 5 years. Narender completed his BSc and MSc at Delhi University.

With Narender's background and experience he is competent to help you with the whole PerkinElmer Instruments product range including: AAS, ICP, FTIR, UV-Visible Spectrophotometry, Fluorescence, GC, GCMS, thermal and elemental analysis.

Narenders contact details are:
Mobile Phone: 021 751008
Email: narender@NZScientific.co.nz

NZAS PRIZE WINNERS 2002

The New Zealand Association of Scientists has announced its 2002 prize-winners and made the awards over two ceremonies, one in Wellington on October 30 and the other in Christchurch on November 7.

Marsden Medal

Dr Howard Wearing, recently retired from HortResearch, was awarded the 2002 Marsden Medal at the ceremony at Lincoln University, Christchurch. This medal was awarded for his outstanding service to horticultural science in the service of industry underpinned by his specialised knowledge of insects.

He has made an enormous contribution to New Zealand society, and especially the horticultural industry, since the 1960s. His personal drive and vision for developing multi-skilled research teams to tackle large and difficult problems has resulted in a range of success stories of international importance. One of his most significant career achievements was to gain access to Japan for cherries and other fruit. This entailed an effective blend of science leadership and country-to-country negotiations over an eleven year period and involved six DSIR Divisions.

Shorland Medal

Dr Hugh Bibby (Institute of Geological and Nuclear Sciences) was awarded the Shorland Medal at the ceremony in Wellington. His outstanding personal lifetime contribution is to developing geophysical methods for exploring geothermal and volcanic systems in New Zealand, and mathematical methods for determining rates of tectonic deformation across New Zealand's plate boundary. A major highlight was the discovery that the Mokai geothermal field, northwest of Taupo, is a major energy resource, whereas it had previously been thought to be only a minor hot-spring area. Geothermal developers can now use Bibby's results to site drill-holes in geothermal fields thereby improving the likelihood that they will encounter hot thermal conditions.

Research Medal

Dr Jack Heinemann (Department of Plant and Microbial Sciences, University of Canterbury) has been awarded the research medal. This is awarded to a scientist aged under 40 for outstanding research work, principally undertaken in New Zealand during the three preceding years. In Heinemann's case it is for his contribution to the knowledge of horizontal gene transfer in bacteria (the movement of genetic material from bacteria to other organisms other than through descent when cells divide) and the biology of genetic elements outside chromosomes.

Science Communicator Award

This is made to a scientists who excels in communicating scientific issues of public interest. This year it went to **Dr Jonathan Hickford** (Senior lecturer in Biochemistry, Lincoln University). He is a molecular geneticist, with professional interests in gene sequencing, gene typing, immunology and genetic analysis but who has also made an outstanding and sustained contribution to the communication of science over seven years. He is an excellent speaker able to pitch his information to the level and interests of different audiences from school children to industry groups. In the last three years, he has been a guest speaker at over 60 public and industry-related meetings.

His involvement with schoolchildren is particularly noteworthy as he motivates them to become interested in science. He has been Chief Judge at the Canterbury-Westland Science and Technology Fair since 1995 and has judged at the Genesis National Science and Technology Fair for five years.

NZ CLIMATE SCIENTISTS: WORLD CLASS

Two leading New Zealand climate scientists from the National Institute of Water and Atmospheric Research have been appointed to senior positions with the international scientific body advising the United Nations on climate change.

Pete Hodgson, Minister of Research, Science and Technology and Convenor of the Ministerial Group on Climate Change, said the positions attained by Dr Martin Manning and Dr David Wratt were further evidence that New Zealand science, including climate research, is world class.

Dr Manning has been appointed head of technical support for the Intergovernmental Panel on Climate Change (IPCC) Group 1 Science

Working Group, based in Boulder, Colorado. He has responsibilities for supporting the next big international assessment of climate change knowledge to be published in 2006 or 2007. These assessments guide policymakers worldwide in determining climate change policy and their approach to international negotiations.

"Dr Manning has led and developed New Zealand's carbon dioxide measuring programme over the last 30 years," Mr Hodgson said. "The results form the most significant record in the Southern Hemisphere and are vital in the assessment of changes in greenhouse gases. Dr Manning and his colleagues are also at the forefront of research into greenhouse gases that lays foundation for future reductions in emissions."

Dr Manning has been has been a member of the IPCC Bureau representing New Zealand and Australia for the last 4 years. The Bureau assesses knowledge about climate change and develops plans for IPCC work.

He will be replaced in the Bureau by fellow NIWA scientist Dr David Wratt, the institute's Principal Scientist for Climate Applications and coordinator of output from NIWA's National Climate Centre. Dr Wratt was a convening lead author for the New Zealand and Australia chapter in the 2001 IPCC assessment of the impacts of climate change and the options for adaptation.

"Dr Manning, Dr Wratt and other New Zealand scientists with IPCC responsibilities will continue to ensure that the world's policymakers have access to the most up-to-date knowledge of climate change and its impacts in the Southwest Pacific," Mr Hodgson said.

NEW APPOINTMENT AT CARL ZEISS

Carl Zeiss is pleased to announce the appointment of C. K. (Frankie) Lee as head of the Microscopy Division.

Having previously been with the Carl Zeiss Far East operation, Frankie Lee brings with him a wealth of experience which he will keenly share with customers in Australia and New Zealand.

Frankie will replace Wolfgang Loeb who will retire from his current position as Divisional Manager at the end of November 2002.

NEW ZEALAND REPRESENTATIVE FOR SYNCHROTRON COMMITTEE

Associate Professor Jim Metson has been appointed the New Zealand representative on the National Scientific Advisory Committee for the Australian Synchrotron project. The appointment follows an invitation last May from Victorian Premier Steve Bracks to New Zealand Prime Minister Helen Clark for a New Zealander to join the Committee.

"We are delighted about this initiative and appreciative of the Victorian State Government's invitation for New Zealand involvement in the Synchrotron project. Professor Metson is already familiar with the Synchrotron project. That, along with his expertise and extensive contacts in New Zealand's research community makes him an ideal New Zealand representative", said New Zealand Minister of Research Science and Technology, Hon. Pete Hodgson.

Mr Hodgson said the arrangement would help ensure New Zealand researchers were aware of opportunities to utilise the Australian Synchrotron. "New Zealand places strong importance on the development of its research and innovation links with Australia. Collaboration between New Zealand and Australian researchers in the Synchrotron and other projects will result in win-win outcomes".

Victoria's Minister for Innovation, John Brumby, warmly welcomed Professor Metson to the committee. "Appointing a New Zealand scientist of Professor Metson's calibre indicates the enthusiasm of researchers and governments beyond Australia for this regionally important project," Mr Brumby said.

"This appointment demonstrates the importance of trans-Tasman science links, and with Professor Metson's input we can design a facility that will meet the broader research needs of both Australia and New Zealand."

A synchrotron is a large and complex machine that produces beams of very intense light. It can be used as a molecular microscope to study the composition of matter. Synchrotrons are invaluable tools for groundbreaking research in biological and life sciences, mining and geoscience, and for manufacturing pharmaceuticals, new age materials and micromachines. The facility in Melbourne will cost an estimated A$157 million and is expected to begin operation in 2007.

Biographical Note
James Metson is an Associate Professor with The University of Auckland Department of Chemistry, Acting Director of the University's Light Metals Research Centre and a past Director of the University's Research Centre for Surface and Materials Science. He gained his chemistry doctorate at Victoria University of Wellington and has a distinguished reputation in the development of surface analytical techniques and in the surface chemistry and smelting technologies for light metals, particularly aluminium.

JOINT RESEARCH PROJECT GETS UNDERWAY

An agricultural scientist from the world's largest manufacturer and marketer of fertiliser arrived in New Zealand last month to begin a joint research initiative with Ballance Agri-Nutrients and AgResearch.

German PhD scientist Frank Brentrup from Hydro Agri, a division of Norsk Hydro which owns 20% of Ballance Agri-Nutrients, met with scientists from AgResearch and Ballance to begin a seven week life cycle analysis study into the energy costs and environmental emissions associated with producing a selected group of fertiliser products.

Warwick Catto, Head of Agro Sciences for Ballance, says the analysis will be an extremely valuable resource accounting tool which will ultimately highlight ways his company can improve the manufacturing efficiency and environmental performance of its products. This information will in turn be used by AgResearch as part of its wider assessment of the resource costs relating to farming systems and related industries.

"The partnership with Norsk Hydro and AgResearch is particularly important for us as we will be drawing on the vast international research expertise of Norsk and also plug that information into AgResearch's Resource Accounting farm system model which will provide useful information for our customers," says Mr Catto.

Mr Brentrup says the study will also enable Ballance to meet international obligations to declare the energy costs associated with the production of food.

"In Europe some food retailers and processing industries are already pressuring suppliers for details on their production systems – including the energy inputs used to manufacture products – so it is important for countries like New Zealand to have this information on hand," says Mr Brentrup.

AgResearch scientist, Stewart Ledgard, says the life cycle analysis project is an innovative and important one.

"This methodology will assist us to more accurately calculate the contribution of fertilisers to the total resource use and emissions from agricultural sectors," says Dr Ledgard.

BIOTECHNOLOGY STRATEGY DISCUSSION PAPER RELEASED

A discussion paper released late last month by Research, Science and Technology Minister Pete Hodgson sets out the framework for a New Zealand Biotechnology Strategy.

"The Government is committed under its Growth and Innovation Framework to supporting biotechnology as a key growth sector," Mr Hodgson said. "New Zealand has a strong track record in adding value to natural products through biological innovation. We have world-class biological knowledge and skills to build on. A stronger biotechnology sector has the potential to accelerate growth in other sectors, including forestry, agriculture, food production and pharmaceuticals.

"This discussion paper offers a vision, goals and guiding principles for the development and use of biotechnology in New Zealand. With new biological knowledge and techniques the opportunities are multiplying rapidly. A sound strategy will help us use biotechnology responsibly in pursuit of those opportunities."

The discussion paper outlines the current state of biotechnology in New Zealand. It notes that although New Zealand has excellent research, with a growing range of applications, the sector is underdeveloped relative to its potential.

Three goals are proposed to support the vision for responsible development of biotechnology:

· build understanding and positive connections between the community and the biotechnology sector;

· manage the development and introduction of new biotechnologies with a regulatory system that optimises opportunities and innovation while safeguarding health and the environment; and

· grow New Zealand's biotechnology sector.

Specific targets and actions for growing the sector are being identified by the Biotechnology Taskforce, a group of ten top biotechnology entrepreneurs, academics and business leaders established in May this year. The discussion paper identifies challenges including retaining and developing talent, funding expensive R&D, commercialising research, supporting clusters, attracting overseas investment and increasing Maori participation.

Development of the Biotechnology Strategy, which was recommended by the Royal Commission on Genetic Modification, is being led by the Ministry of Research, Science and Technology. The ministry will collect and analyse submissions in response to the discussion paper and the Government aims to have a final strategy in place by early 2003.

"All sectors of the community are invited to comment on the development and direction of this strategy," Mr Hodgson said. "Its quality will be directly affected by the quality of the response to this discussion paper, so I encourage everyone to have their say."

Copies of the discussion document are available at www.morst.govt.nz or by phoning 0508 400 805. Submissions close on 30 November 2002 and can be made through the website.

REVISED TIMELINE FOR TRANSFER OF DANGEROUS GOODS TO THE HSNO ACT

The Ministry for the Environment and the Environmental Risk Management Authority have announced today a revised timeline for the transfer of dangerous goods to the Hazardous Substances and New Organisms (HSNO) Act. Dangerous goods include all the common fuels such as petrol, diesel and LPG and many common bulk chemicals such as solvents. The transfer of dangerous goods to the HSNO regime involves a process of properly identifying substances classified as dangerous goods and assigning controls to effectively manage the hazardous properties of these substances.

It was due to be completed by 1 April 2003. This date has been extended to 1 April 2004. The extension by a full year will enable a full round of dangerous goods licensing to occur. Dangerous Goods licenses have a fixed term of one year and are the principal existing means of managing risks.

The delay has been caused because it has taken longer than expected to put in place the regulations for transfer to occur.

The HSNO Act commenced for hazardous substances on 2 July 2001. A transitional period of up to 5 years was put in place within which to progressively transfer existing substances to the Act and to keep existing regulatory regimes in place until transfer has occurred.

The implication for industries handling dangerous goods is that the old rules will continue to apply for a further year with the territorial authorities continuing to provide licensing and enforcement services. Meanwhile the documents outlining the proposed classifications and controls for these substances are out for consultation - the technical work on the transfer of dangerous goods will still keep to the original timetable of completing the technical policy for the transfers by the end of 2002.

NAVMAN STEALS TOP HONOURS AT THE WESTPAC HI TECH AWARDS 2002

Guests didn't need GPS technology to locate the 9th national Westpac Hi Tech Awards 2002 Ceremony dinner held at the International Antarctic Centre in Christchurch.

The Awards ceremony was the pinnacle of three events that also included a launch cocktail function and presentation of the Bright Sparks Awards at CPIT; plus the Hi Tech Forum with guest speakers Jon Labrie, Rod Oram with live links to speakers in the USA.

Turnout at the events exceeded expectations with over 250 at the opening cocktail function, 100 at the Industry Forum and 460 at the Award presentation Ceremony – proof that New Zealand's Hi Tech industry is growing stronger each year and networking more actively than ever before.

Of the 15 company finalists and 6 young achiever finalists, nine companies and one bright young spark proudly walked away with at least one award destined for the most prominent position in the company foyer.

But at the end of the day, only one company could steal the show and hold up the ultimate Westpac Supreme Hi Tech Award for Excellence. This honour went to Navman NZ Ltd.

Navman is an outstanding company that has been making huge waves in the International GPS technology market. A New Zealand owned company, Navman also pocketed the Deal of the Year award and was a finalist in three other award categories: Most Innovative Product of the Year, High Growth Company of the Year and Hi Tech Exporter of the Year. The judges were unanimous in their decision, as Navman had presented an entry that outstripped every other in terms of business excellence.

"They had seen a niche opportunity and propelled the company into the global market through flawlessly executing an audacious business strategy supported by a strong research base," said Chair of the Judging Panel, Marion Rogers.

"Navman not only leveraged off all the opportunities in the Intellectual Property (IP), they also maintained their manufacturing base in New Zealand – an achievement that was particularly highly commended by the judges."

Julian Nalepa, General Manager, Business at Westpac says "Navman are a superb example of an organisation achieving excellence in business across all levels."

The other winners of the Westpac Hi Tech Award categories were:

Broadcast MAP, winner of the Software Company of the Year Award.

Pulse Data International Ltd, winner of the Electronic Company of the Year Award and the Hi Tech Exporter of the Year Award.

IRL Biopharm, Industrial Research Ltd, winner of the Biotech Company of the Year Award.

Connexionz Ltd, winner of the Most Innovative Product of the Year Award and joint winner of the Small Business of the Year Award

iTouch Business Mobility, winner of the Investment in People of the Year Award.

Navman NZ Ltd, winner of the Supreme Hi Tech Company of the Year Award and the Deal of the year Award.

Niche Software Ltd, winner of the High Growth Company of the Year Award.

Prolificx Ltd, joint winner of the Small Business of the Year Award.

Kent Barber of Right Hemisphere Ltd, winner of the Young Achiever of the Year Award.

BIGGEST EVER TECHNOLOGY NEW ZEALAND GRANT FUNDS DRUG DEVELOPMENT IN NEW ZEALAND

Technology New Zealand is giving its biggest ever research and development grant to a project that develops the capability in New Zealand to take newly discovered pharmaceuticals to the point of commercialisation.

The funding, totalling nearly $1.7 million, has been awarded to Auckland company Antipodean Biotechnology Limited, which is working with seven of New Zealand's leading research institutes to develop a new chemical entity, mitoquinone, as a treatment for Friedreich's Ataxia and Huntington's Disease. No treatments currently exist for either disease.

Mitoquinone, which targets mitochondria, the energy source of living cells, was discovered by researchers, Mike Murphy and Rob Smith, at the University of Otago. It is now to be developed to prove efficacy in patients. This is the first time a drug discovered in this country will also be manufactured, formulated into tablets, tested for absorption, metabolism and safety before proceeding to the first patient studies, all within New Zealand.

The research institutes involved in the mitoquinone project are Industrial Research Limited (IRL), Douglas Pharmaceuticals Limited, Process Developments Limited, Massey University, the Institute of Environmental Science and Research Limited (ESR), the University of Otago and the Christchurch Clinical Studies Trust.

The preclinical and clinical development of mitoquinone must meet the demanding standards of regulatory authorities in New Zealand and overseas, such as the United States Food and Drug Administration (FDA). If proved, mitoquinone will qualify for the fast track regulatory approval process given to compounds that target unmet medical needs. This means it could be available to patients in about two years, if it satisfies quality, safety and efficacy standards.

This presents a considerable technical challenge to both the project management by Antipodean and the contributing institutes. If successful, the experience gained is expected to be applicable to other New Zealand pharmaceutical innovations.

The total project is costing $3.34 million, with Antipodean matching dollar for dollar the funds contributed by Technology New Zealand.

Technology New Zealand Investment Manager Lins Kerr describes the project as ‘ground-breaking’ because it links drug discovery in New Zealand with commercialisation for the first time. “New Zealand needs this capability if future drugs are to be commercialised here. We have the raw talent to develop new drugs in New Zealand but the expertise is distributed across a number of organisations.

“By bringing that expertise together Antipodean is creating valuable human capital, raising the profile of our research institutions and putting New Zealand on the map as a source of pharmaceutical innovation.”

Antipodean is a seed venture capital company set up to fund the development and commercialisation of new pharmaceuticals discovered in New Zealand, using New Zealand expertise and facilities. Antipodean will liase with an overseas partner to complete the development process and eventually market the product globally.

Antipodean Chief Executive Ken Taylor says until now New Zealand drug discoveries have been handed over to contract sites or companies for development.

“Getting the project to clinical proof of principle stage in New Zealand delivers a range of benefits. It is less expensive to do the work here and more efficient to have the pre-clinical work close to the source of innovation - people can talk to each other to resolve the technical issues that will arise.

“The step we’re adding here is also the one that contributes the most value to the product, so that’s important for New Zealand.”

While acknowledging that the project is high risk and challenging, Ken Taylor says it is based on science that has been internationally endorsed.

“Having the data accepted and published in a number of top scientific and medical journals is testimony to the excellence of the science involved. That is a credit to the researchers at the University of Otago who took superb chemistry and applied it to a complicated biological process, to come up with a product that has the potential to significantly improve quality of life for people with Friedreich’s Ataxia and Huntington’s Disease.”

Lins Kerr says having Ken Taylor involved in the project was pivotal in Technology New Zealand’s decision to give substantial funding.

Dr Taylor has honours and doctorate degrees in pharmaceutical chemistry and pharmacology from the University of Otago School of Medicine and a postdoctoral fellowship in pharmacology and experimental therapeutics from the John Hopkins University School of Medicine in Baltimore. He held a joint appointment in neurosciences at Princeton University and the Squibb Institute of Medical Research in Princeton before joining the pharmaceutical giant Roche. He has held a number of positions with Roche since then including Medical Director and later Managing Director for the company in New Zealand, and Managing Director of Roche affiliates in the UK and California. He became Chief Executive Officer of Antipodean in October 2001.

Technology New Zealand funding increased this year from $NZ40 million to over $NZ50 million with individual projects eligible, for the first time, for up to $2million under the Technology for Business Growth scheme. The largest previous grant given by Technology New Zealand was funding of $900,000 to Auckland company Navman.

Ken Taylor says the investment from Technology New Zealand is crucial to the project being carried out in this country. Antipodean’s other options for completing the various tasks involved in the mitoquinone project would have seen some, if not all, aspects carried out overseas.

He says Antipodean is looking at investing in a number of other pharmaceutical innovations in New Zealand.

SCIENCE AND TECHNOLOGY DIALOGUE FUND OPEN

The Guidelines and Application form for this fund have now been posted on the Ministry of Research, Science and Technology website at: http://www.morst.govt.nz/society/dialoguefund.html

The closing date for applications is 11 December 2002.

EUROPEAN FUNDING OPPORTUNITES FOR NEW ZEALANDERS

Europe has launched its 6th Framework for Research (FP6 2003-2006). With a budget of EU $17.5 billion, FP6 is one of the biggest research programmes in the world. It will support projects in selected strategic areas and foster a true international market for science. The next step will be for EU Member States to co-ordinate their research policies, and for all players to increase their efforts in the research area. Opportunities exist for New Zealand to bid for certain categories of funding. More information is available from: http://europa.eu.int/comm/research/conferences/2002/index_en.html

INTERNATIONAL COUNCIL OF SCIENTIFIC UNIONS GRANTS PROGRAMME

The International Council for Science (ICSU) is calling for applications under the Grants Programme 2004. Proposals for Programme 2004 must focus on the themes listed below which are similar to those for 2003 and as defined by the ICSU Committee on Scientific Planning and Review. Proposed activities should involve scientists from the global scientific community, across scientific disciplines and national borders. Activities that promote the involvement of young scientists, women, and scientists from developing countries, are encouraged. Activities directly related to follow-up action to the ICSU/UNESCO World Conference on Science and the World Summit on Sustainable Development will also be particularly welcome.

Applicants are expected to develop joint activities and to collaborate with other eligible bodies, as well as with the International Scientific Associates, National Scientific Members and National Scientific Associates in preparing and submitting proposals. Applications from individual ICSU members in isolation are not eligible for funding.

The ICSU Priority Themes for Programme 2004 are: Science and Technology for Sustainable Development Capacity Building and Science Education Science / Policy Interface Dissemination of Data Information on Science and Technology Emerging Science and Technology — Creation of New Knowledge.

Each application must have one lead applicant, who will assume the principal responsibility concerning the proposal, and must collaborate with at least one, or preferably, several supporting applicants. The lead applicant can not be the Royal Society but must be an ICSU International Scientific Union, or one of the Interdisciplinary Bodies and Joint Initiatives.

The ICSU closing date for applications is 1 March 2003. For further information please contact Eddie Davis at the Royal Society of New Zealand
Email: eddie.davis@rsnz.org

SEED FUND FOR PROJECTS BETWEEN ARTISTS & SCIENTISTS

The Ministry of Research, Science and Technology and Creative New Zealand have agreed the terms for a Smash Palace Collaborations Fund. This one-off fund is a part of the response to the Smash Palace forum, which the two agencies co-hosted earlier this year. That forum brought together a range of New Zealand artists, designers, scientists and technologists to explore ways and means of fostering innovation and creativity through greater collaboration between the New Zealand arts and science communities. The Smash Palace Collaborations Fund will be targeted at providing support for a small number of pilot projects based on collaborations between artists and scientists. Further information about the $100,000 fund may be obtained from http://www.morst.govt.nz/smashpalace/fund.html

NZMA CHAIR APPOINTED DEAN AT OTAGO SCHOOL OF MEDICINE

Dr John Adams, Chair of the New Zealand Medical Association (NZMA), is to become Dean of the Otago School of Medicine next year. Dr Adams completed his medical training at Otago, graduating in 1976 and going on to become a Fellow of the Royal Australian and New Zealand College of Psychiatrists in 1984. He is currently completing a two-year term as Chair of NZMA.

2002/2003 NEW ZEALAND SCIENCE & TECHNOLOGY PROMOTION FUND RESULTS

The Science and Technology Promotion Fund has been made available by the Government to support activities that make people enthusiastic about science, mathematics, social science, and technology and excite a desire to find out or experience more. Funds are allocated to projects which demonstrate that they have been developed to achieve this promotion in interesting, creative and innovative ways and impact on an audience that has yet to develop positive attitudes and values to science and technology. Individual projects can seek support from the Fund up to a maximum of $100,000. Projects will be funded for a maximum of two years.

68 applications were received with bids totalling $3,828,989. 26 applications were invited to complete a stage 2 application and 23 stage 2 applications were received with bids totalling $1,284,235. The following 8 projects were selected by the Assessment Panel to receive funding in the year 2002/2003. For more information about them, see http://www.rsnz.org/funding/st_promotion/prom_fund_awards02.php

"Sciboard" New Zealand Association of Science Educators. Project Leader: Jenni Edwards, Awarded 2002/2003: $53,000.00

"Summer of Discovery" Australis Consulting Ltd. Project Leader: Vicki Martin, Awarded 2002/2003: $85,000.00

"Stonehenge Aotearoa" The Phoenix Astronomical Society. Project Leader: Richard Hall, Awarded 2002/2003: $56,500.00.

"Quickest, Strongest, Smartest: New Zealand Robotic Olympics" Massey University. Project Leader: Chris Messom, Awarded 2002/2003: $37,470.00

"Maori in Science Research" University of Waikato. Project Leader: Meto Leach, Awarded 2002/2003: $18,000.00

"Integrated Garden Management : The Science Behind Your Garden" HortResearch Lincoln. Project Leader: Howard Bezar, Awarded 2002/2003: $60,000.00

"Stokes Valley Science Initiative" Stokes Valley Rotary Club. Project Leader: Phillip Hankinson, Awarded 2002/2003: $25,000.00

"Science Role Model Calendar" Capital City Science Educators Association. Project Leader: Doreen Gates, Awarded 2002/2003: $40,000.00

For more information about the Fund, contact Faith Atkins, Phone: (04) 470 5759, Email: faith.atkins@rsnz.org

SCIENTISTS ELECTED FELLOWS OF THE ROYAL SOCIETY OF NEW ZEALAND

The Royal Society of New Zealand has elected 14 new Fellows and 3 Honorary Fellows. Their work covers a wide spread of disciplines and research areas, from the heat stability of milk to infantile amnesia and the underground storage of greenhouse gases.

President of the Academy Council of the Royal Society of New Zealand Professor Paul Callaghan FRS FRSNZ said, "It is very pleasing to see the relatively high number of women scientists coming through. We expect the trend to continue as more women attain senior positions." New Zealand currently has 307 Fellows, 25 of whom are women.

The new Fellows are: John Abrahamson, Associate Professor in Chemical and Process Engineering, University of Canterbury. Patrick Browne, Associate Professor, Geothermal Institute, The University of Auckland. Alan Crawford, Platform Leader, Animal Genomics, AgResearch. Robert Davis, Professor of Civil Engineering, University of Canterbury. John Flenley, Professor of Geography, Massey University. Rosalind Gibson, Professor in Human Nutrition, University of Otago. Harlene Hayne, Associate Professor of Psychology, University of Otago. David Kelly, Associate Professor in Plant and Microbial Sciences, University of Canterbury. Kenneth MacKenzie, Associate Professor in Chemistry, Victoria University of Wellington, and Senior Scientist, Industrial Research Limited. Robert McLachlan, Professor in Mathematics, Massey University. Alison Mercer, Associate Professor in Zoology, University of Otago. Harjinder Singh, Professor of Dairy Science and Technology, Massey University. Robin Smith, Professor in Chemistry, University of Otago. Graham Weir, Team Leader, Applied Mathematics, Industrial Research Limited.

Three new Honorary Fellows were also elected. This honour is given to eminent New Zealand scientists living overseas, who maintain close New Zealand links. They are:

Mark Warner, Professor of Physics, University of Cambridge. Warwick Vincent, Professor of Limnology, Université Laval, Canada. Jillian Evans, Director, Merck/MRL, USA.

BOARD FOR NEW INDUSTRY AND TRADE AGENCY APPOINTED

The Government has approved the framework for the new integrated agency which will replace Trade New Zealand and Industry New Zealand. Cabinet has approved the establishment of a board for the new organisation, which will be headed by Phil Lough. Board members are: Peter Menzies (Auckland); Craig Ellison (Wellington); Michael Andrews (Auckland); Ken Douglas (Wellington); Emily Loughnan (Wellington), Craig Boyce (Christchurch), Wendy Pye (Auckland), and Jenny Morel (Wellington).

One of the board's first tasks will be the appointment of a chief executive designate.

TRACE ELEMENT CENTRE AT OTAGO

A new research centre focused on analysing trace elements is being established at the University of Otago. The Community Trust of Otago has contributed $800,000 towards the purchase of a high-resolution mass spectrometer with an inductively coupled plasma source. Research areas that will be boosted by the centralised facility include human nutrition, medical diagnosis and research, forensic analysis, archaeology, fisheries, and the biological and chemical sciences. For more information on the Community Trust of Otago Centre for Trace Element Analysis, contact Professor Keith Hunter, Phone: (03)-4797917.

MARSDEN FUND APPLICATIONS

The deadline for preliminary proposals for the next round of applications is 14 February 2003. Information, application forms and guidelines are available from research offices at institutions, from the Marsden Fund office, Phone: (04)-4705799, and are on the Royal Society website at www.rsnz.org/funding/marsden_fund

NEW PRO VICE-CHANCELLOR IN INFORMATION TECHNOLOGY AT VICTORIA

Professor Warwick Clegg has been appointed to the newly created position of Pro Vice-Chancellor in Information Technology at Victoria University, Wellington. Professor Clegg, who comes to Victoria from the University of Plymouth in England, will be responsible for academic activities in information technology, Information Technology Services and the Library. He is an expert in novel methods of magnetic data storage and advanced instruments, including lasers, for high-resolution magnetic imaging. Professor Clegg will take up the role of Pro Vice-Chancellor at Victoria University in early 2003.

HAWKE'S BAY ENVIRONMENTAL AWARD

Napier's Faraday Centre won the Community Award at this year's Hawke's Bay Environmental Awards. Their hands-on science exhibition teaches school children about alternative energy sources. Napier's Faraday Centre is the Hawke's Bay Cultural Trust's science and technology centre, and is run by a staff of 20 volunteers on a zero budget. The exhibition combines inter-active displays used in two previous alternative energy workshops, which were funded by the Science & Technology Promotion Fund administered by the Royal Society of New Zealand.

2002 MEDALS AND AWARDS RECIPIENTS

The following medals and awards recipients for 2002 were announced last week by the Academy Council of the Royal Society of New Zealand:

Hutton Medal—Animal Sciences to Professor Roger Morris FRSNZ of Massey University, for outstanding contribution to the advancement of animal sciences particularly in the area of animal health and the control of infectious diseases, including those with human health implications.

Cooper Medal—for the best account of research carried out in New Zealand in physics and engineering to Professor Xiao Dong Chen FRSNZ of The University of Auckland, for cutting edge contributions to food process engineering.

Hamilton Memorial Prize for beginners in scientific or technological research in New Zealand to Dr Adrian Walcroft of Landcare Research in Palmerston North, who has made an important contribution to the area of plant physiology.

Hatherton Award for the best scientific paper by a PhD student at any New Zealand university in physical sciences, earth sciences, and mathematical and information sciences to Mr Robert McCormick, Department of Physics, University of Otago, for his contribution as senior author to "Reconsidering the effectiveness of quasi-static thunderstorm electric fields for whistler duct formation", now "in press" with the *Journal of Geophysical Research.*

TERTIARY INSTITUTION GOVERNANCE REVIEW

Professor Meredith Edwards, Director of the National Institute for Governance at the University of Canberra, is to carry out an independent review of the governance of New Zealand tertiary education institutions. The review fulfils a Labour manifesto pledge to improve the contribution made by governing councils, while guaranteeing stakeholder representation and democratic processes.

