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Chemistry IN NEW ZEALAND

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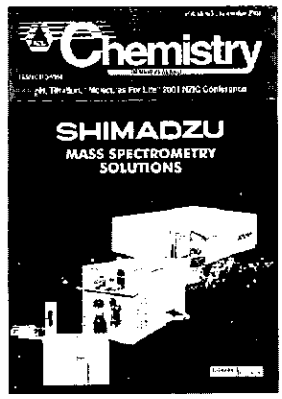


Coming Up ...

March 2002 Balances, Weighing, Filtration, Microscopy, NIR

Deadline for material *1st of the month of publication*

Guest Editorial: Performance-Based Research Funding

Professor Leon Phillips, President NZIC 2001

Recently the Vice-Chancellor's Committee made a submission to TEAC, the Tertiary Education Advisory Commission, on the subject of this editorial, and it appears that the submission was favourably received and will be acted upon. The submission was based on a discussion paper written by Michael Peters, a paper that is mild, sensible and even tentative in its recommendations. Nevertheless, senior administrators of several universities, including Canterbury, are on record as being against it. So what is performance-based research funding and why do I believe it is a good thing?

Performance-based research funding is an extension of the not entirely palatable idea that the research component of the money which universities receive from Vote Education should be separated from the teaching component. Once this idea is accepted, and the usual emotional claims that research and teaching in a university are inseparable are disregarded, it becomes obvious that some means has to be found for deciding what proportion of the research component should go to any given institution. This is a logical and inevitable consequence of our misbegotten EFTS-based system of university funding and it goes a little way towards correcting a few deficiencies of the EFTS system.

Universities are required by their charters to undertake research as one of their two core activities, the other being teaching. The EFTS system does not fund research as such, that being left to FRST, which has no interest in basic research, and to the hopelessly over-subscribed Marsden Fund, which in recent years has degenerated into a lottery. Indeed, the present EFTS system actively penalises universities for doing research. It does this by under-funding graduate students in the experimental sciences, so that the training of such students must be run at a loss, by not recognising the existence of research done by university staff, and by not considering the costs of libraries, laboratories, technical staff or research equipment. Any change in the funding system which provides a positive financial input in response to a healthy research output has to be a good thing, but that is not all.

According to our elected representatives, New Zealand is supposed to be committed to progress based on High-Tec industry, and High-Tec industry (not to be confused with information technology) feeds on the results of scientific research, much of which is done in universities. It also depends on a steady flow of highly qualified graduates, but that is another story. As far as research is concerned, there is no point in investing a lot of time and money in doing 'me too' science, or on dotting i's and crossing t's in somebody else's opus. To get real benefit from an investment in research you have to be working right at the cutting edge, so that you have an expert and up-to-date work force, prompt access to new results and a good idea of what will be possible in the not too distant future. However, cutting-edge work tends to be very expensive because of the way advances in science go hand in hand with advances in instrumentation and technology, and because brand-new technology is always expensive. New Zealand, with a population equal to that of one medium-sized city in the US or Europe, cannot afford to maintain a cutting edge in every field at eight universities plus several polytechnics with research aspirations, so some discrimination has to be exercised. Performance-based research funding is a means of exercising discrimination, and it is probably the only means available as an add-on to the EFTS system.

I don't often have occasion to say kind things about the Vice-Chancellor's Committee, but here I think they are definitely on the right track.

STOP PRESS

Margaret Brimble Professor of Organic Chemistry, and **Graham Bowmaker**, Professor in Chemistry (both) of the University of Auckland have been elected **Fellows of the Royal Society of New Zealand.**

Nobel laureates **Professors Robert Curl** and **Alan MacDiarmid** have been elected **Honorary Fellows**.

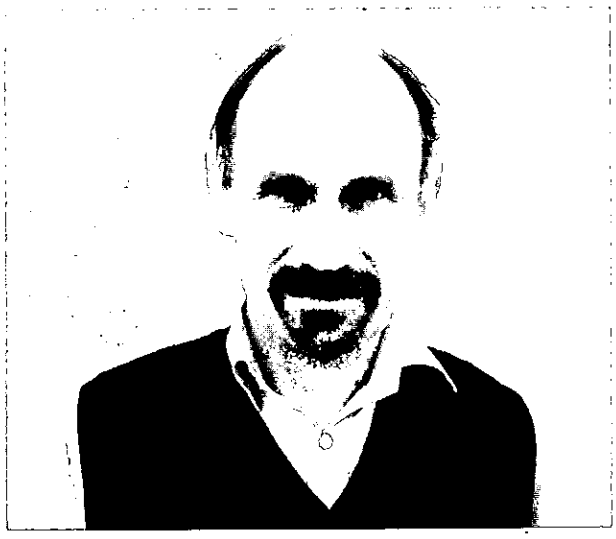
The **2001 Hector Medal** (Chemical Sciences) has been awarded Professor Peter Schwerdtfeger, Department of Chemistry, University of Auckland.

The Royal Society of New Zealand has also announced that the **2001 Rutherford Medal** has been awarded to **Professor Peter Gluckman FRS.**

NZIC NEWS

NZIC Council

2002 NZIC President



Dr Patrick Holland from Cawthron Institute, Nelson takes over from **Professor Leon Phillips** as President of the NZIC for 2002. Pat is a graduate of the University of Canterbury, with Leon one of his excellent tutors (his year included some of our leading 'mature' professionals such as **Brodie, Gainsford, Lane**). He obtained his PhD in radiation chemistry at Queens University, Ontario, Canada in 1970 and then did postdoctoral work with **Dr Al Burlingame** at the Space Science Lab, Berkeley. There he developed his interests in mass spectrometry as a technique for analysis and structural elucidation of organic compounds. This included some analysis of lunar samples brought back by Apollo 12.

Returning to New Zealand, he worked at **Ruakura Research Centre** in Hamilton, moving through the ranks of the research teams of Department of Agriculture, MAF Technology and then into HortResearch. The research had an emphasis on organic-microanalysis applied to toxins in feeds and foods, pesticide residues in soil and crops, and environmental contaminants. He established the mass spectrometry facility at Ruakura and saw it through three generations of instruments that involved a wide range of collaborative research. Some highlights were: helping to set the kiwifruit industry on a sound basis with respect to use of pesticides, uncovering the causal agent of the curious livestock ailments caused by consumption of *Panicum* grass species (transformation of steroidal sapogenins to insoluble bile crystals), and the tracking of persistent environmental contaminants (OCs, PCBs, PAHs) in soils, sediments and estuarine biota. The HortResearch years from 1992 saw the establishment of the Food & Biological Chemistry Laboratory as an accredited commercial operation. This led to a growing interest in laboratory quality assurance.

Throughout the 90s Pat was active in IUPAC, serving as secretary to the Commission on Agrochemicals and more recently to the Division of Chemistry and the Environment. He has found this to be rewarding in the extension of applied research in international forums and the development of long-standing friendships and collaborations.

In March this year Pat moved to Nelson, taking up a Senior Scientist position with **Cawthron Institute**. The key responsibility is to develop and validate to international standards, methods for analysis of marine biotoxins in shellfish using instrumental methods. Ground-breaking work on new LC-MS/MS methods is establishing Cawthron as a leader in international efforts to move quality assurance for shellfish away from use of animal bioassays.

Pat will be attending the NZIC Conference in Napier and will be pleased to meet with members to discuss NZIC matters. He is particularly interested for ideas on the future of the NZIC and cites new services to members as but one example. The in-coming President can be contacted by e-mail at: patrickh@cawthron.org.nz

NZIC Council Report

The Council of NZIC met on Monday, 1 October 2001 at the University of Canterbury.

The following **new members** were welcomed to the NZIC:

Auckland
Dr B Copp, The University of Auckland
Mr S Kennedy, The University of Auckland
Dr K Taylor

Canterbury
Mr N Alexander
Y Feng, University of Canterbury
M Gower
Dr R Hartshorn, University of Canterbury
Dr M Humphries
W Jiao
Dr J Morris, University of Canterbury
Mr R Payne
Mr C Sumby
Mrs A Winter

Manawatu
Mr G Ainge, HortResearch
Mr W Barker
Mr B Fong, New Zealand Dairy Research Institute
R Hardre, Massey University

Otago
A Dixion, University Of Otago
J Hausmann
Mr M Klingee
P Walsh

Waikato
Mr D Deng
Mr M Dines, AgResearch Ltd
Mr D Foster
L Kodikara
Mr B Lee, Forest Research
M Patel
J Sprosen, AgResearch Ltd
Mr R Stratford

Wellington
Ms S Barrs, Victoria University
Mr P Benjes, Industrial Research Ltd
Mr T Davidson, Industrial Research Ltd
Dr C Dickson, Industrial Research Ltd
Mr G Evans, Industrial Research Ltd
J Hart, Industrial Research Ltd
Dr J Hoberg, Victoria University
Mr S Holden
Mr A Jarvis, Industrial Research Ltd
Mr M Kennedy, Industrial Research Ltd
Dr P Northcote, Victoria University
Mr G Painter, Industrial Research Ltd
Mr M Waterland, Industrial Research Ltd
Dr A D Woolhouse, Industrial Research Ltd

The **resignations** of the following members were also received:
Dr J T France, Auckland
Dr C A Bebelman, Auckland
B P Rijkmans, Auckland
Dr D Olgivie, Auckland
Mr D Sidwell, Auckland
Ms C Yateman, Manawatu
Professor S Rumball, Manawatu
Dr G J Shaw, Manawatu
Mrs L Metcalfe, Canterbury
Dr C W Thomson, Otago
Professor P K Grant, Otago
Dr J Herbert, Overseas
Dr W S Hancock, Overseas

Council discussed a number of membership issues and a sub-committee comprising P Holland, A Brodie, and J Spencer was set up to investigate the issues raised and report back to the next Council meeting.

Four **new Fellows** were welcomed to the NZIC (see below for details). They are:
Mr Robert Siebers, Wellington School of Medicine
Associate Professor Bill Henderson, University of Waikato
Dr Richard Haverkamp, Massey University
Associate Professor G Jameson, Massey University

New Zealand Chemistry Olympiad Trust
Council has supported the formation of the New Zealand Chemistry Olympiad Trust. The Trustees are to be; Colin Freeman, Robert Maclagan, Jan Giffney, Sheila Woodgate

IUPAC
Pat Holland spoke to the report of the IUPAC General Assembly (see elsewhere in this issue of *Chemistry in New Zealand*). He and K Powell will co-opt one other person to investigate the formation of a sub-committee to represent New Zealand's interests with the International Union of Pure and Applied Chemistry.

Financial Report for Year Ended 31 December 2000
The audited finacial report for the period 1 January 2000 to 31 December 2000 appears on pages 7-9.

Copies of the minutes of the NZIC Council meeting are freely available from your Branch delegate or on the NZIC web page: www.nzic.org.nz

NEW FELLOWS ELECTED

At the October Council meeting **Dr Richard Haverkamp** and **Associate Professors Bill Henderson** and **Geoff Jameson**, and **Mr Robert Sievers** were elected to the Fellowship of the New Zealand Institute of Chemistry. We congratulate them on their achievements and thank them for their contributions to the profession in New Zealand.

Richard Haverkamp – Manawatu Branch

Richard Haverkamp is Senior Lecturer in the Institute of Technology and Engineering at Massey University with responsibility for the BTech Chemical Technology programme. After obtaining a BSc (Hons) degree from Victoria University in 1982, he worked for a year as Plant Chemist at Colgate-Palmolive Ltd before travelling through Asia for a year. On his return to New Zealand he took up a job with Fletcher Challenge Ltd in Wellington leading to the position of Research/Process Coordinator. Then in 1990 he moved to the DSIR as a Review Secretary for six months before changing to the University of Auckland for PhD studies in chemistry, which he completed in 1992. After two and a half years as a postdoctoral fellow at the University of Toronto, Canada, he returned to Auckland in 1995 to the position of lecturer in the Department of Chemical and Materials Engineering and Technical Director in the Research Centre for Surface and Materials Science. He took up his present position at Massey University in 1998.

Dr Haverkamp has been on the Manawatu Branch committee of the NZIC for two years and is the current Branch Chairman. He is also a member of the Institute of Professional Engineers of New Zealand and serves on the local branch committee of IPENZ and the IPENZ Board. In 2000 he won a Future Director's Award and was also selected as the best teacher of undergraduate papers in his Institute.

His present research interests cover the areas of process sensors, process improvement, surface chemical and electrochemical reactions, and he has published over 40 internationally refereed papers plus a patent and around 100 technical reports. The main techniques he uses in his research are atomic force/scanning tunnelling microscopy, X-ray photoelectron microscopy, electrochemistry and high temperature reactors. Dr Haverkamp is frequently invited

as a consultant and to meetings overseas in countries such as Norway, France, Sweden and Switzerland. Companies extensively consult him and his comments, on topics ranging from "cattle gut racket strings" to "better roads" are often seen in the media.

Bill Henderson – Waikato Branch

Bill Henderson grew up in County Durham in the North East of England. He did his BSc (Hons.) degree in chemistry and geochemistry at Leicester University (in the English Midlands), and stayed there to complete a PhD in organometallic chemistry. He spent two years as a NSF postdoctoral fellow with Du Shriver at Northwestern University in Evanston, Illinois, USA, and this included a period on secondment at Hokkaido University in Japan. This period of research centred on the synthesis of bimetallic metal carbonyl clusters, and their applications as catalyst precursors. Several years in UK industry then followed, working for Albright & Wilson Ltd (now Rhodia) in the West Midlands. His work there concerned applications of organophosphorus compounds, surfactants, and process development. Bill's heart really lay with the academic life however, and in 1992 he accepted a position at the University of Waikato. He has been here ever since and is currently Associate Professor in the Department of Chemistry, with a joint appointment in the Cooperative Education Unit, where he maintains his industry links by finding work placements for BSc (Technology) students. Bill has just been appointed Departmental Chairperson, taking over in the New Year when Brian Nicholson completes his sentence!

Bill has wide research interests that include the chemistry of the platinum group metals and gold, metallacyclic chemistry, applications of electrospray mass spectrometry in inorganic chemistry, and aspects of organophosphorus chemistry, including ferrocene-derived phosphines, and the use of phosphines to immobilise enzymes. He has co-authored over 120 research publications and 2 textbooks. He has also contributed significantly to the Waikato Branch of the NZIC, having been Treasurer for a number of years and two years as Branch President.

Geoff Jameson – Manawatu Branch

Geoff Jameson is Associate Professor in Chemistry in the Institute of Fundamental Sciences and Director of the Centre for Structural Biology at Massey University. He has BSc (Hons) and PhD degrees from the University of Canterbury in the area of small molecule structural chemistry. In 1977 he went to Northwestern University as a postdoctoral fellow and then in 1979 to the University of Zürich. He accepted a position as Assistant Professor at Georgetown University, Washington DC, in 1982, was tenured and promoted to Associate Professor in 1987, and remained there until 1993. He returned to New Zealand and Massey University in 1994 to enable him to develop further his research interests in structural biology.

Geoff Jameson is at present on the Manawatu Branch Committee of the NZIC and is also on the Council of the Society of Crystallographers of Australia. He has been on the International Programme Committee for the 1995 and 1996 Asian Crystallographic Association Conferences and served as a Co-editor of *Acta Crystallographica*, Section C. 1999-2000.

Geoff Jameson has an international reputation in X-ray crystallography and has a broad knowledge of chemical concepts of systems ranging from small molecules to proteins to origin of life studies. His work covers the areas of protein structure and function, milk proteins, proteins of fungal secondary metabolism, biological defences against reactive oxygen species, bioinorganic chemistry, crystal twinning and ultra-high resolution protein structures (manganese superoxide dismutase at 0.9 Å resolution). Recent research includes cloning and expression of genes from a fungal gene cluster, and design, synthesis and high-level expression of a synthetic gene of a milk protein, for protein structure determination by X-ray and NMR methods. He has published around 100 papers in the international literature and often gets asked to sort out structural problems that others have been unable to solve.

Robert Siebers - Wellington Branch

Robert Siebers initially trained as a medical laboratory scientist in both the Netherlands and New Zealand, specialising in haematology, transfusion science, and clinical biochemistry. After senior positions as a medical laboratory scientist in Lower Hutt, Hawera, Hastings and Wellington Hospital laboratories, he took time off as a house-husband looking after his two children, Amanda and Andre, while his wife, Irene, established her medical career. In 1983 he commenced his research career at the Wellington School of Medicine and Health Sciences, primarily in the areas of hypertension and clinical pharmacology research. Since 1995 he has been working in the Wellington Asthma Research Group as Senior Technical Officer and Laboratory Manager, where his main research focus is on house dust mite and other indoor allergens, and asthma and allergy.

He is a Chartered Biologist and Member of the Institute of Biology (London), a Member of the Royal Society of New Zealand, and is a Fellow of the New Zealand Institute of Medical Laboratory Science. Since 1994 he has been Editor-in-Chief of the peer-reviewed biomedical publication, the *New Zealand Journal of Medical Laboratory Science*, and is on the Editorial Board of the *Australian Journal of Medical Science*. He is active in the professional affairs of medical laboratory science, being a Member of their Fellowship Committee, and is on the Board of Studies of the BMLSc degree course at the University of Otago. He is also a member of the Thoracic Society of Australia and New Zealand, and of the Australasian Society of Clinical Immunology and Allergy.

He has authored or co-authored 93 publications in peer-reviewed journals, including several in the *Lancet* and the *British Medical Journal*, as well as in leading allergy journals. Over the years he has successfully obtained research grants from many research bodies, including the Health Research Council, the Lotteries Board, the Asthma and Respiratory Foundation, the Wellington Medical Research Foundation, and the Child Health Foundation.

In his spare time he enjoys the three G's, golf, gardening, and gourmet cooking—and takes a pseudo-scientific interest in the noble grape and its products.

NZIC Branch News

AUCKLAND

NZIC President Leon Phillips visited the branch on October 3 to give his Presidential Address entitled 'Venus, not just a pretty face". The presentation was well attended, and stimulated much discussion. Special thanks go to Professor Graham Bowmaker for looking after Leon during his time in Auckland.

The Department of Chemistry's new NMR facility was officially opened on Thursday 4th October with a small reception and officiated by **Professor Douglas Russell** and **Professor Graham Bowmaker**. The newly acquired Bruker 300 MHz NMR spectrometer is capable of liquid and solid sample analysis.

The University of Auckland will be offering New Zealand's first Medicinal Chemistry degree in 2002. The initial four year BSc (Honours) course aims to produce graduates equipped with the multidisciplinary knowledge and skills for the rapidly expanding pharmaceutical and biotechnology industries. The primary objective of medicinal chemistry is the design and discovery of new drugs. Apart from the obvious chemistry-based organic synthesis, successful drug design also depends on fundamental research into the biological and chemical nature of disease, as well as the development of testing methods and procedures for evaluating new drugs against the target disease. To cover all of these aspects, the new course includes core papers in biology, biochemistry, pharmacology, and physiology, as well as chemistry. Elective courses in computer science, statistics and physics are available. The course is an across-Faculty degree programme overseen by a Board of Studies chaired by **Professor Margaret Brimble**. Continuing the medicinal chemistry theme, The University of Auckland, Chemistry Department has set up a commercial laboratory working for Neuronz Ltd making peptidomimetics. The staff employed are: **Professor Margaret Brimble**, senior scientists **Drs David Callis** (a PhD graduate from Sussex), **Paul Harris** (an Auckland PhD graduate), **Nick Trotter** (an Otago PhD graduate), and research technician **Anoma Ratnayake** (a graduate from Sri Lanka). Meanwhile at New Zealand's largest medicinal chemistry laboratory, the Auckland Cancer Society Research Centre (ACSRC) at the Auckland Medical School, there have been a number of recent staff changes in the Chemistry Section. Recent arrivals have been **Drs Florence McCarthy** (University of Sunderland, UK), **Hamish Sutherland** (an Auckland graduate with post-doctoral experience at the University of Waterloo, Ontario, Canada), **Leesa Swan** (Griffith University, Brisbane), and **Claudette Weir** (Auckland graduate with post-doctoral experience at the University of Alberta, Edmonton, Canada). In addition, two further appointees will be arriving later this year to replace **Drs Jared Milbank** and **Lorna Mitchell**, who have recently departed to take up permanent positions with Pfizer Global Research in Ann Arbor, Michigan, USA. The new arrivals will bring the total number of organic or medicinal chemistry PhD graduates in the ACSRC to twenty.

CANTERBURY

Dr Bryce Williamson is to be the new Head of the Chemistry Department at the University of Canterbury from 1 December 2001 in succession to **Professor John Blunt**.

Drs Greg Russell, Peter Steel and **Richard Hartshorn** are, or shortly will be, on study leave. **Dr Alison Downard** has just returned from study leave.

Professors Ward Robinson and **Kip Powell,** and **Drs. Alan Happer** and **Rod Claridge** have all transferred to half-time appointments in the Department of Chemistry at the University.

Professor Leon Phillips has completed what he describes as a highly agreeable tour of the branches for the purpose of giving an NZIC Presidential Address. Canterbury and Waikato heard 'What is going on at the surface of a liquid?' while the other Branches heard about 'Venus, not just a pretty face'. This latter presentation featured spectacular pictures of the surface of Venus obtained from the Magellan orbiter radar imaging and altimetry, with colouring based on pictures sent back by the Soviet Venera 12 and Venera 13 landers. PhD student, **Glenn Rowland**, whose project formed the basis for the latter part of this lecture, will graduate in December.

Markhams mri Auckland

Chartered Accountants & Business Advisors

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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 2000. 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 2000 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 Council 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 2000 and the result of its operation for the year ended on that date.

Our audit was completed on 20 October 2001 and our unqualified opinion is expressed as at the date.

Markhams MRI Auckland

Markhams MRI Auckland
Chartered Accountants

NEW ZEALAND INSTITUTE OF CHEMISTRY (INC.)

STATEMENT OF FINANCIAL PERFORMANCE
FOR THE YEAR ENDED 31 DECEMBER 2000

			1999
Revenue			
Chem NZ - RSC Subs		15,000	14,000
Chem 13 Exam Fees		12,760	1,028
I. U. P. A. C.		-	320
Publication Sales		-	385
Subscriptions from Members		62,682	69,217
		90,442	84,950
Chemical Olympiad Donations	23,663		7,944
Chemical Olympiad Expenses	27,968		5,472
		(4,305)	2,472
ANC Quiz Fees	-		13,100
ANC Quiz Expenses	-		15
		-	13,085
Chemical Milestones Receipts	(6,462)		29,962
Chemical Milestones Expenses	480		29,962
		(6,942)	-
Gross Revenue from Operation		**79,195**	**100,507**
Operating Expenditure		**86,183**	**86,823**
		(6,988)	13,684
Other Income			
Interest - BNZ	1,636		974
Sundry Income	4,204		1,022
		5,840	1,996
Operating Deficit		**1,148**	**(15,680)**

NEW ZEALAND INSTITUTE OF CHEMISTRY (INC.)

STATEMENT OF FINANCIAL PERFORMANCE
FOR THE YEAR ENDED 31 DECEMBER 2000

			1999
Expenditure			
Accountancy & Audit Fees	3,058		3,323
Branch Expenses - Capitation Fees	13,665		6,315
Branch Expenses - Student Travel	3,000		3,000
Chem NZ Expenses	17,519		7,500
Chem 13 Expenses	7,646		7,980
Conference Expenses	2,215		2,267
Donation	-		563
Depreciation	12		12
Excecutive Office Expenses	16,293		18,675
General Expenses	3,659		6,269
Goods & Services Tax	(2,751)		(738)
Interest & Bank Charges	873		3,098
Projects	4,299		6,340
Overseas Visitors Expenses	-		3,208
Printing & Stationery	4,663		2,897
Prizes	-		1,550
Secretarial Services	-		275
Subscriptions	3,102		5,262
Telephone & Fax Charges	860		800
Travelling Expenses	8,160		5,750
Travelling Expenses - External	-		2,477
		86,183	86,823
Total Operating Expenditure		**86,183**	**86,823**

NEW ZEALAND INSTITUTE OF CHEMISTRY (INC.)

STATEMENT OF FINANCIAL POSITION
AS AT 31 DECEMBER 2000

				1999
Capital Funds				
Chemical Olympiad Reserve			3,923	3,923
Balance at the Beginning of the Year			51,939	36,259
Plus Net Surplus (Deficit) for Year			(1,148)	15,680
			54,714	55,862
Represented by:				
Current Assets				
Accounts Receivable		6,275		29,357
Prepaid Conference Expense		2,500		-
B.N.Z. Current Account		38,850		16,637
B.N.Z. Autocall Account		3,264		3,248
B.N.Z. Term Deposits		16,046		18,824
Chemical Processes in NZ		-		3000
			66,935	71,066
Fixed Assets				
Office Equipment	582			582
Less Accumulated Depreciation	557			545
		25		37
Presidential Chain		360		360
			385	397
			67,320	71,463
Current Liabilities				
Accounts Payable	4,074			8,860
Chemical Education Trust	8,532			6,741
		12,606		15,601
Total Liabilities			**12,606**	**15,601**
Net Assets			**54,714**	**55,862**

NOTES TO THE FINANCIAL STATEMENTS FOR THE YEAR ENDED 31 DECEMBER 2000

1 Statement of Accounting Policies

Reporting Entity

New Zealand Institute of Chemistry (Inc.) is a reporting entity registered under the Incorporated Socities 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.

The University of Canterbury Chemistry Department hosted three outstanding visiting Erskine Fellows this year. One was **Professor Arthur B Ellis** of the University of Wisconsin, whose interdisciplinary work in materials chemistry is largely focused through the University's Materials Science Centre. The Centre is an excellent model for the kind of centres of excellence that we are supposed to be trying to establish in New Zealand at the present time. Since his return to Madison, Professor Ellis has become one of the first recipients of a National Science Foundation Director's Award for Distinguished Teacher-Scholars. The awards, which were announced in the October 1 issue of *Chemical and Engineering News*, provide $US300,000 over four years to enable the recipients to continue and expand their work. The other visiting Erskine Fellows were **Professor Heinrich Lang** of the University of Chemnitz (formerly Karlmarxstadt) whose field is organometallic chemistry and chemical vapour deposition, and **Professor Robert J Donovan** of the University of Edinburgh, whose work involves laser spectroscopy, photochemistry and aerosol chemistry.

The program for **CPC2002 - the RACI/NZIC Physical Chemistry Conference**, will be finalised during the first half of November. Further details, including the preliminary programme can be found via the chemistry department website at: www.chem.canterbury.ac.nz. Registration forms will be available from the beginning of November, and a late-registration fee will come into effect from about December 14. On the basis of numbers of confirmed attendees, the cost of registration will be in the vicinity of $450 (students $250).

Professor Murray McEwan and **Dr Colin Freeman** have been awarded a three-year Marsden grant for their SIFT studies of ion-molecule reactions in relation to ultratrace analysis and interstellar chemistry. A short article about this project appears elsewhere in this issue of *Chemistry in New Zealand*.

MANAWATU

Every year the Branch runs a chemistry quiz for secondary school students. The quiz has two divisions – Junior for years 10 to 11 and Senior for years 12 and 13. It is very popular and goes out to schools nationwide. **Justin Bendall** was the quiz master for the second year running but the whole branch committee will be involved in the marking when the papers are returned.

The Branch congratulates its members **Geoff Jameson** and **Richard Haverkamp** who were elected as Fellows of the NZIC at the October Council meeting and **Carol Taylor** who has been awarded the 2001 Easterfield Medal.

There have been a number of Branch meetings recently. On 13 September Massey University postgraduate students, **Julian Adams**, **Dirk Lenz** and **Jasmine Jury**, talked enthusiastically about their research. On 11 October, Associate Professor **David Officer**, who is the director of the new Nanomaterials Research Centre, gave a fascinating lecture about the new developments occurring in the world of nanotechnology. The branch AGM was on 30 October and was addressed by the Branch Chairman, **Richard Haverkamp** on the topic "Scanning Probe Microscopy Techniques for Chemistry, Materials Science and Other Fields".

HortResearch Ltd

Dilip Ghosh has departed for 6 months to work at the Human Nutrition Research Centre on Ageing, USDA at Tuft's University, Boston learning the tissue culture assays required to validate the neutriceutical effects of anthocyanins. **Daryl Rowan** has been appointed Science Capability Leader for the newly formed Biological Chemistry Group. This new group combines chemists working in the areas of environmental, synthetic and natural products chemistry from HortResearch's sites at both Palmerston North and Ruakura. The group is also responsible for the development of new proteomics capability to extent HortResearch's efforts in plant genomics research. **Tony McGhie** attended the EuroFoodChem XI, Norwich, UK (26-28 September 2001). EuroFoodChem is a series of biennial conferences held at various locations in Europe and supported by the Federation of European Chemical Societies (FECS). Each conference has a different theme. The title of the current conference was 'Biologically-Active Phytochemicals in Food: Analysis, Metabolism, Bioavailability and Function'. This meeting addressed many of the issues the HortResearch team is currently investigating as part of our research into the health-benefits of fruit. The proceedings of the conference have been published in a Royal Society of Chemistry publication entitled 'Biologically-Active Phytochemicals in Foods' editors W Pfannhauser, G R Fenwick and S Khokhar.

Landcare Research

Dr Harry Percival attended the 6th International Conference on the Biogeochemistry of Trace Elements held at the University of Guelph, Ontario, Canada, 29 July - 2 August 2001. He presented an oral paper "Soil solution chemistry of pasture soil amended with heavy metal-spiked sewage sludge". He was also co-author of another oral paper "Biochemical activity as a function of metal concentration in soil amended with heavy metal-spiked sewage sludge", presented by **Tom Speir** (ESR).

The conference attracted just over 600 registrants from 51 countries, and the programme comprised 8 plenary lectures, 8 special symposia and 19 general sessions. The plenary lectures covered chemical modelling and speciation, risk assessment and human health, biological and chemical remediation, and trace element fingerprints for life.

The special symposia covered (1) biosorption of trace elements, (2) bioavailability of metals, (3) natural attenuation of trace element availability in soils, (4) metal speciation and availability, (5) phytoremediation, (6) phyto-, microbial, and chemical remediation tools for metal contaminated soils, (7) geochemical surface controls on trace element fate, and (8) temporal trends of trace metals in biota. The phytoremediation symposium, named the

Brooks Symposium was in honour of the late **Professor Robert Brooks**, Emeritus Professor of Geochemistry at Massey University, who died in January this year.

The general sessions covered a wide range of topics related to trace elements in a variety of ecosystems (such as agricultural, forest, and aquatic) and contaminated environments, along with the more fundamental research into bioavailability, mobility and retention of trace elements. There were 3 field tours associated with the conference, two 1-day tours ("Great Lakes Remediation", and "Biosolids") in the Guelph area, and a 4-day tour "Mine Tailings, Northern Ontario", which included a visit to Sudbury, famous for its nickel mines. Of course, no visit to southern Ontario would be complete without seeing Niagara Falls. Harry reports that he was very pleased to enjoy a fine, warm day there.

Massey University

New postdoctoral fellows in chemistry include **Rachel Williamson** and **Charlie Williams** (with Emily Parker) and **Warwick Belcher** (with David Officer). **Amanda King** has taken up a position as research technician with David Harding. **Jim Jones** (Institute of Technology and Engineering) is going to the University of Birmingham for a month in November to work on a project studying granular flow in bin blenders using a positron emission particle tracking (PEPT) camera. The project is jointly with Clive Davies of IRL, David Parker of the University of Birmingham and John Bridgwater of the University of Cambridge. A PEPT camera is an adapted positron emission tomography camera that tracks a single radioactive tracer as it moves through a bed of granular material. It a powerful technique for examining flows within all sorts of industrial machinery and is able to resolve the tracer motion through metal-walled vessels.

WAIKATO

Professor Leon Phillips visited the Waikato Branch in his capacity of President of the Institute. Leon delivered an interesting lecture about the chemistry on Venus. Leon's talk was well attended and the audience was captivated by his research into this fascinating area of chemistry. The pictures and graphics of Venus left a deep impression on the audience.

Leon took the opportunity to present the **NZIC Waikato Branch J Eric Allan Memorial Prize** to **Ms Susanna Thwaite**. Eric Allan was one of the pioneers of atomic absorption spectroscopy, and **Professor Brian Nicholson** told the group about Eric's contribution to this important analytical technique before Leon presented Susanna with her copy of Cotton and Wilkinson's Inorganic Chemistry.

University of Waikato news centres on completions of graduate degrees. Lately, there have been a good number of research students working with **Dr Chris Hendy** in the geochemistry and environmental chemistry area. **Rebecca Cheatley** completed her MSc in environmental chemistry, concerned with the impact of land use on shallow estuarine groundwater. She is employed now by Environment Waikato, but is taking a bit of R&R first and is on leave of absence to tour Europe. **Reece Harrison** is nearing completion of his MSc also in environmental chemistry (geochemistry of gold mine tailings) and has a job lined up in an analytical chemistry laboratory in Perth. **Levinia Paku** has finished her MSc looking at the influence of Rotorua Sewerage irrigation of Whakarewarewa Forest groundwater. Levinia is now on a joint appointment at the University of Waikato providing student support for Maori students, and in the Cooperative Education Unit, helping find and support students on work placements as part of the BSc(Tech) degree program. **Tracey Adams** has finished her MPhil in geochronology, looking at how to radiocarbon date glacial sediments from a high rainfall area and is presently travelling around Europe. **Jamie Hollands** having finished his MSc, is now doing a PhD in conjunction with Forest Research in Rotorua.

Above: Susanna Thwaite receives the J Eric Allan Memorial Prize from NZIC President Professor Leon Phillips.

Up-coming activities include the annual ChemQuest. With a record number of nearly 70 teams entered from as far away as Whakatane, it promises to be a great event. A report will follow in the next issue.