New Zealand's tertiary education system is undergoing a period of significant change and good governance will be essential in providing a sound foundation. Improved strategic capacity and leadership at both governance and management levels is one of the objectives in the Government's Tertiary Education Strategy 2002-7. Professor Edwards was recently involved with assisting the Commonwealth Department of Education, Science and Training to look at university governance issues as part of its 'Crossroads' review of higher education. Her background includes being the Deputy Vice-Chancellor of the University of Canberra and Deputy Secretary of the Department of Prime Minister and Cabinet. She has served as a ministerial appointee to the University of Canberra's Council for a number of years. She will be assisted by a reference group made up of key stakeholders, including representatives of tertiary institutions, business, unions, and Maori. Her report is due with the Government in March 2003. Review the terms of reference at www.beehive.govt.nz/maharey

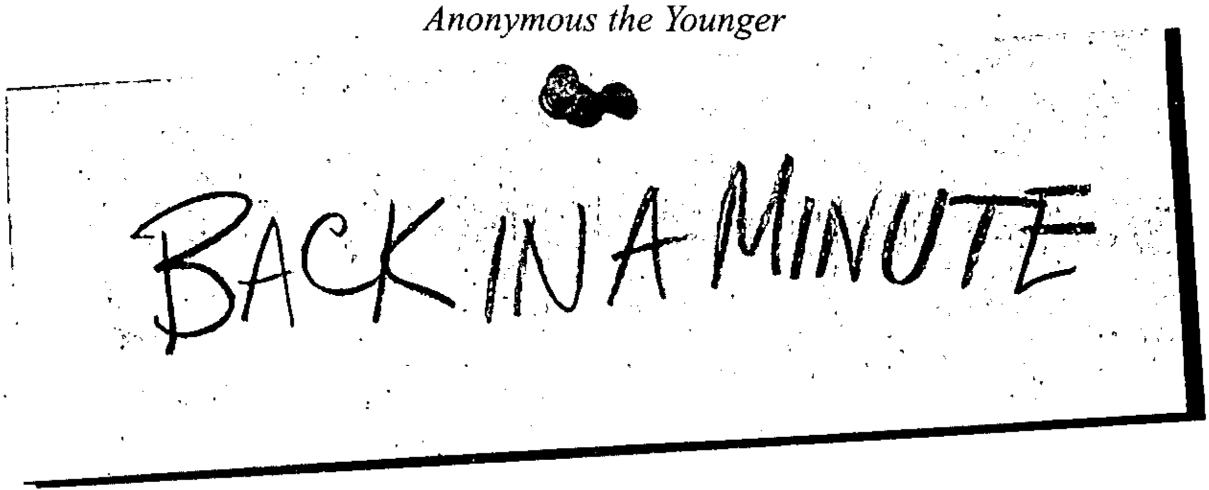
ACADEMY COUNCIL ELECTIONS

The Academy Council of the Royal Society held its Fellows' Annual General Meeting in Wellington on Thursday, 21 November, 2002. Professors Jim Coxon and David Elms both completed terms on Council at this Annual General Meeting. The nominations of Professor Elms, who agreed to stand for a second term, and Professor Anne Smith from the University of Otago were accepted to fill the two vacant positions. Both were elected onto the Academy Council for 4-year terms. The full Academy Council for 2003 is:

President: Professor Paul Callaghan, School of Chemical & Physical Sciences, Victoria University. President-Elect: Professor Carolyn Burns, Department of Zoology, University of Otago. Academy Councillors: —Professor David Elms, Department of Civil Engineering, University of Canterbury. Professor Vernon Squire, Department of Mathematics and Statistics, University of Otago. Dr Stuart Corson, Forest Research, Rotorua. Professor Joyce Waters, Institute of Fundamental Sciences Chemistry, Massey University, Albany Campus. Professor Tony Macknight, Department of Physiology, University of Otago. Professor Patrick Sullivan, Institute of Molecular Biosciences, Massey University. Associate Professor Jenni Ogden, Department of Psychology, The University of Auckland. Professor Anne Smith, Children's Issues Centre, University of Otago.

"Researchmanship", or how to get your PhD without actually working

Anonymous the Younger



The following article is reprinted with permission from *CHEMTECH*, December 1977, (**1977**, *7(12)*, 783-784). Published 1977, American Chemical Society. As such, it reflects the attitudes (the students and professors were all male) and equipment ("I hope I can get at the A60[*] now") of the times. Nevertheless, it contains more than a few words of truth and should be required reading for all budding PhD students.

Allan Blackman, Otago Branch Editor, NZIC.

In theory, getting a PhD involves a research project. If you are an ordinary type of chemist (as distinguished from a theoretical chemist, who is really not a chemist at all), this will involve laboratory work - eight full courses of it, according to the catalogue. Many plodding, unimaginative graduate students actually spend eight to twelve hours a day in the lab - working! But let us see how the true researchman "puts in his time."

It is a fallacy that the two or three years of thesis research are made up of eight- to twelve-hour days. It suffices to make it seem that way. This is called "putting in your time." The true researchman realizes that a chemical research laboratory is not a healthy place and that contact with noxious odours and corrosive chemicals is best taken in small doses. He realizes, from a consideration of the careers of the successful elder statesmen of chemistry, that there is little correlation between success and time spent in the laboratory. What follows are some hints about how to "put in your time" most effectively.

Keep proper hours

Make a point of coming to the laboratory a few minutes before your professor. This is especially important, if, as in the case of James J. Pudvin, the professor works in the same laboratory. If the professor is an early bird and arrives at 9:00 on the button every morning, be in your laboratory by 8:55. Don't bother with shaving, breakfast, etc. – just be there. By 9:00 you should be hard at work. At least make that impression. It need not be research by any means. For instance, Pudvin kept two Erlenmeyers ready all the time, filled with base and phenolphthalein indicator and always had a burette with haphazardly prepared HCl solution ready. When the professor arrived he would run his acid into several samples of base, always exclaiming "Aha, got you that time!" or the like when the indicator changed color. He once explained to his professor that the best analytical results were obtained early in the morning, when one was still fresh and clear-headed.

One can't do this every morning, so sometimes it would do well to reflux a bit of acetone, distil some solvent from a coloured solution, or dump some HCl into a lead nitrate solution. As the $PbCl_2$ precipitated, Pudvin would exclaim triumphantly, "Wait till they read about this in *JACS*" or "Oh boy – another Communication!" An interesting variation was used by another student who did all of his work on the vacuum line. Each morning, the minute he came in, he would turn on the vacuum pump, and leave it chugging away all day. He rarely needed the pump, but he felt, with justification, that the sound of a busy vacuum pump was a reassuring one to his professor. As a clincher he would set up a trap-to-trap distillation, feeling, again with justification, that a Dewar filled with liquid nitrogen was very suggestive of research in progress. The sample of ether that was transferred back and forth was, without doubt, the most well-travelled sample of ether in existence.

By 9:15 the professor usually is deeply immersed in the morning's mail, so it's safe to leave. It would do well to make an appropriate remark on leaving, such as "I hope I can get at the A60 now"[*] or "I hope last year's *JACS* is back from the bindery." Thus, having made your early morning presence known and having clearly stated your

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[*] The A60 was the routine proton NMR spectrometer of the time – *Ed.*

intention of working, it is safe to return to the sack and catch a few more hours of sleep after reading the paper and having a hearty breakfast.

It would do well to come back after lunch, to ask the professor some trivial question, as for instance. "Have you read that article by Bullovsky in the latest *Tetrahedron Letters*?" The professor, being a busy man, will, of course, not yet have laid eyes on the journal. Questions such as these after lunch have several things to recommend them:

- you will have advertised your continued presence in the laboratory;
- you will have made an impression on the professor - he will think that you are a real go-getter, always up on the latest literature; and
- he will feel a trifle ashamed that he's not quite up to date in his field.

Having shown that you're still around, you can safely take in an afternoon movie.

Condition of the laboratory

Closely allied to the "putting in your time" gambit is the condition of the laboratory. Obviously, a neat and orderly laboratory with clean lab benches and spotless equipment would arouse a professor's suspicions. The laboratory must look "worked in," or better yet, "lived in." Pudvin usually kept his laboratory benches littered to make the lab look as if he was madly researching away. On his desk would be sheets of calculations. However, when putting equipment out on the benches, use discretion. The equipment should be rotated periodically. The same flask with the same red solution standing in the same spot for three weeks would do much to cancel any good impression that otherwise might have been made. The morning "work period (9:00-9:15) can be used for equipment rotation. Pudvin usually kept some well-formed crystals under a watch glass on the bench and when the professor made his rounds would remark "they have an interesting NMR spectrum but I'm still waiting for the analysis." Pudvin was quite partial to *p*-dichlorobenzene, azoxybenzene, and ferrocene. Here again, rotation is essential to the success of this gambit. To make the laboratory look "lived in" Pudvin equipped the immediate vicinity of his desk with magazines, selected light fiction, hot plate and coffee pot, alarm clock, a clean shirt and tie; furthermore, he had all of his mail delivered to the laboratory. All this created the inescapable impression that the lab, not his room, was his real base of operations; that his moments of relaxation occurred in the lab, not elsewhere.

Night work

All professors expect a student to have an all-night session in the lab once in a while. Perhaps they feel that if they as students did so, the present generation should suffer in a like manner. Do not disappoint your professor! Pudvin "worked nights" at least twice a month, and his simulation of suffering was so successful that often his professor told him to "go home and get some sleep before you have an accident." Pudvin's approach, which is by no means the only one to take, was as follows.

In the afternoon Pudvin would announce his intention "to make a night of it." He would sign up for the preparative GLC unit for the hours of 8:00 p.m. to 5:00 a.m. {"How else can I get 25 g of starting material?"), and would decline all invitations to go to the movies, play bridge or pool, etc., preferably when the professor was within hearing distance. When everyone was getting ready to go to supper, the professor included, Pudvin was seen carrying flasks, GLC receivers, syringes, coffee pot, radio and a green eyeshade to the GLC room. Next morning at 9:00 when the professor arrived, Pudvin would be found, haggard, pale, noticeably thinner, proudly displaying a 50 mL flask half full of colourless liquid. "100% pure" he'd cheerfully tell the professor. After such concentrated devotion to duty it was not unexpected that Pudvin was not seen in the lab for the next two days.

Actually Pudvin's nightly exertions were spent in strenuous, but pleasurable activities not related to chemistry in the remotest way. At 8:30 the previous evening he had left his laboratory, being careful to leave the lights on and a sign on the door ("BACK IN A MINUTE"). The radio played all night, and the coffee pot remained on "reheat" until Pudvin's return at 8:00 a.m. The flask which he so proudly displayed was filled with 100% pure ethyl acetate.

Choosing a thesis problem

The choice of a thesis problem is second only to the choice of the research professor in terms of its impact on a graduate student's life. Having picked your professor, it is wise not to commit yourself to a thesis topic right away. Get to know your professor a bit better through discussions with the professor's older students. Find out what problems they are working on, and even more important, on what problems they started out their research. The professor's "Pet Problems" - which really intrigue him - are probably those which no one has been able to make work. These are to be avoided: pious words to the contrary, a PhD degree is awarded for completion of a *successful* project.

Pudvin's professor in their first discussion tried to sell him a Pet Problem:

Professor: "Well, I had a little idea the other day that the hydrogenation of boron carbide, if carried out right, should give tetramethyldiborane. That would really make industry look up - we might end up millionaires, to say nothing of the hot papers we'd write..."

Pudvin: (His face showing a mixture of boyish enthusiasm and mournful regret): "Gosh, sir, that sounds real great - it's bound to work. It's really too bad I can't take it on, but in my undergraduate thesis I found that organoboron compounds make me break out in purple blotches."

By way of explanation, Pudvin had found out in his "explorations" in the professor's research group that the professor really had this idea nine years ago and that seven students had already failed at it. Note that Pudvin's excuse allows for no armtwisting by the professor.

Join a going concern; that is, pick a problem that is closely related to work already in progress in the professor's group.

If you do this, the chances are good that you will have minimized both time and effort. There will always be supplies of starting materials around in the research group that can be borrowed, shared, siphoned away in small doses, etc. Also, all required equipment will be on hand in drawers and on drying racks of the more senior graduate students, and expert consultants will be close by at all times - those older students who have come to know more about that particular patch of chemistry than the professor himself. If you do not join a "going concern," you will in truth be a pioneer, entering into unexplored country, the "opening up" of which will require you to carry in your own supplies, and you will tread unmarked paths without a reliable guide. Translated into laboratory terms: you will have to prepare all of your own starting materials and will have only your professor to go to for advice.

Perhaps the best type of problem within this framework is a kinetic study. Here reasonably small quantities of starting materials are required, so that you need never dirty your hands at their preparation. Also, in contrast to a preparative problem, a kinetic study always gets results, *i.e.*, a sackful of numbers, which need not always be meaningful. But that is of no concern to the researchman. Fred Melba, a friend of Pudvin's picked a kinetic problem and worked furiously gathering data during his first summer of research while his professor was lecturing at an NSF Summer Institute. He then fed out all these data in small portions, first in raw form, then in final, refined form, to his professor during the next three years, all the while making his lab look "worked in" and "making nights of it." His professor was at first quite flattered by Fred's pleas for seasoned advice, but after a while got mighty tired of them and soon began avoiding Fred whenever possible. Fred's last two years of "pulling in his time" were pleasant indeed.

We are grateful to Alan Lefor, Hall-Atwater Laboratory, Middletown, Connecticut, USA for this one.

* * * * *

2003 New Zealand Institute of Chemistry Conference First Announcement

Plans are well underway for the 2003 NZIC conference which is to be held in sunny Nelson in the first week of December. We have a great venue lined up at the Rutherford Hotel.

See: http://www.rutherfordhotel.co.nz/ for some details.

The committee is starting to work on the program and more information will follow soon. For now we can let you know that Dieter Seebach (ETH), David Fairlie (Queensland), Chris Abell (Cambridge) and Craig Hawker (IBM) have agreed to present plenary lectures.

Please mark November 30 until December 4, 2003 in your diaries.

Andrew Abell
Chair,
2003 NZIC Conference Committee

Patent Proze

by Jane Calvert and Helen Palmer

METHOD OF TREATMENT CLAIMS - STILL AT ISSUE

You may recall that in earlier issues of ***Patent Proze*** (*Chemistry in New Zealand*, **2000**, *64:1; Chemistry in New Zealand*, **1999**, *63:2; Chemistry in New Zealand*, **1997**, *61:4 and Chemistry in New Zealand*, **1997**, *61:1*) we discussed New Zealand practice in relation to Swiss-style and method of treatment patent claims. These discussions centered on the decisions in *Pharmaceutical Management Agency Limited v The Commissioner of Patents & Ors* [2000] 2 NZLR 529 *(Pharmac)* and *Wellcome Foundation Ltd v Commissioner of Patents* [1983] NZLR 385 *(Wellcome)*.

In *Pharmac*, the Court of Appeal held that Swiss-style claims are allowable in New Zealand. The Court of Appeal in *Pharmac* also considered the issue of patent claims to methods of treating humans, acknowledging that the scope of patentable subject matter has developed over time and that it could no longer be said that a method of treating humans was not an "invention". In other words, *Pharmac* overruled the earlier *Wellcome* decision, in that methods of treating humans could meet the invention requirements of section 2 of the Patents Act 1953.

However, *Pharmac* did not overrule *Wellcome* on the exclusion of methods of treating humans for moral/policy reasons. Nevertheless, an interesting statement was made in the *Pharmac* judgement, to the effect that a logical approach might be to allow claims to methods of treatment, but to require from the patentee a disclaimer of any right to sue a medical practitioner who might use this method of treatment. This would prevent any interference in the well-established protection afforded to medical practitioners by the decision in *Wellcome*.

Despite these comments by the Court of Appeal in *Pharmac*, the Intellectual Property Office of New Zealand (IPONZ) has adopted a practice whereby it continues to refuse claims to methods of treating humans under section 17 of the Patents Act 1953. This section allows the Commissioner of Patents to refuse an application for a patent if the use of the invention in respect of which the application is made would be contrary to morality.

Pfizer, Inc. has recently challenged this practice in a High Court appeal. The Assistant Commissioner of Patents had refused to accept two Pfizer applications directed to mesylate salts of some indole derivates that could be used for treating psychotic disorders. The two applications had been refused on the ground that the claims directed to methods of treating humans were contrary to morality and, if granted, would be in breach of section 17.

The High Court has recently handed down its decision on Pfizer's appeal. In a short judgement, Justice Ellis held that the High Court was bound by the Court of Appeal's earlier decisions, and that "the Assistant Commissioner rightly excluded the claims to a method of treatment of human beings".

We are therefore left with a situation where the *status quo* remains in place. The recent Pfizer decision has not addressed the continuing uncertainty in this area of New Zealand patent law. Thus, some methods of treating humans, such as cosmetic methods, contraceptive methods and non-invasive diagnostic methods, are patentable. The boundary between allowable methods and those that are refused by IPONZ is somewhat blurred.

We are currently waiting to hear whether Pfizer will be able to take the High Court decision on appeal to the Court of Appeal. If such an appeal does not eventuate, or if an appeal is not successful, any alteration to the law in this area will have to come from a legislative change instigated by Parliament. The Government is currently reviewing the Patents Act and has sought submissions from the public on the issues surrounding claims to methods of treating humans.

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

DuPont steps into a new era

Richard Stevenson
Royal Society of Chemistry, Burlington House, Piccadilly, London, W1J 0BA, United Kingdom

DuPont, a company with a 'science engine' at its heart, is transforming itself in readiness for a new era of integrated science.

Reproduced with permission of the Royal Society of Chemistry from *Chemistry in Britain*, **2002**, *38(8)*, 27-30. All images courtesy of DuPont.

The history of DuPont fits into two neat 100-year cycles. From its foundation as a family business in 1802 until its transformation into a conventional corporation in 1902, DuPont was a manufacturer of explosives, supplying the needs of the soldiers and engineers who built the US. In the 20th century, DuPont was a chemical company at the forefront of the global march of new materials. In 2002, as it enters its third century, the company has transformed itself once again, offering not just materials but whole assemblies and services that combine chemistry with biology, electronics and engineering.

The person charged with overseeing this transformation since his appointment as chairman in 1999 is Charles ('Chad') Holliday. He has no doubts about what drives DuPont: 'We have a science engine in this company', he said recently.

The worst of times?

Holliday acknowledges that 2001 was a bad year for the company, as for everyone else in the chemical industry. He prefers to measure the company's progress against its performance in 2000, which he says was a typical year. Although DuPont's turnover is a lot less than it was in, say, 1992 (at the end of the last recession), its structure has changed so much that its underlying profitability is much greater.

In the past five years DuPont has got out of the energy business by selling its Conoco oil subsidiary. It got out of pharmaceuticals when it realised that it couldn't compete with the drug giants. Finally, it put a lot of its nylon and polyester businesses into joint ventures (JVs) with other companies. On the other hand, over the same period DuPont has made a large number of acquisitions. These include Pioneer Hi-Bred and Protein Technologies in the agriculture and nutrition sector, Herberts Paints, and a string of smaller scale acquisitions and JVs in the electronic and communication technologies sector, such as Nobel laureate Alan Heeger's Uniax, which has exciting technology for organic light-emitting diodes (OLEDs). Overall, DuPont's buying and selling deals have been worth around $50,000m (*ca* $NZ120,000m) over the past five years.

In an uncharacteristic understatement, Holliday says that 'we're quite pleased with this adjustment to our company'. The keys to future success, Holliday believes, include R&D 'reinvigoration', together with rigorous control of mergers and acquisitions and disciplined cash management. DuPont's proud boast is that its products go into markets that represent 50% of global GDP. Traditionally, DuPont has aimed its products closer to the end customer than many of its competitors who sell to other chemical companies. Thus DuPont sets great store by its trademarks and brands - it currently has over 2,000 active brand identities that identify it to end-users. But this portfolio of products and

DuPont at a glance

Turnover (2001):	$24,700m
Net profit (2001):	$4300m
Capital spending (2001):	$1600m
R & D spending (2001):	$1200m
Employees:	79,000 (*ca.* 50% outside USA)
Operations:	135 processing and manufacturing facilities in 70 countries
Headquarters:	Wilmington, Delaware, USA
Research:	Over 40 R & D and customer service labs in the USA; over 35 labs in 11 other countries
Research headquarters:	
Global:	DuPont Experimental Station, Wilmington, USA
European:	Meyrin, Switzerland
Research employees:	5100 scientists and engineers

Production sites in the UK:

Bristol:	Microcircuit materials
Dumfries:	Mylar, Melinex and Kaladex PEN polyester films
Gloucester:	Nylon yarns
Humberside:	Dymel aerosol propellants
Maydown, Londonderry:	Lycra and Kevlar fibres
Peterborough:	Soya protein-based consumer food products
Pontypool:	Dacron and other polyester fibres
Ruabon:	Syton and Mazin colloidal silica slurries
Wilton:	Nylon intermediates, specialities and polymer; purified terephthalic acid and resins
Workington:	Cambrelle textiles

brands is constantly being updated: 'We're determined to be the world's leader in innovation in our chosen markets', Holliday remarks.

The best of times?

Holliday has set a goal that by 2005 one-third of DuPont's sales should come from products introduced in the previous five years. Although the company is making progress towards this target (excluding businesses due to be spun off, it achieved 22% in 2000 and 24% last year), it puts considerable pressure on the R&D organisation to deliver, and to continue to deliver in subsequent years.

Science is integral to the 'three pathways to growth' that Holliday has identified for the company. The first of these is 'integrated science', bringing together chemistry, physics, biology and engineering. 'We believe we are uniquely equipped to bring together science teams to solve customers' problems', Holliday said recently, citing DuPont's $35m research alliance with various departments at Massachusetts Institute of Technology as an example of building teams with external partners.

The second pathway to growth for DuPont, Holliday believes, is 'knowledge intensification'. This involves selling 'total systems' to customers and making more use of the company's expertise. For example, DuPont is trading on its reputation for safe plant operation to sell safety-consulting services to transport, automotive and oil companies, alongside the physical products it can sell them. Another example is to combine its expertise in desktop printing inks and textile manufacturing to produce a new system called Artistri for inkjet printing on fabrics. DuPont's research teams working on fuel cells and OLEDs expect the company to be selling complete assemblies, not just the DuPont materials that will go into them.

The third growth pathway is through productivity. DuPont has embraced the 'six sigma' quality and productivity philosophy pioneered by


E. I. du Pont


Wallace Carothers


Roy Plunkett


Paul Morgan


Stephanie Kwolek


Charles Pedersen

DuPont 200 years: a timeline

1802	E. I. du Pont establishes gunpowder works on Brandywine River
1857	Lammot du Pont introduces sodium nitrate blasting powder
1880	DuPont begins producing nitroglycerine-based dynamite and later nitrocellulose-based smokeless powders
1902	Present company formed
1903	Experimental Station established
1904	DuPont expands into cellulose lacquers
1910	DuPont buys Fabrikoid artificial leather
1914-18	DuPont supplies 40% of Allied explosives during WW1
1915	DuPont buys Pyralin nitrocellulose plastics
1917	DuPont expands into dyestuffs to replace German imports
1919	DuPont buys controlling interest in General Motors
1920	DuPont buys viscose rayon process
1921	Shiels and Flaherty discover high nitrocellulose paint (Duco)
1923	DuPont buys cellophane process
1926	DuPont signs patent-sharing agreement with ICI
1930	DuPont-GM JV introduces Freon refrigerants invented by Midgeley
1930	Collins and Carothers discover neoprene
1935	Berchet and Carothers discover nylon
1935	DuPont registers Lucite trademark for polymethylmethacrylate
1938	Plunkett discovers Teflon
1940	Walter Carpenter first non-DuPont family member to be Company President
1942-45	DuPont builds and operates Hanford and Oak Ridge for Manhattan project
1952	Mylar, Dacron, Orlon introduced
1952	US Supreme Court ends DuPont-ICI patent sharing agreement
1957	US Supreme Court forces DuPont to sell GM stake
1962	Lycra introduced
1963	Nomex introduced, based on Paul Morgan's interfacial polymerisation
1967	Tyvek introduced
1969	Corian developed
1971	DuPont introduces Kevlar, developed by Stephanie Kwolek
1981	DuPont buys Conoco oil company
1987	DuPont chemist Charles Pedersen wins Nobel prize for crown ethers
1990	DuPont-Merck JV in pharmaceuticals
1993	DuPont sells Lucite to ICI
1997	DuPont buys Pioneer Hi-Bred and Protein Technologies International
1997	DuPont buys ICI's polyester business (but purchase of ICI's TiO_2 business stopped by Federal Trade Commission)
1999	DuPont buys Herberts Paints
1999	DuPont sells Conoco
2001	DuPont sells pharmaceutical business

General Electric and Holliday claims that in DuPont it is 'practised as well as any company in the world'.

Spun (off) fibres

Holliday sees the growth drivers for the future as being electronics, biotechnology, materials, safety and security. Instead of structuring the company in terms of products - polyesters, fibres, pigments *etc.* - DuPont was reorganised in February 2002 into six divisions or 'growth platforms' that match customer sectors more closely. Five of these are closely linked, but the sixth, DuPont Textiles and Interiors (DTI), is being formed into a separate entity and may be divested.

The notion of spinning off the fibre businesses is shocking to many people inside and outside the company: they have been 'part of the fabric of the company for decades', one executive commented. Holliday acknowledges that the businesses have been critical to DuPont for many years: 'We more than any other company founded the [synthetic fibre] industry', he says. But the industry is migrating from the West to developing countries where low wages and huge markets give textile manufacturers a decisive edge.

'Textiles and Interiors will be ultimately separated to allow it freedom to adapt to the changing needs of its customers', is how Holliday puts it. DuPont executives will not be drawn on exactly how and when DTI will be spun off, but

DuPont's new structure, introduced February 2002

'Growth platforms'	Pro-forma performance 2001 (2000)		
	Sales $m	After-tax operating income $m	%
DuPont Agriculture & Nutrition Crop Protection Nutrition & Health Pioneer Hi-Bred International	4209 (4372)	242 (323)	6 (7)
DuPont Coatings & Color Technologies Performance Coatings Titanium Technologies	4917 (5457)	498 (783)	10 (14)
DuPont Electronic & Communication Technologies Display Technologies Electronic Technologies Fluorochemicals Fluoropolymers Imaging Technologies	2688 (3375)	283 (581)	11 (17)
DuPont Performance Materials Engineering Polymers Packaging & Industrial Polymers DuPont-Dow Elastomers DuPont Teijin Films	4693 (5334)	277 (578)	6 (11)
DuPont Safety & Protection Advanced Fiber Systems Chemical Solutions Enterprise: Specialty & Performance Chemicals Industrial Chemicals Nonwovens Safety Resources Surfaces	3574 (3694)	485 (593)	14 (16)
DuPont Textiles & Interiors* Fibers Intermediates Industrial Nylon Fibers, Resins & Intermediates DuPontSA	6477 (7722)	70 (709)	1 (9)
Other Bio-Based Materials† Intellectual Assets Business† Corporate Ventures† Pharmaceuticals‡			

* To become separate entity by 1 January 2003.

† Reporting to Chief Science and Technology Officer.

‡ DuPont Pharmaceuticals sold to Bristol-Myers Squibb 2001; DuPont retained its interests in Coxaar and Hyzaar, licensed to Merck.

if the company follows the route it took when it divested Conoco, it will probably choose a separate stock market listing for DTI and sell off a proportion of the company, maybe 20% in the first instance. That would give Dupont the chance to get a better price for the rest. (With DTI's profits crumbling from $709m in 2000 to only $70m in 2001, now is a good time to tell the stock market it is being dumped, but a bad time actually to sell).

Solid platforms

While DTI serves commodity markets where labour costs are important, the other five DuPont platforms serve growing high-value markets. The company does not anticipate many job losses in these areas, rather the reverse. Holliday points out that for DuPont 'purchasing costs are three times payroll costs, so the opportunities for savings are on the purchasing side'.

DuPont Agriculture & Nutrition, led by Howard Minigh, combines DuPont's long-standing business in crop protection chemicals with recent acquisitions in seeds and genetics and in soya protein food ingredients. It also includes the BAX system for pathogen screening, and the RiboPrinter system that applies the polymerase chain reaction to microbial screening, both with a food safety emphasis.

DuPont Coatings & Color Technologies, led by Ed Donnelly, concentrates on dispersions and particle technologies, coatings and colourants. It includes businesses such as titanium dioxide, paints and powder coatings, and digital inks, with markets ranging from cars and paper to industrial coatings, paints and plastics. Although the world market for digital inks may be tiny compared to that for paints (around $1000m-3000m pa as against $60,000m-70,000m), it has a high growth potential at around 12% pa. Donnelly says that DuPont wants to expand the coatings and colour business into the 'white spaces' where it didn't have a presence, such as textile and photographic printing opportunities for digital inks, antimicrobial coatings, and new aerospace coatings.

DuPont Electronic & Communication Technologies, under the leadership of Diane Gulyas, is perhaps an unexpected area to find DuPont operating in, but from a base in providing polymers for wiring and printed circuit boards it has grown into the world's No 2 supplier of materials to manufacturers of electronic devices. The impetus for speed, miniaturisation and lower cost in this industry opens up big opportunities for the suppliers of materials and the sector offers high profit and growth levels. Gulyas says that DuPont 'aims to build a significant business with double-digit growth'. DuPont has a leading R&D position in OLEDs, which will begin to replace liquid crystal diodes in display devices this year, and in fuel cells based on its own membrane technology.

DuPont Performance Materials, led by Craig Naylor, is perhaps the business with closest links to DuPont's history. Its products cover engineering and industrial resins, elastomers and films, with markets in the automotive, construction, electronic and packaging industries. Its most exciting opportunities lie in technologies such as PEN films for OLED displays, new markets for engineering polymers such as Caltrel or elastomers such as the metallocene-based Engage, and in specialist products like the new BioMax biodegradable polyester.

DuPont Safety & Protection, under Ellen Kullman, is a completely new business grouping, bringing together well-established materials for safety equipment, such as Kevlar, Nomex and Tyvek, with medical fabrics and equipment, and consulting and training services offered to the chemical, oil and transport industries.

Despite (or because of) the likelihood of being sold off, DuPont Textiles & Interiors is playing up its strengths. "We intend to use this separation event as a catalyst to dramatically improve the performance of this business", is how Richard Goodmanson puts it. Australian-born Goodmanson is DuPont's Chief Operating Officer and has been given the job of leading DTI. He points out that DTI will be the largest integrated manufacturer of fibres and fibre intermediate chemicals. It has an annual turnover of $6000m-plus and a 'deep technology base', with R&D centres in nine countries. With Lycra and Cordura fibres, Stainmaster carpet treatments, and many others, 'We have the only meaningful consumer brands' in the sector, Goodmanson says. It is operating in a large, fragmented industry, yet 75% of its sales come from businesses where it is the world's No 1 (and in some cases is an order of magnitude larger than the No 2 supplier). DTI 'will generate a lot of cash for the owners, whoever they are', Goodmanson concludes.

Growth businesses

There are some anomalies in this new structure. For example, some products like fluoropolymers being split across several platforms, so the manufacturing plants will have multiple customers within the company. Also there are some ventures based more on intellectual property than physical production, such as technology licensing, and new start-ups such as bio-based materials. These fall naturally under the direction of Tom Connelly, DuPont's Chief Science and Technology Officer.

The heart of Connelly's realm is the famous Experimental Station at Wilmington, Delaware, in the USA, but DuPont has scientists in many other labs around the world. With a PhD from Cambridge, UK (where he was a Winston Churchill scholar) and experience of running businesses in the UK and Hong Kong as well as heading the European Technical Centre in Geneva, Connolly has a broad background. He needs it, because DuPont's 5100 scientists and engineers are spread across 12 countries and a bewildering array of technologies.

Current high priority research areas for the company include biotechnology (both for plant breeding and industrial production), electronic materials, and nanotechnology. All these are treated as enabling technologies – for example, the work on nanoparticles could find outlets in many areas including electronics and coatings. An example of bringing together different strands of technology is Sorona, a new fashion fibre now being test marketed, which has remarkable stretch recovery properties. Sorona is polytrimethylene terephthalate, known to DuPont scientists as 3GT. The molecule has been known for decades, but commercialisation has been

Above: *The DuPont Experimental Station.*

held back by the cost of propane-1,3-diol (the three-carbon glycol referred to in the 3GT nickname). However, DuPont scientists have been working with the biotechnology specialist Genencor to make 3G by a fermentation route. This has involved taking four separate genes from various species of bacteria and yeasts and splicing them into *E. coli*, the bacterial workhorse. In partnership with Tate & Lyle's US subsidiary, DuPont's scientists have shown that the engineered *E. coli* can then make the 3G molecule from glucose derived from cheap corn syrup. DuPont's Scott Nichols points out that the project is an excellent example of the new ways of thinking that Holliday champions for DuPont, both by setting up teams (with Genencor and Tate & Lyle), and by 'reducing the environmental footprint' by using a renewable resource in place of a fossil feedstock.

From family firm to global giant

When the du Pont de Nemours family fled Revolutionary France for the new United States of America at the dawn of the 19th century, they took with them some valuable assets from Europe: contacts, and an enlightened way of doing business. Young Eleuthère Irénée du Pont, who had studied under Lavoisier at the French national gunpowder works, decided that he could make better gunpowder than the Americans. In 1802 'E. I,' established a powder works on the banks of the little Brandywine River outside Wilmington, Delaware. Soon the river was powering a whole series of powder mills as Du Pont became the biggest gunpowder supplier in the US. Much of the firm's success was due to access to capital and technology from the family's French contacts, and their commitment to quality, safety and worker welfare. Technical innovation was a hallmark of the company: in 1857, Lammot du Pont developed a way to use cheap Chilean sodium nitrate to break the British government's stranglehold on the saltpetre (potassium nitrate) trade. Lammot also introduced the company to dynamite production (though he was later killed in a plant explosion). Dynamite (based on nitroglycerine) and guncotton (based on nitrocellulose) not only kept the DuPont company in the forefront of explosives but introduced it to real chemistry. As well as the military, DuPont supplied the hunters, railway engineers and miners who opened up the American West. At the end of the 19th century the network of shareholdings among E. I.'s descendants became too cumbersome: the family partnership was turned into a conventional company, and in 1902 three du Pont cousins led a management buy-out. The second century for the company ushered in a new era as a chemical company. A year later DuPont established its famous Experimental Station, which went on to become one of the world's premier industrial research laboratories. At first this research was based on DuPont's expertise in nitrocellulose, chemistry and on technology transfer from France: quick-drying Duco cellulose paints transformed the motor industry. DuPont licensed cellophane from France and improved it. Between the two world wars - when war work naturally dominated - DuPont introduced a string of new materials that helped to establish the modern affluent society. Carothers invented neoprene and nylon, Midgeley invented Freon, Plunkett discovered Teflon. The company's proud motto was 'Better things for better living - through chemistry'. Like an imperial power, DuPont divided up the world through agreements (later broken up as anti-competitive) with its European rivals IG Farben and Imperial Chemical Industries (ICI), and with General Motors (GM), a major customer. During World War I DuPont's engineers had built an enormous new factory (Old Hickory in Tennessee) at record speed to supply the Allied war effort. In World War II they topped the feat by building the Hanford and Oak Ridge complexes to supply the atom bomb project. As a result, the company could have moved into nuclear energy - 'it could have become Westinghouse', as a company historian puts it. Instead, DuPont chose to stick to chemistry. The post-war years saw the stream of new materials continuing, with Lycra, Nomex and Kevlar among them, and all kinds of other chemical products being introduced. DuPont was one of the most successful diversified chemical companies of its day - it even bought an oil company (Conoco) to secure its feedstocks. By the 1990s, the commercial environment for chemical companies had changed. Like many others DuPont has put itself through a vigorous process of transformation in the past decade. It has sold its oil and pharmaceutical

Above: *Dupont materials are used today used in products as diverse as hi-tech sporting equipment, safety clothing, paints and furniture.*

operations - both of them good businesses, but too small to compete with global rivals - and it has sold off, swapped, or put into joint ventures most of its commodity plastics. Although the sense of history is strong at DuPont, there is little sentimentality about selling off famous brands: even synthetic fibres, a sector that DuPont virtually invented and has been described as 'part of the fabric of the company', is being groomed for some kind of future separation. Today, DuPont is based not just on polymer chemistry but a broader range of sciences - organic and inorganic materials, biotechnology, electronics - and on business units aligned with market sectors rather than organised by the shape of the molecules they make. The old motto of 'Better things ... through chemistry' has been replaced by 'The miracles of science'.

About the author

Richard Stevenson has recently completed 25 years on the staff of Chemistry in Britain, the magazine of the Royal Society of Chemistry. He has been Editor since 1991 and is a former Chairman of the Association of British Science Writers.

XX1st International Carbohydrate Symposium

Cairns, July 2002

Robin Ferrier and Richard Furneaux

Industrial Research Limited, LowerHutt

Australia established its premier reputation as a conference country amongst the international carbohydrate community in 1980 when the ninth of this biennial series, run under the auspices of IUPAC and IUBMB, was held in Sydney - surely a city endowed with everything dreamt of by chemical tourists (except of course inexpensive fares). That meeting has since been considered the standard against which the successors have been measured. The Cairns symposium this year, therefore, had very much to live up to, but with the fantastic natural advantages of the location and a new conference centre rated in the top ten in the world, and with strongly appealing chemical and social programs, it seemed to succeed admirably. Professor Stephen Angyal's anniversary history of the meetings, which all attendees received, identified the special significance of the 21st. New Zealand shared a little in the responsibilities and privileges, with our Royal Society being an official sponsor, in particular of two of the main speakers Professors Roush (USA) and Tietze (Germany) who gave outstanding and different lectures both in Cairns and at the 14th IUPAC Conference On Organic Synthesis held in Christchurch the following week. The present reporters were invited to share fully in the work of the Cairns organizing committee, chaired by the irrepressible Bob Stick of the University of Western Australia; altogether 19 New Zealand based chemists attended.

Reflecting the dramatic increase in the recognition of the significance of the carbohydrates in fundamental biological processes, and the arrival of glycobiology as an accepted discipline, numbers at international carbohydrate meetings have been rising appreciably in recent years, and Cairns provided yet more evidence: three times as many registrants travelled there as the 220 who were in Sydney in 1980. The nature of the invited and contributed lectures and the posters clearly illustrated the newfound importance of the subject. While interest remains strong in basic synthesis using sugars as starting materials, in their organic chemistry and in industrial and biotechnological aspects of carbohydrates, more and more effort is going into all manner of biological and medical topics as evidenced by some of the section titles: carbohydrates in molecular and biomolecular interactions, carbohydrates and cellular development, biosynthesis of carbohydrate polymers, bioengineering of carbohydrate-active enzymes, carbohydrates in immunology and cancer, carbohydrates and microbial pathogens.

Before the welcome reception on Sunday evening Professor Adrienne Clark, one of Australia's foremost women scientists (botanist with strong chemical leanings) and with extraordinary prominence also in administration, politics and business, gave a talk of general relevance and of interest to both registrants and accompanying visitors of whom there were 80. This initiative we would recommend to other programme committees; it acted as an appetizer for the plenary lectures that were to follow. Phrases like anti-toxin oligosaccharides,glycoconjugates and the immune systems, synthesis of antibiotics, detection of lysosomal storage disorders, anti-tumour vaccines, anti-parasite drugs and automated synthesis of oligosaccharides to address medical problems give an indication of the themes of the 10 splendid plenary lectures given by leaders in the field from USA (3), Japan (2), Canada (2), Australia (1), Germany (1) and UK (1). About 120 other talks and 500 posters were presented.

On the Wednesday, as the main feature of a full social programme, we had a day free to visit either the Great Barrier Reef or inland wonders and, if a whole day off seems extravagant, no-one complained about that - or indeed anything else about a memorable and productive week.

As a postscript to the above we wish to explain (as opposed to offer excuse for) the delay in its submission: we felt no responsibility to report via *Chemistry in New Zealand* as it was until recently, and had temporarily overlooked the major change that has occurred. Now we are delighted to contribute, and we hope many will feel the same way and supply appropriate material to support the new Editor and Editorial Board. They have set themselves such high standards in recent issues by providing professionally presented, interesting and informative mixes of news and chemical material, as well as retaining a tolerable proportion of advertisements, that the quality will be difficult to maintain. We hope NZIC members will take pride in the new product, as we do, and volunteer their contributions and assistance as generously as they can. (See *Chemistry in New Zealand*, **2002**,*66:3*, 9 for evidence of the importance of *Chemistry in New Zealand* to the membership).

The 2002 Nobel Prize in Chemistry

Fenn and Tanaka, and Wüthrich

Allan Blackman & Brian Halton

John B. Fenn

Koichi Tanaka

Kurt Wüthrich

Synopsis

The announcement of the 2002 winners of the Nobel Prize in Chemistry was made on October 9. The prize has been divided into two, going to scientists in the important fields of mass spectrometry (MS) and nuclear magnetic resonance spectroscopy (NMR), specifically for *"the development methods for the identification and structure analyses of biological macromolecules"*.

The Laureates for mass spectrometry are **John B. Fenn** (Virginia Commonwealth University, USA) and **Koichi Tanaka** Shimadzu Corporation, Kyoto, Japan) each gain one quarter of the prize whilst Laureate **Kurt Wüthrich** (ETH, Zürich, Switzerland, and The Scripps Research Institute, La Jolla, USA) gains the other half for his work on NMR. Each of the three has contributed in different ways to the further development of these methods to embrace biological macromolecules.

Fenn and Tanaka "developed soft desorption ionisation methods for mass spectrometric analyses of biological macromolecules" whereas Wüthrich "developed nuclear magnetic resonance spectroscopy for the determination of the three-dimensional structure of biological macromolecules in solution". These advances provided the revolutionary breakthrough to make chemical biology into the "big science" of our time. We can now rapidly and reliably identify what proteins a sample contains and also produce three-dimensional images of proteins in solution. Thus the chemist can both "see" the proteins and better understand how they function in cells.

John Fenn was born in New York City in 1917. He obtained an A.B. from Berea College (Kentucky) in 1937 and his PhD from Yale in 1940. After a dozen years working in process development at Monsanto and Sharples Chemical he was appointed Director of Project SQUID, a US Navy program of basic and applied research in Jet Propulsion administered by Princeton University. He became Professor of Aerospace and Mechanical Sciences at Princeton in 1959. Fenn joined the Yale faculty in 1967 as Professor of Chemical Engineering and Chemistry, a post he held for 13 years. From 1980 until his retirement in 1987, he was Professor of Chemical Engineering, remaining there as a Research Scientist after becoming Emeritus. In 1993 he moved to Virginia Commonwealth University as Research Professor. He has served as a visiting Professor at Trento University in Italy, the University of Tokyo, the Indian Institute of Science at Bangalore, and the Chinese Academy of Science in Beijing and as a distinguished lecturer at several other institutions. He has authored one book and over 130 papers, and he is sole or co-inventor on 19 patents.

Somewhat surprisingly, Fenn's Nobel Prize-winning research was carried out in the 1980s towards the end of his academic career, and at the age of 85, he becomes the oldest person to be awarded the Nobel Prize in Chemistry. A lifelong interest in molecular beam research led him to investigate the electrospray process first observed by John Zeleny in 1914. Sadly, he has a tragic connection with Dunedin - while visiting there in 1992 to give a seminar, his wife sustained ultimately fatal injuries in a car accident on the peninsula.

Koichi Tanaka is undoubtedly the least well known of this year's laureates and his is a remarkable story. He is not a trained chemist, is only 43 years old, and is not a university professor and he doesn't even have a doctorate - in fact, he is the first person to win the Nobel Prize in Chemistry having only a bachelor's degree. Tanaka was born in 1959 and obtained a bachelor's degree in electrical engineering from Tohoku University in 1983. He started work that year in the Central Research Laboratory at Shimadzu Corporation in Kyoto, and he now serves as a Chief Researcher in the company's Life Science Business Unit. During this time he spent five years in the life sciences department of Kratos Analytical, Shimadzu's subsidiary in Manchester, England, returning to Japan in May of this year.

At the same time as Fenn was working on the electrospray method of soft ionisation, a number of other groups were trying to use lasers to gently ionize large molecules. The concept of soft laser desorption applied to small molecules was successfully demonstrated in the mid 1980s but Tanaka made the breakthrough with reports of the mass spectra of intact chymotrypsinogen, carboxypeptidase A and cytochrome C. In stark contrast to John Fenn, Tanaka had completed his prize-winning research at the age of 28. Shimadzu commercialised his findings in 1989, paying him 10,000 yen (about NZ$170 at current rates) for obtaining the patent; last year the company earned some $NZ66 million in sales from his invention. Shimadzu are reportedly planning to present Tanaka with a hefty bonus and promote him. However, Tanaka appears uninterested in promotion, saying at a news conference that he had deliberately failed company exams designed to test employees' managerial aptitudes so he could concentrate on his research projects. Scifinder® lists Tanaka has having authored only 9 papers and one must wonder about his promotion chances if he were in academia!

Kurt Wüthrich was born in Switzerland in 1938 and undertook his undergraduate education at the University of Bern. He obtained his PhD from the University of Basel in 1964 and did postdoctoral work at both Basel and Berkeley. After two years at Bell Telephone Labs in New Jersey, he was appointed Privatdozent at the Eidgenössische Technische Hochschule Zürich in 1970. Here he was promoted to Assistant Professor (1972), Associate Professor (1976) and Professor of Biophysics (1980). He became Chairman of the Biology Department in 1995 and, in 2001, he accepted the position of Cecil H. and Ida M. Green Visiting Professor of Structural Biology at the Scripps Research Institute in California. Currently he holds Professorships at Zürich and Scripps and plans to move his laboratory to the USA because Swiss law requires him to retire at the age of 65.

Wüthrich began his career as an inorganic chemist - the first four of his 621 papers concerned Cu^{2+} complexes of phenylenediamine - but gained an interest in NMR during his time at Berkeley and Bell Labs. Two 1968 papers titled "High resolution proton magnetic resonance spectra of sperm whale cyanometmyoglobin" and "Proton magnetic resonance studies of human cyanomethemoglobin" published in the *Proceedings of the National Academy of Sciences* signalled the start of his interest in the NMR of biological molecules. Since this time, Wüthrich has been instrumental in developing new methods of analysis of NMR data by the application of multidimensional NMR techniques to biological systems. In 1985, he had refined the method to a sufficient degree to allow the determination of the solution structure of the small protein proteinase inhibitor IIA from bull seminal plasma. This was the first protein to have been structurally characterised solely by NMR. Since then, NMR has become a tool of ever increasing importance in biological chemistry, and currently about 20% of the protein structures in the Protein Data Bank have been determined using the technique.

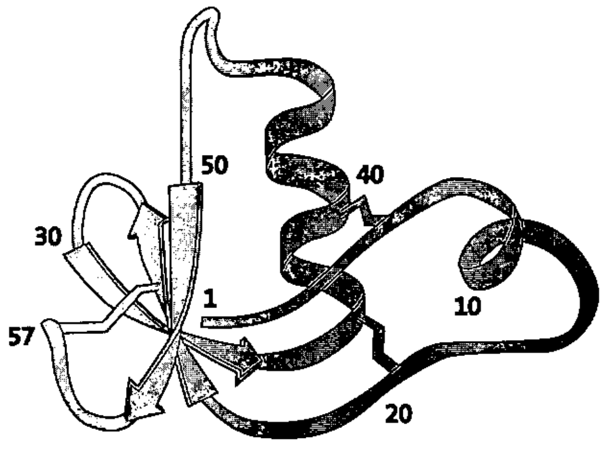

Figure 1. This protein consists of a long chain of amino acids that is pleated, folded and wound together like a ball of wool. It is this three-dimensional image of the protein that one needs to achieve to understand the function of the protein. This protein, one of the first to have its structure determined with NMR, has a diameter of approximately 10^{-8} m.

Revolutionary analytical methods for biomolecules

Why study biological macromolecules?

All living organisms – bacteria, plants and animals – contain the macromolecules that are responsible for what we call life. Events in the cells are controlled by nucleic acids (such as DNA) that may be termed the cells' "directors", while the various proteins are the cells' leading actors. Each protein has a biological function that may vary with its environment, as is well known for haemoglobin that transports oxygen to all the cells in the body.

Protein research itself is not new, but proteomics, *i.e.* studies of how different proteins and other substances act together in the cell, is a relatively new field of research that has grown enormously in the past few years. As the gene sequences of more and more organisms have been mapped and the research frontier advanced, new questions have cropped up: how can it be that man's 30,000-or-so genes code for hundreds of thousands of different proteins? What happens if a gene is damaged or is missing? How do diseases such as Alzheimer's or mad cow disease originate? Can the new chemistry be used to diagnose and treat more quickly the diseases that are threatening mankind?

To be able to tackle questions such as these the chemist must be in constant pursuit of new knowledge of proteins and how they function together with each other and with other molecules in cells. This follows from the fact that small variations in protein structure determine function (Figure 1). It is also critical to be able to see what protein molecules look like at the very moment when they interact with one another and what happens at the decisive moments.

Mass spectrometry – a method of identifying molecules

Mass spectrometry allows the rapid identification of a component in a sample on the basis of its mass. The foundations of mass spectrometry were already in place at the end of the nineteenth century. The first analyses of small molecules were reported in 1912 by Joseph J. Thompson. Several of the Nobel Prizes of the twentieth century depended directly on mass-spectrometric analysis. Examples are Harold Urey's discovery of deuterium (Nobel Prize in Chemistry 1934) and the discovery of the fullerenes, "carbon footballs" that gave Robert Curl, Sir Harold Kroto and Richard Smalley the Nobel Chemistry Prize in 1996. This long used, very sensitive technique formerly could only be applied to small and medium-sized molecules gaining routine application in doping and drug tests, foodstuff control and environmental analysis.

The goal of using mass spectrometry for macromolecules long attracted the scientist. During the 1970s a number of successes were achieved in transferring macromolecules to ions in the gas phase. These, termed desorption technology, have formed the basis for the revolution in the field during the past twenty years.

Although macromolecules are large in comparison with other molecules they are, nevertheless, still remarkably small. A haemoglobin molecule, for example, has a mass of 10^{-19} g. In order to measure the mass of such entities the mass spectral technique requires the individual protein molecules to become ionised thereby separating from each other and spreading out as a cloud of freely hovering, electrically charged protein ions. The ions are then accelerated in a vacuum chamber to reach the target in an order determined partly by their charge and partly by their mass—the time of flight (TOF) is measured with the fastest ions being those that are lightest and have the highest charge.

Today there are two procedures that allow proteins to transform into ions in the gas phase without losing their structure and form, and it is the discoverers behind these methods that are rewarded jointly with half the 2002 Nobel Prize in Chemistry. In one of these methods, of which John B. Fenn is the originator, the sample in solution is sprayed using a strong electrical field to produce small charged droplets, which desolvate in vacuum to form freely hovering ions. In the other, an intense laser pulse is applied under suitable conditions (energy, structure and chemical environment of the sample) to the sample under examination whereupon some of it gains energy from the laser beam and molecules are ejected as free ions. The first person to show that this phenomenon, known as *soft laser desorption*, could be used for large molecules such as proteins was Koichi Tanaka.

Fenn's contribution – hovering through spraying

During 1988 John B. Fenn published two articles that were to mean a breakthrough for mass spectrometry by employing *electrospray* for macromolecules. The first of these showed that polyethylene glycol molecules of unknown mass could be handled; large molecular masses with high charges were detected. The second publication reported the use of the method on medium-sized whole proteins. The release of ions is achieved by spraying the sample in an electrical field such that charged droplets are formed. As the solvent gradually evaporates from the droplets, freely hovering "stark naked" protein molecules remain. The method came to be called *electrospray ionisation* (ESI) (Figure 2).

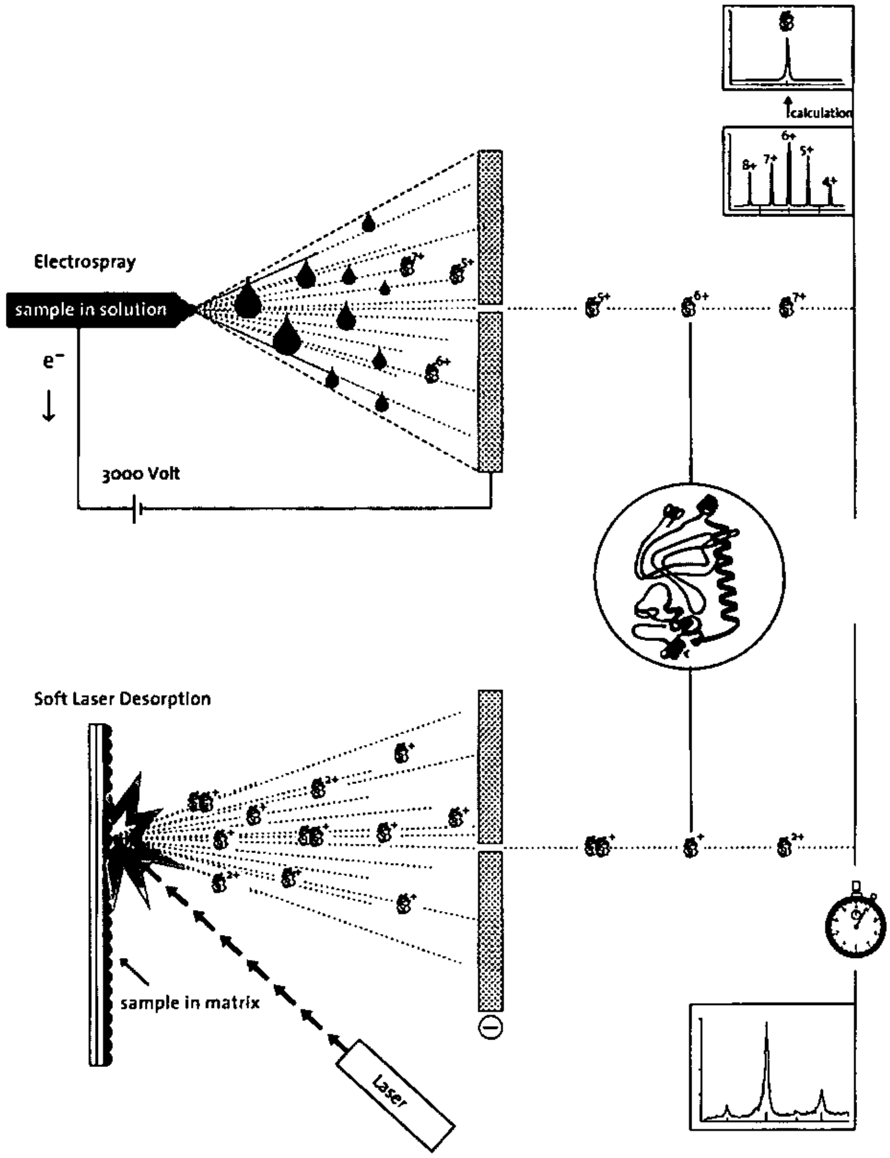

Figure 2. Principles for biomolecule mass spectrometry. In ESI biomolecules are released as multiply charged ions from small charged droplets. By ionisation with SLD the energy from the laser light is transferred to the biomolecule so that it enters the gas phase.

As the molecules take on multiple positive charges, the mass/charge (*m/z*) ratio becomes small enough to allow the substances to be analysed in a normal mass spectrometer. Moreover, the observation of a series of peaks that depend upon the number of positive charges present makes identification easier.

Tanaka's contribution – hovering through blasting

At the same time as Fenn reported his work exciting things were happening at the Shimadzu Instrument Company in Kyoto, Japan. A young Japanese engineer, Koichi Tanaka, reported an entirely different technique for the ionisation of the sample. At a symposium in 1987 and a year later in print, Tanaka showed that protein molecules could be ionised using *soft laser desorption* (SLD) (Figure 2). Here, a laser pulse strikes the sample which, unlike in the spray method, is in a solid or viscous phase. When the sample takes up the energy from the laser pulse it is released as intact hovering molecular ions with low charge, which are then accelerated by an electrical field and detected by recording their time of flight. Tanaka was the first to demonstrate the applicability of laser technology to biological macromolecules. The principle is fundamental to many of today's powerful laser desorption methods, particularly the ones known as MALDI (*Matrix-Assisted Laser Desorption Ionisation*) and also SELDI (*Surface Enhanced Laser Desorption Ionisation*) and DIOS (*Direct Ionisation on Silicon*).

Applications of mass spectrometry

Both electrospray ionisation (ESI) and soft laser desorption (SLD) have many fields of application. Sophisticated biochemical analyses, but dreams a few years ago, are now routinely possible. The interactions between proteins, very important in understanding the signal systems of life, can be examined with ESI. The method is superior to others in its rapidity, sensitivity, and identification of the actual interaction. Mass spectral analyses employing ESI are relatively cheap and spread quickly to laboratories around the world. Today soft laser desorption (in the form of MALDI) and electrospray have become standard methods for structure analyses of peptides, proteins and carbohydrates which make it possible to quickly analyse the protein content of intact cells and living tissue.

The versatility of applications generated by this year's Nobel Prize winners' fundamental studies include:

Pharmaceuticals development

The early phase of pharmaceuticals development has undergone a paradigm shift. Combined with fluid separation, ESI-MS has made possible the analysis of several hundred compounds per day.

Malaria

Scientists have recently discovered new ways of studying the spread of malaria. Early diagnosis is possible thanks to application of the soft laser desorption method to blood samples. Here the oxygen-bearing component of human haemoglobin absorbs the energy of the laser pulse.

Ovarian, breast and prostate cancer

New methods for the early diagnosis of different forms of cancer have been reported at a rapid rate during the past year. By employing a surface that cancer cells adhere to and then analysing the film with soft laser desorption cancer can be detected more rapidly than by a medical practitioner.

Foodstuff control

ESI technology has also made progress in the analysis of small molecules. Very recently we have learned that preparation of the food we eat can give rise to a number of substances hazardous to health, *e.g.* acrylamide which can cause cancer. Mass spectral analyses at various stages in food production can provide the essential information for suitable temperature control or a change in the ingredients and the avoidance or minimization of harmful substances.

NMR for biological macromolecules

Whereas mass spectrometry gives answers to questions such as "what?" and "how much?" about, *e.g.* a protein, NMR in one sense answers the question "what does it look like?" By interpreting the peaks in an NMR (*Nuclear Magnetic Resonance*) spectrum one can draw a three-dimensional picture of the molecule under examination. Since the sample under study is usually in solution, the protein is in its natural environment in the cell.

Before the advent of NMR, X-ray crystallography was the only method available for determining the three-dimensional structure of the substance. In 1957 the first true three-dimensional structure of a protein, myoglobin, was presented. This was rewarded with a Nobel Prize in Chemistry to Max Perutz in 1962. As a complement to X-ray crystallography, chemists long sought a method that would also function in a solution, *i.e.* an environment that better resembles the natural environment of the biomolecule.

The physicists Felix Bloch and Edward Purcell discovered as early as 1945 that certain atomic nuclei absorb radio waves of a particular frequency (through their nuclear spin) when placed in a powerful magnetic field. This was rewarded with the Nobel Prize in Physics in 1952. A few years earlier it had been discovered that the frequency for NMR depended not only on the strength of the magnetic field and the type of atom but also on the chemical environment of the atom. In addition, the nuclear spins of different nuclei interact with each other thereby generating fine structure, *i.e.* further peaks in the spectrum (Figure 3).

The applicability of the NMR method was initially limited by its low sensitivity that demanded concentrated solutions. However, in 1966 the Swiss chemist Richard Ernst (Nobel Prize in Chemistry 1991) showed that the sensitivity could be increased dramatically by exposing the sample to short and intense radio frequency pulses, instead of slowly varying the frequency. Moreover, during the 1970s he contributed the development of determining which nuclei were adjacent to each other in a molecule. By interpreting the signals in an NMR spectrum it thus became possible to gain an idea of the appearance of the molecule, *viz.* its structure. The method was successful for relatively small molecules but not for larger ones because it was not possible to differentiate between the resonances of the different atomic nuclei. The scientist who finally solved this problem was the Swiss chemist Kurt Wüthrich.

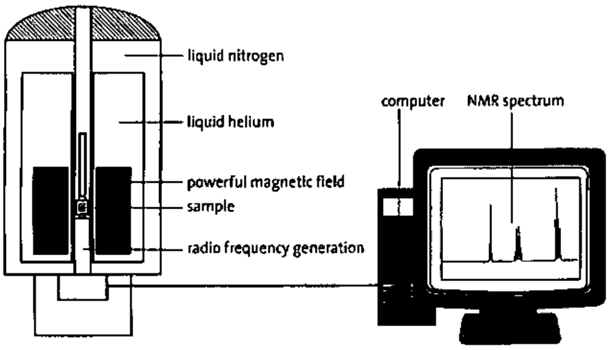

Figure 3. The sample to be examined is placed in a very strong magnetic field. The figure shows a super-conducting magnet cooled by liquid nitrogen and helium. Pulses of radio frequency waves are sent into the sample, which emits a radio wave "answer". This response is analysed electronically and the result is an NMR spectrum.

Kurt Wüthrich – showed that NMR was possible for proteins

At the beginning of the 1980s, Kurt Wüthrich developed an idea of how to apply NMR to biological molecules such as proteins. He invented a systematic method of pairing each NMR signal with the relevant hydrogen nucleus in the macromolecule (see Figure 4). The method, called sequential assignment, is today a cornerstone of all NMR structural investigations. Wüthrich also showed that it was subsequently possible to determine pairwise distances between a large number of hydrogen nuclei and use this information (with a mathematical model based on distance-geometry) to calculate the three-dimensional structure of the molecule (Figure 4).

The first complete determination of a protein structure with Wüthrich's method came in 1985. At present some 15-20% of all known protein structures have been determined with NMR. The majority have been determined by X-ray crystallography and a few with other methods such as electron diffraction or neutron diffraction.

Areas of application for NMR with macromolecules

In many respects, the NMR method complements X-ray crystallography for structural determination. If the same protein is investigated with both methods, in the one case in solution and the other in the crystal, the same result is generally obtained. Differences occur for certain superficial areas that are affected by the environment – in the crystals by the tightly packed protein molecules and in solution by the surrounding solvent. While the strength of X-ray crystallography lies in being able to determine accurately very large three-dimensional structures, the NMR method has other unique advantages. The fact that the investigation takes place in a solution means that physiological conditions can be approximated, and unstructured and very mobile parts of a molecule examined. It is possible to elucidate the mobility and dynamics of a long a protein chain. Isotope labelling can also be used to facilitate atom identification.

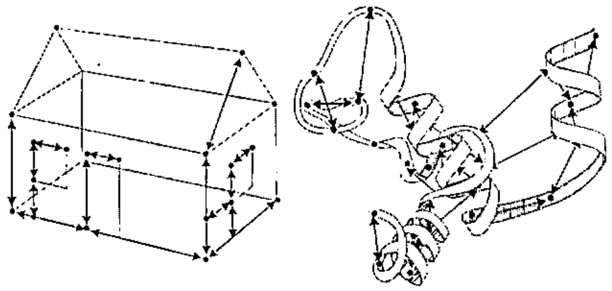

Figure 4. If one knows all the measurements of a house one can draw a three-dimensional picture of the house. In the same way, the measurement of a vast number of short distances in a protein makes it possible to create a three-dimensional picture of its structure, as shown schematically above.

One example of an NMR-determined protein structures comes from prions that are involved in the development of dangerous diseases such as mad cow disease (Nobel Prize in Medicine to Stanley Prusiner in 1997). Here Wüthrich and coworkers have used NMR methodology to show that the healthy form of prion proteins consists of two parts. Approximately one half of the protein chain assumes a well-ordered, fairly rigid three-dimensional structure in water (121-231 in Figure 5), while the other half is without structure and very mobile (see 23-120 of Figure 5). From such information it is hoped that an understanding of the process that brings the transition from the benign to the disease-related scrapie form can be gleaned. NMR can also be used in studies of structure and dynamics of other biological macromolecules such as DNA and RNA.