WELLINGTON

The Wellington Branch was saddened at the death of **Dr Frank Hurst** who retired from DSIR a number of years ago. Frank had held responsibility for the Forensic Section as it was and, in the very early days, handled all the blood alcohol analyses himself – but that might have been only two or three samples a week. A full obituary appears elsewhere in this issue of *Chemistry in New Zealand*. **Dr Alan Browne**, a VUW PhD graduate of 1976 (supervisor **Professor B Halton**) and former NZIC member, died in at his home in Maryland on October 1. He last visited New Zealand in August and was a long-standing employee of the US Department of Energy as Program Manager, Environmental Technology Development – Energetics.

Professor Brian Halton is the recipient of the 2001 **Shorland Medal** awarded by the New Zealand Association of Scientists in recognition of a person's outstanding lifetime contribution to basic or applied research that has added significantly to scientific understanding. Brian's

contribution is to basic research (more aptly described as fundamental research) and has involved what was a little known class of compounds – the cycloproparenes – that now command significant international attention.

The Branch AGM was held prior to the October meeting. The Chairman's annual report and the Branch annual accounts were accepted with surprisingly little discord or comment—save from the writer (who else but the Editor of *Chemistry in New Zealand*) who questioned the implication of "All 2000 committee members ..." in the minutes of the 2000 AGM.

Professor John Spencer and **Ms Sue Freitag** are stepping down after two years as Branch Chairman and a long spell as Branch Secretary, respectively. They were thanked by acclamation for their dedication and contribution to the life of NZIC in Wellington. For the first time in quite a while the number of volunteers willing to serve on the 2002 committee was more than enough to ensure that the Branch moves forward with vigour.

Above: Outgoing Wellington branch Chairperson Professor John Spencer at the branch AGM.

The new Committee is:

Chairman: **Emeritus Professor Neil Curtis** (VUW)
Secretary: **Dr Catherine Dickson** (IRL)
Treasurer: **Mr Alan Turner** (Consultant)
Members: **Dr Suzanne Boniface** (Queen Margaret College), **Ms Elizabeth Douch** (Tawa College), **Ms Sue Freitag** (Opus International), **Dr Graeme Gainsford** (IRL), **Dr Vincent Gray** (Consultant), **Professor Brian Halton** (VUW), **Dr W E (Ted) Harvey** (Consultant), **Mr Rob Keyzers** (Student Representative), **Dr Peter Northcote** (VUW), and **Dr Helen Palmer** (Baldwin Shelston Waters).

The October meeting was held at NIWA, Evans Bay, and consisted of a dual presentation by **Dr Jill Cainey** and **Mr Antony Gomez** (a chemist and mathematician, respectively) on the topic of "Baring Head – New Zealand's Clean Air Station". The need for and use of the atmospheric measurements that have been made at Baring Head (on the southeast coast of the Wellington harbour entrance) since 1970 were presented and discussed. The focus has been on tracking atmospheric species in strong onshore southerly winds (on the evening in question the remote sensor indicated a southerly of close to 60 knots). Under these conditions the air is derived from well south of New Zealand and is representative of that over the Southern Ocean. The measurements have credence as being from "clean air". The routine monitoring shows CO_2 at 367 ppm, CH_4 at 1730 ppb, CO at 50 ppb and non-methane hydrocarbons at a mere 10-100 ppt.

Apart from monitoring carbon dioxide levels Jill has a distinct interest in ozone levels and in the sulfur cycle given the ability of plankton to eject dimethyl sulfide. The audience of almost 30 was finally treated to a demonstration of the remote handling capabilities at the station by the computer-controlled instrumentation.

BRANZ

Senior technician **Bryan Keen** has spent five weeks at the NIST Building and Fire Research Laboratory in Washington on a BRANZ Travel Scholarship. He has been learning about their latest techniques for concrete characterisation and testing.

Peter Haberecht, now stationed in the BRANZ Melbourne office, has followed up his success in winning the 2000 A C Kennett Award (a joint award of NZIC and the Australasian Corrosion Association for work on degradation of non-metals) with a paper on corrosion of glass. This has led to the **2001 Westinghouse Prize** (for the best paper in 2000-2001) from the UK Institute of Metal Finishing, for work on defining the mechanisms of protection of steel by cadmium brush-plating.

The BRANZ capability to test and model effectively the performance of materials in fire is currently being extended by the creation of a room-corridor installation capable of testing to ISO 9705. This accompanies the Vertical Channel Test commissioned earlier in 2001, and together they complement the cone calorimeter and the large fire test furnaces that have been in place for a number of years.

Cawthron Institute, Nelson

Cawthron has revamped its website at:
http://www.cawthron.org.nz

Nico Van Loon has taken up the position of Laboratory Manager. Nico has an MSc in Analytical Chemistry and Environmental Geochemistry from University of Utrecht, and an MBA from University of Waikato. He comes from laboratory management positions with R J Hill Laboratories and AgriQuality. **Veronica Beuzenberg** is commissioning a new facility for bulk culturing of micro-algae. The primary goal is production of marine biotoxins for metabolism and toxicology research and for use as analytical standards. **Jenny Smith** has obtained a FiRST Award for her research at Massey University on plant

defence mechanisms and is well into her Post Doctoral Fellowship at Cawthron. The research is on the production of sulfated oligosaccharides of medical interest from seaweed and is with **Lesley Rhodes** and **Doug Mountfort** and in collaboration with **Ruth Falshaw** of IRL.

Industrial Research Ltd

On 15th October, **Dr Geoff Page** announced his resignation as CEO of Industrial Research Limited to take up the position of Managing Director of ANUTECH, a wholly owned company of the Australian National University, Canberra. Dr Page will leave IRL on 31st January 2002.

Student **Ulrike Wolf** from the Technical University of Clausthal in Lower Saxony, Germany, has joined the Applied Inorganic Chemistry team for four months. He is working with **Dr Tim Kemmitt** on the preparation of TiO_2 and SiO_2 thin films.

Dr. Graeme Gainsford (a stalwart of the Wellington Branch) is currently on one month's leave working at the Brookhaven National Laboratory in New York. Graeme is utilising the National Synchrotron Light Source and is being funded through the International Science and Technology (ISAT) Linkages Fund.

Gabriel Ossenkamp attended the *Silica 2001* conference in Mulhouse, France, from September 3 to 6, 2001. Four days of the scientific and technological aspects of silica use, characterisation, modification, and synthesis combined with French food and wine; Alsacian hospitality made the width of scientific endeavour in the field clear, without letting it become too dry. Gabriel presented a poster entitled "Towards functional materials through surface esterification of silica".

Dr Ken Mackenzie of the Ceramic section has had a busy time in recent months. Not only has he recently been appointed as Associate Professor in Materials Science at Victoria University, in a joint appointment between VUW and IRL but also he completed a one-month BRAP study award. This was spent investigating the preparation of advanced ceramics by *mechanochemical* synthesis (high energy milling) that was split between the Tokyo Institute of Technology and Warwick University (England). He has also completed and submitted for publication a book on "The Applications of Solid State NMR to Inorganic Materials".

Fred Lecarpentier has recently completed a two month BRAP study award at the Mechanical Metallurgy Laboratory of the EPFL in Lausanne (Switzerland), where he was researching the fabrication and evaluation of a new sialon-aluminium metal matrix composite (MMC) body. **Mark Bowden** and **Vaughan White** attended the European Ceramic Society Conference in Bruges, Belgium from September 9-13, 2001. Both made follow-up industry and institutional visits in the UK. Mark then travelled on to Sweden where he worked for three weeks at the Swedish Ceramic Institute, Gothenburg, funded by a BRAP travel award.

Dr Ian Brown gave an invited lecture entitled "*Use Of IBA Techniques For The Measurement Of Oxidation Processes In Sialon Ceramics*" to the "Advanced Materials Produced and Analysed with Ion Beams International Conference" in Wellington in July. Together with **Ching-Zen Han** he attended the 8th NZ Engineering & Technology Postgraduate Conference, at the University of Waikato in late August. Ching-Zen presented a paper on her current PhD research on Ti-Al_2O_3 composites.

Juliane Heiber (Technical University of Ilmenau, Germany) is working with **Dr Marc Daglish** and other members of the Electroceramics group for a five-month period.

B Dent Global

The Gracefield firm B Dent Global (www.bdg.co.nz) celebrated its 5th anniversary with the arrival of two additional synthetic organic chemists to join **Drs Dennis Page** and **Barry Dent**. **Neil Beare** (PhD Otago – **Professor Rob Smith**) comes from a successful postdoctoral period at Yale with **Professor John Hartwig** and **Susan Maddock** (PhD Auckland – **Professor Warren Roper**) joins after extensive work in the USA, most recently with 2001 Nobel Laureate **K. Barry Sharpless** (see elsewhere for a summary of the 2001 Nobel Prize in Chemistry). The firm has consolidated its leadership in the synthesis of drug metabolites and isotope labelled standards with the awarding in October of a 2 FTE contract from a US bioanalytical company.

Victoria University

In conjunction with Victoria University the Branch ran a Titration Competition and its annual 6th and 7th form Chemistry Quiz on the same day. The titration competition had some 40 entrants from 10 colleges. **Dr David Weatherburn** with considerable assistance from **Mrs Jackie King** and **Dr Gordon Heeley** organised the event. The outright winner was **Nathan Smith** of **Heretaunga College**, but David found it difficult to separate the next five place-getters and so five second prizes were awarded. This year a very challenging titration was set but the standard was high and the contestants appeared to enjoy themselves.

The Quiz was even more popular than last year with 33 four person teams (132 contestants) from 15 colleges. It was encouraging finding that teams had travelled from

Levin (Waiopehu College) and the Wairarapa (Wairarapa and Kuranui Colleges) as well as from Wellington and the Hutt Valley. The contestants appeared to have a great evening and enjoyed the opportunity of testing their chemical knowledge against their peers. About 20 teachers accompanied the students and they seemed also to enjoy the evening. PhD graduate students **Rob Keysers** and **Laine Cousins** did a great job in organising the event from beginning to end. They were able to muster a committed group of helpers from SCPS, namely **Kirsten Edgar, John Ryan, Andrew McFarlane,** and **Thomas Borrmann**. There were also three helpers from outside: Rob's friend, Lucy, Duncan Henry, and Lynne Gallie (VUW publicity). Lynne has been very supportive to Rob and Laine throughout, and was a big help on the night. Not only did she distribute some VUW advertising but she also persuaded the Dean of Science to part sponsor the evening with $600 to offset costs The event was at the University Staff Club.

Above: *Quiz organisers Rob Keysers and Laine Cousins.*

Above: *Titration Competition winner Nathan Smith of Heretaunga College.*

The event was won by the **Scots College "The Chemistry Kings"** team, a seventh form team returning from last year when they were placed second as 6th formers (beating their 7th form team in the process!). Second place went to **Hutt Valley High School** with third place going to the **"Legion of Tom"** team from **Upper Hutt College**. It was an excellent day.

Above: *Kings of chemistry, quiz winners "The Chemistry Kings" from Scots College.*

Carissa Jones, the recipient of RSNZ and Wellington Branch travel assistance to Pacifichem 2000, has completed her PhD degree (supervisor **Professor Brian Halton**). She is now gainfully employed as a postdoctoral fellow with Professor Jay Siegel at the Chemistry Department of University of California-San Diego. Her PhD studies centred on the cycloproparene work of the Halton group and involved the synthesis of new and novel functionalised derivatives that have formed the basis of her five publications.

On October 15, 2001 a recently renovated part of the Laby Building was commissioned as the "Magnetic Resonance of Materials Laboratory" at a formal opening by the Minister of Science **Rt. Hon. Pete Hodgson**. The laboratory houses two 300 MHz multinuclear NMR spectrometers that are the work horses for the materials studies of **Professor Paul Callaghan FRS.**

Above: *Minister of Science, Rt. Hon. Pete Hodgson cuts the ribbon to officially open the "Magnetic Resonance of Materials Laboratory" at Victoria University.*

Toward Sustainable Chemistry

Terry Collins
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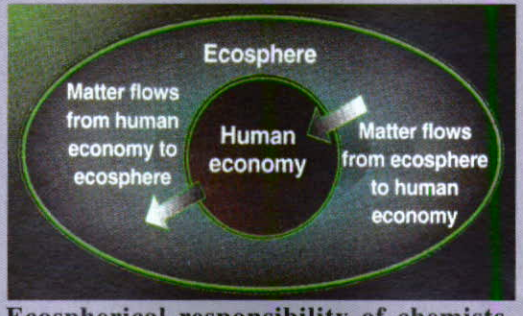
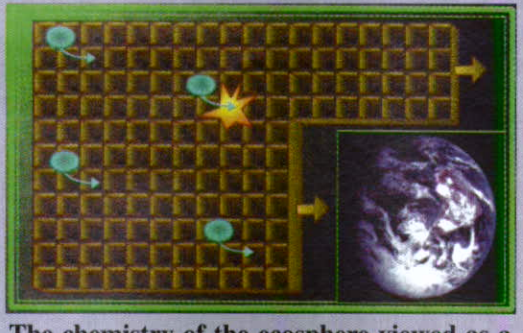
Chemistry has an important role to play in achieving a sustainable civilisation on Earth. The present economy remains utterly dependent on a massive inward flow of natural resources that includes vast amounts of nonrenewables. This is followed by a reverse flow of economically spent matter back to the ecosphere. Chemical sustainability problems are determined largely by these economy-ecosphere material flows (see the figure, below), which current chemistry education essentially ignores. It has become an imperative[1] that chemists lead in developing the technological dimension of a sustainable civilization.

When chemists teach their students about the compositions, outcomes, mechanisms, controlling forces, and economic value of chemical processes, the attendant dangers to human health and to the ecosphere must be emphasized across all courses. In dedicated advanced courses, we must challenge students to conceive of sustainable processes and orient them by emphasizing through concept and example how safe processes can be developed that are also profitable.



Ecospherical responsibility of chemists. Diagram based on ideas of Herman E. Daly.



The chemistry of the ecosphere viewed as a mail sorter's network.

Green or sustainable chemistry[2] can contribute to achieving sustainability in three key areas. First, renewable energy technologies will be the central pillar of a sustainable high-technology civilization. Chemists can contribute to the development of the economically feasible conversion of solar into chemical energy and the improvement of solar to electrical energy conversion. Second, the reagents used by the chemical industry, today mostly derived from oil, must increasingly be obtained from renewable sources to reduce our dependence on fossilized carbon. This important area is beginning to flourish, but is not the subject of this essay. Third, polluting technologies must be replaced by benign alternatives. This field is receiving considerable attention, but the dedicated research community is small and is merely scratching the surface of an immense problem that I will now sketch.

Many forces give rise to chemical pollution, but there is one overarching scientific reason why chemical technology pollutes. Chemists developing new processes strive principally to achieve reactions that only produce the desired product. This selectivity is achieved by using relatively simple reagent designs and employing almost the entire periodic table to attain diverse reactivity. In contrast, nature accomplishes a huge range of selective biochemical processes mostly with just a handful of environmentally common elements. Selectivity is achieved through a reagent design that is much more elaborate than the synthetic one. For example, electric eels can store charge via concentration gradients of biochemically common alkali metal ions across the membranes of electroplaque cells. In contrast, most batteries used for storing charge require biochemically foreign, toxic elements, such as lead and cadmium. Because of this strategic difference, manmade technologies often distribute throughout the environment persistent pollutants that are toxic because they contain elements that are used sparingly or not at all in biochemistry.

Persistent bioaccumulative pollutants pose the greatest chemical threat to sustainability. They can be grouped into two classes. Toxic elements are the prototypical persistent pollutants; long-lived radioactive elements are especially dangerous examples. New toxicities continue to be discovered for biologically uncommon elements. The second class consists of degradation-resistant molecules. Many characterized examples originate from the chlorine industry[3] and are also potently bioaccumulative. For example, polychlorinated dibenzo-dioxins and -urans (PCDDs and PCDFs) are deadly, persistent organic pollutants. They can form in the bleaching of wood pulp with chlorine-based oxidants, the incineration of chlorine-containing compounds and organic matter, and the recycling of metals. The United Nations Environmental Program (UNEP) International Agreement on persistent organic pollutants lists 12 "priority" pollutant compounds and classes of compounds for global phaseout. All are organochlorines.

Imagine all of Earth's chemistry as a mail sorter's wall of letter slots in a post office, with the network of compartments extending toward infinity (see the figure,

below). Each compartment represents a separate chemistry so that, for example, thousands of compartments are associated with stratospheric chemistry or with a human cell. An environmentally mobile persistent pollutant can move from compartment to compartment, sampling a large number and finding those compartments that it can perturb. Many perturbations may be inconsequential, but others can cause unforeseen catastrophes, such as the ozone hole or some of the manifestations of endocrine disruption.[4] Most compartments remain unidentified and even for known compartments, the interactions of the pollutant with the compartment's contents can usually not be foreseen, giving ample reason for scientific humility when considering the safety of persistent mobile compounds. We should heed the historical lesson that persistent pollutants are capable of environmental mayhem, and treat them with extreme caution. In cases where the use of a persistent pollutant is based on a compelling benefit, as with DDT (dichlorodiphenyltrichloroethane) in malaria-infested regions, chemists must face the challenge of finding safe alternatives.