NMR is also used routinely in the pharmaceuticals industry to determine the structure, and hence the properties, of proteins and other macromolecules that can be interesting targets for new pharmaceuticals. A pharmaceutical is best designed to fit into the structure of the protein like a key in a lock. Perhaps the most important industrial use of NMR is in the search for small potential pharmaceuticals that can interact with a given biological macromolecule. If the small molecule binds to the larger one, then the NMR spectrum of the large molecule is changed and this may be used to "screen" a large number of candidates at an early stage of the development of a new drug.

The Nobel Foundation and host sites have freely provided this information. Further details are available at:
Nobel Foundation: www.nobel.se
Fenn: http://www.has.vcu.edu/che/people/fenn.html
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http://www.scripps.edu/mb/wuthrich/people/kw/kw.html

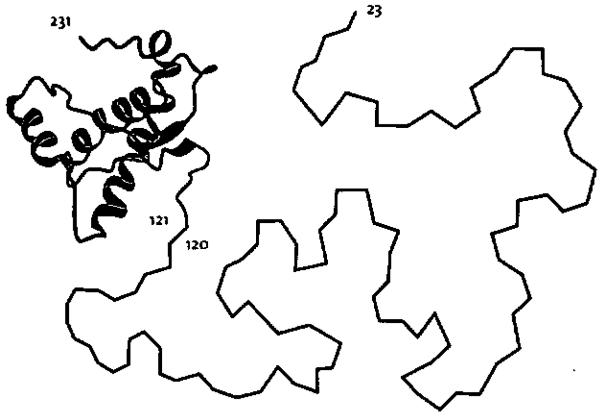

Figure 5. Structure of a prion protein determined with NMR. Half of the protein chain (23-120) is disordered and quite flexible in aqueous solution.

THE BREWING PROCESS – A BRIEF REVIEW

David Meads
Speight's Brewery, Dunedin

Brewing is one of the oldest professions known to man – the earliest known records are from Mesopotamia/Sumaria around 4,000-5,000 years ago. Archaeologists have recently unearthed 3,800-year-old Babylonian beer making instructions on cuneiform tablets at a dig in Syria. Beer was also an important part of the diet for Egyptians throughout the time of the Pharaohs.

The brewing skills from Egypt and the Middle East were adopted by the Greeks and Romans and soon spread to the rest of Europe. Brewing was predominantly a household task but it moved to the monasteries in medieval times. With the decline in the influence of the church after the Reformation, brewing subsequently became a commercial enterprise on a much larger scale.

Captain Cook brewed the first beer in New Zealand at Dusky Sound in 1773 to help offset the effects of scurvy amongst his crew. It was made from molasses and rimu and manuka leaves.

Brewing was one of the first enterprises to appear in the new colony of New Zealand in the mid-to-late 1800s. Messrs McKinnon and Wickins established Otago's first brewery in 1856 and with the discovery of gold in Otago in the 1860s, it was not long before more breweries sprang up producing beer for the thirsty miners. Other breweries included the Dunedin Brewery, Water of Leith Brewery, Red Lion Brewery, Strachan's Victoria Brewery, J Speight & Co., and the Well Park Brewery. One of these breweries is still brewing today – Speight's Brewery in Dunedin (Figure 1)*.

British settlers to New Zealand brought with them their traditions and techniques. William Dawson was a renowned brewer who, after training at Burton–upon-Trent in England and working briefly for Wm. Younger & Co. in Edinburgh, arrived in Dunedin in 1873; he founded Speight's Brewery along with James Speight and Charles Greenslade in 1876. Dawson used his knowledge to produce a range of fine ales and stouts. The quality of these beers was ultimately recognised with a gold medal from the Melbourne Exhibition in 1880.

At the time of Speight's establishment, the science of brewing was in its infancy with pioneers such as Louis Pasteur discovering the importance of yeast and its role in fermentation, and Emil Hansen developing methods for growing pure yeast cultures. Simple instruments such as thermometers, saccharometers, and hydrometers were introduced to enable more consistent control of the process. The first microscopes were used to reveal the hitherto "invisible " world of yeast and bacteria, and brewing laboratories were established.

Although equipment has changed and the brewing process is more clearly understood, the basic chemistry remains the same. The conversion of starches into sugars takes place in the malting process and the mash tun while the complex hop chemistry occurs in the kettle, and the associated biochemistry accounts for the conversion of fermentable sugars into ethanol, carbon dioxide, and around 400 flavour compounds.

The raw materials for the production of beer are water, malted barley, hops, and yeast. Each of these materials has a fascinating chemistry, which becomes even more interesting with the interactions that occur during the brewing process. Malt, the primary raw material, is a product of the degradation of barley endosperm by the naturally occurring enzymes found in the aleurone layer of the grain. Large and small starch granules are embedded in a protein matrix. Germination produces enzymes that break down the cell structure surrounding the starch granules during the mashing process. The extent of this enzymatic breakdown in the barley endosperm is known as modification.

Kilning of the malt is a heating process that initiates reactions, which form colour and flavour compounds. Some of the principal reactions are the Maillard reaction (non-enzymatic browning), Strecker degradation (the reaction of dicarbonyl compounds with amines), formation of dimethyl sulfide and the thermal degradation of phenolic acids. The maltster and the kilning regime govern the degree to which these reactions affect the final malt flavour. A range of coloured malts is available to the brewer to provide both colour and flavour variations to the beer.

Water is a key component of any beer and the mineral content has a huge influence on the final beer quality. Historically, breweries were sited where the water best suited the style of beer being produced – hence hard, calciferous water at Burton-upon-Trent produced superb pale ales while the soft water at Pilsen produced classic lager. Nowadays, we have the ability to treat and adjust water to brew particular styles of beer at any location. The water used to brew Speight's range of beers is sourced from an aquifer some 70 metres below the brewery.

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* *All figures appear at the end of the article.*

Mineral ions in water influence the p*H* and play a part in the biochemical process of brewing and fermentation, and the final taste of the beer.

Hops have been used to flavour beer since the Middle Ages. They were prized for conferring aroma, flavour and preservative properties, and their use spread rapidly through Europe from the 12th century onwards. Hops are hardy, climbing perennial herbaceous plants that grow only in specific latitude ranges in both the northern and southern hemispheres. The hop cones, which are produced by the female plant, are used in brewing (Figure 2).

Very little was known about the chemistry of hops until the early 1800s when gallic acid was isolated from hop tannin. More work followed but it was not until the 1950s when developments in separation and identification techniques finally allowed detailed understanding of hop chemistry and its contribution to beer quality. The breeding program established by Hop Research in Nelson in the 1950s is responsible for the quality triploid hops that are now available, and which have high α-acid levels to provide bittering yet retain aromatic qualities.

Yeasts are simple, single celled fungi, which bring about the complex biochemical changes involved in the conversion of sugars produced in the brew-house into alcohol, carbon dioxide, and flavour compounds. The brewer is interested only in one particular strain, *Saccharomyces cerevisiae.* Typically, each brewery has its own unique pure (or mixed) strain of yeast that is propagated on a regular basis. Yeast needs carbohydrates, nitrogen, vitamins, and trace elements to grow, along with oxygen for cell-wall production that is essential for reproduction. The role of yeast is explored further in the discussion on fermentation below.

The brewing process consists of a number of steps as illustrated in Figure 3. Firstly, malted barley is crushed in dry or wet mills to produce grist, which is mixed with warm water to facilitate the action of enzymes. This process is known as mashing. The resulting sugar solution, or *wort*, is then separated from the husk in the lauter tun. The wort is then boiled and hops are added to provide flavour and aroma.

The wort is cooled and mixed with yeast in a fermentation tank. Under carefully controlled conditions, fermentation and yeast growth occur over a period of 7 – 10 days during which time alcohol and carbon dioxide are produced, along with small amounts of other organic compounds. The resultant product is beer. Batch fermentation predominates in the industry. However, New Zealand brewers pioneered the process of continuous fermentation that is still used commercially today. The beer is transferred from the fermenter to a storage tank and is allowed time to mature. The final step of filtration clarifies the beer ready for packaging into bottles, cans and kegs, or for despatch via tanker to hotel tanks.

Many chemical and biochemical reactions occur during the brewing process. The chemistry of mashing involves the interaction of enzymes, mineral ions and the substrate provided by the malted barley. The starch in the malted barley is further broken down in the brew-house during mashing by hydrolysing enzymes (principally α- and β-amylases) after the granules have been gelatinised. This is achieved by using carefully controlled temperature rises and rests that are designed to optimise enzyme activity and the correct conditions of p*H*.

Calcium ions cause a drop in p*H* during mashing by reacting with phosphates and polypeptides to release H^+ ions. In addition, the calcium ions help protect the amylase enzyme from heat during mashing, assist with both protein precipitation and oxalate removal, limit colour formation during boiling, and help with yeast flocculation. Magnesium ions act similarly to calcium and are a co-factor for some enzymes during fermentation. Sodium ions influence palate sweetness, zinc ions are a vital yeast nutrient, while chloride ion increases palate fullness and sulfate ion contributes to dryness and bitterness.

The main changes, which occur during wort boiling, are sterilisation, concentration, hop acid isomerisation, removal of volatiles, colour increase, and reduction of p*H* and nitrogen levels. Wort boiling involves some complex reactions that result in colour and flavour development similar to those found in the malt kilning process. In addition, there is a contribution of hops to both flavour and aroma from hop oils and resins, which undergo transformation during boiling.

Hop oils and resins are located in the lupulin glands of the hop cone. The soft resins consist of α- and β-acids, which provide the bittering principals. These acids are isomerised during wort boiling to form *cis*- and *trans*-iso-α-acids that are considerably more soluble. The three main acids humulone, cohumulone and adhumulone give rise to isohumulone, isocohumulone and isoadhumulone, respectively (Figure 4). The essential oils in hops give beer its characteristic aroma. These are very volatile and are almost completely lost during the boil – the late addition of aroma hops results in more fragrant character beers.

Fermentation is perhaps the most fascinating part of brewing. Yeast metabolism involves the breakdown of fermentable carbohydrates into ethanol and carbon dioxide. Hexose sugars are catabolised via the Embden-Meyerhof-Parnas (EMP) pathway (Figure 5) to form pyruvic acid, which is in turn decarboxylated to form acetaldehyde and CO_2. The acetaldehyde acts as an electron acceptor to oxidise NADH and forms ethanol. Some pyruvate also contributes to the production of organic acids via a limited Krebs cycle (Figure 6). Diacetyl and pentane-2,3-dione are minor products of carbohydrate metabolism with important flavour implications if yeast does not further metabolise them to less flavourful diols. Yeast also produces two storage polymers, trehalose and glycogen, which are used during yeast storage for maintenance metabolism.

Wort nitrogen metabolism contributes to fusel alcohol production using the Ehrlich pathway. These alcohols impart an alcoholic, warming effect on the palate. They can also react with organic acids to produce esters which impart a fruity, solvent character to beer. Esters make up the largest family of aroma compounds produced by yeast.

Volatile sulfur compounds with low flavour thresholds are produced by yeast metabolism and also make a significant contribution to beer flavour. Sulfate is reduced biosynthetically to sulfite and then to sulfur dioxide and hydrogen sulfide as part of the synthesis of cysteine and methionine. Dimethyl sulfide levels from brewhouse reactions can be affected by losses in the gases that are given off during fermentation.

At the end of the fermentation we have a wonderfully complex mixture known as beer. Beer contains around 400 chemicals, which combine to give flavour, aroma and mouthfeel. The yeast can be used again and when no longer required is usually sold to yeast extract manufacturers.

The maturation process allows these beer flavours to reach the final balance. Beer is cooled to sub-zero temperatures and stored for an appropriate time. Residual yeast activity helps to modify the flavour intensity of many compounds – some remain unchanged, some increase and others decrease. The reactions that occur are not completely understood. The high molecular weight proteins and tannins combine to form colloidal haze, which is removed during the storage process by gravity sedimentation. This process can be enhanced by the use of fining agents such as isinglass.

The beer is filtered to give the clarity and brilliance required by the consumer. The predominant technique used by most brewers is diatomaceous earth filtration. The brewer takes the opportunity at this stage to standardise the beer and to add back some of the carbon dioxide collected during fermentation to achieve a precise level of carbonation.

Beer is a dynamic substance and subtle changes in flavour and appearance begin from the moment it is filtered. Heat treatment (pasteurisation), light, oxygen, and time all influence the flavour and appearance of beer. As with most chemical reactions, pasteurisation (heating) reduces reaction times and can accelerate beer flavour changes caused by the interaction of oxygen and beer constituents. Heat can also impair the physical stability and appearance of beer. The reaction of light with hop iso-α-acids and sulfur-containing amino acids in beer, forms prenyl mercaptan, 3-methylbut-2-ene-1-thiol ($Me_2C{=}CHCH_2SH$) (Figure 7). This compound has a very low aroma threshold and causes lightstruck flavour, which is most unpleasant. It is described as skunky. The brewer protects his beer from lightstrike by packaging in cans and brown bottles. Oxygen is an enemy of packaged beer – oxidation reactions produce carbonyl compounds that are significant in their contribution to the aging of beer and are associated with the papery, cardboard characters found in old beers.

Beer is a cereal-based beverage with a balanced package of carbohydrates, vitamins and minerals, which make a positive contribution to a healthy diet. Carbohydrates are in the form of complex dextrins that help in the maintenance of blood sugar levels. Many of the vitamins survive the brewing process and these include vitamin B6, niacin, vitamin B2 (riboflavin), pantothenic acid, biotin, and folate. Minerals such as silicon are available in hydrated form, which the human body can readily utilise. Some of the phenolic compounds such as ferulic acid from barley, and prenyl flavanoids from hops are antioxidants and may well work in the same manner as antioxidants from red wine.

Beer is the result of many chemical and biochemical reactions, and the utilisation by yeast of organic carbon compounds. Today's brewers have a greater scientific understanding of the process, which has allowed a degree of control, and therefore consistency, in the beers produced.

At Speight's Brewery, the proud tradition of brewing continues 126 years on using well water, dry milling, copper brewing vessels, batch fermentation in both modern tanks and kauri gyles by a team that is passionate about the beer they brew. Beer which is truly "The Pride of the South".

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$$2\ \mathrm{ATP} + \mathrm{glucose} + 4\ \mathrm{ADP} + 2\ \mathrm{P_i} + 2\ \mathrm{NAD^+} \rightarrow 2\ \mathrm{ADP} + 2\ \mathrm{pyruvate} + 4\ \mathrm{ATP} + 2\ \mathrm{NADH}$$

Figure 5. The Embden-Meyerhof-Parnas (EMP) pathway.

Figure 1. Speight's Brewery, Dunedin.

Figure 2. Hop cones.

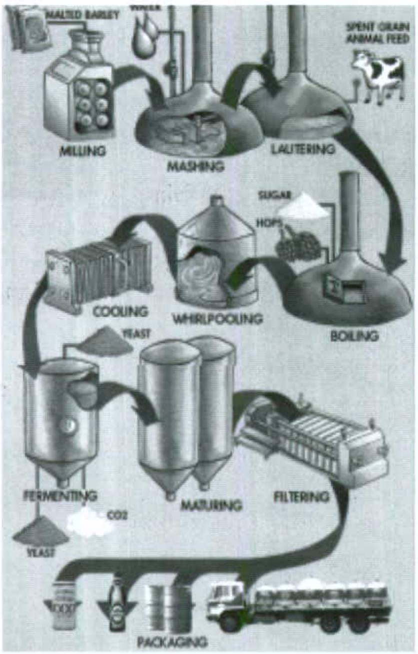

Figure 3. The brewing process.

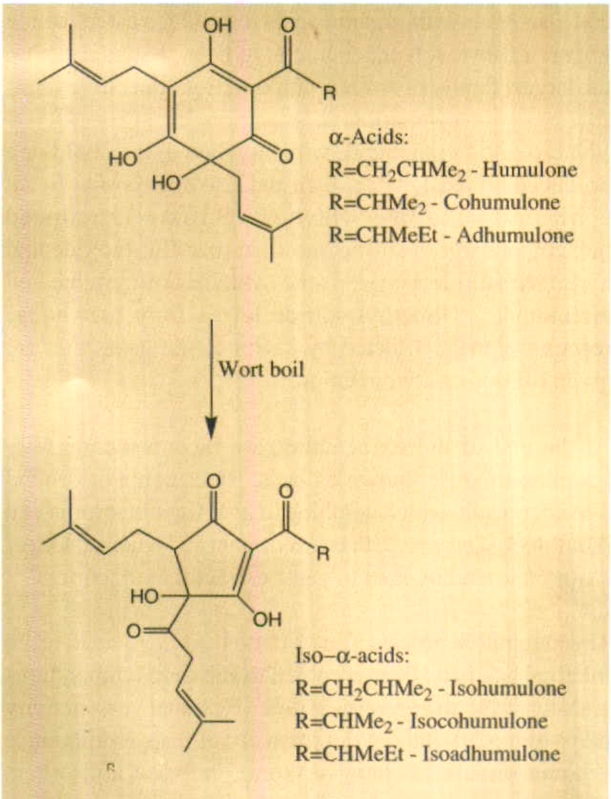

Figure 4. The structure of α- and iso-α-acids.

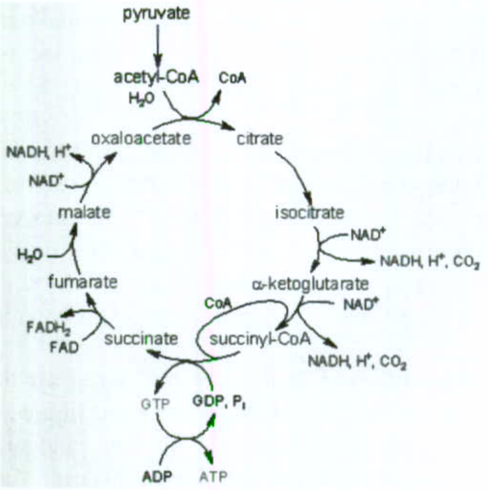

Figure 6. A Krebs cycle.

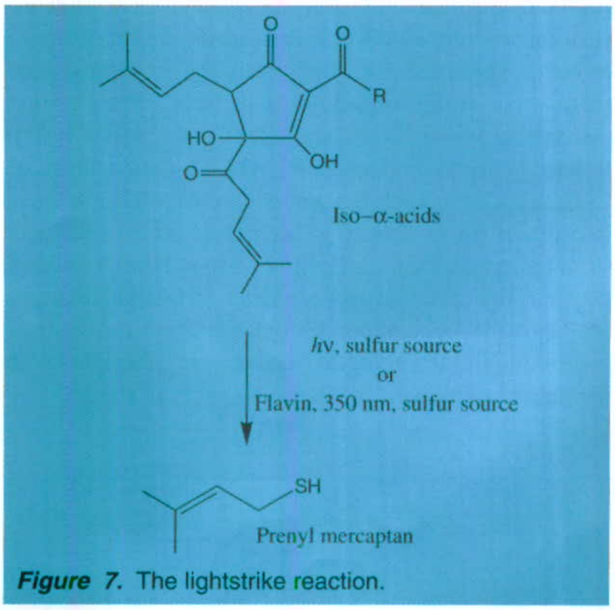

Figure 7. The lightstrike reaction.

Studying Chemistry!

Paula Caradoc-Davies
Department of Chemistry, University of Otago, P O Box 56 Dunedin

Dr Paula Caradoc-Davies, a New Zealander educated at Otago, has recently started a FRST Postdoctoral Fellowship with Dr Lyall Hanton. In the following article she tells us a little about her background, her motivations for studying chemistry, and the work in which she is currently involved.

Coming from an extended family where no one had ever gone to University, and with parents who earned somewhere in the middle–to–low income range, you might not expect that I would end up doing what I am doing. But here I am, 20 years of education later, with a Doctor of Philosophy in Chemistry and working as a New Zealand FRST postdoctoral fellow designing and making *'smart boxes and cages for advanced molecular devices'*. I guess I started on this road in the seventh form at Queens' High School in Dunedin, where I had the good fortune to be taught by a young and truly inspirational teacher, Andrea Lorimer. Not only was chemistry fun, it had yes and no answers—or so I thought. This was great news considering my efforts in the much-hated English classes.

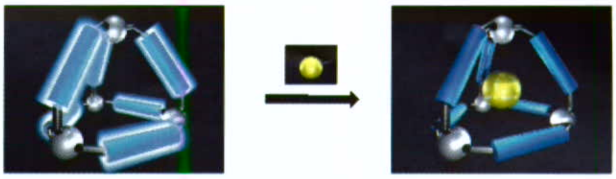

Figure 2. Schematic showing (left) an empty cage 'switched on' and (right) a cage containing an entrapped.

I never really looked back from there and went on to complete my BSc(Hons) at the University of Otago. After more years of being broke than I like to think about, but with a thankfully small student loan (on the scale of things) I decided I was sick of study and was going to get a job. Several interviews, no job and an offered University PhD Scholarship later, I decided that maybe getting to spend a few more years in a lab was a good idea. So I started my PhD with Dr Lyall Hanton at Otago. Originally, I was to start investigating the complexes of some new flexible acyclic ligands. However, when Lyall went on sabbatical leave to the University of Nottingham during the first year of my PhD, he discovered that my project was perfectly set up to be part of one of the fastest growing areas of inorganic chemistry, namely supramolecular chemistry. Up until this time, most work in the area had focused on making complexes with metals that had strong geometric preferences and rigid *N*-donor ligands, such as pyrazine and 4,4'-bipyridine. By complexing labile metals, *e.g.* Ag(I) and Cu(I), with flexible oligopyridine-thioether

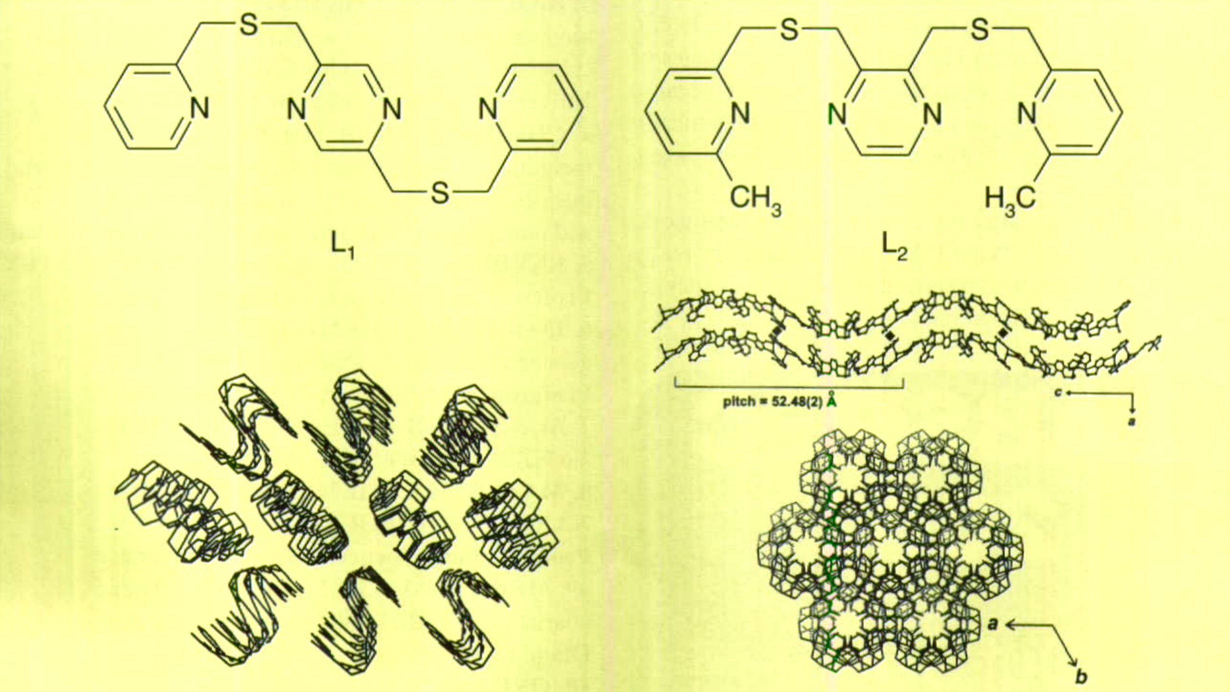

Figure 1. (Left) The $AgNO_3$ complex of (L_1) viewed down the [110] axis showing packing of the two different polymeric chains present in the single crystal. (Right) The $AgClO_4$ complex with (L_2): (Upper) A view of the helix. The crystal was homochiral, with only the *M* enantiomer observed throughout. (Lower) A view down the crystallographic *c*-axis showing the hexagonal packing of the helices.

ligands that we had designed, we hoped to generate coordination polymers with properties that the rigid ligand complexes did not display. As it turned out I ended up making some really interesting supramolecular polymers as illustrated in Figure 1. I have to say that I really enjoyed the time during my PhD working with Lyall. His approach was (and is) the perfect balance of asking how your work is going and knowing when not to ask!

Somewhere in the middle of my PhD I met Tom and decided to get married. Since Tom was finishing his PhD in biochemistry at Otago and I was still interested in doing research, I worked for a year as a research assistant on an Otago Research Grant with Lyall. This was when I started to become more interested in discrete complexes that might be capable of unique functions. These ideas were developed and led to the proposal for the current postdoctoral work, namely making new functional materials by designing and synthesising "smart" boxes and cages (Figure 2). The boxes and cages are molecular containers nanoscale in size, which are constructed by connecting metal vertices and ligands (that act as the container edges) to give the desired box and cage shapes. They are "smart" because the ligand edges of these containers are designed with extended conjugation and fluorescent units so that they will emit light (or switch on) when the cage/box is empty and not emit light (switch off) when a small molecule becomes trapped within the cage/box. In addition the ligands are designed to form intermolecular interactions with certain types of guests, *e.g.* aromatic compounds, in order to trap molecules within the cage or box.

There are a number of possible applications for these types of containers. They can act as molecular sensors and/or entrapment agents, *i.e.* both sensing and removing specific undesirable compounds. Also if these cages/boxes could be laid down on a surface in an ordered fashion they could behave as information storage devices in electronic systems. At the moment I am in the very early stages of the project and on a steep learning curve of organic synthesis. Thankfully the gradient has been dramatically lowered with the help of a kind and patient Dr Dave Larsen.

As to what happens after my current post-doctoral work, I'm not really sure. What I do know is that I am really excited about this research and am enjoying the challenge, some days more than others!

The planning for Pacifichem 2005 announced earlier this year has progressed. Not only are the dates for the Congress in Honolulu confirmed as December 15-20, 2005 but the congress web site has been officially launched and proposals for congress symposia are now being accepted at: **http://www.pacifichem.org**

Pacifichem 2005 will cover the **11** thematic areas listed below. For certain areas NZIC has appointed Area Coordinators and they are also included:

1. AGROCHEMISTRY - including agriculture, carbohydrate, cellulose, food, pulp and paper chemistry.
2. ANALYTICAL CHEMISTRY - including clinical, electrochemical sensors, and trace analysis. **Professor Keith Hunter, University of Otago.**
3. BIOLOGICAL CHEMISTRY - including biotechnology, genomics, microbial, and proteomics chemistry. **Professor John Cutfield, Biochemistry, University of Otago (with Dr E W Tan, Chemistry).**
4. CHEMISTRY AND THE COMMUNITY - including chemical education, chemical economics and business, chemistry and the law, and public education and outreach. **Dr Richard Coll, University of Waikato.**
5. ENVIRONMENTAL AND GREEN CHEMISTRY **Professor Keith Hunter, University of Otago.**
6. INORGANIC CHEMISTRY - including geochemistry and nuclear chemistry. **Professor John Spencer, Victoria University.**
7. MACROMOLECULAR CHEMISTRY **No NZIC representative.**
8. MATERIALS CHEMISTRY AND NANOTECHNOLOGY **Professor John Spencer, Victoria University**
09. MEDICINAL CHEMISTRY - including pharmaceutics. **Dr E W Tan, Chemistry, University of Otago (with Professor John Cutfield, Biochemistry).**
10. ORGANIC CHEMISTRY **Professor Brian Halton, Victoria University.**
11. PHYSICAL AND THEORETICAL CHEMISTRY.

Contact details follow:

Professor Keith Hunter
Department of Chemistry
University of Otago
P O Box 56 Dunedin
New Zealand
Tel: +64-3-4797917
Fax: +64-3-4797906
Mobile: +64-25-2243609
Email: khunter@alkali.otago.ac.nz

Dr Eng Wui Tan
Chemistry Department
University of Otago
P O Box 56 Dunedin
New Zealand
Tel: +64-3-4797926
Fax: +64-3-4797906
Email: ewtan@alkali.otago.ac.nz

Professor John Cutfield
Biochemistry Department
University of Otago
P O Box 56 Dunedin
New Zealand
Tel: +64-3-4797836
Fax: +64-3-4797866
Email: john.cutfield@stonebow.otago.ac.nz

Dr Richard Coll
Department of Chemistry
School of Science & Technology
The University of Waikato
Private Bag 3105, Hamilton
Tel: +64-7-8384100
Fax: +64-7-8384218
Email: r.coll@waikato.ac.nz

Professor John Spencer
Department of Chemistry
Victoria University
P O Box 600 Wellington
New Zealand
Tel: +64-4-4635119
Fax: +64-4-4635241
Email: john.spencer@vuw.ac.nz

Professor Brian Halton
Department of Chemistry
Victoria University
P O Box 600 Wellington
New Zealand
Tel: +64-4-4635954
Fax: +64-4-4635241
Email: brian.halton@vuw.ac.nz

There are three deadlines for individuals to submit a proposal to run a congress symposium. The first round is now open and runs to March 31 next. Thus anyone wishing to organise and *RUN A SYMPOSIUM* within any of the 11 areas is encouraged to submit their proposal now (the requisite form is available at the website) as some 75% of the available session time is likely to become committed from this first proposal round. Each proposal requires three coorganisers to represent ***ANY THREE*** Pacific Basin countries but it is presumed that the majority by far will emanate from the countries of the six sponsoring societies. New Zealand has had a poor reputation for organising symposia though a good number of members acted as coorganisers. *For 2005 it is vital that this number be markedly higher if the Institute is to retain its role in the Pacific basin movement through this organization. I trust that my academic colleagues will become far more proactive than in the past.* After a proposal is accepted for a specificed number of congress sessions the organizers will have ample time to set their programme to include invited speakers and to seek any additional sponsorship should they so wish. The essential deadlines for symposia are:

March 31, 2003 for first round symposium proposals for decision by June 15, 2003.
September 15, 2003 for second round proposals with decision by January 15, 2004.
September 15, 2004 is the FINAL DEADLINE FOR PROPOSAL SUBMISSION with decision by January 15, 2005.

Contributed papers WILL be accepted for presentation in both SYMPOSIA and GENERAL SESSIONS—the deadline for Abstract submission will be in APRIL 2005.

Proposals received after the first deadline will be handled as indicated by the timetable above until all the congress sessions are filled.

The organizing committee has significantly increased the fund to sponsor Scholars from developing countries of the Pacific Basin to the Congress. The New Zealand delegate has refined the programme and will convene the selection panel; essential details are available on the web site. In addition, the highly successful "Student Papers Competition" has been retained and it is hoped that the additional sponsorship sought for this will enhance the prizes awarded. Pacifichem 2005 is now only three years away—plan to be there.

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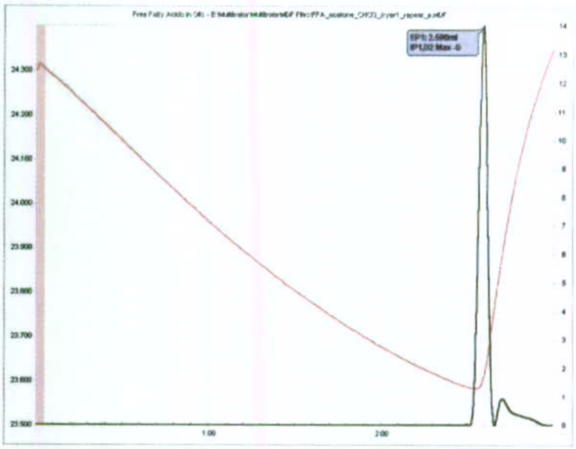
Breakthrough In Free Fatty Acid Analysis Of Edible Oils

A new automated thermometric titration method permits the rapid, high precision, high accuracy analysis of Free Fatty Acids (FFA) in edible fats and oils. The procedure is much superior to conventional coloured indicator and potentiometric methods. A simple, zero-maintenance thermometric probe is used to determine the titration endpoint. Analytical precisions of 0.001% w/w FFA (as oleic acid) for fresh oils, and 0.003% w/w FFA for used fryer oils have been recorded. The method has been validated by analysis of high purity oleic acid. Results are unaffected by sample colour or turbidity. The titration is carried out in polypropylene beakers under ambient laboratory conditions using 0.1M KOH in isopropanol as titrant. After the free fatty acids have been neutralized, the endpoint is signalled when the first excess of hydroxyl ion catalyses a strongly exothermic reaction between components of the solvent mixture. For more information please go to http://www. multitrator.com



Above: *Thermometric titration plot of determination of free fatty acids in used fryer oil.*

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Metrohm Introduces Their New 780 p*H* Meter And 781 p*H*/Ion Meter

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New Mini-Spray Dryer From Büchi

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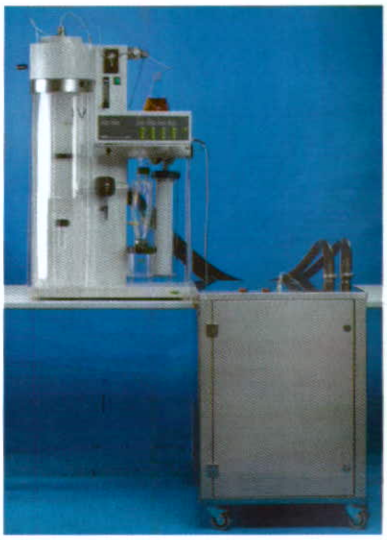

The system is well suited to spray dry small sample volumes down to 50 mL. Increasing the yield was a main target in development of the new system by optimising the two-fluid nozzle geometry (embedding a ruby stone for precise nozzle opening), the fluid behaviour in the glassware and by introducing new filter materials for particle recovery. Further innovations are the RS-232 serial port for on-line documentation, the integrated nozzle cleaning system and the versatile glass assemblies for different modes of operation.

In the past, the instrument was restricted to use with aqueous solutions only. With the new Inert Loop B-295 accessory, the system can be configured to safely work with organic solvents. The principle is based on a closed loop under inert gas, normally nitrogen. After loading the gas stream with solvent in the spray dryer, it is cooled down to condense the solvent and separate it. The cleaned gas stream is recovered to the Mini Spray Dryer. The oxygen concentration is permanently monitored to detect any possible malfunctions and the pressure is monitored to detect leakage or malfuction. This novel accessory expands the application range especially in the pharmaceutical and chemical industries.

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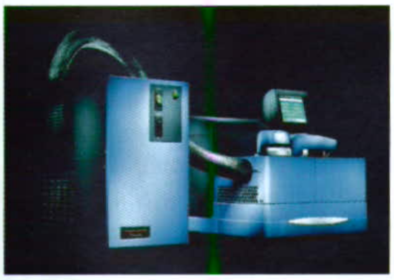
TA Instruments Introduces The RCS, A High-Efficiency Refrigerated Cooling System For Q Series Differential Scanning Calorimeters



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From Adsorption To Bioadhesion At Hydrous Metal (Oxide) Surfaces.
What Does *in situ* Infrared Spectroscopy Reveal?

Jim McQuillan
Department of Chemistry, University of Otago, P O Box 56, Dunedin

> *"There are therefore Agents in Nature to make the Particles of Bodies stick together by very strong attractions. And it is the Business of experimental Philosophy to find them out."*
> Isaac Newton, Opticks, 1704

Abstract

Probing chemical reactions at surfaces is an active area of modern research. Internal reflection infrared spectroscopy with particle films provides a simple but powerful *in situ* means of revealing molecular processes occurring at solid surfaces under aqueous solutions. Examples from recent research studies carried out at the University of Otago are given below. These include adsorption and adhesion to stainless steel, the binding of arsenate ions to iron oxides, the adhesion of *Pseudomonas aeruginosa* bacteria to metals, and the adhesion of marine molluscs to surfaces.

Molecules at Wet Surfaces

Chemistry is a relatively mature scientific discipline and has spawned many new areas of research activity that are vigorously challenging the dominance of the traditional sciences. Chemists have developed and refined techniques primarily for investigating the solid, liquid, and gas phases. However, the general properties of bulk phases are now well understood and there is an increasing need for chemistry to embrace interdisciplinary areas where the special skills of chemists can provide new insights and knowledge advances. What happens to molecules at the boundaries between bulk phases is not so well characterised and surface studies have become a very active part of modern physical chemistry. Furthermore, there are many interesting surface phenomena in nature that await more detailed chemical analysis and understanding.

One might expect the field of surface science,[1] which bridges physics and chemistry, to provide some answers. However, surface science is dominated by electron spectroscopic techniques, which are limited mainly to studies of single crystal solids under high vacuum conditions. Frequently the surface phenomena of interest in nature—and in technology—involve interfaces between polycrystalline or particulate solids and aqueous solutions. A number of exciting new surface techniques have emerged which can address the surfaces of such solids under solutions. These include surface-enhanced Raman spectroscopy (SERS),[2] scanning tunneling microscopy (STM),[3] atomic force microscopy (AFM),[4] and sum-frequency vibrational spectroscopy.[5] While the microscopic techniques (STM and AFM) have been valuable in indicating surface morphology and measuring interfacial force fields, only the spectroscopic techniques are capable of providing the molecular details which are needed to adequately model and predict interfacial behaviour. The high sensitivity of SERS has been very useful in metal surface and electrode studies but the technique is restricted to highly dispersed silver, gold, and copper.

Infrared (IR) spectroscopy occupies a venerable position in the history of chemical spectroscopy and has contributed significantly to our understanding of heterogeneous catalysis at the gas/solid interface. IR spectroscopy has been generally overlooked in studies of aqueous systems because of the strong IR absorption of water. This problem is overcome by using internal reflection spectroscopy, also known as *a*ttenuated *t*otal *r*eflection (ATR) spectroscopy, which provides a powerful means of examining chemical reactions at solid/solution interfaces.[6] The now widespread use of Fourier transform IR spectrometers has also simplified ATR-IR methods. In this article the principles of the *in situ* ATR-IR technique using solid particle films in aqueous media[6] is outlined and selected examples of recent adsorption and adhesion studies carried out at the University of Otago are presented. *Adsorption* is a term applied when small molecular species with few interaction centres attach to surfaces, whereas *adhesion* is a term used for larger species and macroscopic systems where there are multiple attractive interactions with a surface.

ATR-IR Spectroscopy of Solid/Solution Interfaces[6]

The simplest experimental ATR-IR arrangement involves a single internal reflection 45° zinc selenide (ZnSe) prism with its largest face horizontal as shown schematically in Figure 1a. With such an arrangement total internal reflection occurs if the refractive index of the medium in contact with the upper face of the prism remains below about 1.7. This condition is met for aqueous solutions and for porous films of solid particles with refractive indices as high as 2.6, *e.g.* TiO_2, provided the film has enough porosity to give a small enough effective refractive index. The evanescent wave arising from the total internal reflection decays exponentially into the less dense medium over a distance of a few micrometres. Thus those molecules closest to the ZnSe surface make the largest contribution to the spectrum. When the particle film thickness matches the penetration depth of the evanescent wave and the film is immersed in solution the wave can interact with infrared active species adsorbed from the solution onto the particle surfaces (Figure 1b).

Almost all metals are covered in thin metal oxide films. Thus the interaction of a solution species with a metal

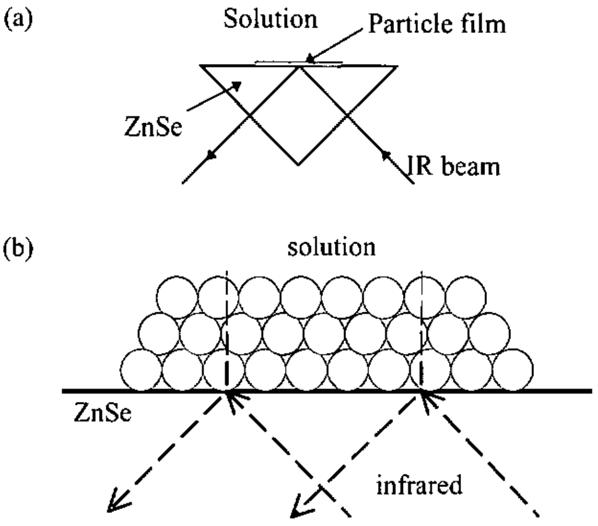


Figure 1. Single internal reflection at a ZnSe prism coated with a thin particle film and immersed in solution (a) general view, and (b) decay of evanescent wave through the film.

surface is normally with its metal oxide and an oxide film can model the metal surface. The oxide may correspond to a naturally occurring mineral, *e.g.* boehmite (AlOOH) at aluminium surfaces or hematite (Fe_2O_3) at iron surfaces. Chemical interactions of solution species with metal surfaces are, therefore, very similar to such interactions with minerals in nature. Particle films have usually been formed on ATR prisms by dip-coating colloids or drying aqueous suspensions of sub-micron particles. Such films can have an increase in area of about two orders of magnitude over the projected area and give spectra with high sensitivity from a single internal reflection. Oxides so far studied at Otago include TiO_2, ZrO_2, Al_2O_3, AlOOH, Fe_2O_3, FeOOH, Ta_2O_5, and Cr_2O_3. Zinc selenide is the most favoured ATR prism material because it has a wide spectral window and is stable from highly alkaline solutions down to p*H*=2. Alternative prism materials for acidic media are Ge and diamond-coated ZnSe.

Spectra of adsorbed species are normally obtained by flowing dilute solutions of the adsorbate over the particle films. These spectra are then compared with that from the corresponding solution in the absence of the adsorbing species. Variation of solution concentration provides absorbance data that can be used to construct adsorption isotherms and to determine adsorption constants that indicate the strength of adsorption.[7] The extent of adsorption and adhesion are usually p*H* dependent due to the variation of metal oxide surface charge with p*H*, and each oxide has a characteristic isoelectric point (zero charge p*H*). The p*H* dependence of adsorption and the determination of isoelectric points can be made using ions such as the tetramethylammonium cation or the perchlorate anion which do not interact chemically with metal oxides and respond only to surface charge.[8] Irradiation of metal oxide films can induce interfacial photocatalytic reactions, and infrared spectral changes from reacting adsorbates can be observed *in situ* with this technique.[9]

What sticks to metals such as stainless steel?

The existence of attractive interactions between the metal oxides at the surfaces of metals and molecular species in solution make the solution species 'surface active'. Surfactants are surface-active species with a hydrophobic tail, which drives their tendency to escape from aqueous solutions. However surfactant adsorption or adhesion to surfaces is based on weak interactions where no strong chemical bonding occurs. Significantly stronger adsorption occurs when the solution species has ligand properties and can form coordinative covalent bonds to the metal ions at the metal (oxide) surface. We have carried out many studies with TiO_2 which is an important material in diverse contexts such as dye-sensitised solar cells,[10] titanium implants,[11] photocatalytic remediation of waste waters, sunscreens, and paint pigments. Our experiments, and those of others, have shown that many bidentate ligand species such as oxalate, carboxylic acids, and phosphate adsorb strongly to TiO_2 surfaces forming coordinative bonds. This is simply coordination chemistry in two-dimensions and many principles from coordination chemistry can be directly applied to metal (oxide) surface reactivity.

Stainless steel is very important in technology, but we do not have a good understanding of its surface chemistry despite protein and bacterial adhesion being significant problems in our dairy food industry plants. The passive surface of stainless steel is essentially *c*hromium(III) *o*xide-*h*ydroxide (COH) and we have utilised a monodisperse colloid film of this material (Figure 2) in model adsorption studies.[12] Both oxalic and lactic acids are known to induce corrosion of stainless steel and our studies of the adsorption of oxalic acid at low concentrations on COH-coated ZnSe have shown that the oxalate ion coordinates to the Cr(III) surface ions. Although this study has not been extended to high oxalic acid concentrations, it seems very likely that under such conditions species such as $Cr(Ox)_3^{3-}$ will be formed with consequent dissolution of the protective passive film and corrosion of the underlying metal.

The adhesion of bacteria leading to biofilm-induced corrosion of stainless steel is also of industrial concern. Glucuronic acid is a monosaccharide component of the polysaccharide protective slime exuded by bacteria adhering to surfaces. The ATR-IR spectrum of D-glucuronic acid adsorbed onto COH from dilute aqueous acidic solution is shown in Figure 3b and the ATR-IR spectrum of a high concentration D-glucuronic acid solution recorded without the COH film on the ZnSe appears in Figure 3a. The solution spectrum (Figure 3a) shows a prominent carbonyl absorption at 1731 cm^{-1} from

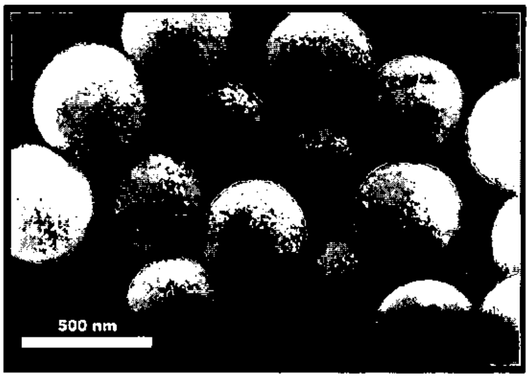


Figure 2. SEM image of chromium(III) oxide-hydroxide (COH) colloid particles.

the -COOH group. The spectrum of the adsorbed species differs dramatically in this part of the spectrum as the 1731 cm^{-1} band is lost and strong bands emerge at 1582 and 1415 cm^{-1} that are readily identified as due to the carboxylate group. Thus the carboxyl group is deprotonated upon adsorption, indicating that coordinative bonding occurs with the Cr(III) surface ions. The nature of the surface species is indicated by **1** and such bonding from polysaccharide terminal groupings are likely to contribute significantly to the adhesion of the slime to stainless steel and to other metal surfaces.

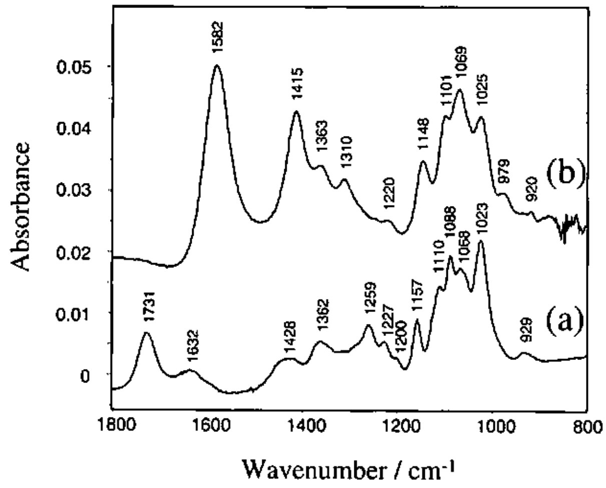
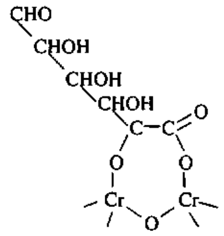


Figure 3. ATR-IR spectra of D-glucuronic acid (a) 0.25 M solution at p*H*=2.2, and (b) adsorbed on chromium(III) oxide-hydroxide from 10^{-3} M solution at p*H*=3.

Arsenate Binding to Iron Oxides at Macraes Mine

The mining of gold-bearing ores inevitably brings oxidisable minerals into contact with the atmosphere and minerals such as pyrite (FeS_2) and arsenopyrite (FeAsS) are oxidised with an accompanying release of acid. The high acidity gives increased dissolution of metal oxides and 'acid mine drainage' of metal ions. The end products of FeAsS oxidation are hydrous Fe_2O_3, AsO_4^{3-} and SO_4^{2-}. The arsenate is of particular concern because of its toxicity, but little arsenate is found in the leachate (pH ~6) from the tailings dam at the Macraes gold mine in North Otago. The arsenate ion has bidentate ligand properties and this suggests it should adsorb to hydrous Fe_2O_3.

Adsorption experiments with films of hydrous Fe_2O_3 recovered from the tailings dam, and with its synthetic equivalent, showed that arsenate binds strongly to this substrate and is only very slowly washed from the surface in the absence of arsenate in solution.[13] The suggested structure for arsenate strongly bound on the iron oxide surface is shown by **2**. Scorodite ($FeAsO_4.2H_2O$) is the most common natural form of iron(III) arsenate. In its structure the arsenate ions link two Fe(III) octahedra in a similar manner to that indicated in **2**. It is fortunate that the arsenic and the iron from the oxidation of the arsenopyrite are once again chemically bound together and the toxicity of the released arsenic consequently much reduced. This chemistry is also applied in the iron oxide filters being used to purify the arsenate-contaminated bore waters found in Bengal and Bangaladesh.



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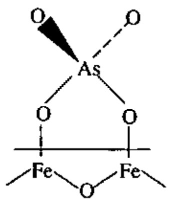

2

How do bacteria adhere to metals?

Most bacteria exist in nature attached to surfaces within biofilms which are complex communities containing large numbers of cells. Adhesion of bacteria to surfaces and their subsequent production of polysaccharide slime creates the biofilm which is hard to remove and the bacteria within it are less susceptible to antibiotic agents. Bacterial biofilms are a significant contributor to disease and infection related to surgical implants, a source of contamination in food processing environments, and also contribute to biofouling in marine and aquatic environments. Determining the principal factors favouring bacterial adhesion to surfaces is a key aspect of strategies aimed at inhibiting or preventing biofilm formation.

ATR-IR spectroscopy can be used to study the adhesion of bacteria to the surfaces of ATR prism materials and to prisms coated with thin films of other materials such as metal oxides. Using this approach the adhesion behaviour of *Pseudomonas aeruginosa* has been studied[14,15] by flowing aqueous suspensions of bacteria across the surface of ZnSe and ZnSe coated with about 50 nm of colloidal TiO_2. To increase sensitivity a multiple reflection prism was used with a thin TiO_2 film to bring the bacteria-TiO_2 interactions closer to the strongest part of the evanescent field. *Pseudomonas aeruginosa* is cylindrical with length ~ 2 μm and diameter ~ 0. 5 μm so the ATR-IR spectrum of the attached bacterium comes from the entire cell. The decay of the evanescent wave away from the ZnSe surface results in the parts of the attached cell closest to the TiO_2 surface, and involved in the attachment, making the largest contributions. Figure 4 shows the ATR-IR spectrum of the bacteria freshly attached to the TiO_2 coated prism surface. The prominent absorptions at about 1650, 1550, and 1250 cm^{-1} arise from the amide bonds of the bacterial proteins. The ragged top of the amide peak about 1650 cm^{-1} is due to interference from the bending mode of water in multiple reflection experiments.

When the spectrum in Figure 4 is compared with that of the same bacteria attached to a bare ZnSe surface the peaks

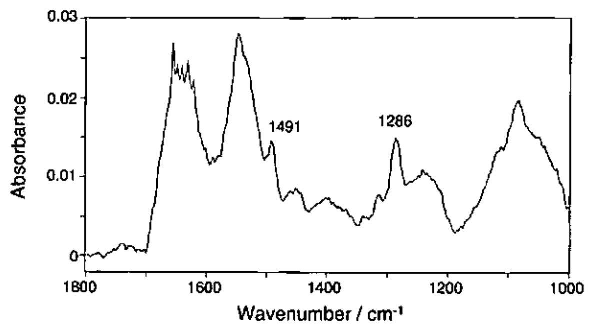

Figure 4. ATR-IR spectrum of *Pseudomonas aeruginosa* attached to TiO_2-coated ZnSe multiple internal reflection prism under aqueous solution.

at 1491 and 1286 cm^{-1} are absent. These peaks have been identified as arising from catecholate ligands in pyoverdine, a siderophore of *Pseudomonas aeruginosa*.[16] The catecholate ligands bind to the Ti(IV) ions in the TiO_2 surface accounting for the relative prominence of the 1491 and 1286 cm^{-1} bands in the spectrum of Figure 4. Very similar spectra have been obtained when a thin iron oxide coating is used. Siderophores are metal chelating molecules involved in sequestering iron, which is essential for bacterial metabolism. It is not surprising that bacterial siderophores are involved in bacterial adhesion to metal (oxide) surfaces, although this spectrum was the first such observation. The siderophore-related adhesion to iron oxides may therefore play a role in iron uptake by *Pseudomonas aeruginosa* in soils, the environment where they are mostly commonly found.

Observing the Chemistry of Marine Shellfish Adhesion

The blue mussel, *Mytilus edulis*, is the world's most common in nature and in aquaculture. However, in this country it is the native green mussel, *Perna canaliculus*, which is widely farmed and forms the basis of a significant export industry. The industry has largely used seed mussels (spat) collected from wild sources such as Kaitaia beach. Presently, a number of studies are being carried out by the industry and research groups to produce mussel larvae under controlled conditions so as to obtain a better understanding of the spat adhesion processes. For some time it has been known that mussels adhere to surfaces using adhesive proteins[17] secreted at the ends of the hairy byssus threads that a mussel grows when it finds a favourable location.

We have recently begun to use the ATR-IR technique to observe the adhesion behaviour of live mussels and other molluscs. Small mussels have been studied in a flowing seawater environment and the secretions of the mussel foot, which it uses to move over surfaces, as well as the secreted adhesive proteins from the anchoring byssus threads, have been readily monitored. Figure 5 shows the spectra of water insoluble residues remaining after (a) blue mussel and (b) topshell adhesion experiments were carried out with a ZnSe prism. The spectra are similar showing the strong amide absorptions about 1650 and 1550 cm^{-1} that are characteristic of proteins, and also strong absorptions in the 1100–1000 cm^{-1} region mainly from polysaccharides. The adhesion chemistry of marine molluscs is clearly heavily based on proteins. Detailed analysis of these spectra and their *in situ* time-evolution is expected to clarify understanding of the adhesion processes.

Conclusions

Although frequently overlooked in surface analysis, infrared spectroscopy is now readily applied to investigations of solid surfaces immersed in aqueous solutions. Using micron thick particle films of solids on internal reflection prisms, the nature of adsorption and adhesion reactions at the solid/liquid interface may be deduced. This method is applicable to wet metal (oxide) and mineral surfaces and has wide potential for application to the many poorly understood such systems surrounding us in nature and in technology.

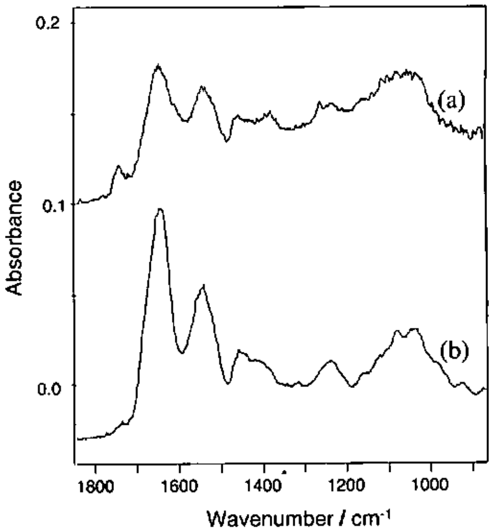

Figure 5. ATR-IR spectra of adhesive residues from attachment to multiple reflection ZnSe prism of (a) blue mussel *Mytilus edulis*, and (b) topshell *Diloma arida*.

Acknowledgements

Invaluable contributions to the work reported in this paper have come from Kevin Dobson, Paul Connor, Jens Degenhardt, Alisa Roddick-Lanzilotta, Michael McWhirter and Juliet Gao. Special thanks are also due to my colleagues Phil Bremer, Dave Craw and Iain Lamont. The work has been supported by the University of Otago, Industrial Research Ltd, and the New Economy Research Fund (NERF).

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26-30 November 2003

Expressions of interest are invited for participation in this meeting which is to take place immediately prior to the **NZIC Conference** in Nelson 1-4 December 2003.

The meeting has been organized in response to the highly successful first workshop held in Nelson in February 2000 following the 9th International Conference on HABs in Hobart, Tasmania. Themes on analytical methods, standards and reference materials for marine biotoxins will address outcomes of an APEC project (2000-2003) that is designed to facilitate trade and investment in seafood products. HABs are a significant threat to aquaculture in the Asia-Pacific region and improved technologies for management of toxins have been the subject of intensive international research over the period of this project.

Aim

The workshop will provide practical information on new developments in analytical methods for harmful algal species and for marine biotoxins in shellfish and other seafood products. The aim is to increase awareness and technical capabilities for ensuring the safety of seafood with an emphasis on monitoring programmes. It is aimed at laboratory personnel, scientists and seafood quality regulators from government and industry.

Venue

Rutherford Hotel, Nelson

Programme Format

Days 1 and 2:

Invited and contributed papers on marine biotoxins, hazardous alga, and techniques for their monitoring and analysis. Poster sessions, round-table discussions and a trade display are to be included.

Days 3 and 4:

Hands-on demonstration and training workshop covering test methods for algal identification and analysis of marine biotoxins. Emphasis on emerging techniques, *e.g.* gene probes, LC, LC-MS, *in vitro* biochemical tests, and ELISA.

Demonstrations will include:

- Sample preparation – seawater, shellfish
- Gene probes: whole cell and sandwich hybridisation format oligonucleotide probe assays for identification of phytoplankton
- ELISA assays for toxins
- Protein phosphatase inhibition assays for DSP toxins
- Cytotoxicity assays for PSP and NSP toxins
- LC procedures for ASP and PSP toxins
- LC-MS (electrospray) assays for toxins (multi-residue)
- Calibration standards and reference materials – sources, preparation, storage, use and documentation.
- Laboratory accreditation (ISO17025) – specific issues for monitoring labs.

Bring Your Own!

Participants are encouraged to bring their own practical demonstrations and displays:

- Poster presentations on techniques and findings
- New technologies for demonstration, *e.g.* test kits
- Reference materials, *e.g.* toxin standards
- Managements tools for HABs, *e.g.* monitoring protocols and sampling techniques

Expressions of Interest

The second circular, to be released mid-February 2003, will contain more details on the programme, registration details, and a call for poster presentations and demonstrations. ***Please notify us of your interest prior to this date.***

Contacts:

Direct personal contact may be made to:
Dr PatrickHolland, Mr Lincoln Mackenzie, or **Dr Lesley Rhodes** at the **Cawthron Institute**.
Ph: +64-3-5482319; Fax: +64-3-5469464
Email: HabTech2003@cawthron .org.nz
Additional information is available at the Cawthron web site: **http://www.cawthron.org.nz/habtech03**

Advanced Level Chemistry Students' Concepts Of Chemical Bonding †

Richard K. Coll [a] *and Neil Taylor* [b]
[a] Department of Chemistry, The University of Waikato
[b] School of Curriculum Studies, The University of New England

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Introduction

Chemistry as a discipline is dominated by the use of models and modelling.[1] Chemists use models to explain data, to predict events and to help understand chemical reactivity.[2] As a consequence, chemistry teaching, especially at the advanced level, is also dominated by the use of models. These models, being highly abstract in nature are referred to as mental models. An understanding of students' mental models is important because teachers employ increasingly complex models throughout the degree program.[3,4] However, there are many reports in the literature indicating that students' understanding and use of mental models is limited in comparison with desired teaching outcomes.[5-8]

Chemical bonding is a key concept in chemistry and is a topic area where understanding is developed through diverse models that are built upon a range of physical principles. In addition, students are expected to interpret a variety of representations standing for chemical bonds. The central importance of chemical bonding to the subject is well recognised,[9] and it is considered a core topic in many chemistry curricula at the school and university level. It is also well known that the topic of chemical bonding is one for which students' commonly develop a wide range of alternative conceptions.[10] As such, it is notable that there have been few studies of students' mental models for chemical bonding. The few studies that have been reported are mostly, but not exclusively,[11] confined to the secondary school level. What research that does exist suggests that students hold consistent alternative conceptions, *i.e.*, conceptions that are in disagreement with the taught models or currently accepted scientific view, across a range of ages and cultural contexts. Intermolecular bonding in particular is often problematic for students[12,13] and, for example, students' often think intermolecular bonding is stronger than intramolecular bonding[14,15] and invoke intramolecular bonding in inappropriate circumstances, *e.g.*, in ionic compounds.[16-18] Others believe that intermolecular bonding is absent in polar molecular substances such as water.[19] Another highly prevalent alternative conception is that students think continuous covalent or ionic lattices contain molecular species,[12,19,20] and many students appear to have little appreciation of the underlying electrostatic nature of chemical bonding.[15,17,21,22] Many students, likewise, have a poor understanding of the bonding in metals, seeing it as weak or in some measure inferior to other forms of bonding.[12,18,23] Similarly, alternative conceptions have been reported for covalently bonded substances with, for example, some students believing that the number of valence electrons and number of covalent bonds are one and the same, and others confusing resonance forms with molecular structures, or believing that covalent bond formation involves the transfer of electrons.[11,20,24]

Background Theory and Methodology

The background for this inquiry is based on Norman's typology of mental models[25] and is that used in a prior exploratory study reported elsewhere.[26] Chemical bonding has been classified into a series of three *target systems*, namely, *metallic*, *ionic* and *covalent* bonding and a series of mental models associated with each target (see below). The *sea of electrons* and *octet rule* are introduced into the New Zealand curriculum at high school Year-11 and Year-12, the *band theory*, *valence bond approach* and an introduction to *molecular orbital theory* in the first two years of university, and the *ligand field theory* and advanced molecular orbital theory in the final year of the undergraduate degree. There were two models for ionic bonding identified; one we have termed the *electrostatic model* - a model based on the Octet Rule, in which bond formation is based on the attraction of a cation and anion,[26] and a second based on computation of attractive and repulsive forces in an ionic lattice that we have termed the *Theoretical Electrostatic Model*. Of these models, the former is introduced in high school, the latter usually in second year undergraduate chemistry courses. Advanced molecular orbital theory and ligand field theory are also treated in fourth-year Honours and Masters level papers. Examination of curriculum material, that is, text books, lecture notes, and so forth[27] shows that whilst some of these models are highly abstract, *e.g.*, the molecular orbital theory, they are presented in a highly consistent manner, that is, there is considerable consensual agreement about how scientists view and use these models and the manner in which they are presented to students in lectures.