Consider, for instance, the alarming reproductive damage that can be inflicted by minute quantities of endocrine-disrupting chemicals (EDCs), such as PCDDs, polychlorobiphenyls (PCBs), and the pesticides endosulfan and atrazine.[3] EDCs disrupt the body's natural control over the reproductive system by mimicking or blocking the regulatory functions of the steroid hormones or altering the amounts of hormones in the body. Uncertainty still clouds our understanding of their full impact, but mass sterilization is one limiting conceivable outcome of ignoring the demonstrated dangers of EDCs. Our present knowledge strongly suggests that anthropogenic EDCs should be identified and eliminated altogether.

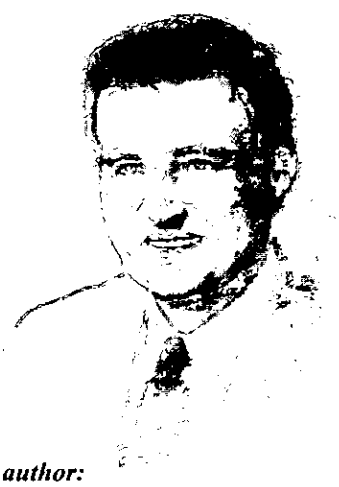
Stringent regulations based on the precautionary principle and the principle[3] of "reversed onus" should be developed to guard against the release of new environmentally mobile persistent compounds; a precise definition of persistence also needs to be developed. This would provide a regulatory foundation for weeding persistent bioaccumulative compounds out of all technology, and highlight where research is needed to find safe alternatives. Groundbreaking legislative proposals toward this goal are about to be considered in the Swedish Parliament.

In their current formal training, all chemistry students will learn that the chlorination of phenol proceeds by a mechanism known as electrophilic aromatic substitution. But very few will learn of EDCs and their dangers or come to know that prime examples of EDCs, namely PCDDs, are produced in trace quantities whenever phenol is chlorinated. This hazardous omission illustrates one important type of content that is simply missing from the conventional curriculum.

Green chemistry can dramatically reduce environmental burdens of both classes of persistent pollutants by moving the elemental balance of technology closer to that of biochemistry. Significant reductions in the dispersal of many persistent pollutants have already been achieved. By the late 17th century, the use of lead oxide as a correcting agent for acidic wine was banned on pain of death in Ulm in the duchy of Wurtemburg.[5] More recently, large reductions in lead pollution have been achieved in what are recognizable examples of green chemistry, for instance, by replacement of lead additives in paint with safe alternatives, by the development of cleaner batteries, and by the as yet unfinished and sometimes flawed progression away from tetraethyl lead toward safer combustion promoters in fuels. PCDDs and PCDFs have been greatly reduced in the pulp and paper industry by the replacement of chlorine with chlorine dioxide as the principal bleaching agent.

Nevertheless, much more can and must be done. For example, chlorine-based oxidations such as pulp bleaching, water disinfection, household and institutional cleaning, and clothing care continue to produce huge volumes of organochlorine-containing effluent. Despite industry efforts to reduce pollutant concentrations, some of the inescapable trace contaminants are persistent, bioaccumulative carcinogens and/or EDCs. Chlorine-based oxidation technologies could be replaced with alternatives based on catalytic activation of nature's principal oxidizing agents, oxygen or hydrogen peroxide. My research group has patented TAML activators, which are potent but selective peroxide-activating catalysts comprised of biochemically common elements for these and other fields of use. Environmental considerations also underpin the worldwide investigation and development of supercritical and near-critical carbon dioxide as a clean solvent. The present search for safer solvents in the green chemistry community is distinguished by a remarkable burst of creativity that perhaps reaches its zenith in ionic liquids. These solvents have unique properties such as the absence of any vapour pressure under standard conditions.

Pollutant production can also be reduced by improving process selectivity, reducing energy intensity, and minimizing the flow of matter to and from the ecosphere via atom economic processes, that is, processes optimized to reduce per unit of product the quantities of chemicals employed in the reactions as solvents and reagents or produced as by-products.



About the author:

Terry Collins teaches green chemistry at Carnegie Mellon University in Pittsburgh, PA, USA. He was born and educated in New Zealand. His group has invented "green" substitutes for processes producing persistent bioaccumulative organochlorides. He has received several awards including the Presidential Green Chemistry Challenge Award (USA).

To achieve such sustainable chemistry requires a sea change in the chemical community. The principles of green or sustainable chemistry must become an integral part of chemical education and practice. However, there are several obstacles to overcome. First, chemists need to comprehensively incorporate environmental considerations into their decisions concerning the reactions and technologies to be developed in the laboratory. These questions need to become as important as those associated with the selectivity of the technology and how it works. Principles upon which to base these decisions have already been developed.[2] Second, it is critical that chemistry that is not really green does not get sold as such, and that the public is not misled with false or insufficient safety information. For example, certain chlorine industry companies have sought to protect their profits by distorting scientific data to make dioxins appear to be less harmful to humans than they actually are.[3] The general trust that chemical risk is treated in a fair and reasonable manner must be strengthened. Third, since many chemical sustainability goals such as those associated with solar energy conversion call for ambitious, highly creative research approaches, short-term and myopic thinking must be avoided. Government, universities, and industry must learn to value and support research programs that do not rapidly produce publications, but instead present reasonable promise of promoting sustainability. Fourth, chemistry exerts a near boundless influence on human action and is thus inextricably intertwined with ethics. An understanding of sustainability ethics is therefore an essential component of a healthy chemical education.[1]

The all-encompassing challenge lying before green chemists is to understand the ethical forces, chemical-ecosphere relations, educational needs, and research imperatives that sustainability brings centre stage and to reconcile this understanding as much as possible with economic maxims. If chemists increasingly direct their strengths to contributing to a sustainable civilization, chemistry will become more interesting and compelling to people, and may lose its "toxic" image. It will become more worthy of public support and spawn exciting economic enterprises that nurture sustainability.

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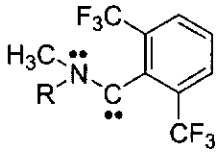
Snippets

The heaviest chemistry

Element 108, hassium (Hs), is now the heaviest element to have had its chemistry studied. Scientists from Germany, Norway, Russia, Switzerland, UK, and the USA carried out the first chemical studies of the element using techniques developed at Lawrence Berkeley National Laboratory and the Paul Scherrer Institute in Switzerland. The research shows that hassium forms a gaseous oxide similar to that of osmium and confirms that it should be placed directly under osmium in group 8 of the periodic table. Preparation and constant monitoring of the experiments required many hours of accelerator time and lots of people power, remarks Heino Nitsche, Chemistry Professor at the University of California, Berkeley, who directed the development of a new, very low temperature technique for simultaneously separating and detecting group 8 oxides. The system was installed at the UNILAC heavy-ion accelerator at the Heavy-Ion Research Center (GSI) in Germany, where element 108 was discovered in 1984. In the experiments, the team bombarded curium-248 targets with high-energy atoms of magnesium-26. The resulting hassium atoms were heated with oxygen. Six oxide molecules, carried singly through the system by a stream of helium, were condensed on detectors.

Stable carbenes with spectator substituent

Stable carbenes - neutral molecules in which a carbon atom is surrounded by only six electrons - are difficult to achieve. Usually an electron-active substituent is needed on either side of the carbene to stabilize it. A team led by Guy Bertrand of Paul Sabatier University in Toulouse, France has synthesized stable singlet carbenes containing amino and aryl groups (below) [*Science*, **2001**, *292*, 1901]. The amino group, which has both p-donor and s-acceptor electronic character, ensures that the carbene centre remains neutral. X-ray data indicate that the aryl group, which contains *o*-trifluoromethyl groups, does not interact with the carbene lone pair of electrons and serves as a spectator. These carbenes can be isolated at room temperature at close to quantitative yields. Because these carbenes don't require two strongly interacting substituents, the number and variety of such carbenes should increase, Bertrand and colleagues write, which will lead to new synthetic developments and applications.



NZIC Remuneration Survey 2000

G Boston and S van Eyk, Manawatu Branch, NZIC

Summary

The median remuneration of chemists surveyed was $70,000. The median annual salary increase was 2.0%

Last year, as one of the special grants to Branches, the Manawatu Branch organised a survey of the remuneration of NZIC members. This was the eleventh survey and the first in over ten years. In the past ten years employment conditions have changed dramatically and we designed the survey to try to capture the effect of benefits on total remuneration. Based on similar surveys from the RACI and IPENZ, we included questions on job responsibility to try and assess the impact of job performance on remuneration.

Survey forms were sent to all waged NZIC members. Of the 261 replies received, 230 were from males and 31 from females. As the NZIC no longer collects gender information we cannot tell if these numbers represent the gender distribution of the NZIC membership.

The median age of the respondents was 50 years with the males noticeably older (median age 52 years) than the females (median age 38 years). Again, as the NZIC no longer collects age data we cannot tell if this is representative of the NIZC membership but the "general feeling" is that the NZIC has an ageing membership.

Data were collected on respondents' base salary and the value of other benefits towards their total remuneration package. Some 14% did not receive any additional benefits, 23% chose not to answer (or did not know what benefits they received?), while 63% of respondents did receive a benefit in addition to their base salary. However, of the 165 people who received benefits, 38 were unable to put a value to the benefits indicating that remuneration was possibly not a key issue in their job.

Gender variation

The plot of remuneration by gender (Figure 1) shows that the median remuneration for females over 31 years old was less than that of similarly aged males. Only at ages less than 30 was the remuneration for males and females equivalent. However, the small number of females in the sample (24 females versus 223 males over 30) cautions against drawing any firm conclusions from the data. Due to the small number of females no further gender-based analysis has been done. Note that the plots have been limited to a maximum of $200,000; 5 people – all from private industry – reported earning more than $200,000.

Age variation

The median remuneration for the survey was $70,000 with half of the respondents earning between $56,000 and $89,000.

The total remuneration increased with age (Table 1), between 31 and 60 years old this was approximately a linear increase with age of about $10,000 per cohort. Below 30 years old the remuneration is proportionally lower, reflecting the fact that more highly qualified people have yet to enter the work force.

The median increase in base salary was 2%, which matches the 2% rise in the Consumer Price Index between 1999 and 2000. The CPI for 2001 is currently running at 3.2% - did you get a salary increase to match it?

The percentage increase in base salary was markedly higher for younger chemists. We do not propose to speculate on the reasons.

The absolute amount of total benefits was similar across all age groups. However, this means that benefits form a larger proportion of total remuneration for the younger chemist and may be an indication of the trend towards performance-based remuneration.

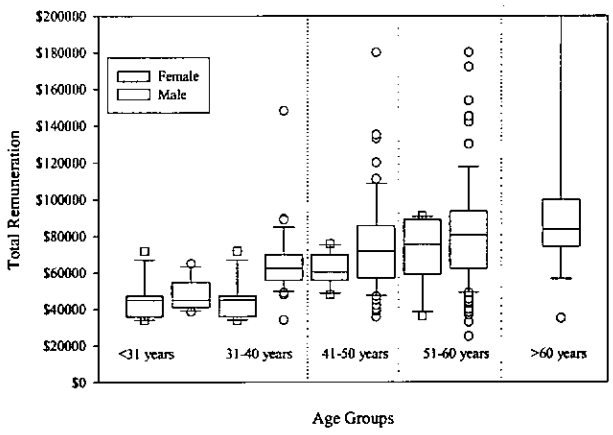


***Figure 1:** Total Remuneration by gender.*

Regional variation

The median remuneration in the three main centres was noticeably higher than other areas (Table 2). Of the main centres, Wellington had the highest median remuneration of $78,592 while Auckland had the lowest at $75,500.

There was a large number of respondents from other North Island locations reflecting the strong science communities in Palmerston North, Hamilton and Taranaki. The median remuneration for these areas was $65,000. The median remuneration in the South Island, excluding Christchurch, was $58,500.

Regional variations in salary increases were not marked except that the rest of the North Island received a noticeably lower median increase of 1% than did the other locations (2.6%).

The median size of benefits paid was higher in the three main centres and it is noticeable that benefits are more common in the North Island (53% of chemists) than in the South Island (40% of chemists).

Qualifications

A doctorate degree is held by 58% of respondents and their median remuneration of $79,500 (Table 3) is markedly higher than the $62,500 of those with Masters level qualifications. The median remuneration of those with NZCS was $62,000, higher than the $56,000 of those with Bachelor level qualifications. There were only 6 respondents with NZCS aged between 36 and 57 whereas there were 57 respondents with Bachelor level qualifications aged between 23 and 74 years. While the large difference may reflect the extra value placed on experienced laboratory staff over a basic degree qualification, the sample size is too small to draw any firm conclusions.

There was considerable variation in the rates of salary increase and benefits paid between qualification groups.

Employment sector

The plot of remuneration by sector (Figure 2) clearly shows that total remuneration in the private sector is generally higher than in both the education sector and the public sector. Conversely, the median base salary is highest in the education sector (Table 4). The difference is a reflection of the fact that 71% of chemists in the private sector receive a benefit that comprises a large portion of their total remuneration (median of $9,000). By contrast only 28% of chemists in the education sector and 55% of chemists in the public sector receive additional benefits which comprise a smaller portion of their total remuneration (median of $3,000 and $5,000 respectively).

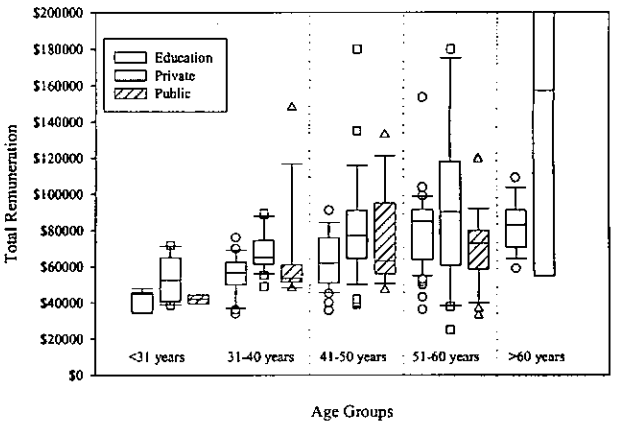


Figure 2: Total Remuneration by sector.

The remuneration of private sector chemists is presumably more closely related to market success and risk taking, none more so than the owners of companies. The risks and rewards were shown in this survey where the owners of two companies received the maximum ($340,000) and minimum ($25,000) remuneration recorded.

Job responsibility

In general, respondents' assessment of their job responsibility was not reflected in their remuneration and the data have not been shown. There were large differences in assessment of apparently the same job. For example, of two Senior Lecturers of the same age earning around the median salary of $70,000 one scored his job as 14 out of 35 and the other as 27 out of 35. The same scatter was also observed in other sectors.

The design and use of these questions must be reassessed for future surveys. We welcome feedback from readers, please contact:
Secretary@nzic.org.nz

Table 1. Variation in remuneration by age.

		Base salary			Total remuneration		
Age group	Sample size	Lower quartile	Median	Upper quartile	Lower quartile	Median	Upper quartile
<30	14	$38,400	$44,500	$48,500	$38,650	$45,000	$50,300
31-40	44	$52,625	$57,250	$65,750	$53,925	$59,545	$67,750
41-50	74	$55,600	$64,250	$78,625	$56,000	$69,000	$84,250
51-60	114	$58,875	$75,500	$89,000	$61,750	$80,500	$92,250
>60	15	$68,600	$81,000	$100,000	$68,600	$83,000	$100,000
All ages	261	$54,000	$66,000	$83,167	$56,000	$70,000	$89,000

		% annual Base salary increase			Total benefits			
Age group	Sample size	Lower quartile	Median	Upper quartile	Sample size	Lower quartile	Median	Upper quartile
<30	14	1.4	6.1	9.2	4	$1,750	$4,500	$12,500
31-40	44	0	3.8	7.3	21	$1,550	$4,000	$7,750
41-50	74	0	1.8	4.3	38	$4,300	$6,000	$12,500
51-60	114	0	1.6	4.0	59	$3,000	$4,452	$14,000
>60	15	0	0	2.5	5	$1,200	$3,000	$23,250
All ages	261	0	2.0	4.6	127	$2,500	$6,000	$11,000

Notes on the data presentation

The data were analysed using Minitab Statistical Software Release 13 (Minitab Inc., Pa, USA) and the median, upper and lower quartile data are shown.

The data were graphed in a box plot using Sigmaplot version 4 (SPSS, Il, USA). The box plot shows the range of data; the base of the box indicates the lower quartile, a line within the box marks the median, and the top of the box indicates the upper quartile; that is 50% of the results lie within the box. Whiskers above and below the box indicate the 90th and 10th percentiles, outlying points are graphed individually.

Table 2. Variation in remuneration by location.