Data collection comprised two distinct stages as reported in the earlier study.[26] First a description of the above models was produced from an examination of curriculum material: lesson plans, lecture notes, textbooks, and workbooks used by students, combined with informal interviews with the instructors involved in the inquiry. Second, the students' mental models were investigated using semi-structured interviews, including the use of an *Interviews About Events* (IAE) approach. In this approach students are shown line drawings that depict the use of models in some way, for example, salt being crushed, the malleability of a metal or the conductivity of a molten salt. The data from this latter part of the study helped develop an understanding of students' use of their mental models and the alternative conceptions students held about their models: the results of these latter data are reported elsewhere.[26,28-30]

There were a total of 30 student participants involved in two complementary studies. A pilot study was based in Australia (six students) and a larger study in New Zealand (24 students) with a total of 10 students from each of senior secondary school (Year-12 and 13, aged 17-18 years), undergraduate (second and third year of a three-year degree program - aged 19-20 years) and postgraduate levels (with even numbers of Masters - aged around 21-22 years - and Doctoral level candidates - aged 23-25 years). As might be expected the postgraduates students were high academic achievers but generally the participants were chosen so as to provide a range of abilities and reasonably even gender balance. All of the participants described themselves as being of European ethnicity and pseudonyms have been used to protect their identities.

Research Findings

Students' Mental Models for Metallic Bonding

The data for secondary school students showed that most preferred the sea of electrons model, with a few possessing no clear mental model or being highly confused. For example, June described electrons as "moving around" and "attracted by the positive centres," Nigel talked about "electrons flowing around," and Frances said, "you cannot actually see where the electrons are." Hence, most students seemed to hold the view that the valence electrons are not associated with a given metal ion, but others tried to utilise the octet rule - invoking the formation of covalent bonds. Having drawn two aluminium atoms and describing the dots and crosses in his drawing as electrons, Keith stated: "The aluminium ion there needs three more electrons to satisfy its full outer shell so it's bonding with that which has got three full ones." Two students, Anne and Anita appeared not to possess a coherent mental model for metallic bonding, their descriptions consisting of listing macroscopic physical properties of metals rather than a description of metallic bonding. This aspect is illustrated by Anne's description of the bonding in aluminium foil, claiming that "it's held together quite strongly" but when asked if she had a model in mind of the way it would be held together she replied "Um...not really."

The undergraduate students shared similar views to their secondary school counterparts, with, for example, Steve, Alan, Reneé, and Jane, specifying the sea of electrons model for metallic bonding. The undergraduates who chose the sea of electrons model, provided similar explanations as illustrated by Steve's response: "[drawing rows of Al^+ inside circles with negative signs also inside circles]. This is a row of monovalent cations in a delocalised sea of electrons. That's the metal bonding [drawing lines linking negative charges with Al^+]."

The remaining undergraduates held a variety of mental models for metallic bonding. For instance, Phil, Bob, and Mary, had no clear picture of the bonding in metals, as seen in Bob's response: "I honestly don't have much of an idea except that, in some way I see the atoms of the metal as being close together in regular fashion, they are bonded together, I don't know whether it's been that well explained to me."

The preferred mental model for the postgraduates was the sea of electrons model. Although the postgraduates overall provided more complete descriptions than did their secondary school counterparts, two struggled. Grace appeared to possess no model for metallic bonding stating: "I don't know" and Christine provided a rather vague description: "I think I don't actually think of them as being bonded." Some of the postgraduates' descriptions of their preferred model incorporated ideas and terminology from other models, such as 'electron cloud,' 'molecular orbital'.

The secondary school students mostly failed to recognise that steel (used as a prompt during interviews) was an alloy containing iron as a base metal, with a variety of other metals substituted into the lattice, and also containing interstitial carbon as a hardening agent. More of the undergraduates than secondary school students identified steel as an alloy but they were often vague about details. For instance, Reneé and Steve both showed an appreciation of the interstitial nature of the alloy steel, Reneé indicating that carbon is "in the middle" of the metallic lattice. The postgraduate students, like undergraduates, routinely identified steel as an alloy but several students were unable to provide much detail about the bonding in the alloy steel. Christine, for example, struggled to explain the bonding in steel in a similar way to that for aluminium, but she did recognise that it was a mixture of metals.

Students' Mental Models for Ionic Bonding

The secondary school students possessed a number of mental models for ionic bonding with the preferred target model for the bonding in ionic compounds being the electrostatic model. Anne stated that "these have an electrostatic attraction between the two [ions]", Neil similarly viewed the bonding as involving charged species and he related the bonding to an attraction between charged species "because the sodium ions are positively charged and the chloride ions are negatively charged they are attracted to each other". David's mental model seemed better defined. He related the bonding in sodium chloride to electron transfer and the resultant electrostatic attraction between oppositely charged species and stated:

> " I know it's ionic bonding and that's where they donate electrons and receive electrons, the two things. So the way I would see that is the Na is the positive one and then Cl is the negative one. So because there's the attraction between the positive and negative charge, they are bonded together."

The undergraduate students' preferred mental model for ionic bonding was the electrostatic model and they placed greater emphasis on lattice structure and the use of nomenclature specific to models of ionic bonding. Steve, for example, seemed to feel that he could be expected to remember the specific lattice structure for sodium chloride:

> "Well once again you have got a regular repeating, a regular sort of repeating structure in an infinitely extended network of sodium plus [draws rows of Na^+ ions in a cuboid arrangement] ions, ah, sodium plus cations and chloride minus anions [draws Cl^- in centre of Na^+s]. So you have, I can't quite remember what the exact structure is. I should remember that. But you have got a regular array of say Na^+ and then they have a Cl^- and they have a repeating thing in three-dimensional units. I can't quite remember, it's either face-centred cubic or body-centred cubic".

The postgraduate students' preferred mental model for ionic bonding was the electrostatic model, their explanations being similar to those of the undergraduate and secondary school students, with James saying "It's mainly ionic, just having positive and negative sort of spheres packing together," and "when you have a positive charge and a negative charge, and it's the charges which sort of attract each other rather than sharing the electrons."

Students' Mental Models for Covalent Bonding

The secondary school students did not appear to hold any clear preferred mental model for the bonding in molecular iodine (I_2). The single consistent idea was that bonding in iodine involved covalent bonding and that covalent bonding involved sharing, although views on what was actually shared were highly variable. So, for example, Anne, said that the bonding in molecular iodine is "pure covalent" and her drawing of the bonding in I_2 simply consisted of two 'I' symbols with no links between the symbols.

The secondary school students' preferred mental model for the bonding in chloroform was much clearer, and almost all described the octet rule although some initially simply stated that the bonding in chloroform was "similar to that of iodine." Anita, to illustrate, said "they, *i.e.*, chloroform and iodine, are similar because they are both covalent," whereas Claire said that the carbon and chlorines "are sharing two electrons." However, overall the students explanations were clearly based on the octet rule and Neil's view is typical: "You'd have your carbon and it's got room for like another, it's got four electrons in its outer thing. So it's got room for four more, and it can get one from, like share one with Cl who only wants one more."

Like their secondary school counterparts, the undergraduates appeared to hold a variety of views for the bonding in I_2. However, most students expressed a preference for the octet rule. The undergraduates see the bonding in I_2 as covalent in nature, which they described as involving the sharing of electrons, Phil as an example, saying "the valence electrons they'd probably have an electron out on it's own looking to share with another one. So another iodine will come along and they just share electrons, quite happily share with each other."

The undergraduates' views of the bonding in chloroform were pretty much the same as those that they held for molecular iodine. Bob, for example, used a combination of ideas from the octet rule with those from molecular orbital theory.

> "Similar to iodine, the fact that it's covalent, made up of atomic orbitals again. In that case from what we established in the last one then between the carbon and [drawing CH_2Cl_2 structure in planar arrangement]. Those anions are going to want to be as far away, and the hydrogen obviously, they are not, I shouldn't call them anions. These groups on the carbon are going to want to be as far away from each other as possible. Because, chloride, because of their electron clouds around them repelling each other. Therefore adopts a tetrahedron obviously".

The postgraduates' preferred mental model for the target covalent bonding was clearly the octet rule, with all students describing covalent bonding as consisting of the sharing of electrons and going on to relate this directly to the notion of full-shell stability. The postgraduates were, however, highly emphatic about the molecularity of I_2 and spontaneously introduced the concept of van der Waals forces between molecules.

James Just covalently bonded dimers, and sort of van der Waals as weak forces holding all those dimers together in a big crystal.
Interviewer That's dimers was it?
James Yeah.
Interviewer So what's holding it together within the dimers?
James Oh that's sort of covalent bonds between the two iodines. Sort of like the electrons are shared in the middle.
Interviewer Ok could you just tell me what you mean by van der Waals forces?
James Um...it's where you have...sort of like a momentary polarisation or something of the dimers and the other dimer beside is polarised the same as that, so they polarise at the same time and they sort of attract.

The postgraduates generated descriptions for the bonding in chloroform ($CHCl_3$) that were identical in nature to those they provided for molecular iodine, as seen in Jason's response.

> "Ok so you have a carbon, which has four electrons a proton has one, and each of these, each of the chlorines, about it has eight, oh seven sorry. Ah, they want eight OK. So this configuration satisfies the valence requirements of each of the elements. Because hydrogen can only have a 1s orbital. It only needs two to fill its valence shell, but carbon and the chlorines, all need eight, and they can form eight by sharing an electron each. This sharing is very strong so these four bonds are all very strong. But the bonds between each chloroform is quite weak".

This description is typical of the postgraduates, in that it contains much the same ideas, but considerably more detail than that provided by the undergraduates and secondary students.

Summary and Conclusions

The data gathered in this inquiry regarding students' mental models for chemical bonding supports the preliminary findings from an earlier study[26] and are briefly re-capped here. The present work suggests that students from all three academic levels prefer simple mental models of the target systems for chemical bonding. The advanced level students typically provided more detailed explanations for their models and some of the postgraduate students were aware of the limitations of mental models. The extra depth of explanation for the models of bonding by undergraduates and postgraduates compared with secondary school students is probably simply a reflection of their learning experiences. As such, the findings of this study are consistent with those of other studies involving abstract chemistry concepts like atomic structure for which students showed a preference for realist, *e.g.*, space-filling, models of atoms and molecular species.[6,18,31] What is of particular interest and importance is that the advanced level-students including PhD students retained clear images of simple models like the sea of electrons and octet rule that they encountered many years previously. This is rather surprising given, for example, the vast differences between the octet rule and the molecular orbital theory. But this finding does suggest that the mental models preferred by the students in this study are very stable.[25]

Implications for Teaching and Learning

The present work was concerned with students' *preferred* mental models and suggests that despite competence in the description and use of sophisticated mental models for chemical bonding (as evidenced in their performances in examinations), these students at least, prefer simple models and relate to more abstract models only in particular contexts.[32,33] The fact that the students clung to these models even when they broke down in some way provides some cause for some concern in that their lecturers might well have expected their students to chose or more quickly adopt at least some of sophisticated mental models for chemical bonding that possess more explanatory power. The interviews did provide plenty of opportunities in which the simple models were in fact inadequate, and it is not desirable that students were so reluctant to draw on the more advanced models. As mentioned, there was some evidence that senior level students appreciated the limitations of the simple models they preferred to use – but this was pretty limited.

If the students show such a strong preference for simple models, this begs the question as to the advisability of teaching sophisticated abstract mental models for the concept of chemical bonding. In fact some authors argue that instructors for general or introductory level chemistry should concentrate their efforts on descriptive chemistry and materials chemistry.[34-36] This might be reasonable for undergraduates, but really only serves to place emphasis on rote learning and is hardly challenging. It is not obvious that 'dumbing down' a course will achieve very much. Lecturers use sophisticated abstract mental models of chemical bonding for much more than just describing the bonding in substances. Clearly, such models underpin much of chemistry, and are used to develop other concepts such as spectroscopy and chemical reaction schemes. Consequently, in our view, and as suggested in our earlier work,[26] we do not think it makes sense to remove complex models from the curricula purely because students prefer to use simple models. What we recommend instead is that tertiary level instructors consider limiting the teaching of such models until the advanced levels of the undergraduate degree. This suggestion is offered, since non-majors in chemistry will have little need for models in their subsequent studies.

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Spectroscopy and solid state properties of drugs: Will femtochemistry meet pharmacy?

Keith Gordon[a] and Thomas Rades[b]
Departments of [a]Chemistry and [b]Pharmacy, University of Otago, P O Box 56, Dunedin

In the pharmaceutical industry, solid state properties of drugs and drug-formulations are of great importance as more than 75% of all pharmaceutical products are administered as solid dosage forms.[1] It is crucial to be able to monitor and quantify the presence of different manifestations of the solid state, *e.g.* different polymorphs or amorphous versus crystalline forms. Traditionally, X-ray powder diffraction (XRPD) and differential scanning calorimetry (DSC) have been used for this purpose, but both techniques are time consuming and do not render themselves for in-process control, during drug and dosage form development. In recent years there has been a growing interest in the use of spectroscopic techniques to identify and potentially to quantify properties of pharmaceutical solids.[2] Although the vibrational spectroscopic techniques determine properties of a drug on the molecular level, the spectra may show differences depending upon which solid state the drug is in. Whilst infrared spectroscopic techniques such as near infrared spectroscopy (NIR), diffuse reflectance infrared spectroscopy (DRIFTS) and attenuated total reflection IR spectroscopy (ATR) are increasingly used, the potential of *Raman spectroscopy* in this field is only now beginning to be realized.

Raman spectroscopy

Raman spectroscopy measures vibrational spectra through the inelastic scattering of monochromatic photons, normally from a laser.[3] It differs from IR spectroscopy in a number of aspects. Firstly, it is a scattering technique, thus the intensity of the Raman photons strongly depends on the excitation wavelength used (photons at 400 nm scatter almost 40 times more efficiently than those at 1000 nm). Raman signals are much weaker than IR spectral signals; this is one of the reasons why Raman spectroscopy has been less utilized than IR. Secondly, the intensity of Raman transitions is governed by the change in polarisabilty with molecular vibration, as opposed to change in dipole, as with IR. This means that vibrations that are weak in the IR may be strong in Raman spectra and *vice-versa*. Perhaps the most important example of this is shown by the IR and Raman spectra of water. The IR spectrum of H_2O is dominated[4] by very strong transitions at 3756, 3652 and 1595 cm^{-1}. The Raman spectrum of water also has these bands but they are very weak.[5] For this reason Raman spectroscopy has been very widely used in biological chemistry and biospectroscopy where water is a major component of the samples of interest.[6] However, many solid dosage forms also contain water either adsorbed or as crystalline water.

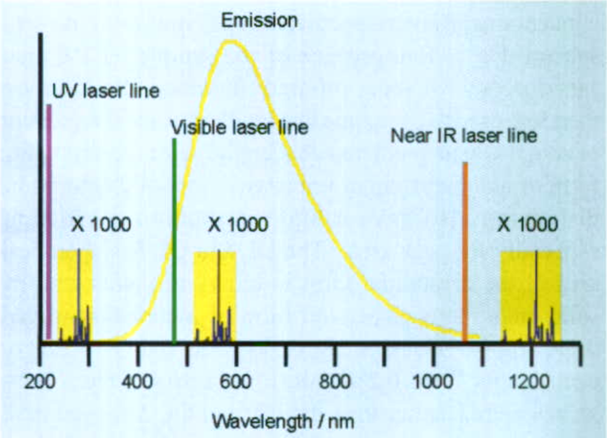

Figure 1. Raman spectrum (black in yellow boxes) of a sample measured at 3 excitation wavelengths. In the UV, the Raman scattering occurs at shorter wavelengths than molecular emission (yellow line). The scattering generated with visible excitation is swamped by the emission signal. The scattering generated by far-red excitation lies at longer wavelengths than the molecular emission.

Some of the practical limitations of Raman spectroscopy flow from the inherent paucity of the signals. The requirement for a laser as an excitation source and very sensitive detectors increases the cost of the experiments. Other impediments include the need for critical optical alignment and optical phenomena such as chromatic aberration. These tend to increase the difficulty of doing Raman spectroscopy and have hampered its widespread uptake as an analytical technique.[7]

An additional problem that may occur is emission from the sample. Many materials emit light quite efficiently under photoexcitation and this can swamp the Raman scattering. Figure 1 shows that a Raman signal (black within yellow box) generated using a visible wavelength laser will appear in the visible region, at about 570 nm. Luminescence (yellow band) from most molecular materials will occur in the visible region. As luminescence is 10^6 times more intense than the Raman signal, the Raman signal is obscured. However, with a long wavelength (red) laser the signal is generated at about 1200 nm (black with yellow background); very few molecular materials are emissive at such near IR wavelengths. Commercial Raman

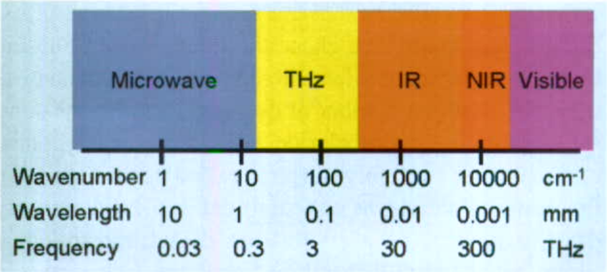

Figure 2. The wavenumber, wavelength, and frequency in THz for the electromagnetic spectrum (from microwave to visible).

instruments use red excitation to avoid emission. An alternative solution is to use a UV laser that generates Raman scattering below 350 nm, which is at shorter wavelengths than most molecular emissions. This methodology requires the use of UV lasers that are still primarily in the domain of spectroscopy research laboratories.[8]

Off-the-shelf instruments now exist that present Raman spectroscopy as a "user-friendly" non-specialist technique. Such instruments cost about $100,000 - $200,000 and may be based on diode lasers or Fourier-transform (FT) methods. Raman spectroscopy offers a serious alternative solution to analytical problems with solid state drugs or dosage forms in the pharmaceutical industry.

Solid state properties of drugs and drug-formulations are of highest importance in the pharmaceutical industry as most pharmaceutical products are administered as solid dosage forms (as tablets, polymer and sugar-coated tablets and capsules). This is mainly for reasons of high patient compliance, high chemical drug stability and the availability of fast and economical ways of mass production.[1]

Solid drugs may exist as crystalline, supercooled liquid crystalline or amorphous forms. Crystalline forms may exhibit polymorphism and the drug may thus exist in a thermodynamically stable or metastable form. Different polymorphic forms of a drug will almost certainly show differences in their dissolution rate and solubility, thus potentially affecting the bioavailability and efficacy of the drug, as well as differences in its chemical and physical stability. With the advent of combinatorial chemistry in the drug discovery process, drug molecules will become larger and contain more functional groups. The likelihood of polymorphism occurring will therefore increase in the future. However, already today, most drugs and new drug candidates show crystalline polymorphism. In 1995 four of the top five selling drugs showed polymorphism.[2]

Supercooled liquid crystalline and amorphous forms will be increasingly produced in the future, to improve the solubility of poorly water-soluble drugs. This approach is especially useful if the dissolution rate of the drug rather than its membrane permeability is limiting its bioavailability. As supercooled liquid crystalline and amorphous forms are thermodynamically unstable states, they may undergo recrystallisation under certain conditions. Therefore it is important to monitor and quantify the presence of these different manifestations of the solid state.

For a recent study,[9] we chose the three drugs ranitidine hydrochloride, fenoprofen calcium, and indomethacin as they can exist in a number of different forms in the solid state. Ranitidine hydrochloride, an H_2-receptor antagonist, can exists as two polymorphs (called form I and II), fenoprofen calcium, a non-steroidal anti-inflammatory drug, can exist as a crystalline dihydrate and in a supercooled liquid crystalline form, and indomethacin (another non-steroidal anti-inflammatory drug) can be produced crystalline and in the amorphous state, which is fairly stable when produced as a solid amorphous dispersion in an amorphous polymer, *e.g.* polyvinylpyrrolidone.

The different forms of the three drugs were initially qualitatively characterised by XRPD, DRIFTS, and Raman spectroscopy. The resulting spectra and diffractograms of the different manifestations of the solid state of the drugs differed characteristically, and thus allowed the identification of these forms. The main purpose of this study however, was to evaluate the use of Raman spectroscopy in the quantitative analysis of three types of solid-state mixtures: polymorph plus polymorph, supercooled liquid crystalline plus crystalline, and solid amorphous dispersion plus crystalline.

The application of univariate methods of analysis based on Raman spectroscopy was found to be inadequate for quantitative analysis. Therefore we used a multivariate method of analysis, namely principal components analysis (PCA) of the Raman spectroscopic data. The PCA was based on both peak areas and heights of peaks in the Raman spectra of binary mixtures of the different solid-state forms. Multiple linear regression was carried out using the concentration of one form as response and an adequate numbers of principal components as predictors.

Linear regression of actual versus predicted concentration of one form of ranitidine hydrochloride in the presence of the other gave good linear relationships. PCA of corresponding data for ranitidine hydrochloride form I in tablets of form II, and for form II in tablets of form I also gave good linear relationships. The detection limit (DL) and quantitation limit (QL) of ranitidine hydrochloride form I and II in binary mixtures, and in mixtures with tablets of the other polymorph, were 0.6% and 1.8%, respectively. These values were smaller than those found by DRIFTS and XRPD using artificial neural networks in an earlier study which gave DL and QL values for ranitidine hydrochloride form II in binary mixtures with form I of 1.5% and 5.2%, respectively.[10]

In the studies of indomethacin and fenoprofen calcium, conventional Raman spectroscopy did not result in useful spectra due to fluorescence of the samples. FT-Raman spectroscopy with near-infrared emission of the laser was therefore used to overcome this problem. Linear regression of actual versus predicted concentration of the crystalline form of indomethacin as impurity in the solid amorphous dispersion also gave a high correlation coefficient, especially for peak area. The DL and QL based on peak area of the crystalline form in binary mixtures with the solid amorphous dispersion form of indomethacin were 0.1% and 0.4%, respectively. The DL and QL based on peak height were 0.2% and 0.7%, respectively. These values were smaller than the DL and QL achieved in an earlier study by Seyer *et al.*[11] using multivariate analysis of second derivative near-infrared spectroscopy. However, linear regression of actual versus predicted concentration of the crystalline form of fenoprofen calcium as impurity in the supercooled liquid crystalline form only gave a fairly good correlation coefficient for peak area but not for peak height. Quantification of the crystalline form of fenoprofen calcium in binary mixtures with its supercooled liquid crystalline form gave much higher DL and QL compared to the previous studies of ranitidine hydrochloride and indomethacin (4.1% and 13.5%, respectively). The reason for this finding was most likely that the Raman spectra of the two forms were fairly similar. It was found that the DRIFTS spectra showed more pronounced differences, and it is likely the PCA of DRIFTS data in this case will provide a better means of quantitation of the different forms in binary mixtures.

In conclusion however, the study has shown that the combination of Raman spectroscopy and PCA provides a sensitive method for the quantitative analysis of mixtures of different solid-state forms of drugs, alone and in combination with pharmaceutical excipients. No sample preparation is needed for Raman or FT-Raman spectroscopy thus minimising the risk of solid-state transformation upon sample preparation. The method used in this study is a useful and potentially favourable technique to complement or replace existing methods.

In another study, Niemczyk *et al.*[12] were able to measure the drug bucindolol, a nonselective beta-adrenergic blocker, in a capsule formulation - indeed it was even possible to analyse for the drug from capsules encased in blister packs. The Raman technique was non-destructive and rapid (60 s per measurement). The spectrum of the active drug is complex as aromatic character generally increases the Raman cross section. The excipients in most capsule formulations are cellulose–based and do not show strong Raman signals. This is in contrast to IR spectroscopy, which possesses strong signals from active component and excipients alike and is thus more complex. It was possible to detect as little as 3 mg of bucindolol in a 1 g capsule with an accuracy of about 10%. This level of accuracy in quantitation is certainly sufficient for on-line monitoring and quality assurance.

FT-Raman, in conjunction with other techniques, has been used to clarify the properties of samples of the drug carbamazepine by McMahon *et al.*[13] Carbamazepine, a drug used in the treatment of partial and tonic-clonic seizures, exists in a number of polymorphic forms. The conversion between these forms was believed to be facilitated by humidity via a dihydrate form of the drug. McMahon *et al.* demonstrated[13] that the dihydrate could interconvert polymorphs in one direction (from form III to I), but not *vice-versa*. The Raman data used by this group focused on the low wavenumber spectral region below 200 cm^{-1}. In this region many of the most interesting features were observed. IR spectroscopy struggles at these low wavenumber regions. A new technique is emerging that may offer insight at even lower wavenumbers—this is the realm of *THz spectroscopy* (terahertz; 1 THz = 10^{12} Hz).

Femtochemistry meets pharmacy

The THz region of the electromagnetic (EM) spectrum sits between the near infrared and the microwave regime (see Figure 2) anywhere from 300 GHz to 20 THz (15 μm - 1 mm). This corresponds to 10 cm^{-1} and greater, and this turns out to be a very useful region of the EM spectrum. One of the main commercial drivers for the development of THz spectroscopy is medical imaging. The majority of current medical imaging technology relies on the two ends of the EM spectrum, one is magnetic resonance imaging, using photons at 0.4 μeV and the other is X-ray imaging, using 30,000 eV photons. There are a number of reasons for the paucity of methods relying on the intervening photon energies; IR radiation is very aggressively attenuated by water which is present in most medical samples, visible radiation is scattered as $(1/\lambda)^4$ so that blue light has difficulty providing sharp images. If we consider Figure 2, green light at 500 nm (20,000 cm^{-1}) scatters 10^{16} times more efficiently than microwave radiation at 2 cm^{-1}. Microwave radiation may be used for imaging, but the problem with these photons is that their wavelength is so great (0.3 and 30 cm) that imaging fine structure is difficult. The THz region lies between the microwave and the IR region. It provides better resolution than microwaves because of the shorter wavelengths of the photons used but does not suffer from scattering problems of IR and visible light because of its comparatively long wavelength. Furthermore, the THz region of the spectrum provides a unique opportunity to probe a variety of molecular interactions that are otherwise difficult to detect.

What types of interactions lie in this part of the EM spectrum? Figure 3 shows some of the interactions. In the microwave region molecules interact by increasing rotational energy. In the IR region the interactions are absorbed through vibrational energy changes. The THz regime is at lower energies than most internal vibrations associated with individual molecules. However, in the condensed phase, motion on the picosecond time-scale can give rise to absorption processes. The collective motion of many atoms and molecules in a coherent sense can give rise to such phenomena. This means that THz absorption profiles are very sensitive to the collective molecular environment of probed samples and thus of are potentially great importance in the investigation of different solid state forms of drugs. Subtle changes for example in solvation of intramolecular bonding will perturb the THz absorption profile whereas the IR spectrum may be rather insensitive to these changes.

Proteins are a very good example of the potential of THz spectroscopy. Proteins are well known to possess structural fluctuations on the picosecond timescale.[14] These low frequency motions have been connected to protein function.[15] For example the proteolytic enzyme α-chymotrypsin has a low frequency mode at 29 cm^{-1} that originates from intramolecular motion of the structure of the protein and disappears when the protein is denatured. Many other protein samples show dramatic changes in their THz spectra when hydrated.[16-18] The interactions between adjacent molecules (Figure 3) can result in motion on the picosecond timescale and THz absorption phenomena, but these motions are quite different in nature from typical molecular vibrations also shown in Figure 3.

The generation of THz light is achieved by using ultrashort laser pulses and "photoconductive emitters". When a visible light pulse of 10^{-12} s duration strikes a sample of a photoconductive emitter electron-hole pairs are created in

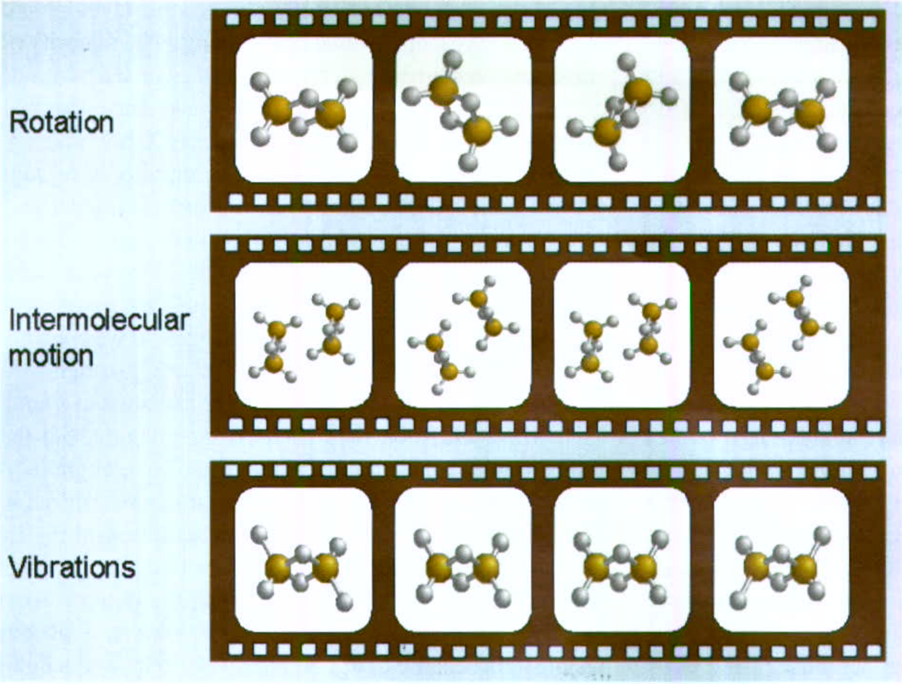

Figure 3. Molecular motion of B_2H_6. Changes in rotational energy (top reel) may be brought about by microwave radiation interactions. Motion between molecules (middle reel) may be brought about by THz absorption. A change in vibrational motion (lower reel) may be achieved with IR absorption.

the surface layer of the semiconducting device. These charge carriers are then accelerated by a bias voltage (that exists as a consequence of band bending at interfaces) and the current surge gives rise to emitted photons.[19]

A second way of thinking about this is to consider it as a frequency-difference generation mechanism. Again ultrashort light pulses, about 70 fs in duration are used. By virtue of their short time duration these pulses have very high peak *E*-field strengths. They also possess broad spectral ranges. As a light pulse strikes the material the electron cloud within the material oscillates. The dipole generated (*P*) from this oscillation is related to the electric field strength of the radiation (*E*) by the following equation:

$$P = \chi^{(1)}E + \chi^{(2)}E^2 + \chi^{(3)}E^3 \text{ and higher terms.}$$

If the *E*-field of the photon is given by $E = E_0\cos(2\pi\nu t)$, where *n* is the frequency,

then it is clear that *P* will oscillate at ν Hz. However, it will also oscillate at 2νHz as a consequence of the second term $\chi^{(2)}E^2$.

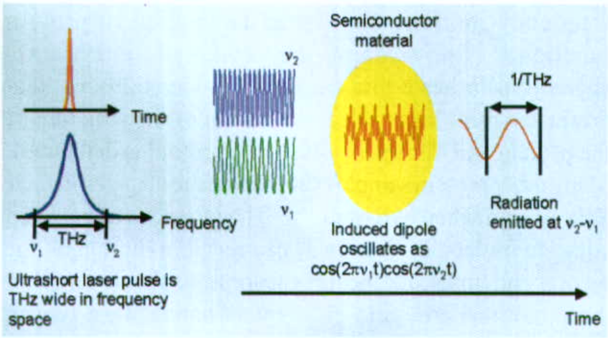

Figure 4. Schematic of THz generation. A light pulse of short time duration must have broad spectral width. Spectral components of the pulse (ν_1 and ν_2) induce dipole oscillations in a semiconductor material that follow $\cos(2\pi\nu_1t)\cos(2\pi\nu_2t)$. One of the beat frequencies from this is ν_2-ν_1. This corresponds to a THz frequency.