		Base salary			Total remuneration		
Region	Sample size	Lower quartile	Median	Upper quartile	Lower quartile	Median	Upper quartile
Auckland	62	$58,375	$68,450	$88,125	$64,375	$75,500	$92,500
Wellington	39	$50,000	$72,500	$90,028	$58,550	$78,952	$95,000
Christchurch	42	$57,525	$74,500	$85,900	$59,900	$76,350	$89,625
Rest of NI	78	$52,025	$62,859	$75,000	$55,150	$65,000	$80,625
Rest of SI	40	$45,250	$58,250	$73,263	$45,750	$58,500	$79,572

		% annual Base salary increase			Total benefits			
Region	Sample size	Lower quartile	Median	Upper quartile	Sample size	Lower quartile	Median	Upper quartile
Auckland	62	0	2.3	4.8	34	$5,000	$6,300	$12,000
Wellington	39	0	3.1	6.0	24	$3,000	$6,226	$9,500
Christchurch	42	0	2.7	4.1	18	$1,450	$6,800	$14,250
Rest of NI	78	0	1.0	3.9	36	$2,125	$5,000	$13,750
Rest of SI	40	0	2.5	6.4	15	$1,500	$2,500	$8,000

Table 3. Variation in remuneration by qualification.

		Base salary			Total remuneration		
Qualification	Sample size	Lower quartile	Median	Upper quartile	Lower quartile	Median	Upper quartile
None	6	$44,800	$47,750	$59,500	$45,375	$50,400	$70,750
NZCS	14	$49,878	$58,750	$67,375	$51,053	$62,000	$69,575
BSc & Hon	57	$42,500	$54,000	$67,857	$48,000	$56,000	$78,750
MSc & Hon	31	$53,000	$59,000	$71,000	$53,000	$62,500	$73,633
PhD	153	$60,750	$75,000	$88,200	$63,359	$79,500	$90,750

		% annual Base salary increase			Total benefits			
Qualification	Sample size	Lower quartile	Median	Upper quartile	Sample size	Lower quartile	Median	Upper quartile
None	6	0	1.0	2.8	2		$10,800	
NZCS	14	0	2.6	4.5	10	$1,188	$5,200	$7,100
BSc & Hon	57	0	2.9	7.4	29	$4,000	$12,000	$19,763
MSc & Hon	31	0	3.5	4.2	12	$1,400	$6,000	$23,750
PhD	153	0	1.7	4.6	74	$2,500	$5,000	$9,000

Table 4. Variation in remuneration by sector.

		Base salary			Total remuneration		
Sector	Sample size	Lower quartile	Median	Upper quartile	Lower quartile	Median	Upper quartile
Education	118	$55,600	$69,196	$85,225	$56,000	$70,196	$86,750
Public	51	$50,000	$61,000	$78,000	$51,071	$64,000	$80,000
Private	91	$54,000	$66,000	$82,000	$59,600	$73,633	$97,000

		% annual Base salary increase			Total benefits			
Sector	Sample size	Lower quartile	Median	Upper quartile	Sample size	Lower quartile	Median	Upper quartile
Education	118	0	2.0	4.1	33	$1,750	$3,000	$5,592
Public	51	0	1.7	4.7	28	$2,125	$5,000	$7,450
Private	91	0	2.3	5.2	65	$4,750	$9,000	$17,250

Report on the 41st IUPAC General Assembly and the 41st IUPAC Council Meeting Brisbane, Australia, June 29-July 8 2001

Kip Powell
NZIC IUPAC Representative, Department of Chemistry, University of Canterbury

IUPAC's Mission is to advance the world-wide aspects of the chemical sciences and to contribute to the application of chemistry in the service of mankind. In so doing IUPAC promotes the norms, values, standards, and ethics of science and advocates the free exchange of scientific information and unimpeded access of scientists to participation in activities related to the chemical sciences.

1. The changing face of the chemical sciences

IUPAC is undergoing a major restructuring in an effort to increase its visibility, to enlist input to its traditional activities from a wider geographic base and to improve its accountability to industry and to its National Adhering Organisations.

This comes at a time when there is

- Rapid expansion in international communication, which facilitates the access to, and exchange of scientific information.
- Greater interaction and dependency between the disciplines within the chemical sciences and technologies, and a re-drawing of the borders between the traditional areas of research.
- A merging between the traditional areas of academic, basic and industrial research.
- An increased public and scientific awareness of the importance of materials, health and environmental science.

2. The restructuring of IUPAC

In response to the above factors and objectives, IUPAC is terminating all of its working Commissions, Working Parties and Sub-committees which have served under the seven Divisions and from whose membership came the major flow of new projects.

In future, IUPAC projects can be initiated by any interested party worldwide who can form a Task Group. The Task Group will present a Project Submission to IUPAC for internal and external review to seek approval and subsequent funding. The role of the Division Committees will be to identify growth areas, solicit project proposals, moderate the review process, approve funding and manage their portfolios of approved projects.

This will be a more inclusive process than in the past, although New Zealand has, for its population and level of subscription to IUPAC, had a very high level of involvement in the Divisions, Commissions, Working Parties and Task Groups of IUPAC in recent years - see Appendix 1.

3. Where can New Zealand chemists find a role in the new IUPAC structure?

3.1 Directory of Expertise

With the demise of Commissions, IUPAC has lost the structured involvement of, and links to, many world leaders in the different chemical disciplines, both academic and applied. The secretariat recognises that the identification of potential new projects that meet the IUPAC goals, and the review of the project proposals and of the final documents will require a large pool of experienced chemists. Further, some Task Groups when preparing project proposals, or Divisions when reviewing proposals, will recognise the need for additional expertise or geographic representation.

To this end, both the Divisions and the secretariat are in the process of establishing a Directory of Expertise that will capture the names of both experienced and emerging scientists who have the necessary skills to contribute to the IUPAC programs.

It is important that New Zealand scientists – industrial, research and academic - are adequately represented on this database. This is a task that could be appropriately undertaken by the Council of NZIC.

3.2 Project proposals and formation of Task Groups

The restructuring of IUPAC offers a unique opportunity for scientists to address global problems that affect their science and industry and possibly, by inference, their negotiations and trade with the worldwide community.

IUPAC does not support scientific research *per se*. Its projects are of global rather than national interest and they often seek a consensus position on matters of terminology, method, validation, traceability etc. IUPAC also places priority on the dissemination of outputs by its Task Groups.

This report does not attempt to identify specific issues for a Task Group, rather it provides examples that illustrate the type of project that would be consistent with IUPAC goals:

- Approved, validated methods for measurement of p*H* in organic tissue, *e.g.* meat carcasses.

- Harmonisation of quality assurance schemes for the measurement of pesticide residues on fruit.
- Recommendations for terminolgy in the application of magnetic resonance imaging techniques.

The formation of Task Groups to address such problems, in association with other interested parties from the global community, may be the outcome of a symposium or workshop at an international scientific or industrial conference.

During the General Assembly two of the New Zealand delegates (Dr Pat Holland, Cawthron Institute; Professor Kip Powell, University of Canterbury) attended workshops that covered the initiation and formulation of projects and the Project Submission procedure. Kip Powell also attended a workshop on the review, funding and management of projects.

They would be willing to share this knowledge with prospective Task Groups or at appropriate conferences or symposia.

Appendix 2 gives examples of IUPAC projects and Task Groups in which New Zealand scientists are currently involved.

3.3 As serving members of IUPAC Divisions, Operational Committees and Working Parties

It will be to New Zealand's advantage to have direct representation on IUPAC's Divisions and key committees. These representatives can promote New Zealand interests as appropriate. It is essential for New Zealand chemists to be kept in front of the international chemical community. This may also be achieved through:

- Active participation in the work of Task Groups and the production of authoritative outputs.
- Nominations for positions as National Representatives linked to the Divisions and Operational Committees, when these are requested from the New Zealand National Adhering Organisation (NAO; RSNZ for New Zealand).
- Nominations for positions on the Division Committees, when these are requested from the New Zealand NAO.

The latter is extremely important. The Nomination Committees should contact NAOs for each of the seven Divisions. Further, the responsibility of 'National Representatives' will be significantly enhanced under the new structure. They will have full voting rights on a Division. However, nomination of National Representatives should be taken seriously: they should be eminent scientists and be prepared to contribute voluntary work to the Union. I feel that it is also incumbent on the NAO to make some provision for the attendance of its nominated National Representatives (NR) at biennial IUPAC meetings.

4. The Young Scientists Awards

At the opening session of the 38th Congress, held in parallel with the General Assembly, presentations were made to the winners of the Young Scientist Awards. These graduates, four each for 1999 and 2000, had recently completed PhD degrees and had been judged on the basis of 1000 word synopses of their research accomplishments. The winners came from India, Australia, Italy, Germany, USA and Japan. It would be good to see young New Zealand scientists represented there in future, something that may be fostered through the GRIF or Marsden programmes.

5. IUPAC Subscriptions

IUPAC is in a sound financial position. For this reason it was only necessary to increase the average subscription rates by 1%.

It is unfortunate for New Zealand (or it has been fortunate for several years) that the CT value available to IUPAC in recent years has been severely out of date. The calculation for 2002-03 subscriptions, based on the more recent 1998 CT figure for New Zealand, leads to a 70% increase in the New Zealand dues. At this stage one must assume that IUPAC has the correct CT value, but it is imperative that when New Zealand receives its account for IUPAC dues that it closely scrutinises the validity of the CT value used in the calculation.

New Zealand's concern about the dues increase was conveyed personally to both the Treasurer (Christoph Buxtorf) and the Executive Director (John Jost). It was made clear by both that, should New Zealand have significant financial difficulties in meeting its dues, then it is expected that we would present a case for an interim adjustment for one biennium. As indicated by the tenor of his letter to the Royal Society, Dr Buxtorf is encouraging New Zealand, and some ten other nations so affected, to seek a bridging arrangement. He understands, as do we, that it is essential for both IUPAC and New Zealand that we remain an active participant. I recommend the adoption of this approach from the Royal Society to the IUPAC Treasurer.

5.1 Future direction

The Czech delegation to the Council meeting presented a proposal that would change the formula by which dues are calculated, to the significant benefit of small nations and significant detriment of large nations. There was considerable sympathy for the plight of small nations who, under the present formula, do pay an over-weighted subscription. However, it was also appreciated that a rapid correction could see the loss of one of the major nations and with it severe implications for IUPAC's future viability. It was also noted that small nations receive disproportionate voting rights at Council, *e.g.* New Zealand has 2 votes and the USA has only 6, and both have equal access to all of IUPAC's scientific output.

There was a strong directive to the Bureau that it should reconsider the fairness of the current formula used for

calculating dues. Council directed the President to form an *ad hoc* working party to consider the relevant issues.

New Zealand will be represented on this working party along with the Treasurer, Canada, Japan, Czech Republic, India, Germany, Brazil, Sweden and USA.

Appendix 1

New Zealand involvement in IUPAC Divisions, Commissions, Committees and Working Parties, 2000-01

Dr Pat Holland, Titular Member, Chemistry and the Environment Division.
Dr Richard Hartshorn, Titular Member, Commission on Nomenclature in Inorganic Chemistry.
Dr Greg Russell, Working Party on Modeling of Polymerisation Kinetics and Processes.
Professor Jim McQuillan, National Representative, Commission on Electrochemistry.
Professor Kip Powell, Secretary and Titular Member, Analytical Chemistry Division.
Professor Ken Marsh, Subcommittee on Thermodynamic Data, Subcommittee on Liquid Solubilities (Commission V.8)
Dr Wayne Temple, Associate Member, Commission on Toxicology.

As part of the restructuring process, in 2000 IUPAC brought together several Strategy Development Committees to advise the Bureau on priorities and changes. New Zealand was represented on the Education Strategy Development Committee (Kip Powell).

Appendix 2

IUPAC approved projects in which New Zealand chemists are currently involved.

Dr Greg Russell, Modeling of Polymerisation Kinetics and Processes.
Professor Kip Powell, Updating of the IUPAC Stability Constants Database.
Dr Richard Hartshorn, revision of "Red Book I", the IUPAC text on nomenclature of inorganic chemistry.
Professor Kip Powell, Chemical speciation of environmentally significant heavy metals and ligands.

The IUPAC Prize for Young Chemists

The IUPAC Prize for Young Chemists has been established to encourage outstanding **young research scientists** at the beginning of their careers. The prize will be awarded for the **most outstanding PhD thesis** in the general area of the **chemical sciences**, as described in a 1000-word essay.

Awards

IUPAC will award up to *four* prizes annually. Each prize will consist of $US1000 cash and travel expenses to the next IUPAC Congress. In keeping with IUPAC's status as a global organization, efforts will be made to assure fair geographic distribution of prizes.

Prizes will be presented biennially at the IUPAC Congress (the next of which is to be in Ottawa, Canada in August 2003). Each awardee will be invited to present a poster on his/her research and to participate in a plenary award session.

Applications may be submitted, as described below, to the IUPAC Secretariat and will be judged by a committee of eminent scientists appointed by the President of IUPAC.

Procedures for the 2002 Prize:

a. Entrants must have received their PhD (or equivalent) degree, or completed all PhD requirements including successful defense of the doctoral thesis, **during calendar 2001** in any of the 60 countries that are Members or Associate Members of IUPAC. Entrants need not be citizens or residents of one of these countries at the time the application is submitted.

b. The research described in the entrant's thesis must be in the field of the **chemical sciences**, defined as "chemistry and those disciplines and technologies that make significant use of chemistry."

c. The IUPAC Prize recognises only work that was performed while the entrant was a graduate student.

d. Application requires submission of a completed entry form, together with the material listed in items *e* and *f*. The entry form and supporting material should be submitted by e-mail whenever feasible. Additional material may be sent as needed by fax or mail.

e. An **essay** must be submitted by the entrant that describes his or her thesis work and places it in perspective relative to current research in the chemical sciences. The essay must be written in English by the entrant and may not exceed **1000 words.** For applications submitted through a National Adhering Organisation or Associate (NAO), a national language may be permissible, and the NAO will assist in translation to English. The announcement by the appropriate NAO should be consulted.

f. Two supporting letters (sent by e-mail if feasible) are required from the thesis adviser and/or chairman of the thesis committee and one additional faculty member. These letters should comment on the qualifications and accomplishments of the applicant and the significance of the thesis work.

g. Complete applications must be received at the IUPAC Secretariat by **February 1, 2002**. If submitted through an IUPAC National Adhering Organization or Associate NAO, the deadline established by the NAO must be met. Early submission is strongly encouraged so any questions may be resolved before the deadline date.

IUPAC Secretariat
P O Box 13757, 104 T. W. Alexander Drive, Building 19,
Research Triangle Park, NC 27709-3757, USA
Fax: (+1-919)-485 8706
Email: secretariat@iupac.org
URL: http://www.iupac.org

"Molecules for Life"

NZIC, NZSBMB, NZBA & BIOTENZ Conference
4-7 December 2001
War Memorial Centre, Marine Parade, Napier, New Zealand

CONFERENCE PROGRAMME

Please Note: At the time of publication of this issue of *NZ BioScience*, some speakers, times etc. for this conference programme were still being finalised, and are subject to change. Further details including registration fees, transportation and accomodation and the conference venue are available on the worldwide web at http://hort.cri.nz/nzic

Conference Contact: Stan Moore (s.moore@massey.ac.nz)

WEDNESDAY, DECEMBER 5TH

Time	Century	Breakout 1	Breakout 2	Exhibition	Founders'
8.20	Opening Remarks				
8.30	P1-Imperiali				
	Glycotechnology	*Analysis of Bioactives*	*Inorganic Chemistry*	*Fats & Oils/ Food and Health*	*Biotechnology*
9.30	GT1-Slim	AB1-Ross	IC1-Powell	FO/FH1-MacGibbon	BT1-France/Maddox
9.50	GT2-McJarrow	AB2-Anderson		FO/FH2-Melton	
10.10	GT3-Kröger	AB3-Holland	IC2-Dickinson	FO/FH3-McKenzie	NZBA Distinguished Biotechnologist Award
10.30			MORNING TEA		
11.00	P2-Collins				
12.00			LUNCH		
		Green Chemistry	*Molecular D & C*	*Fats & Oils*	*Biotechnology*
1.00	NZSBMB Applied	GC1-Collins	MDC1-Spicer	FO4-Catchpole	BT2-McKenzie
1.20	Biosystems Award	GC2-Wright	MDC2-McKeown	FO5-Hirst	BT3-Marsh
1.40	Scott	GC3-Wingate	MDC3-Tercel	FO6-Robinson	BT4-Tagg
		C & M Biology	*Glycotechnology*	*Food and Health*	*Biotechnology*
2.00	Easterfield Award	CMB1-McInnes	GT4-Lenz	FH4-McGhieBT5-Hein	
2.20	Brooker	CMB2-Edwards	GT5-Evans	FH5-HarcourtBT6-Taylor	
2.40		CMB3-Jordan	GT6-Blattner	FH6-MucaloBT7-Yorke	
3.00			AFTERNOON TEA		
3.30	P3-Demain				
	Biotechnology	*C & M Biology*	*Molecular D & C*		*Inorganic Chemistry*
4.30	BT8-Kennedy	CMB4-Askarian-Amiri	MDC4-Morris		IC3-Workman
4.50	BT9-Farrell	CMB5-Magan	MDC5-Furkert*Ca		IC4-Morgan
5.10	BT10-Welman	CMB6-Hood	MDC6-Larsen		IC5-Spencer
5.30	BT11-Demain	CMB7-Muratovska	MDC7-Hoberg		IC6-Curnow
6.00			ART DECO WALK		
7.00			POSTERS - GALLERY		