This is how frequency doubling occurs in pulsed laser systems. For a very short, in-time, light pulse there are a range of frequencies, say from ν_1 to ν_2 as shown in Figure 4. Now the second term for *P* will include mixed frequency terms such as $\cos(2\pi\nu_1t)\cos(2\pi\nu_2t)$. The oscillations of the electron cloud then beat against each other and one of the resultant emitted frequencies will be the frequency difference between the beats, *i.e.* $\cos[2\pi(\nu_2 - \nu_1)t]$. These frequencies lie in the THz regime because $\nu_2 - \nu_1 = \nu(\text{THz})$. As the original laser pulse contained a range of frequencies the emitted THz radiation also spans a frequency range.[20,21]

Having generated a THz signal it is necessary to measure its interaction with a sample. In a typical experiment the broadband signal is imaged through a sample and then into a Michelson interferometer (Figure 5). The interferometer acts to spectrally discriminate the various frequencies from which the signal is composed. The THz photons are detected using a Ge bolometer.

The potential of THz spectroscopy in the study of different solid-state forms of pharmaceuticals is considerable. Polymorphs exist through subtle changes in the packing of molecules within a structure. The bond lengths and angles of the individual molecules may be unperturbed

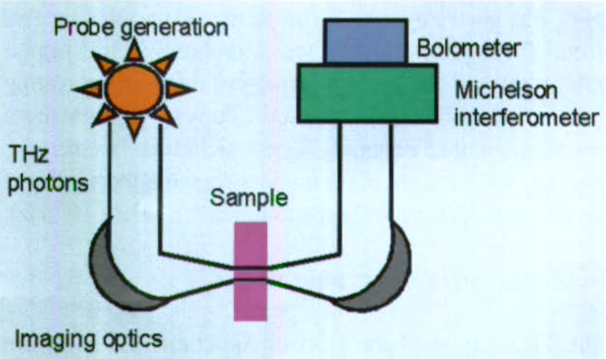

Figure 5. Schematic of a THz absorption experiment. THz photons across a range of frequencies are focused through a sample. The spectral information is separated in a Michelson interferometer and detected using a bolometer.

and hence the vibrational spectrum, as measured by IR or Raman is very similar for each polymorphs. However, as the motions probed by THz radiation may be caused by intermolecular motion, the packing parameters have a profound effect on the THz spectrum. Future work must show what role THz spectroscopy can play in the qualitative and quantitative investigation of solid drugs.

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NEWS

CHEMICAL EDUCATION TRUST FUND DISTRIBUTION 2002

The distribution of funds from the NZIC Chemical Education Trust (CET) to secondary schools in 2002 was realised in early October following calls for applications in both this *Journal* and *CHEM NZ*.

Because of declining interest rates, the CET Fund income was less over the past year than for some while. This resulted in three grants each of $550 being made this year -for the CET Annual Accounts see *Chemistry in New Zealand*, **2002**, *66:3* (September 2002). From the range of applications received the Trustees awarded grants to:

Katikati College (*Anderley Middleton*) – towards the cost of a commercially available colourimeter.
Nelson College (*David Fairley*) –towards the cost of conductivity testers and parts for a colourimeter.
Taradale High School (*Martyn Williams*) – towards the cost of an electronic balance.

Further interaction of NZIC with the chemists of the future in this way can only become effective if members support the Trustees financially. Donations to the Chemical Education Trust are tax deductible (over $5) and can be made to the NZIC Office; receipts will be issued. The fund need support the support of as many members and friends as possible.

B. Halton
Treasurer
15 October 2002

2003 NZIC OFFICERS

The 2003 NZIC Office holders elected at the November 6, 2002 Annual General Meeting in Wellington are:

President:	Dr David Bibby IRL, Gracefield
1st Vice-President:	Professor Andrew Brodie Massey University
2nd Vice-President:	Professor Graham Bowmaker, The University of Auckland
Treasurer:	Dr Colin Freeman University of Canterbury
Hon. General Secretary:	Mr Grant Boston Fonterra Research Institute, Palmerston North

A profile of the in-coming President will appear in the first issue of *Chemistry in New Zealand* in 2003.

New Zealand National Crystal Growing Competition 2002

The competition, divided into Primary/Intermediate and Secondary school section, is run by the Waikato Branch on behalf of NZIC. This year it attracted 34 entries in the junior competition and 37 in the senior competition. The judges are pleased to announce the winners as listed below.

Primary/Intermediate Competition
1st Prize **Teagan Matthews** Kaitaia Intermediate $60
2nd Prize **Theo Nates** Kadimah College $50
3rd Prize **Geoffrey Connell** Kadimah College $40
4th Prize **Leanne Usher** Kaitaia Intermediate $30
5th Prizes:
Rafi Lawrence Kadimah College $10
Edward Bates Manurewa Central School $10
Lisa-Marie Griffin & **Megan Naidu** Manurewa Central School $5 each.

Secondary Competition
1st Prize **Maxine Skilton** Waiopehu College $60
2nd Prize **Ryan Chadwick** Nayland College $50
3rd Prize **Lauren Penney** Nayland College $40
4th Prize **Nikita Scott** Nayland College $30
5th Prizes:
Jenni Moffatt Nayland College $10
Paddy Sinclair Nayland College $10
Chantelle Lawson Motueka High School $10

Associate Professor Bill Henderson
Chairperson, Department of Chemistry
University of Waikato
On behalf of the Waikato Branch,
New Zealand Institute of Chemistry

NEW ZEALAND INSTITUTE OF CHEMISTRY (INC.)

STATEMENT OF FINANCIAL PERFORMANCE
FOR THE YEAR ENDED 31 DECEMBER 2001

			2000
Expenditure			
Accountancy & Audit Fees	$3,009		$3,058
Branch Expenses - Projects/Capitation Fees	$30,956		$13,665
Branch Expenses - Student Travel	$500		$3,000
Chem NZ Expenses	$9,108		$17,519
Chem 13 Expenses	$8,170		$7,646
Conference Expenses	$2,714		$2,215
Donation	$3,500		-
Depreciation	$12		$12
Excecutive Office Expenses	$18,081		$16,293
General Expenses	$715		$3,659
Goods & Services Tax	$2,951		($2,751)
Interest & Bank Charges	$817		$873
Projects	$3,050		$4,299
Printing & Stationery	$3,321		$4,663
Prizes	$604		-
Production Costs - *Chemistry in New Zealand*	$8,775		-
Subscriptions	$4,890		$3,102
Telephone & Fax Charges	$962		$860
Travelling Expenses	$10,147		$8,160
Travelling Expenses - External	$3,518		-
		$115,800	$86,183
Total Operating Expenditure		$115,800	$86,183

NEW ZEALAND INSTITUTE OF CHEMISTRY (INC.)

STATEMENT OF FINANCIAL PERFORMANCE
FOR THE YEAR ENDED 31 DECEMBER 2001

			2000
Revenue			
Chem NZ -RSC Subs		$17,045	$15,000
Chem 13 Exam Fees		$13,345	$12,760
Subscriptions From Members		$59,017	$62,682
		$89,407	$90,442
Chemical Olympiad Donations	$18,182		$23,663
Chemical Olympiad Expenses	$22,295		$27,968
		($4,113)	($4305)
Chemical Milestones Receipts	-		($6,462)
Chemical Milestones Expenses	-		$480
		-	($6,942)
Gross Revenue from Operation		$85,294	$79,195
Operating Expenditure		$115,800	$86,183
		($30,506)	($6,988)
Other Income			
Interest - BNZ	$1,544		$1,636
Sundry Income	$889		$4,204
Pacifichem	$2,558		-
		$4,991	$5,840
Operating Deficit		$25515	$1,148

NEW ZEALAND INSTITUTE OF CHEMISTRY (INC.)

STATEMENT OF FINANCIAL POSITION
FOR THE YEAR ENDED 31 DECEMBER 2001

				2000
Capital Funds				
Chemical Olympiad Reserve			-	$3,923
Balance at the Beginning of the Year			$50,791	$51,939
Plus Net Surplus (Deficit) for Year			($25,515)	($1,148)
			$25,276	$54,714
Represented by:				
Current Assets				
Accounts Receivable		$4,435		$6,275
Prepaid Conference Expense		-		$2,500
B.N.Z. Current Account 00		$2,135		$38,850
B.N.Z. Autocall Account 25		$5,830		$3,264
B.N.Z. Term Deposits		$16,994		$16,046
B.N.Z Current Account 02		$6,731		-
			$36,125	$66,935
Fixed Assets				
Office Equipment	$582			$582
Less Accumulated Depreciation	$568			$557
		$14		$25
Presidential Chain		$360		$360
			$374	$385
			$36,499	$67,320
Current Liabilities				
Accounts Payable	$11,223			$4,074
Chemical Education Trust	-			$8,532
		$11,223		$12,606
Total Liabilities			$11,223	$12,606
Net Assets			$25,276	$54714

The accompanying notes form part of these financial statements.

NOTES TO THE FINANCIAL STATEMENTS
FOR THE YEAR ENDED 31 DECEMBER 2001

1. Statement of Accounting Policies

Reporting Entity

New Zealand Institute of Chemistry (Inc.) is a reporting entity registered under the Incorporated Societies Act 1908. The financial statements of the Institute have been prepared in accordance with generally accepted accounting practice and the Framework for Differential Reporting.

Measurement Base

The accounting principles recognised as appropriate for the measurement and reporting of earnings and financial position on a historical cost basis are followed by the Institute.

Specific Accounting Policies

The following specific accounting policies which materially effect the measurement of financial performance and financial position have been applied:

- Accounts Receivable are stated at their net realisable value after allowing for all bad debts.
- Fixed assets are stated at cost less aggregate depreciation. Depreciation has been calculated using the maximum rates permitted by the Income Tax Act 1994.
- Investments are valued at the lower of cost or net realisable value at balance date.
- The financial statements have been prepared on a GST inclusive basis. Accounts Payable and Accounts Receivable are stated inclusive of GST. All other assets and liabilities have been stated GST exclusive.
- Subscriptions are accounted for in the period they are receipted.
- The Institute qualifies for differential reporting as it is not publicly accountable and it is not large. Total revenue is less than $5 million, assets are less than $2.5 million and there are less than 20 employees. The entity has taken advantage of all available differential reporting exemptions.

Changes in Accounting Policy

There have been no changes in accounting policies. All other policies have been applied on bases consistent with those used in previous years.

Markhams mri Auckland

Chartered
Accountants &
Business Advisors

6th Floor, 369 Queen Street. P.O. Box 2194, AUCKLAND. Telephone: 09 309 6011, Facsimile: 09 366 0261, Email: mail@markhams-akl.co.nz

AUDIT REPORT

TO THE MEMBERS OF NZ INSTITUTE OF CHEMISTRY (INC.)

We have audited the financial report attached. The financial report provides information about the past financial performance of the Institute and its financial position as at 31 December 2001. This information is stated in accordance with the accounting policies attached.

Executive Council's Responsibilities
The executive council is responsible for the preparation of a financial report which gives a true and fair view of the financial position of the Institute as at 31 December 2001 and of the results of operations for the year ended on that date.

Auditor's Responsibilities
It is our responsibility to express an independent opinion on the financial report presented by the Board and report our opinion to you.

Basis of Opinion
An audit includes examining, on a test basis, evidence relevant to the amounts and disclosures in the financial report. It also includes assessing:

- the significant estimates and judgements made by the Executive in the preparation of the financial report, and
- whether the accounting policies are appropriate to the Institute's circumstances, consistently applied and adequately disclosed.

We conducted our audit in accordance with generally accepted auditing standards in New Zealand. We planned and performed our audit so as to obtain all the information and explanations we considered necessary. We obtained sufficient evidence to give reasonable assurance that the financial report is free from material misstatements, whether caused by fraud or error. In forming our opinion we also evaluated the overall adequacy of the presentation of information in the financial report. In common with other organisations of a similar nature, control over revenue prior to it being recorded is limited and there are no practical audit procedures to determine the effect of this limited control, and our audit opinion below is subject to this comment.

We provide accountancy service to the Institute. We have no other relationship with or interests in the Institute.

Unqualified Opinion
We have obtained all the information and explanations we have required.

In our opinion:

- proper accounting records have been kept by the Institute as far as appears from our examination of those records; and
- the financial report attached:
  - complies with generally accepted accounting practice;
  - gives a true and fair view of the financial position of the Institute as at 31 December 2001 and the result of its operation for the year ended on that date.

Our audit was completed on 4 November 2002 and our unqualified opinion is expressed as at the date.

Markhams MRI Auckland

Markhams MRI Auckland
Chartered Accountants

CHARTERED ACCOUNTANTS
A member of Moores Rowland International, an association of independent accounting firms throughout the world. Affiliated offices throughout New Zealand. The firms practising as Markhams MRI and Moores Rowland are independent. They are affiliated only and not in partnership.

NZIC Branch News

CANTERBURY

The Canterbury-Westland Science Fair took place in the last week in August at the Convention Centre. On Sunday 25 August Jan Wikaira and Meryn Bowen judged the chemistry entries of which there well over 300. Each one was looked at to assess its chemistry content.

The top NZIC award went to **James Bull**, a Year 13 pupil from Riccarton High School. His entry, Smoke or Coke not only won the NZIC prize but was also third overall in the fair, won the UC prize for best year 12/13 exhibit, and took third place in the Environment Canterbury prize for maintaining or improving our environment. The study he undertook was a comparison of the harmful emissions when coal and coke are used as solid fuels. It was a very original project that had been well planned and researched. The standard of experimentation was impressive and the results very well presented. James demonstrated an especially good understanding of the chemistry involved. The second award went to **Robert Adriaens**, a Year 12 pupil from Cashmere High School. He investigated a method of prolonging the life of car batteries. Each winner received the NZIC book *NZ is Different* and a generous cash prize from the Branch; the prizes were presented later at school assemblies.

The September Meeting: *The Science of Fireworks*, was given by **Anthony Leland** (Firework Professionals) and was a joint effort by the NZIC and the Outreach Programme of the University Chemistry Department. It was promoted to students from high schools and there was an excellent turnout, despite the meeting being postponed (due to the unfortunate ill health of Anthony) to a time during the school holidays. An audience of approximately 250 enjoyed an informative and lively presentation from Anthony, with assistance from several members of his fireworks company. Illustrations of fireworks from the past (accompanied by a real "Green Man") led on to a discussion of the physics and chemistry of fireworks manufacture, propulsion, and especially colour (a convincing green seemed to be the Holy Grail). Periodically Anthony would pause to blow something up, which he enjoyed as much as the audience. The evening concluded with a spectacular indoor display, which challenged the air conditioning extractor system. Given the popularity of the topic, the Outreach Programme has consulted Anthony with a view to developing a talk that can be used in schools. The Branch will also be looking at having a fireworks event on a regular basis in a collaboration that allows Anthony to concentrate on the pyrotechnics while we give the talk.

Twelve teams of year 11 students from high schools in the greater Christchurch area took part in the annual chemistry competition at Christchurch Polytechnic Institute of Technology (CPIT) in September. The competition involved two qualitative analysis exercises, preparation of a buffer solution, and measurement and interpretation of water conductivity. The four activities had a very tight 60-minute time limit. "To succeed, a team needs to be good at working as a team as well as having a good knowledge of chemistry. The top teams win or lose the competition on team work", said **David Hawke**, the CPIT lecturer who organised the competition, which is part of a series for high school chemistry students organised by the local Branch of the New Zealand Institute of Chemistry.

This year, **Shirley Boys' High School** won the competition with a score of 102 points out of a possible 150. Close behind was a team from **St. Margaret's College** (99.5 points). Each member of these teams received CD vouchers, donated by CPIT. All competition participants received a certificate of participation, and a healthy supper.

University of Canterbury

Visitors: Dr. Muna Al-Mandhary has returned to Sultan Qaboos University in Oman after a very productive research year collaborating with **Peter Steel**. **Dorothea M. Luedecke** (Professor of Physical Chemistry, University of Applied Sciences at Furtwangen, Germany) is visiting the Departments of Chemistry and Chemical Engineering. Dorothea's fields of interest are thermodynamics, metallurgy, material science and semiconductors. While at Canterbury she wishes to learn about the Science Outreach Programme and is contributing to its extension to Chemical Engineering. **Professor Jane Nelson** (School of Chemistry, Queens University, Belfast, Northern Ireland) has completed her two months as Erskine Fellow in the Department. During her stay she taught a course in inorganic spectroscopy.

Professors **Piergiorgio Casavecchia** (University of Perugia, Perugia, Italy) lectured on Spectroscopy and Molecular Dynamics while **Chris Easton**, an ex-member of the Department's academic staff now at the ANU, presented lectures on topics in physical organic chemistry **Dr Paul Anastas** spent a month in the Department lecturing on aspects of green chemistry.

Franziska Meier, from the Free University of Berlin, Germany is working on a special project with **Owen Curnow**. **Dave Beer** is attached to the Science Outreach Programme for the second half of this year whilst **Jim Hudson** is back working with **Peter Harland's** research group. **Philip Borsting** (University of Southern Denmark) is to work in **Peter Steel's** group for the next 6 months. **Ekkehard Unger** has joined the MarinLit operation for a few months. Ekke, whose PhD was completed in Germany, has been working at the Cawthron Institute for a few years.

Postdoctoral Fellows: Todd Clements, a Marsden Postdoctoral Fellow from the University of California, San Diego, has arrived for one year of work, also with the **Harland** group. **Shigeru Miyamoto** (Tokyo Institute of Technology) is working with Andrew and Jim on a FiRST-funded project developing inhibitors of the calpains associated with cataract formation. This work will be conducted in conjunction with Lincoln University, which has developed a line of sheep genetically disposed to cataracts.

PhD News: Congratulations to **Chris Knox** and **Chris Fitchett** who have both recently passed their PhD oral exams. We wish them well in their future endeavours.

University of Canterbury Council: Dr Robin Mann (a graduate of the Chemistry Department) has been appointed (as the unchallenged candidate) Chancellor-designate for 2003. **Jim Coxon** has been elected as Academic Staff Representative on the University Council for a further term of four years, having already served two years on Council.

Marsden success: Congratulations to **Alison Downard, Andrew Abell, Jim Coxon** and associates on their successful bids to the Marsden Fund. Andrew Abell and Alison Downard received a Marsden Grant to work on the design and synthesis of new conformationally-constrained peptidomimetics for incorporation into oligomers, both in solution and attached to surfaces, ranging from large surface area solid supports to nanoscale materials. It is intended that these systems will form the basis of new approaches to isolation, purification and sensing of important biomolecules. The work involves collaboration with **Richard Blaikie** (Canterbury), **Jim Coxon** (Canterbury) and **Kate McGrath** (Otago)

Congratulations: Sam Yu, has been awarded a University of Canterbury Summers Scholarship and will be working with **Alison Downard** over the holidays. The following students have been awarded Department of Chemistry Summer Scholarships: **David Bones, Meryn Bowen, Neroli Eggeling, Michelle Hamilton, Tim Heaton-Burgess, Victoria Hewitt, Jared Panther** and **Emma Turner. Richard Payne** has been awarded a Gates Scholarship to undertake PhD studies at the University of Cambridge (UK) starting in 2003. It has been announced that **Richard Hartshorn** will be a recipient of a University of Canterbury teaching award at December graduation.

On Saturday 5 October **Susie Meade** gave birth to (probably) identical twins, Jacob Meade Hartshorn (2.705 kg, 15.55) and Todd Meade Hartshorn (2.770 kg, 16.05). Congratulations Susie, Richard and the grandparents.

Internal Grants Round: Successful applications to the University internal grants round were: Peter Steel for 2-year post doc; Bryce Williamson for research into magneto-optical properties of magnetic nano-devices; and the biodiscovery consortium (fronted by Murray Munro) for equipment related to bio-prospecting and the development of bioactive compounds.

141 Years of Excellence in Chemistry: Four gentlemen of the Chemistry Department, **Ward Robinson, Kip Powell, Rod Claridge** and **Alan Happer** have recently gone onto half-time contracts. To celebrate this event the quartet organised a dinner for some of their past and present academic colleagues. Ward noted that during the past year the quartet, who have clocked up 141 years of combined service, have become gentlemen in the field of chemistry. Strictly they are only half gentlemen since they have opted for half-time positions that allow them access to the building, and library cards, so that they can go on as they have over the last century!

The Chemistry Department Ball: Several weekends ago saw the social event of the Christchurch ball season, when over a hundred guests attended the combined chemistry-biology ball within the salubrious surrounds of the Newberry Lodge. Organised by **Antonia Miller**, one of the 'chemically-minded' in the PAMS Department, the guests were greeted at the door with a glass of champagne. While the DJ played some of the solidest gold hits of the eighties the assembled scientists let their hair down and let it all hang out. By all accounts all who attended or at least could remember attending enjoyed the evening. Among the debs and young pretenders it must be said there was a good representation of more senior (in years anyway) fellows showing the youngsters how to have a good time.

Hot Papers: For the second time this year, a paper from the Department has been selected by the ChemWeb magazine *The Alchemist* as one of the week's two 'Hot Papers in Chemistry'. Recently **Dave McMorran's** "self-complementary molecular cleft", published in *Chem. Commun.* received such accolade as did **Chris Sumby's** "silver platter" paper earlier in the year. Both Dave and Chris work in **Peter Steel's** research group.

MANAWATU

The NZIC President, **Pat Holland**, visited the Branch on September 12. After being entertained at a local restaurant he spoke on *Endocrine Active Substances in the Environment*. On October 29, the 2002 Royal Society of Chemistry Australasian Lecturer, **Bill Kitching** from the University of Queensland, addressed the branch on *The Organic Chemist in Biological Chemistry: Structure, Synthesis and Biosynthesis*.

A number of local branch members were persuaded by Manawatu Science and Technology Fair Chief Judge, **Tony Wright**, to assist with judging the event. **Susannah Neild**, Monrad Intermediate School, won the Manawatu Branch Prize with her entry *Enzyme Power*, and **Melissa Joe**, Awatapu College, was awarded the Massey University Chemistry Prize for her investigation into *Calci-in-Water*. Interaction with high schools is also **Geoff Jameson's** forte - he has compiled the Annual Chemistry Quiz that the Branch mails to high schools in the region with profits (if any) going to the Branch's Chemical Education Trust for redistribution to schools.

The Branch thanks its Chairman, **Richard Haverkamp**, for his leadership as he has decided it is time for him to step down. The committee has appreciated his laid back, but efficient style of chairing meetings over the last two years – they never lasted more than an hour!

AgResearch

Nutrition and Behaviour Research Chemist **Lucy Meagher** attended the ACS fall meeting in Boston in August 2002.

She presented a poster on the *Mass Spectrometry of Condensed Tannins from Pasture Legumes: Chemical Characterization Links with Nutritional Properties* at the Agriculture and Food Chemistry Division reception. Sessions of interest to current research alignment at AgResearch included flavour chemistry, bioactives in foods and molecular biology of secondary metabolites. The Biotechnology division held sessions of interest on advances in bioseparations, chromatography scale-up, fermentation process development, bioprocess monitoring and control. On her return to New Zealand, she stopped at the Henry A. Wallace Beltsville Agricultural Research Center (BARC) in Beltsville, Maryland. Beltsville, near Washington DC, is the headquarters of the US Department of Agriculture, Agricultural Research Service. The stop involved visits to researchers in the Human Nutrition Research Center (BHNRC), Animal and Natural Resources Institute (ANRI), Animal Waste Pathogen Laboratory (AWPL), Growth Biology Laboratory, Immunology and Disease Resistance Laboratory and the Parasite Laboratory to discuss common areas of research interest.

Central Environmental Laboratories

The Palmerston North City Council Laboratory has relocated recently to the Batchelar Centre adjoining the HortResearch site in Tennent Drive. Its Manager, **Jim Anderson**, has noted that the 10 full-time staff members have welcomed the move from its previous Civic Complex basement location to larger, and windowed, premises. The move has allowed work expansion, and also separation of "clean" and "wastewater" chemistry testing areas. The laboratory, which has been operating for some 40 years, is now identified as Central Environmental Laboratories to reflect its wider client base and range of testing activities.

Fonterra Research Centre

Kevin Pearce is leaving the Fonterra Research Centre (FRC) after joining the then, New Zealand Dairy Research Institute in 1968. He is taking up a new position with Westland Milk Products, Hokitika, as their R&D Manager. During his time with FRC his research interests included: the physical chemistry of milk and dairy products; protein chemistry; milk minerals; natural and processed cheese; milk and protein powders. As a keen outdoor enthusiast, Kevin will no doubt be pursuing the opportunities the South Island offers for mountaineering, orienteering, photography, sea kayaking, speleology, and tramping.

Massey University

Three Marsden Grants were awarded to Massey chemists in the recent round. **Geoff Jameson** gained $645,000 for the project *Hydrogen atoms in protein structures: invisible agents of biological activity* whilst **Eric Ainscough** and **Andrew Brodie** were awarded $570,000 for the project *New metal-rich scaffolds;* **David Harding's** project *Design and synthesis of biodegradable hydrogel scaffolds to support liver cell growth* captured $575,000. David has also had his contract with Fonterra Tech Ltd, which pays the salaries and expenses for 2.5 staff, renewed for another year. **Carol Taylor** and **Geoff Jameson** have been awarded funding for postdoctoral fellowships from the Massey University Research Fund. Third year chemistry students, **Robyn Abernethy** and **Tania Mramor**, have been awarded Summer Scholarships to work at the Australian National University.

David Parry was elected Vice-President of the International Council for Science (ICSU) at the ICSU General Assembly in Rio de Janeiro. David is the first New Zealander to be appointed to this position on the international executive that represents about 5 million scientists from 27 unions and 103 countries worldwide. "We will be undertaking a review of international interdisciplinary activity in particular regard to the environment and sustainable development, data and information and capacity building of the scientific capability in third world countries." He says a second focus is the administration of $2 million in funding grants aimed at areas of scientific importance and, thirdly, assessing new and emerging areas of science to determine where to focus resources.

Geoff Jameson has been appointed as the 2003 Royal Society of Chemistry Australasian Lecturer, which means he will have to visit major centres in New Zealand and Australia next year. Previous New Zealand recipients of this prestigious award have been **Ted Baker** and **Bill Denny**.

The Richard Dean Batt Memorial Lecture, which was established in 1994 in memory of the Foundation Professor of Biochemistry, Professor Batt, has become an important event of Massey University. The Fifth lecture in the series was delivered by the **Honourable Pete Hodgson** on September 12. His topic, *Exploring Innovation*, contained a timely message and was well received by a capacity audience (it is to be published in full in the next issue of *Chemisty in New Zealand*). **Richard Haverkamp**, Institute of Technology and Engineering, has recently returned from overseas. He collaborated and visited with colleagues in South Africa (Rhodes University, University of Pretoria and Technikon Pretoria), Ireland (Dublin City University), The Netherlands (Technical University of Eindhoven and Hogeschool Brabant), and the UK (University College London) and as well attended two conferences. On his return, at the Final Year Technology and Engineering Dinner, the students awarded him the 2002 Techensoc Excellence Award for the *Lecturer most likely to get distracted and go off the topic*!

Ken Jolley celebrated his 35 years of employment at Massey University by delivering a lecture entitled *Magnetic Moments* but said an alternative title could be *From Holiday Camp to Gulag*! He reviewed his research over the years and added comments on the huge changes that have occurred in the university system over this period – hence the subtitle. Some of his comparisons of the past with the present provided amusement for younger staff and students, and a state of terminal nostalgia in the elderly! Ken will formally retire at the end of the year but has negotiated two part-time contracts – one with the Nanomaterials Research Centre and one with the University to continue some lecturing.

We are very sorry to have lost **Tony Wright**, who has taken up a position at the University of Queensland. The newly established position is a cross-faculty appointment between Science and Education and he will be responsible for establishing a science education programme on the new campus at Ipswich (which is housed in the old mental asylum) as well as working with the Chemistry Department at St Lucia in Brisbane. Tony presented a public lecture to the University entitled, *Chemistry: In Your Face – Like it or Not*, in which he provocatively explored the huge gulf between the education experts and the chemistry experts. As always with Tony's lectures, it was illustrated with practical demonstrations, including one of his favourites, burning phosphorus. This lecture also formed part of the October high school chemistry teachers' meeting. Other activities included hands-on experiments for teachers to try in the laboratory based around perfumes and lipsticks and an exciting lecture from **David Officer** on *The Chemistry of Nanotechnology*. Other staff leaving Massey University for overseas are technicians **Michelle Eccleshall**, who has been working in the Centre for Separation Science and **Emma Smith** who has been in the Nanomaterials Research Centre. **Simon Hall** is spending several months working at the Los Alamos National Laboratory with former Massey staff member, **Tony Burrell**.

Joe Beckman (Alma College, Michigan) is spending 3 months working with **Trevor Kitson** and **Paul Buckley**, on rapid kinetic experiments using the stopped flow spectrometer. Other new arrivals in chemistry include PhD students, **Ben Mulchin** (with **Emily Parker**) and **Fabio Lodato** (with **David Officer** and **Warwick Belcher**). **Mark Vigneswaran** has moved from HortResearch to work in the Nanomaterials Research Centre. Congratulations to **Slavica Pavlinic** and **Michael Liu** who have recently defended their PhD theses successfully. Slavica worked with **Tony Wright** and **Paul Buckley** and now has moved to Hamilton. Michael, supervised by **Simon Hall**, now has a position in the Nanomaterials Research Centre.

OTAGO

The news from Otago is highlighted by **Keith Gordon's** recently announced elevation to the rank of Associate Professor. Keith arrived in the department in 1993 with an unintelligible Belfast accent that still manages to keep him clear of lecturing the 1100-strong CHEM112 class. Over the intervening years he has set up a truly world class Raman facility in the Department which he has used to study a wide variety of chemical systems. Whoever would have thought that Raman spectroscopy could be so useful? Keith is looking forward to the reduction in lecture load his promotion will bring....

Elise McGale is working as a research assistant with **Keith Gordon's** group. Her research focus is on organic light-emitting diodes that she has fabricated with some success. **Sarah Howell** is off to Germany shortly to attend a series of courses run by instrument manufacturer Bruker. These will provide training in how to develop step-scan time-resolved FTIR spectroscopy and in FT-Raman spectroscopy. It is hoped that Sarah's expertise will allow us to make full use of the newly purchased FT-Raman and IR bench. **Keith Gordon** will also be attending these courses. **Clare Strachan** has joined the group and is doing a PhD in pharmacy (with **Dr Thomas Rades**). She is looking at developing new spectroscopic techniques to quantify drug polymorphism. She is also investigating modeling of the vibrational spectra of such drugs using computational quantum chemistry. **Tracey Clarke** finished her Honours project with the group but is coming back after her exams to join as a research fellow for 2003.

Dr Guolun Zhong arrived to take up a postdoctoral position with **Keith Gordon** in October. He received a BSc in Analytical Chemistry from Jilin University and his MSc and PhD degrees from Shandong University. He has worked as a lecturer and associate professor in several Chinese universities. During April 2001 and August 2002, he was a research assistant professor at Korea University. His research interests include gas chromatography and electrochemical analysis, electrochemistry, organized molecular films, chemical vapour deposition (CVD), light-emitting diodes (LED) and multi-step synthesis of conjugated polymers. He will be working on Raman spectroscopy of new materials as part of the MacDiarmid Institute for Advanced Materials and Nanotechnology.

The Gordon group commissioned a medium-frame krypton ion laser in October. This was funded through the MacDiarmid Institute for Advanced Materials and Nanotechnology and provides a range of excitation wavelengths for resonance Raman measurements. The Chemistry Department at the University also provided funding to upgrade the CCD-spectrograph and built a number of high-quality laboratory spaces for the new system to be housed in. These improvements have greatly improved the flexibility and sensitivity of the Raman facility at Otago and we are looking forward to the new research that will come from this. The MacDiarmid Institute has also funded a PhD scholarship to study the optical and electrical properties of functionalised nanotubes and fibres. This is in collaboration with the Nanomaterial Research Centre at Massey University. Further information on research group activities may be found at:
http://neon.otago.ac.nz/chemistry/research/kcg/kcg-res.htm

Two students have recently been awarded their PhD degrees. **Dr Anna Barlow** was jointly supervised by **Rex Weavers** of the Department of Chemistry and **Nigel Perry** and **Steve Lorimer** of the Plant Extracts Research Unit, and she is currently acting as a First Year tutor in the Department before taking up a postdoctoral post at Exeter. **Dr Zimei Rong** worked with **Henrik Kjaergaard** and is now doing postdoctoral work in France. The Department welcomes **Dr Gurmit Singh Gill** from Guru Nanak Dev University in Amritsar, India, as a postdoc with **David Larsen**. **Dr John Daniel** is visiting the Department from the NOAA in Boulder, Colorado for three months, working with **Henrik Kjaergaard**.