THURSDAY, DECEMBER 6TH

Time	Century	Breakout 1	Breakout 2	Exhibition	Founders'
8.20	Opening Remarks				
8.30	P4-Sander				
	Computational Biology	*Nanomaterials*	*Green Chemistry*	*Electrochemistry*	*Molecular D & C*
9.30	COM1-Collins	*Symposium*	GC4-Hillary	EC1-Kilmartin	MDC8-Smith
9.50	COM2-Stojmirovic		GC5-Robinson	EC2- Tizzard	MDC9-Sumby
10.10	COM3-Tweedie		GC6-Langdon	EC3-Dana	MDC10-Tan
10.30			MORNING TEA		
11.00	P5-Tasker	*Nanomaterials*			
		Symposium			
12.00			LUNCH		
	Inorganic Chemistry	*Nanomaterials*	*Structural Biology*	*Chemical Education*	*Analysis of Bioactives*
1.00	IC7-Murray	*Symposium*	SB1-Gonen	CE1 - Exploring the Learning Potential of New Technologies	AB4-Meagher
1.20			SB2-Jameson	Discussion Forum	AB5-Holroyd
1.40	IC8-Brodie		SB3-Baker		AB6-Tavendale
	Inorganic Chemistry		*C & M Biology*	*Chemical Education*	*Biotechnology*
2.00	IC9-Evans*		CMB8-Glover	CE2-Dalgety	BT12-Quinn
2.20	IC10-Otter		CMB9-Robertson	CE3-Salter	BT13-Lorimer
2.40	IC11-Brothers		CMB10-Stowell	CE4-France	BT14-Davis
				CE5-Carlisle	
3.00			AFTERNOON TEA		
3.30	P6-Quinn				
	Natural Products	*Physical Chemistry*	*Fats & Oils*	*Publish & Perish*	*X-Ray Crystallography*
4.30	BT15/NP1-Webb	PC1-McGrath	FO7-Eyres	PP1-Jackson	XR1-Gainsford
4.50	BT16/NP2-Northcote	PC2-Phillips	FO8-Franich	PP2-Penny	XR2-Adams
5.10	BT17/NP3-Blunt	PC3-Waterland	FO9-Shaw	PP3-Watson	XR3-Wikaira
5.30	BT18/NP4-Pasco	PC4-Smith	FO10-Sun	DISCUSSION	XR4-Davidson
6.00		NZBA AGM	NZSBMB AGM	NZIC AGM	
7.30			PRE-DINNER DRINKS		
8.00			DINNER		

FRIDAY, DECEMBER 7TH

Time	Century	Breakout 1	Breakout 2	Exhibition	Founders'
8.20	Opening Remarks				
8.30	P7-Wilson				
	Molecular Basis of Disease	*Nanomaterials Symposium*	*Inorganic*	*Green Chemistry*	*Biotechnology*
9.30	MD1-Brader		IC12-Ward	GC7-Weatherburn	BT19-Buchanan
9.50	MD2-Harper			GC8-Rate	BT20-Haines
10.10	MD3-Palmer		IC13-Edie	GC9-	BT21-TBA
10.30			MORNING TEA		
11.00	P8-Easton	*Nanomaterials Symposium*			
12.00			LUNCH		
	Structural Biology	*Nanomaterials*	*Molecular D & C*	*Electrochemistry*	*Biotechnology*
1.00	SB4-Welham	*Symposium*	MDC11-Fielder	EC4-Hall	BT22-Ward
1.20	SB5-Pytel/Clark		MDC12-Dixon	EC5-Downard	BT23-Rades
1.40	SB6-Dobson		MDC13-Edmonds	EC6-Miskelly	BT24-Severn
	Biochemistry		*Molecular D & C*	*Electrochemistry*	*Biotechnology*
2.00	BC1-Berridge		MDC14-Martyn	EC7- Havercamp	BT25-Snowball
2.20	BC2-Vissers		MDC15-Lee	EC8- McQuillan	BT26-Lanzon
2.40	BC3-Gerrard		MDC16-Denny	EC9-Hart	BT27-Buddle
3.00			AFTERNOON TEA		
	Biochemistry	*Nanomaterials*	*Molecular D & C*	*Natural Products*	*Biotechnology*
3.30	BC4-Brittain	*Symposium*	MDC17-Rewcastle	NP5-Prinsep	BT28-Dempster
3.50	BC5-Parker		MDC18-Miller	NP6-Mitchell	BT29-Heath
4.10	BC6-Templeton		MDC19-Abell	NP7-Bendall	BT30-Brenton-Rule
4.30	Closing Remarks				
7.30			BUS TO CLEARVIEW		
8.00			WINERY VISIT		

Update

BENZYNES

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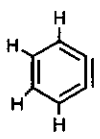
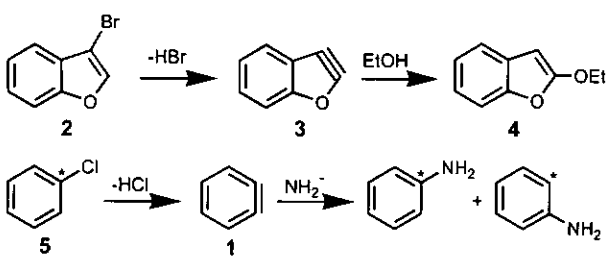
The occurrence of benzynes—or didehydrobenzenes, e.g. (**1**), as they are commonly termed—is something that most chemistry graduates are aware of from even the briefest study of reactive intermediates in organic chemistry.



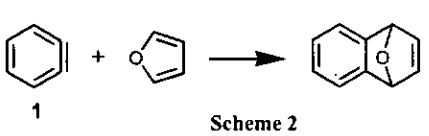
1

What will be surprising to many is that the first suggestion of the possibility of an aromatic molecule having two hydrogen atoms *fewer* than the number required for conventional bonding was made almost exactly 100 years ago. On April 2, 1902 Stoemer and Kahlert submitted a paper to *Berechte* reporting that 3-bromobenzofuran (**2**), a *non-benzenoid* aromatic, gave the 2-ethoxy derivative **4** upon treatment with strong base in the presence alcohol.[1] They suggested that 2,3-didehydrobenzofuran (**3**) was the likely intermediate but, despite this, it was not until 1942 that the existence of a benzene species was proposed. The original pronouncement was made by Wittig[2] and then substantiated by Roberts and coworkers some 11 years later.[3] These authors showed that the label (*) in [1-^{14}C]chlorobenzene (**5**) was scrambled to the 1-, 2- and 6-positions upon reaction with potassium amide as a 1:1 mixture of [1-^{14}C]- and [2-^{14}C]aniline is formed; *o*-benzyne (**1**) is the obvious intermediate (Scheme 1).



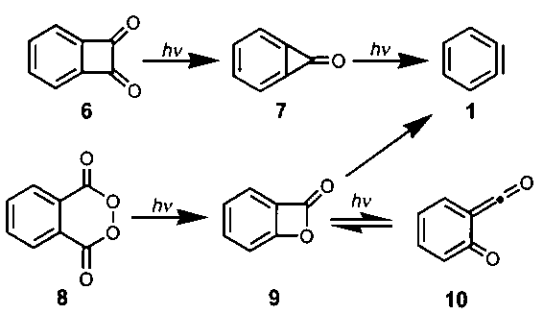
Scheme 1

Since those times the availability of simple and straightforward routes to *o*-benzyne (**1**) have led to it commanding considerable attention from the chemical community. In large part, this stems from the ease by which **1** acts as a dienophile and undergoes Diels-Alder cycloadditions with dienes that allow for the direct incorporation of a benzene ring into larger molecules as illustrated in Scheme 2.



Scheme 2

While trapping of a proposed reactive molecule implies the possible presence of that species it does not actually prove its existence, rather it demonstrates unambiguously that something with the symmetry of the proposed intermediate was present. Thus, there has been much effort directed to gain physical evidence to support the formation of benzynes usually by use of spectroscopic methods. Additional direct evidence for the existence of **1** came in the 1960s when its ultraviolet[4] and mass spectra[5] were recorded. However, in 1973 specific spectroscopic proof for the existence of **1** as an isolable albeit reactive intermediate came from matrix isolation and the observation of the infrared (IR) spectrum of the molecule. Chapman and his group[6] showed that, upon photolysis, the two substrates **6** and **8** (Scheme 3) lose carbon monoxide and carbon dioxide and generate **1** (via **7** and **9**, respectively), a process that has received considerable further attention (*vide infra*).



Scheme 3

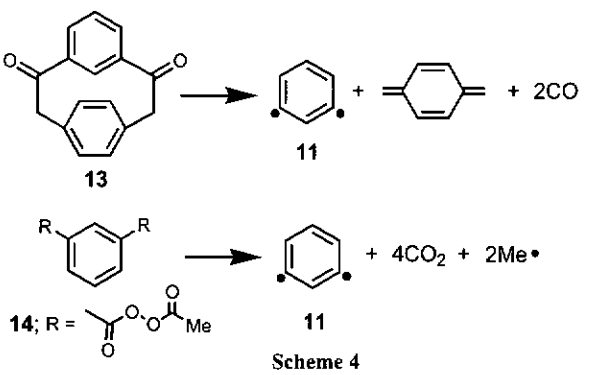
Matrix isolation is employed because this technique allows for the trapping of the reactive molecule in a rigid and inert environment. This prevents diffusion of the 'reactive' species and so minimises the possibility of any subsequent intermolecular reaction. Under low temperature conditions—generally 4-77 K—a unimolecular reaction is inhibited when the activation barrier is less than about 10 kJ mol^{-1}. The IR spectrum recorded for a molecule trapped in a low temperature matrix is remarkably similar to that obtained in the gas-phase and this allows for direct comparison of the observed spectrum with that calculated for the compound. IR spectroscopy is the most important spectroscopic tool for inert matrix work. Because of the dramatic improvements in computer capacity and the ready availability of quantum chemical programs, high level *ab initio* calculations of molecular vibrational frequencies are now almost routinely performed. The use of such calculations when coupled with state-of-the-art experimental techniques allows for confident characterisation of highly reactive molecules. Benzyne

(**1**) was revisited in 1992 and a complete set of the molecular vibrational frequencies was obtained.[7]

The state of knowledge concerning *m*- (**11**) and *p*-benzyne (**12**) is much less developed than for **1** because the reactivities are higher and the number of possible preparative routes is much smaller.

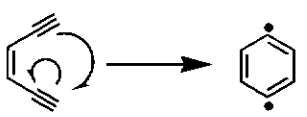
1 **11** **12**

The heats of formation for the three isomers **1**, **11** and **12** have been calculated[8] as ca. 446, 510 and 574 kJ mol^{-1}. However, despite the challenges, spectroscopic evidence for **11** was obtained in 1996 and this information came from matrix studies using the cyclophane **13** and the bis-perester **14** as precursors (Scheme 4).[9]



Scheme 4

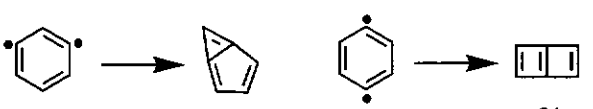
In contrast, thermolysis of the enediyne **15** gave rise to *p*-benzyne **12** by way of the well-known Bergman cyclisation (Scheme 5).[10] Enediynes are potent anticancer drugs and the recent understanding gained in their mode of action[11] has created much interest in the benzynes **12**, **11** and **1**. The isolation and better characterisation of these species is expected to be of much assistance in the study of enediyne antitumor drug action.[12]



15 **Scheme 5** **12**

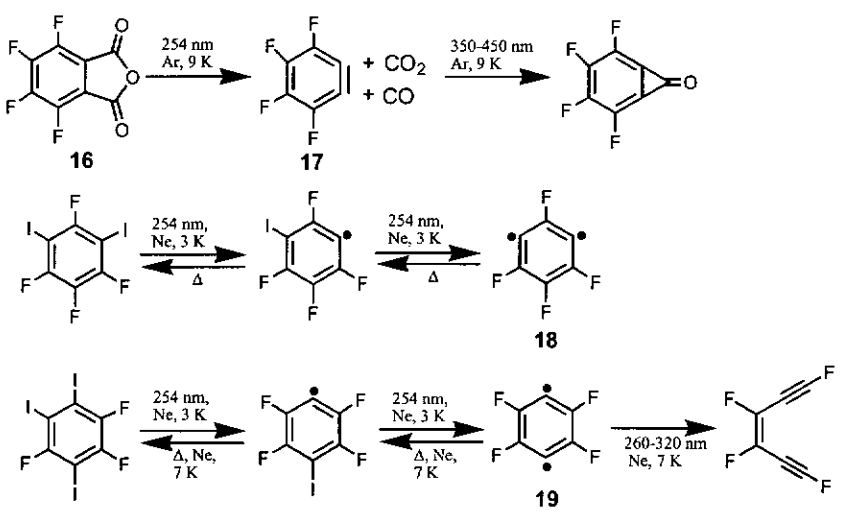
Despite the spectroscopic characterisation of **11** and **12**, all attempts to isolate and characterise derivatives had failed until quite recently. Sander and his students in Bochum[13] now have isolated the perfluorinated derivatives of **1**, **11** and **12**. Photolysis of matrix isolated perfluorophthalic anhydride (**16**) gives perfluoro-1,2-didehydrobenzene (**17**) in a clean reaction that has allowed not only for its isolation and characterisation, but also for its cycloaddition and insertion chemistry to be studied at the low temperatures involved.[13] Reaction with carbon monoxide contained in the matrix, under long wavelength irradiation, gave the cyclopropenone shown. In like manner, but using di-iodo precursors, the 1,3- (**18**)[13] and 1,4- (**19**)[14] analogues have been obtained by sequential (but thermally reversible) loss of iodine atoms in the matrix (Scheme 6). Calculations have suggested that fluorinated **19** should be *more* stable than its ring-opened enediyne isomer and this has proved to be the case. Once formed, it takes irradiation at a wavelength slightly longer than that used for the formation of **19** (>260 nm) to bring about the ring opening.[14]

The isolation and characterisation of derivatives of **11** and **12** promotes the question of whether *m*- and *p*-benzyne exist as the open shell diradicals depicted or whether there might be a preference for the bicyclic forms **20** and **21**. Hess and others have addressed these issues.[15] Detailed density functional *ab initio* calculations lead to the conclusion that *m*-benzyne (**11**) and its bicyclic isomer **20** have very similar energies and it seems that **11** might well exist in the bicyclic form **20**. In similar vein, while the ring-closed form **21** of *p*-benzyne (**12**) is expected to be strongly antiaromatic, Hess[15] has concluded that it is a strong candidate for low temperature isolation in a matrix; no doubt time will tell.



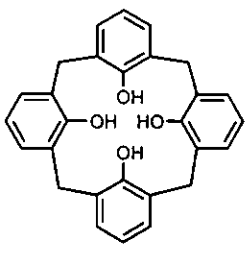
11 **20** **12** **21**

In parallel with the developments in matrix isolation discussed above there has been an upsurge of interest in host-guest chemistry as pioneered by the late Professor Cram at UCLA.[16] The synthesis of the first molecular container compound by his group[17] initiated the concept of stabilising a reactive molecule by incarceration inside

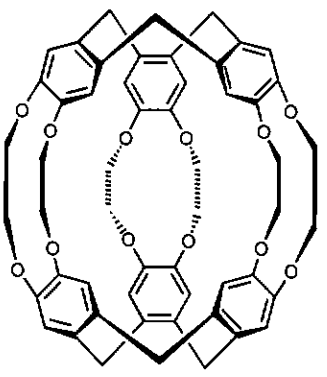


Scheme 6

such a species. A container molecule is hollow, often spherical in shape and with interior cavities that can hold a single guest molecule. The guest is unable to exit from the host because there is no 'hole' large enough in the outer shell for it to pass through. If the guest is a permanent prisoner and cannot escape even at high temperature, the host is termed a cryptophane or, more correctly a *carceplex*, but if the outer shell expands sufficiently to provide a hole large enough for the guest to exit (or exchange) then it is a *hemicarceplex*. The calixarenes[18] as illustrated by **22**, provide the spherical shape and find use as host "end caps" that can be tethered together by appropriate chains to provide a cryptophane, *e.g.* **23**. What is more, the non-covalent binding of the host within the guest has provided for 'chemistry within the host'.[19]



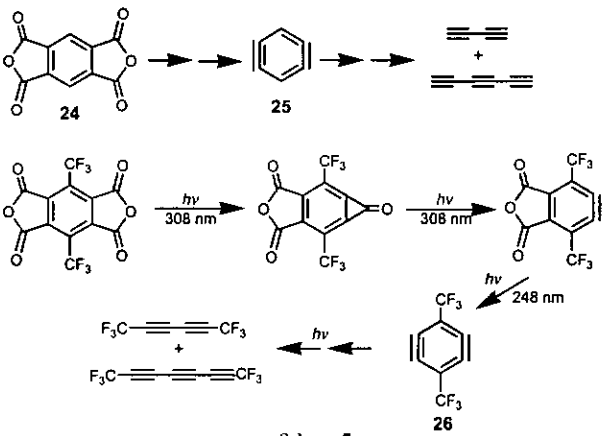
22, a calix[4]arene



23, a cryptophane or hemicarceplex

In the context of the didehydrobenzenes, progenitor **6** (Scheme 3) has been incarcerated inside an appropriate calix[4]arene molecular container and its photochemistry studied.[20] This is illustrated in Figure 1. Photodecarbonylation leads firstly to **7** and then to **1** each of which is unable to escape from the container. Because reagents cannot reach these entrapped reactive molecules they have relatively long lifetimes.[20] Benzyne (**1**) undergoes reaction with the container wall but remained long enough for its ^{1}H and ^{13}C NMR spectra to be recorded *in situ*. Comparison with data for similarly incarcerated benzene shows the aromatic ring current to remain intact in **1** and the coupling pattern matches theory. Precursor **7** is unstable above ca. –75 °C in solution but it is held tightly in the hemicarceplex and it is sufficiently stable in the solid state that an X-ray crystal structure has been obtained at room temperature although the data have yet to appear.[20]

The possible existence of a bis-benzyne *within the same benzenoid ring* has also been addressed in recent times. 1,2-Eliminations coupled with trapping experiments invariably lead to products that result from sequential benzyne generation with the first benzyne trapped before the second is generated.[21] Studies by Yabe and his group[22] in 1995, employing matrix techniques, implied that **25** was formed during photolysis of the di-anhydride **24**. More recently, the same authors isolated the trifluoromethyl-substituted derivative **26** and provided spectroscopic evidence in support of it.[23] Even more recent theoretical studies support their conclusion.[24]



Scheme 7

The study of the didehydrobenzenes has provided a wealth of fascinating chemistry. While much has been accomplished in the 50 years since Roberts proved the existence of *o*-benzyne, it is clear that this fascinating area of organic chemistry has much to offer from further investigation.

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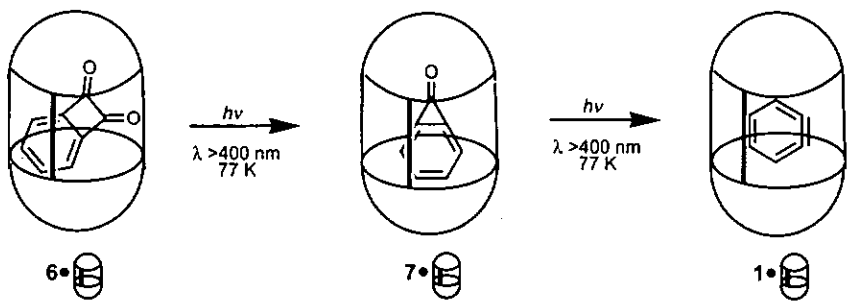

Figure 1. 1,2-Didehydrobenzene formed inside a host.

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2001 New Zealand Association Of Scientists Awards

The New Zealand Association of Scientists has announced its 2001 awards with a ceremony on October 18 at the Foundation for Research, Science and Technology. The **Rt. Hon. Pete Hodgson, Minister of Research, Science and Technology**, presented the certificates and medals.

The New Zealand Association of Scientists Certificate for Science Journalism, sponsored by the Association of CRIs, was awarded to **Kim Hill** of Radio New Zealand especially for her interviews with the New Zealand Nobel Laureates Professors Alan MacDiarmid and Maurice Wilkins and that with Professor Brian Wynne covering "science and society" with reference to stem cell research. **Lisa Glass** of Television New Zealand's **Assignment** programme brought flair and imagination to health science reporting on news programmes while **Anne Beston** of the *New Zealand Herald* was commended for quality reporting that reflected a good understanding of the subject matter.

The Communicator Awards, sponsored by FoRST, are made to two scientists and one freelance writer or professional science communicator. The scientist prizes went to **Dr Chris De Fretas** of the University of Auckland Geography Department on the Tamaki Campus for a variety of topical issues related to global warming, and to **Mr Graham Shepherd** of Landcare Research in Palmerston North for his communications on soil management and in particular visual soil management. **Caroline Cook** of Dunedin won the professional science communicator award for her work as Director of the International Festival of Environment Science and Technology in Dunedin and the Auckland Regional Science Festival, events that attracted high attendances well publicised in the popular media.

The New Zealand Association of Scientists **Research Medal**, awarded to an under 40 year old, this year went to **Dr Robert Poulin** of the University of Otago's Zoology Department for his outstanding contribution in the area of evolutionary ecology of parasites.

The **Shorland Medal** is in recognition of an outstanding lifetime contribution to basic or applied research that has added significantly to scientific understanding. Named in honour of the late **Dr Brian Shorland**, the third such award has gone to **Professor Brian Halton** of Victoria University of Wellington's School of Chemical and Physical Sciences. It recognises his contribution to fundamental research in organic chemistry that has taken the class of molecules known as the cycloproparenes from relative obscurity to widespread recognition. From beginnings in the early 1960s, these highly strained organic compounds have novel yet potentially important properties. Professor Halton's work has led to some 115 of his 145 publications in major international journals dealing with this area.

The **Marsden Medal** is awarded for a lifetime of outstanding service to science. This year the medal went to **Dr Ian Speden** of the Institute of Geological and Nuclear Sciences for outstanding service to earth sciences, and science in general. He made a specialist contribution to knowledge of New Zealand fossils and had a long-term interest in applying geology to practical problems that led to many multi-disciplinary studies. He was Director of New Zealand Geological Survey and has had many administrative roles in science management; currently he is Vice-President of the International Union of Geological Societies.

Ed.

Travels with a lap-top, August-September 2001

Leon Phillips
Department of Chemistry, University of Canterbury, Private Bag 4800, Christchurch

I was in Italy for four weeks, in the United States for most of a week, and in aeroplanes the rest of the time. I owe this trip to the generosity of the University of Canterbury's Erskine fund. The final week was affected by the terrorist outrages with great uncertainty about when flights from Europe to the US would resume. Eventually I found myself on the first flight from Frankfurt to O'Hare. This was after a long wait in Rome while Lufthansa made sure the connecting flight existed, so that they wouldn't have to put me up at a hotel in Bad Homburg or somewhere, Frankfurt already being full of undelivered passengers. Once underway, there were much more tedious airport security checks, several flights cancelled without warning, and no private vehicle access at Los Angeles airport (LAX). Nevertheless, my schedule of visits was completed essentially as planned.

In Italy I used the University of Perugia, where I had worked previously, as a base for visits to Bologna, Firenze (both Università di Firenze and the associated European Research Centre for Lasers and Spectroscopy), Roma (La Sapienza) and Napoli. The consensus among my friends in Perugia was that a visit to Bari would involve a very long rail journey for little purpose, because almost nothing of interest was going on there, so I yielded to time-pressure and cut the University of Bari from the itinerary. My friends at Perugia included Piero Casavecchia who is to be a Visiting Erskine Fellow at Canterbury during 2002. He was very helpful in contacting people to arrange suitable times for my visits — not an easy task during August in Italy. It probably helped that he could say I was President of NZIC! Near the end of my stay, Vincenzo Aquilanti, an eminent theoretician with many better things to do, cheerfully spent more than an hour on the telephone before he succeeded in finding a human operator at the United Airlines office in Milan who could state, with some degree of certainty, that my flight from Frankfurt to Chicago had not been cancelled.

I gave my more popular seminar, "*Venus - not just a pretty face*", at most of the places I visited and also spoke at two conferences. One was a workshop on the hydrogen bond at the University of Bologna, where I talked about the structure of a liquid surface and my host Walther Caminati made sure I knew that their first degree (in law) was awarded in 1088. He also produced an extraordinary outdoor meal for workshop participants — and assorted friends and relations — at a partly restored villa on some hectares of land he owned in the hills around Bologna. A variety of salads and pastas, wine from his own grapes, and prosciutto crudo con fichi with ripe figs plucked from the nearby trees formed the offering. At the other conference, the 26th International Symposium on Free Radicals held in Assisi, near Perugia, I gave a brief talk summarising my poster about free radical processes in the clouds of Venus and I also chaired a session. This was a major meeting and new results were presented by leading experimentalists from places where it is understood that advances in scientific knowledge and instrumentation go hand-in-hand, so that it is essential to have an adequate source of contestable funding for research equipment. The first paper at this meeting was by Xie-Ming Yang from Taiwan, recipient of the H. P. Broida Award for Free-Radical Research, in recognition of his highly sophisticated molecular-beam studies of chemical reaction dynamics. He is also to be a plenary lecturer at CPC2002, the joint RACI/NZIC meeting that will be held in Christchurch during February 2002 (for further information, see the University of Canterbury, Chemistry Department web page).

One of the stated objectives of the trip was to visit universities in Italy and learn what they are teaching in chemistry, what is happening to their degree structure, and how they are doing in general. The question about teaching can be answered very quickly. They try to teach essentially the same material as we do but, like us, are finding it necessary to lower standards. Expectations are reduced because of a general dilution of the secondary-school curriculum, an increase in the number of students without a corresponding increase in the number of really capable students, and a fall in the proportion of students who are motivated to study fundamental scientific disciplines relative to those who attend university solely in order to secure their entry into a money-making profession. The question about degree structure is more interesting.

Before 1 October 2001 the Italian degree structure comprised a 5-year Laurea, with no restriction on entry, after 13 years of elementary and secondary schooling from age 6. The Laurea could be followed immediately by a fixed-duration 3-year Ph.D. Potential academics would then be expected to spend two or three years gaining experience as a postdoctoral fellow before entering the academic ladder in their thirties as a research assistant in an established research group. Completion of the Laurea entitled a graduate to be called Dottore, which is the reason most professional people in Italy have this title. From my own acquaintance I know that Laurea graduates in chemistry are very knowledgeable and well-prepared for a career in research, but are not necessarily highly motivated and are probably over-qualified for a career in industry.

This system has some obvious disadvantages. Five years is much too long for a first degree. The extra year of schooling (compared with the rest of Europe) means that students are fairly mature and liable to have been rendered mentally inflexible from much rote-learning by the time they enter university. The unrestricted entry means that there is no way of assessing the ability of entering students, so subjects like chemistry have a very high failure rate in the first year. Also, students are liable to enter university for political rather than academic reasons and, when the number of students reaches 150,000, as it does in Rome

and several other large centres, the political consequences of angering the student body are not to be taken lightly.

The problem of the extra year of schooling (and, I would say, the late start at age 6) has still to be addressed, but since October 1st there has been a new degree structure, with a 3-year Laureate, which brings Italy more into line with the rest of the European Union. This should provide the necessary flow of graduates at a suitable level to enter employment. A further two years of work will lead to a diploma roughly equivalent to our master's degree, and make the diploma-holder eligible to undertake research for a PhD Different institutions will work out the details in their own individual ways and it will probably not be any easier than it is now for students to transfer between institutions or even departments — for example, in one major university the chemistry department teaches and examines on a semester system, while the physics department operates a three-term system, so a joint degree is practically impossible. At the same institution, from this year onwards the chemistry department plans to teach all their students at a given level on only three days a week, albeit more intensively, so they can study at home on the other two days and so reduce the amount of time wasted on travelling, typically an hour each way. Other departments might decide to follow suit in later years, but in Italy there must always be scope for individual flair.

The question of how well they are doing in general does not have a simple answer, but I would judge that they are doing rather better than we are. In chemistry, their past low level of support for experimental research, at least relative to the more affluent countries of western Europe, has caused them to be very strong and active in theory at the present time. There are now signs that this emphasis is changing, with many groups working in the more expensive areas such as molecular beams, and significant major facilities such as the synchrotron at Trieste and the laser laboratory at Firenze. The European Union provides generous funding to encourage co-operation between researchers with the exchange of postdoctoral fellows among different EU countries. One incidental consequence of this is a trend towards greater uniformity in the standard of research equipment in the various countries, although Spain and, to a lesser extent, Italy have quite a lot of catching up to do. In contrast to the present situation in New Zealand, in Europe there appears to be wide general recognition of the importance of basic research in universities as a source of graduates and ideas for society and industry. Here, in contrast, the universities are severely under-funded for the training of graduate students in the physical sciences, so this work has to be done at a loss, and the existence of research by staff is not even recognised. Possibly the current proposals from Vice-Chancellors Committtee to TEAC for performance-based research funding will improve the lot of our experimental research schools relative to private providers, polytechnics, and paper-based university disciplines, but that remains to be seen.

In the United States I visited the University of Wisconsin, in Madison, and the University of California at Irvine. At both of these (admittedly relatively well-endowed) places there is more and better equipment in the undergraduate teaching laboratories than we have in our best research laboratories. It is also worth pointing out that in the USA it is generally acknowledged that it makes no sense whatever to appoint an academic on the basis of his or her capacity to do original research and then deny the appointee the means to carry out said research. At Wisconsin they were complaining that they recently lost out on appointing an outstanding candidate as a new assistant professor in organic chemistry (not normally a field in which individuals require a lot of expensive dedicated equipment, as opposed to having access by their students to expensive general facilities) because they could not quite match the $US750,000 start-up grant that Berkeley were offering.

At Wisconsin I interacted mainly with the group of Gil Nathanson, a recent visitor to Canterbury, who does highly original molecular-beam experiments on liquid surfaces. I also did my best not to look too downhearted while touring the multi-laser dynamics laboratories of Fleming Crim, and delivered my seminars about what goes on at a liquid surface and photochemical reactions in the clouds of Venus. At Wisconsin I was interested to meet several faculty members a decade or more older than I am and still going strong. A notable feature of physical chemistry at Wisconsin is the number of people who are working on protein dynamics, lipid membranes and other biologically-oriented topics.

At Irvine, where there is a big emphasis on atmospheric chemistry, I mainly visited the group of Barbara Finlayson-Pitts, who with her husband Jim Pitts has written what promises to be the definitive text in this field for many years to come. By great good fortune I had just written an enthusiastic review of their book for the *Journal of Atmospheric Science*. Ralph Cicerone, Chancellor of the University of California at Irvine and a distinguished atmospheric scientist himself, is the person who first pointed out the likely deleterious effects of chlorine release in the stratosphere in connection with the Thiokol rocket fuel that was initially chosen for the space shuttle. The building in which Barbara has her laboratory is now called Rowland Hall, after F. Sherwood Rowland, a Visiting Erskine Fellow at Canterbury during the late 1970s who, together with his student Mario Molina, was awarded the Nobel Prize in Chemistry for discovering the effect of halocarbons on the ozone layer. At the time of my visit Sherry Rowland was out of town, doing something important in his capacity as International Vice-President for the US Academy of Science, but he sent his regards to his friends at Canterbury.

Nowadays, visits to laboratories in the United States manage to be simultaneously stimulating and depressing — no mean feat.

Apology

Credits for the photographs of Professor MacDiarmid used in the last issue were inadvertently omitted. We are grateful to Victoria University (Image Services) (cover - upper) and Massey News (cover – lower) for permission to reproduce these photographs.

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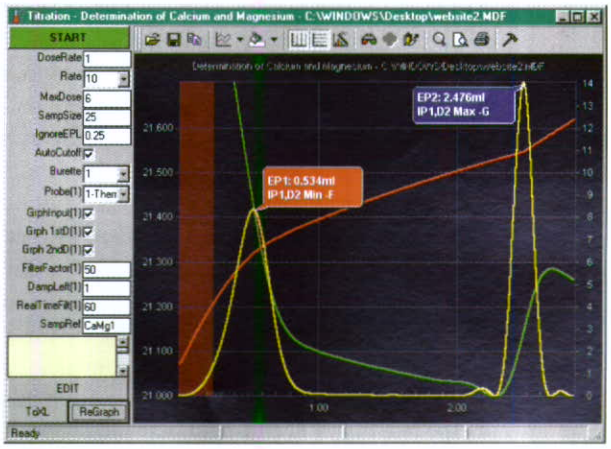

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For further information on the Oakton range of products or to request a catalogue:

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NEW SULFUR-IN-OIL ANALYSER

In response to the recent increases in regulatory standards regarding sulfur content in diesel fuel as well as heavy and light oil, Ai Scientific introduces a new series of sulfur-in-oil analysers from Horiba - the SFLA-2800/2100 range. Based on the technique of non-dispersive X-ray flourescent analysis, the SLFA-2800/2100 units have an analysis range of 0 - 5 % sulfur with a detection limit of 5 ppm sulfur. The measurement time is set during the preparation of calibration curves at any value between 10 and 600 seconds (in accordance with required precision). The instrument's memory holds up to 5 different calibration curves for different sample types which can be manually or automatically selected during each sample measurement. Samples are presented in "no mess" disposable cells and results are displayed on an easy-to-read LCD screen.