Seven staff members from the Department of Chemistry were successful in the latest round of Marsden grants. **Keith Hunter and Philip Boyd** (NIWA Centre for Chemical and Physical Oceanography, housed in the Department of Chemistry) are the principal investigators for a $600,000 grant over three years, entitled "Dust up from the Red Heart — does trans-Tasman aerosol transport alter New Zealand's oceanic biota?". **Jonathan Kim** of the Department of Chemistry is an associate investigator on the grant, as is **Associate Professor Grant McTainsh** (Griffith University, New South Wales).

Jim McQuillan is a principal investigator, along with **Iain Lamont** (Department of Biochemistry) and **Phil Bremer** (Department of Food Science) on a $617,000 grant investigating "How do bacteria stick to metals?".

Russell Frew is an associate investigator on a $570,000 grant, "Food web connectivity in the Fiordland ecosystem: an investigation of trophic links across ecotone boundaries", headed by **Steve Wing** (Department of Marine Science); **Catriona Hurd** (Department of Botany) is also an associate investigator.

Kathryn McGrath is an associate investigator on a $600,000 grant headed by **Andrew Abell** and **Alison Downard** from the Department of Chemistry, University of Canterbury, entitled "Conformationally constrained and immobilised bioactives".

Keith Gordon is an associate investigator on the fast-start grant of $100,000 over two years won by **Mark Waterland** (Industrial Research Ltd - and a PhD graduate of the Department of Chemistry in 1998), "Understanding molecular interactions in solid polymer solutions: a combined theoretical and experimental investigation. **Dave Phillips** (University of Hong Kong) is also an associate investigator.

Allan Blackman has been responsible for soliciting the Otago-based articles for this issue of *Chemistry in New Zealand.* His other claim to fame comes from the magic shows that he does – and I am told that it is not as painful as the photo at right might imply.


Allan Blackman 'disappears' during one of his recent magic shows.

Thanks to the exhaustive efforts of **Kathryn McGrath**, the University of Otago Chemistry Department recently launched its new interactive alumni network. Former graduates and staff should have all received our first magazine by now - if not please contact us at the address below and we will get a copy sent to you. The aim of having an alumni network is to keep track of our graduates and former staff, and for the Department to act as a conduit through which everyone can keep in touch. The network will operate predominantly through the alumni web page (http://www.otago.ac.nz/chemistry/alumni/) and all those who have had any association with the Department are encouraged to participate. We would like to develop news pages, job pages, information pages and question pages on the web to which anyone can submit. We have already had an excellent response - so if you want to know whatever happened to all your classmates, or you just want to know a little about what's happening in the Department now, please register at the web site or email us (chemalumni@alkali.otago.ac.nz) and feel free to send us information, photos or anything you think may be of interest (within reason!) and help us to establish a viable alumni network.

CONTACT DETAILS:
Otago Chemistry Alumni Network,
Department of Chemistry,
University of Otago,
P O Box 56 Dunedin, New Zealand.
Phone: +64-3-4797932, Fax: +64-3-4797906
Email: chemalumni@alkali.otago.ac.nz
Internet: http://www.otago.ac.nz/chemistry/alumni/

WAIKATO

University News
CHEMQUEST 2002, the annual quiz for sixth form students run by the Chemistry Department at the University of Waikato was held on Wednesday 23rd October. Invitations were sent to schools in the Waikato/Bay of Plenty region to send teams of three students to the University for a fun packed night of chemical questions, ranging from *Periodic Puzzlers* to *Demon Demos*. A total of 48 teams entered this year, with students coming from as far afield as Whakatane to compete for the James and Wells trophy, medals and cash prizes. After each of the four rounds of questions, it was *Teachers' Turn* with four teachers per round competing for a small prize for themselves and $120.00 of book tokens for their school, generously donated by the Waikato Branch. It was a most enjoyable night for contestants, presenters and spectators and the following prizes were awarded:
1st Prize to *Three Blind Mice* from St. Paul's Collegiate (**Matthew Wells, Paul Lu, William Kelton**).
2nd Prize to *Y12* from Fairfield College (**Alastair Waller, Chris Collins, Fatrian Rusydy**)
3rd Prize to *Holden's heroes* from Tauranga Boys' College (**Andrew Hayward, Kevin Lai, Robert Fleury**)
4th Prize to *Bob Marley and the Wailers* from St. Paul's Collegiate (**Anthony van der Engel, Rex Wu, Sachi Fernando**)
5th Prize to *Team X* from Fairfield College (**John Revell, Michael van Kampen, Natalie Scott**)
Teachers turn:
Round 1: **Lisa Janek** (Fairfield College)
Round 2: **Andrew Ryan** (Hamilton Boys' High School)
Round 3: **Andy Horsfield** (Waihi College)
Round 4: **Anderley Middleton** (Katikati College)

Richard Coll and **Michèle Prinsep**, presented the quiz with **Bill Henderson** running "*demon demos*". Numerous other people contributed to the success of the occasion including many of the staff and students of the Chemistry Department and School of Science and Technology. Thanks go to the University of Waikato for organisation, marking and publicity, and **Sam Pearson** (James and Wells) and **Bob Wilcock** (NZIC) for prize presentation and especially the sponsors of the quiz James & Wells

Patent Attorneys, Hamilton, School of Science & Technology and the Department of Chemistry, University of Waikato, the New Zealand Institute of Chemistry, and finally bit not least, Exscite Science Centre, Hamilton.

Jacinta Dalgety working with **Richard Coll** is nearing the end of the write-up for her PhD. Jacinta has just had a paper from her thesis accepted for publication in the prestigious *Journal of Research in Science Teaching* and a conference paper based on the same work has been short-listed for the best paper award from the USA-based National Association for Research in Science Teaching. **Richard Coll** is staying on at Waikato with plans to move to Oxford falling through due to lack of funding. He is now 0.7 in Waikato's Centre for Science & Technology Education Research, and retains teaching duties in Chemistry contributing to chemical technology, and with **Michael Mucalo** also looks after work placements for chemistry students in the BSc(Technology) program.

Lyndsay Main attended the Merck Lectureship Reunion at Cambridge in September, a celebration to mark the retirement of Tony Kirby, Jim Staunton and Ian Fleming. The annual Merck Lectureship was set up at Cambridge in 1987 and all but one of the previous distinguished recipients of the award (a who's who of modern organic chemistry) were back on hand to present lectures on their current research. The retirees (who seem to have a lot of chemistry planned for retirement!) gave lectures replete with fascinating historical information and amusing anecdotes, and their chosen favourite sons (respectively Alan Fersht, Chris Abell and Ian Paterson, all of Cambridge) also presented current research lectures.

Professor Bill Kitching, the Royal Society of Chemistry Australasian lecturer from the University of Queensland gave a well attended and fascinating seminar on Friday 25th October at the University entitled *Insect Chemistry and Chirality*.

NIWA News
As this is the first contribution to the NZIC Branch News for the NIWA-Hamilton chemistry group for sometime, this 'news item' will serve as largely an introduction for the new faces, and an introduction for some of the not-so-new faces, that make up the Hamilton chemistry group.

Bob Wilcock was elected President of the Waikato Branch of the NZIC in March, and since that time has initiated major changes, perhaps the most important being the strategic decision to serve pizza at the traditional NZIC barbeque. This accompanied the Presidential address to the branch from **Pat Holland** on 17th September. In the laboratory, Bob has been using gas tracers to examine how aquatic plants alter hydraulic conditions and modify water chemistry in lowland streams. Bob is continuing his collaboration with **Professor Steve Chapra** from Tufts University, USA, on modelling diurnal changes in p*H* and dissolved inorganic carbon in streams.

Burns Macaskill is currently collaborating with **Keith Hunter's** research group at Otago to characterise ocean/atmosphere exchange of carbon dioxide in the southern ocean. **Craig Depree**, a Waikato graduate, joined NIWA in November 2000 after postdoctoral studies with **Eric Ainscough/Andrew Brodie** at Massey and **Sally Brooker** at Otago. Craig's main research emphasis has been on understanding the source, distribution, and fate of polycyclic aromatic hydrocarbons in aquatic environments, and in particular the role of colloidal and sedimentary organic carbon.

Trevor Mathieson, also a Waikato graduate, joined NIWA at the start of 2001 following an Alexander von Humboldt Fellowship working with **Professor Schmidbaur** at the Technical University of Munich. Trevor has been investigating the pore-water/sediment partitioning of metal contaminants in estuarine environments, with the contention that results will provide a more accurate basis for contamination assessment.

Michael Ahrens, (PhD, SUNY Stony Brook, NY, USA, 2000) joined NIWA in Oct 2000 as an ecotoxicologist, but with considerable interest in environmental organic chemistry. Michael's recent research has centred on the bioavailability and toxicology of polycyclic aromatic hydrocarbons (PAHs) to sediment-dwelling marine organisms, which will enable a more accurate estimation of environmental risk from contaminated sediments. Other research has investigated UV photoactivated toxicity of PAHs to marine animals, and the characterization and synthesis of digestive surfactants of marine invertebrate organisms.

Michael Ellwood, a NZS&T Postdoctoral Fellow, arrived at NIWA in November 2001. Michael is an Otago graduate and comes to NIWA having completed postdoctoral research with **Professor Stan van den Berg** at the University of Liverpool, UK and **Associate Professor Bill Maher** at the University of Canberra, Australia. Michaels's research focuses on zinc and cadmium speciation in the waters east of New Zealand. Since arriving, Michael has been out to sea on the NIWA research vessel Tangaroa on two occasions, and is currently preparing for his third voyage departing in November.

WELLINGTON

The Wellington Branch was associated with a meeting on September 2, arranged, by the Royal Society of New Zealand, at which **Professor Pierre Laszlo** spoke on *'Technology and Advancement of Science; the Second Chemical Revolution'*. Professor Laszlo was in New Zealand to lead a weeklong course for scientists on communicating science. This was organised by the French Embassy with assistance from the Royal Society of New Zealand.

He described the transformation of laboratory equipment from "tools", with which direct measurements were made, to increasingly complex "instruments" where the measurements require increasingly sophisticated interpretation. The ready availability of structural information led to a fundamental change in chemical understanding during the last century, from a basis of "substance" to one of "structure". However, he warned of a danger in this progression. The development of "centres" with more powerful, expensive, technician operated and complex software-driven instruments leads to the possibilities of incorrect interpretations and of missed (but significant) anomalies. Instead, he advocates the wider distribution of less sophisticated (and cheaper) instruments, directly accessible by researchers who should be able to experiment with instrument settings and performance. The researchers will then have a more direct understanding of the meaning of output of the instruments, and be more likely to spot instrumental or software nonsense, or the anomalies which might lead to novel developments.

Pierre Laszlo was Professor of Chemistry at Liège and at the Ecole Polytechnique and held both positions until taking early retirement in 1999. His main research interests have been in the catalysis of organic reactions by inorganic solids such as the clay minerals; studies of molecular interactions in solution, and multinuclear magnetic resonance spectroscopy. He has contributed more than 200 primary publications and 15 published monographs and textbooks to the scientific literature. As a science writer, he has also authored more than 15 books, and has published a number of essays on the popularisation of science. The award of the Maurice Pérouse Prize by Fondation de France recognized this activity in 1999.

NZIC President Dr Patrick Holland (Biotoxins Section, Cawthron Institute, Nelson) visited the Branch over September 11-12 and gave his Presidental Address *Endocrine-Active Substances in the Environment.* Moreover, he has agreed to provide a summary of the address for a future issue of *Chemistry in New Zealand.* He reviewed the current status of research and regulation for endocrine active substances (EASs) and described a wide range of natural and synthetic compounds that have the potential to exert adverse effects on higher organisms through interactions with the endocrine system. This can occur by interfering with signalling pathways and control systems at a genetic transcription level. The wide range of EASs include organochlorine compounds such as the polychloro- and polybromo-biphenyls, dioxins and dioxin-like substances, ethers, phenolic-*xeno*-estrogens, phthalates, organotin compounds, steroidal hormones, and phytoestrogens. The effects on wildlife from exposure to EASs have been well documented but effects on man are controversial. Some recent advances in analytical methods for some of the key classes of EASs were described and included determinations based upon GC-MS, LC-MS, ELISA and bioassays. The growing importance of receptor-based *in vitro* bioassays was also highlighted.

October 9 saw the Branch's AGM and Chairman's address. The AGM re-elected **Emeritus Professor Neil Curtis** as Branch Chairperson for his second year, but currently the Branch has no Secretary. Our long serving (and suffering) Treasurer Alan Turner retains his role.

The 2003 Wellington Branch Committee is:
Chairman: **Neil Curtis**
Secretary: **Vacant**
Treasurer: **Alan Turner**
Committee: Suzanne Boniface and Elizabeth Douch (half-time each), Kirsten Edgar and John Ryan (half-time each), Vince Gray, Brian Halton, Ted Harvey, Peter Northcote, Helen Palmer plus one to be nominated by Graeme Gainsford as his replacement.

The touring Royal Society of Chemistry lecturer, **Professor Bill Kitching**, visited Wellington in late October and his address *Insect Chemistry and Chirality* attracted a small but dedicated audience of 21. From the 1959 structure determination of bombykol – an achiral C_{16} *Z,E*-diene – that required the sacrifice of half a million female moths to provide adequate material for compound characterization, Bill took us through the fascinating world of insect pheromones of species detrimental to the life blood Queensland's economy. He showed how modern synthetic chemistry and forefront chromatographic and instrumental analysis has been used to identify chiral insect *semio*-chemicals in the fruit-spotting bug (*Amblypelta nitida*) –chiral ocimenes – and the Scarab beetle. The occurrence of bicyclic lactones with defined side chain geometry, and the more recent determination of spiroacetal linkages (in fruit fly) and their likely biosynthetic pathway (from studies with up to a dozen flies only) completed a fascinating discourse.

Cawthron Institute

Doug Mountfort returned after four months in Europe, mainly at the University of Cambridge. He completed his tour with visits to IGV Institute, Potsdam and APO Lbs, Wageningen to look at facilities for large-scale culturing of microalga for secondary metabolite production. **Gretchen Skea,** a PhD student from University of Auckland, is working with Doug on the enzymology of the digestive processes in fish herivores - important for polysaccharide degradation. **Paul McNabb** and **Veronica Beuzenberg** attended the 10th International Conference on Hazardous Algal Blooms, in Tampa, Florida (October) and presented recent research on LC-MS of marine biotoxins and production of key toxins by culturing and extraction of alga.

Patrick Holland (2002 NZIC President) attended the AOAC International annual meeting in Los Angeles in September and presented a paper on validation and use of LC-MS methods for regulatory testing of shellfish. Pat has also completed his presidential tour of the North Island NZIC Branches that included the Rotorua sub-branch; he was pleased to find us all in good heart.

Industrial Research Ltd

After a long and distinguished career in DSIR Chemistry Division and latterly IRL, **Neil Milestone** is leaving in December to take up an Associate Professorship at the Immobilisation Laboratory of the Engineering Materials Department at University of Sheffield, England on February 1, 2003. He will finish on-site at IRL at the end of November 2002, but will continue with project links for some time. His role at Sheffield, a five-star UK University, is to develop a group to investigate the use of cementing materials to help in the clean up of wastes. It will be primarily a research role looking after postgraduate students but will also allow Neil to indulge his secret desire to do "a little teaching".

Neil Milestone

Neil joined Chemistry Division as a bursar in 1964 whilst completing undergraduate studies at VUW (BSc 1968). The DSIR bursary paid the princely sum of £150 per year and required the bursars to work at Gracefield during the summer vacation. Along with that privilege came compulsory membership of government superannuation and arrears in the year's contributions took care of the first two weeks pay! He completed his MSc (Hons) in 1969, majoring in coordination chemistry under **Professor N.F. Curtis**. In 1973, he graduated DPhil in soil chemistry from the University of Waikato, studying under **Professor A .T. Wilson**.

Neil returned full-time to DSIR Chemistry in 1973, working as a scientist in the Cement and Concrete Section, investigating effects of additives on cement hydration—the first concrete trucks carried a bag of sugar in the cab to stop the concrete hardening if they got caught in a traffic jam! One company was very upset when, after it requested a way of removing a load of hardened concrete from the bowl of a truck which had gone over a bank, it was suggested its use as a boat anchor was appropriate. A year's postdoc at the University of Illinois in 1976 studying cement hydration helped Neil become one of the leading researchers in this field. Standards Association (NZ) requested he be a member of the committees on cements, admixtures, and pozzolans. He is currently revising the guidelines for alleviating Alkali Aggregate Reaction, the reaction between volcanic aggregates and cement, for the New Zealand concrete industry.

In 1987, Neil became Section Leader of the Inorganic Materials team conducting research on cement and catalysis. This section was expanded in 1991 with incorporation of scientists in the paint and petroleum field. On the formation of IRL in 1992, Neil was appointed to run the Team which, eventually through Team mergers, became Applied Inorganic Chemistry; this was amalgamated at the end of last year into the Materials Technology Group.

Neil has played a vital and pivotal role in developing suitable cementing systems for exploitation of New Zealand's geothermal fields. During 1984-89 and again in 1994-96, he led a team examining a new hydrothermal cementing system needed to develop the Ohaaki geothermal field. Overseas formulations typically lasted around 6 months in the aggressive environment at Ohaaki and Rotokawa. Segmented trays held test samples recovered from the wells, or rather the holes where some of the US-sourced test samples should have been if they had survived! Neil describes the only "pure white Maori" he has ever seen when one of the wells blew out wrapping the samples around the top of the derrick. This work also included study at Brookhaven National Laboratory (USA) in 1985-86 on a prestige DSIR fellowship. Currently, he is working with CHH and FR in examining some of the requirements for cellulose fibres in autoclaved cement products.

Neil became a key member of the team investigating options based around zeolite catalytic transformations of methanol to gasoline. He visited Mobil in 1980, the first technical person they had encountered from New Zealand, as they tried to sell their new MTG process. His visit prompted a redesign of the Motonui plant after he pointed out there was CO_2 in our natural gas; this removed the need to acquire extra gas to make CO_2 for the correct C/H ratio needed for methanol synthesis. Neil's zeolite research extended to include aluminophosphates and their properties (the submitted patent on metal substitution missing by 4 months) as well as industrial uses of zeolites. He led the team that showed that Methanex could save considerable money by using catalyst manufacturers other than Mobil (IRL's biggest contract in the first 2 years of its existence).

Neil's contacts with industry have meant he has handled a number of unusual projects outside these areas. These include sorting out why calcium hypochlorite can go bang or catch fire (the bin for residues carried the scorch marks for months!), synthesis of silicate fibres in Malaysia (working temperatures of around 35 °C and 98% humidity), and the logistics and economics of the use of tallow (difficult to convince industry that it's not sensible to use a product now being sold for ~$500/tonne for conversion to products such as detergents or bio-diesel at around $200-300 tonne).

Neil has supported the NZIC at local and national levels throughout his career. He joined as a student member and won the 1972 student prize! He has held every position on the Branch Committee – Chairman 1985 and Interview Panel 1979-1990 are but two for which we have dates – most of the others were in the 1979-1985 period (as an aside, this Editor recalls Neil's careful persuasion that led to his nomination to Vice-Presidency in 1985). He assisted with conference organisation whenever the NZIC conference was hosted by the Branch, *e.g.* the last NZIC and IC'99 in 1999. He has been recognised with many awards: the NZIC Industrial Chemistry Prize twice - in 1991 for zeolite research and then again in 1994 for cement chemistry, and in 1996, the New Zealand Royal Society Science and Technology Award for his work in silicate and catalysis science. For his research into silicates he was awarded a DSc by Victoria University in 2000. Appointed an IRL Distinguished Scientist in 1999, Neil has been a Councillor and Chairperson of the Royal Society Executive Committee playing a significant wider role in New Zealand science. The Wellington Branch is particularly sorry to see Neil depart for it is from members of his stature – with NZIC blood circulating in his veins – that others have been encouraged to follow his example with support. We wish him well in his new venture and will welcome his return at any time.

Victoria University

Dr Carol Taylor (Palmerston North Campus - Massey University) visited the School on October 4 to meet with staff and deliver her lecture "Hydroxyproline: Molecular Hinge and Fine-Tuning Device". The work forms the basis of Carol's NZICV/RSC Easterfield Medal Award. The formal Easterfield Lecture will be delivered at the 2003 NZIC Conference in Nelson. On November 8, **Professor Mordecai Rabinovitz** of the Hebrew University of Jerusalem, a long-time friend and colleague of Professor Halton lectured on *Polycyclic Anion Chemistry*.

* * * * *

George W Emerson

A tribute on behalf of his academic colleagues, former students and friends

George Emerson graduated in chemistry from the University of Otago in the late 1950s and was the holder of a prestigious Sir George Grey Scholarship. He switched his attention to biochemistry working on the biochemistry of tuberculosis, started a PhD, and soon became a lecturer in the Department. This began a long era of dedicated service, commitment, and extreme loyalty to the Biochemistry Department at Otago that was to last through four decades. He also gave great service to the New Zealand Institute of Chemistry in the roles of Otago Branch Treasurer, Chairman, and Council Delegate, and also to the New Zealand Biochemical Society. George was a Fellow of the Institute of Chemistry.

George was renowned for being a rigorous and effective academic, and for those things he was passionate about; he exhibited integrity, a depth of knowledge and a sense of purpose that was admired by all. George regularly assumed the conscience of the Department of Biochemistry at Otago, particularly in times of rapid change, because he had a unique sense of the value of the past. It was natural and appropriate that he stepped forward to take charge of the organisation for the Department of Biochemistry's 50th year celebrations in 1999. With typical meticulous care he attempted to contact every former graduate to ensure they had an opportunity to be part of the celebrations. His latest project, alas unfinished, was a written history of the Department through these 50 years, but, under the guiding hand of Merv Smith—a long time colleague—this work will be finished and it will be dedicated to George.

I was personally made aware of George's high standards and discipline soon after I arrived at the University of Otago as a new postgraduate student in the late 1960s. I had been assigned as George's demonstrator for a student undergraduate laboratory that was to start at 2 pm. The doors closed on the strike of two, and those students who had dallied at the Medical cafeteria and were still straggling upstairs missed out that day. Needless to say, the next week *everybody* was there on time, including this newly arrived postgraduate student demonstrator from Wellington.

George's great love in biochemistry was for metabolism and he held strong—one could say almost fierce—views on how it should be taught. Contrast this though with his willingness to spend hours with the most hapless student exhibiting great patience and sensitivity until he could get the student up to speed. As a former (and not hapless) student now in Dallas, Texas, said, "George truly was a great teacher, the guy taught me a lot. I often find myself repeating his words of wisdom ...". George was also a very practical and skilled experimenter, and he loved being around fermentors and culture equipment. Many times over the years he would be seen bedecked in lab coat helping a poor soul who was bamboozled by the many parts.

George had an excellent sense of humour but it required engagement and understanding. For those without prior warning it could be daunting. George could be gently mocking or quite provocative, but he expected a response and was happy when he got it. He particularly went for the 'trendies' and I personally experienced a few choice and acerbic comments when I arrived in the Department with a beard. I smiled to myself when returning to an academic position in 1975 to meet George resplendent with beard; the accompanying photograph of George is a beautiful example of this. George survived the arrival of molecular biology in the mid-to-late 1960s, albeit with a barrage of scornful comments. With a twinkle in his eye, he frequently gave his opinion that DNA was merely a figment of the imagination (a bit daunting for the new arrival from Wellington who had come to work on DNA).

Perhaps George did not get the academic recognition he deserved for his skill, service and dedication, but George moved to the beat of his own drum. He balanced his academic life with a service to the community and to Dunedin, and to issues that he was passionate about in a way that was quite different from that of his colleagues. Particularly noteworthy have been his role in preserving rail heritage, among which was the saving of part of the Central Otago Railway Line and the establishment of the Taieri Gorge Railway as a major tourist venture. For these activities he received a QSM and a certificate of appreciation from Dunedin City. George's deep and unparalleled sense of the value of the past is illustrated with his captivation for preserving the heritage of Dunedin city gasworks - he was chairman of the Dunedin Gasworks Museum Trust, with an aim of bringing into being a working gasworks museum.

When George decided to take early retirement in 1997, while retaining a connection to the Department, we were sad at Otago to lose such a valued and valuable colleague. At the same time we were happy that he was going to assist his son Richard at the now famous, Emerson's brewery, to pursue one of his passions. Brewing in fact was one of the threads that had gone through George's career - he took under his wing several students that were seen as more practically oriented, foreseeing the era of biotechnology, and schooled them in the applied aspects of metabolism. Several of these are now industry leaders in the brewing and wine industries. In the mid 1980s George had a study leave at the University of Heriot Watt in Edinburgh in the Department of Brewing and Biological Sciences - but he was anxious to communicate that he still was pursuing rigorous biochemistry. He wrote in his leave report "... The title Brewing and Biological Science reflects the history of the Department and is now somewhat misleading. . . "! A true personality, the very best of another era, George will be missed by his many friends and colleagues.

Warren Tate, 17 September, 2002.

CONFERENCES & SEMINARS

6-10 January 2003
10th International Symposium On Deep Seismic Profiling Of The Continents And Their Margins
Taupo, New Zealand
http://www.gns.cri.nz/news/conferences/seismix2003

3-5 February 2003
Royal Society Communications Training Workshop
The Mass Communication and Journalism Department
University of Canterbury , Christchurch
Contact: Catherine.ibell@rsnz.org

2-7 February 2003
ICPP 8th International Congress Of Plant Pathology
Christchurch Convention Centre, Christchurch, New Zealand
Contact: John Fletcher
New Zealand Institute for Crop & Food Research
Private Bag 4704, Christchurch, New Zealand
FletcherJ@crop.cri.nz
www.lincoln.ac.nz/icpp2003/

4-7 February 2003
Australasian Quaternary Association (AQUA) Biennial Conference in Association with the New Zealand Friends Of The Pleistocene
www.geo.vuw.ac.nz/conferences/aqua03/index.html

9-14 February 2003
AMN-1: Advanced Materials And Nanotechnology Conference
Te Papa Tongarewa, Museum of New Zealand, Wellington
www.macdiarmid.ac.nz

15-16 February 2003
Canterbury Sustainability Expo
Christchurch
www.gosolar.co.nz

17-19 February 2003
Royal Society Communications Training Workshop
Te Manawa, Palmerston North
Catherine.ibell@rsnz.org

24-26 March 2003
Fifth International Conference on Electromagnetic Wave Interaction With Water And Moist Substances
Organised by the International Society for ElectroMagnetic Aquametry (ISEMA)
Novotel Hotel, Rotorua
k.thakur@irl.cri.nz

24-28 March 2003
7th International Conference On Southern Hemisphere Meterology And Oceanography
Wellington
New Zealand
Meterological and Marine Sciences Societies

6-11 July 2003
"Windows On A Changing World" - 22nd Conference Of The New Zealand Geographical Society
The University of Auckland, Auckland
Contact: J Logie
The University of Auckland
nzgs2003@sges.auckland.ac.nz
www.geog.auckland.ac.nz/nzgs2003/

7-11 July 2003
Fifth International Conference On Industrial And Applied Mathematics
Sydney, New South Wales, Australia
http://www.iciam.org

9-11 July 2003
The New Zealand Insitute Of Physics Conference and Physikos 2003
Massey University, Palmerston North

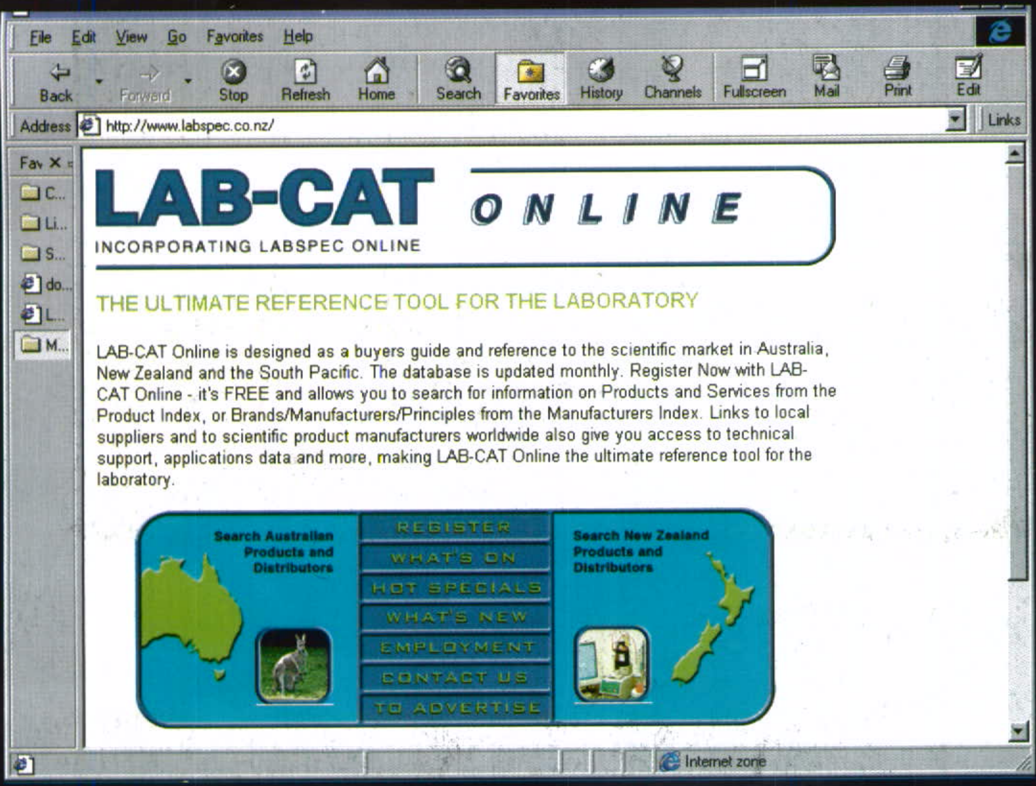
17 - 22 August 2003
21st IIR International Congress Of Refrigeration
Washington DC, USA
Contact: joanna@airah.org.au
www.airah.org.au

1-5 September 2003
The 18th International Radiocarbon Conference
Te Papa, Museum of New Zealand, Wellington
Details, registration and abstract submission forms at
www.14Conference2003.co.nz

20-23 October 2003
Tenth Asian Chemical Congress (10 ACC 2003) Joint Conference with Eighth Eurasia Conference On Chemical Sciences (EuAsC$_2$S-8)
Hanoi, Vietnam
Contact: Professor Dr Huynh Van Trung
Chemical Society of Vietnam
2, Pham Ngu Lao Str., Hanoi, Vietnam
Tel/Fax: +84-4-8267498
Email: csv@netnam.vn

30 November-4 December
2003 New Zealand Institute Of Chemistry Conference
Rutherford Hotel, Nelson, New Zealand
Contact: Dr Andrew Abell
Department of Chemistry
University of Canterbury
Private Bag 4800 Christchurch
a.abell@chem.canterbury.ac.nz

1-5 December 2003
3rd International Wildlife Management Conference
Christchurch, New Zealand
www.conference.canterbury.nz/wildlife2003



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