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NEW VISCOMETER COMPLIES TO ASTM D445

NEW PRODUCTS

Ai Scientific announces the release of the new MINIVIS II from Grabner. The MINIVIS II features a new ball detection principle with reflection sensors which extends its application to both clear and dark samples. The viscosity range is expanded from 0.2 to 1,500 mPas/cSt across a temperature range of 0-100 °C. The MINIVIS II gives an easier alternative to measuring viscosity by glass capillaries. The precision of the results obtained are the same as specified in ASTM Method D445 but the measuring time only takes 3 to 10 minutes (depending on viscosity). Additional advantages are the use of a very small sample volume (0.4 mL) and a cleaning procedure that takes only a few minutes. The only interaction by the user with the instrument after the introduction of the sample is to enter the sample's density which is required to calculate the viscosity. The MINIVIS II also has an accessory valving system that is mounted on the back panel to control sample flow. This enables it to be connected as an at-line analyser for pre-programmed analysis.

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BIO-RAD ENHANCES KNOWITALL™ ANALYTICAL SYSTEM WITH IUPAC NAMING

Bio-Rad Laboratories, Inc., Informatics Division (www.bio-rad.com, www.sadtler.com) announced the addition of IUPAC naming and drawing functionality to their KnowItAll™ Analytical System. The integration of this new software plug-in is the result of Bio-Rad's collaboration with a third-party software vendor ChemInnovation Software, Inc., (http://www.cheminnovation.com), based in San Diego, CA.

The KnowItAll system's new IUPAC NameIt™ and IUPAC DrawIt™ facilitate the process of naming structures or creating structures based on systematic rules set forth by the International Union of Pure and Applied Chemistry (IUPAC) that are accepted internationally as the standard for chemical nomenclature. With Bio-Rad's IUPAC NameIt and IUPAC DrawIt, the user simply enters a structure or a name and the software automatically generates respectively either the systematic IUPAC name or structure. Generating names and structures this way not only saves time, but also ensures accuracy and standardisation of both communication and data mining within the laboratory.

Users can draw structures directly in the KnowItAll system or import structures from popular file formats. The IUPAC NameIt™ and IUPAC DrawIt™ software plug-ins support systematic and common names from most common organic compounds and can designate E,Z descriptors for double bonds and R,S configurations for chiral centers.

The new IUPAC plug-ins are part of Bio-Rad's KnowItAll Analytical System, a fully integrated, scalable environment that combines the power of Bio-Rad's software and analytical databases and allows chemists to search and analyze spectral data, build databases, draw structures, and generate high-quality reports. Since IUPAC NameIt™ and IUPAC DrawIt™ work within the KnowItAll environment, generated names and structures can easily be imported into KnowItAll databases.

Eric Melanson, Bio-Rad's Worldwide Marketing Manager comments, "Because of KnowItAll's unique architecture, software from third parties, like IUPAC NameIt and IUPAC DrawIt can be quickly and easily integrated into the KnowItAll system. As future customer input dictates the addition of new features and capabilities, the KnowItAll system is capable, through its benefit of 'plug-in's' of quickly adding value-added functionality that meets the growing needs of the chemistry community. We are pleased to work with ChemInnovation Software, Inc. to implement IUPAC naming and look forward to working with other third party software providers in the future."

For additional information on Bio-Rad Laboratories, Informatics Division, Sadtler Software and Databases:
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KnowItAll, NameIt, and DrawIt are trademarks of Bio-Rad Laboratories. Bio-Rad's IUPAC NameIt and IUPAC DrawIt software generate names and structures, respectively, based on systematic IUPAC rules. Use of the term IUPAC with these marks does not imply that Bio-Rad is affiliated with IUPAC.

Patent Proze

by Jane Calvert and Greg Lynch

CIPROFLOXACIN BUNGLE IN CANADA

Over the past month, Canada's Ministry of Health (Health Canada) and its officials have faced criticism over a debacle involving what appears to be a complete disregard of Canadian patent law.

The situation arose after Health Canada officials approached Bayer Inc., the Canadian subsidiary of the international group Bayer AG (Germany), to purchase the antibiotic Ciprofloxacin (Cipro). Health Canada was attempting to stockpile Cipro to protect Canadians in the event of an emergency should anthrax reach Canada.

It has been reported that Health Canada officials contacted Bayer by telephone about obtaining one million tablets of Cipro. Bayer reportedly said that it could not supply the quantity of Cipro that was requested. This prompted Health Canada to approach the Canadian pharmaceutical generics company Apotex Inc. to supply the one million tablets at a cost of Canadian $1.5 million. Unfortunately, it seems the Minister of Health and Apotex ignored the fact that Cipro was still the subject of a Canadian patent owned by Bayer.

Bayer denied that an order had been placed with them by Health Canada and insisted that it could supply the required number of tablets of Cipro to Health Canada. Bayer then threatened to sue for patent infringement.

At this threat, the Canadian Government proceeded to negotiate a deal with Bayer. The result was that Bayer agreed that it would supply one million tablets of Cipro within 48 hours of a request from Health Canada. Health Canada agreed to purchase all supplies of its Cipro requirements from Bayer, while Bayer's Canadian patent was in force. The patent will expire in 2004.

However, Health Canada was still not out of trouble. It had signed a contract with Apotex for a supply of Cipro, which it still had to honour. Although, the cost of solving this problem with Apotex has not been disclosed, it has been reported that Apotex will be paid by Health Canada for producing the Cipro tablets. But, rather than supplying the tablets to Health Canada, Apotex will supply them to Bayer. Bayer has agreed to hold the Apotex tablets in case Bayer cannot meet Health Canada's demand.

To make matters worse, the whole situation could have been avoided if Health Canada had made use of the provisions in the Canadian Patent Act that authorise the Governmental use of a patented invention in situations of national emergency or extreme urgency.

Under Canadian law, the Government can make an application to the Commissioner of Patents for authorisation to use technology covered by a patent. The Commissioner may authorise the use of a patented invention on the following principles:
(a) the scope and duration of the use shall be limited to the purpose for which the use is authorised;
(b) the use shall be non-exclusive; and
(c) any use shall be authorised predominantly to supply the domestic market.

It is easy to appreciate that these principles could have been satisfied by Health Canada if it had made an application under this provision. You may recall that similar provisions exist in New Zealand's patent legislation, which was the subject of *Patent Proze* - Crown Use of A Patented Invention *Chemistry in New Zealand*, **2000**, *65:2*.

Other issues in this saga have added to Health Canada's problems. Health Canada has not yet granted approval for the use of Cipro for the treatment of inhalation anthrax. It appears that Health Canada does not see that formal approval is necessary at this stage when its aim is to stockpile Cipro.

With the FDA having recently approved the use of Cipro for inhalation anthrax in the United States, it is likely that Canada will fallback on the FDA's position, if necessary. It is interesting to note that, to date, there have been no reported studies on the use of Cipro to treat inhalation anthrax in humans. All known clinical studies have only been carried out on animals.

Not surprisingly, the credibility of the Canadian Minister of Health has been the subject of much debate. His credibility has not been helped by the fact that some years ago he was legal counsel for Apotex. One would have thought that experience as legal counsel in a generics pharmaceutical company would have given rise to a healthy knowledge Canada's patent legislation.

If you have any questions please direct these to:
Patent Proze, P O Box 852 Wellington
or E-mail@bsw.com

Jane Calvert

Jane Calvert and Greg Lynch are both patent attorneys and solicitors at Baldwin Shelston Waters, where they specialise in chemistry and biotechnology patents. Jane joined BSW after completing a PhD in chemistry at the University of Canterbury in 1994. Greg also joined BSW in 1994 after three years research at Industrial Research Limited in Wellington. Following completion of a PhD in chemistry at the University of Otago in 1989, he spent two years as a post-doctoral researcher at Oxford University.

Greg Lynch

The Analysis Of Trace Levels Of Gases In Complex Mixtures By Gas Phase Sampling Using Selected Ion Flow Tube-Mass Spectrometry

Colin G Freeman and Murray J McEwan
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The human nose is an extremely sensitive olfactory organ, detecting some odoriferous compounds at concentrations as low as a few ppt (parts per trillion by volume). Unfortunately it is not quantitative and neither can it recognise the individual components of many mixtures of trace Volatile Organic Compounds (VOCs). For some considerable time the scientific community has experimented with a number of different sorts of olfactory devices with varying degrees of success. *The advent of the technique of Selected Ion Flow Tube-mass spectrometry* (SIFT/MS) *has changed the way of thinking in trace gas detection, both in the simplicity of operation and in the sensitivity of detection.*

Interstellar Clouds:

The experimental system being used at the University of Canterbury has been developed during the last two decades with the express intention of studying reactions between ions and neutral molecules in the gas phase. Such ion-molecule reactions are of fundamental importance in the chemistry of *interstellar clouds*. About 35 years ago, practitioners of the rapidly developing field of radioastronomy discovered that molecular species were present in the tenuous clouds of gas that exist between stars. At the time it was suggested that ion-molecule reactions could account for much of the chemistry that was occurring in those regions of space where it was once thought that no chemistry was possible. Close to 120 different molecules and ions have now been identified in the interstellar medium (about 70% of these observed are organic compounds). By virtue of the enormous size of these interstellar clouds, it is reasonable to suppose that ion-molecule processes together with some neutral-radical reactions, make up a substantial fraction of all the chemistry that occurs in the Universe. Although the interstellar clouds (ISCs) are tenuous (10^3-10^6 particles cm^{-3}) and cold (10-50 K), ion molecule reactions thrive under these conditions where conventional chemistry virtually ceases because of activation barriers. Sequences of ion-molecule reactions that are known to occur from laboratory studies, along with some neutral-radical reactions, have been included in synthetic models and account quantitatively for the number densities observed by radioastronomy. The question of how these complex molecules are synthesised has been, and is still, a major theme of the current research programme being undertaken in the ion-molecule laboratory at the University of Canterbury.

Trace Gas Analysis:

An unexpected outcome of the very high sensitivity of the instrument we use [which, strictly speaking, is described as a Flowing Afterglow-Selected Ion Flow Drift Tube (FA/SIFDT)] is its ability to detect volatile chemicals at trace levels in surrounding air. In the normal mode of operation of the FA/SIFDT instrument, small measured flows of a neutral reactant are introduced into the SIFDT flow tube and all ions derived as products are recorded. The rate coefficient for reaction is found from the rate of disappearance of the reactant ion with increasing neutral flow. This procedure can, however, be made to work in reverse. If the rate coefficient and product profile for the reaction of an analyte are known and the flow rate of the gas mixture containing the analyte is monitored, then the product ion signals give a direct measure of the neutral analyte concentration in the gas mixture. This application of SIFT technology (or SIFT/MS as this application is called) is quite recent and was first reported by groups in Britain[1] and Austria.[2] Detection limits as low as a few parts per billion (ppb) and even parts per trillion (ppt) are quoted for real-time measurements. Because SIFT/MS technology has only recently been developed it is a burgeoning new field with enormous and exciting potential. Applications as diverse as identifying breath indicators for renal failure, the monitoring of plant volatiles, and the detection of formaldehyde in cells that had been subject to chemotherapy following breast cancer have already been discovered.

Application of the FA/SIFDT to studying ion-molecule reactions:

Ions formed by a microwave discharge in the ion creation region are mass selected by a quadrupole mass spectrometer and drifted into the reaction flow tube against a pressure gradient through a Venturi orifice. Under typical operating conditions in the flow tube there is a helium carrier gas ("solvent") present at a partial pressure of *ca.* 0.5 Torr, flowing at a velocity around 100 ms^{-1}. All products formed by reaction of the mass-selected ion with an added neutral are monitored by a second quadrupole mass spectrometer located at the downstream end of the flow tube. The product channel ratios are found by extrapolating the observed product ion ratios to zero neutral flow. Rate coefficients for reaction are found from the slope of the semilogarithmic decay of the reactant ion with neutral flow.

Measurement of VOCs at trace levels:

The gas mixture containing the VOC, *e.g.*, human breath, a headspace gas sample, or a mylar bag containing an atmospheric sample, is added through the heated capillary inlet shown in Figure 1. The precursor ion, which must not react with the main ingredients of the atmosphere (N_2, O_2, CO_2, Ar), reacts only with the VOC to generate product ions, all of which are monitored. Provided the concentration of the VOC is low and the flow of the gas mixture through the capillary and the ion chemistry are known, then the size of the product peaks are a direct measure of the number density of the VOC in the gas mixture. The precursor ions that are commonly used are

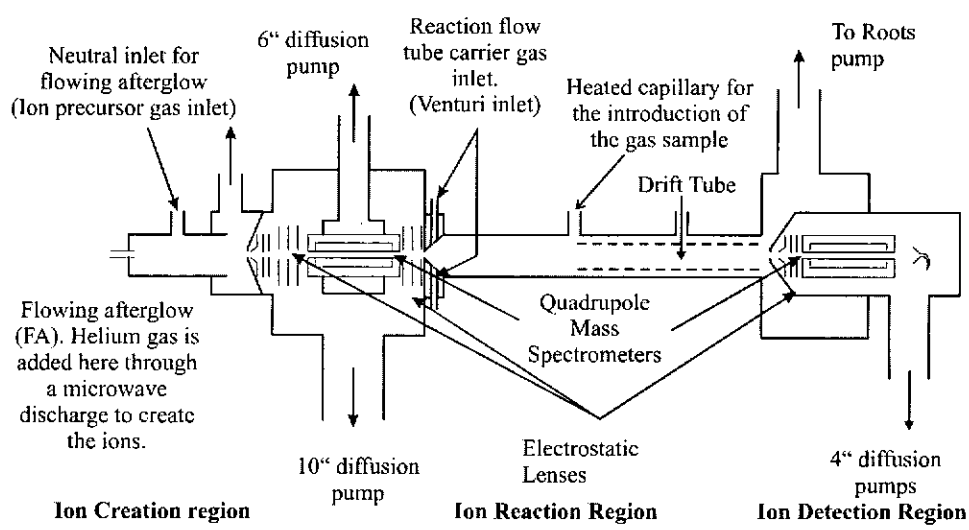
H_3O^+, O_2^+ and NO^+. Used in this way, the SIFT/MS technique can, for example, profile all the trace metabolites from a single breath in about 3 seconds at concentrations down to a few ppb. The sensitivity of the SIFT/MS analytical method depends on the time allowed for data acquisition. Several molecules can be quantified in a few seconds if their partial pressures are above a few ppb. Alternatively a single gas can be quantified at the 100 parts per trillion level in about 10 seconds of integration.

Our work in this area is new and exciting, and it presents countless opportunities for expansion. In experiments undertaken during the past 18 months, we have investigated the breath of athletes to see how their metabolism has changed under stress. We have also looked at the release of nitrogen in the form of nitrogen oxides, ammonia and amines, from nitrogenous fertilizers applied to soils. In addition, we have studied the rate of ethanol metabolism in breath and blood after drinking. The results from these examples have been published elsewhere.[3] We have since embarked on other applications of the SIFT/MS technique and work currently in progress includes: the examination of the volatile species released from unsmoked cigarettes and unsmoked marijuana; the residence time of industrial solvents in the human body; the identification of amines in metabolised blood samples from Antarctic Weddell seals; and the examination of grain for evidence of rancidity. In each of these new applications it is first necessary to establish the reaction chemistry of the target analyte with each possible ion precursor, *e.g.*, H_3O^+, O_2^+ or NO^+. In other words, the SIFT has to be "trained" to detect each new analyte. For each analyte, in each application, it is necessary to measure the complete product channel ratios as well as rate coefficients. This data is a fundamental requirement of the SIFT-MS technique in order for it to be used as an analytical tool.

The sensitivity and specificity of the SIFT/MS technique in the detection of volatile VOCs gives it a number of advantages over conventional analytical methods such as GC/MS, electronic "noses", and spectroscopic techniques in that it is done in *real time* without the need for pre-concentration steps. It is absolute without the need for calibration standards, it is not subject to contamination from different chemical species, and it is easily changed from one analyte to another. The successful application of the SIFT/MS method relies on the fact that the reactivity of the precursor ion with a particular analyte is known.

In theory both positive and negative precursor ions may be selected for SIFT mass spectrometry. However, the reactions of three positively charged precursor ions with a large number of organic compounds have been studied. Precursor ions H_3O^+ detect and quantify polar molecules, *e.g.*, ammonia, acetone, methanol, ethanol and dimethyl sulfide, as well as carboxylic ("fatty") acids. The O_2^+ ion reacts mainly by charge transfer to produce M^+ and fragment ions. The usefulness of this second precursor ion is that it reacts with some VOCs that are unreactive with H_3O^+ such as small hydrocarbons. The NO^+ ion can also be generated and is reactive with a wide range of trace species. While in many instances a trace VOC can be identified by a single precursor ion, in some circumstances the mass of the ion is not sufficient and it is useful to obtain the pattern of product ions from all precursor ions for identification. The use of these three precursor ions is therefore an enormous advantage in both the identification of the trace gases, especially when isomeric forms are possible, and also in verifying the accurate identification of a putative target trace gas.

At present all our measurements are made on an experimental system which is laboratory-based—more accurately, "anchored" since it weighs several tonnes! For many applications it would be a considerable advantage to have a portable instrument that could be taken to the air sample. This is obvious for clinical situations and for most environmental analytical applications, where there is the possibility of change in the composition of the trace gas mixture during storage through either chemical reaction or interaction with the walls of the sample container. We are at present in the process of designing and constructing a *ca.* 200 kg portable trolley-mounted version of the SIFT/MS. Once the largest energy barrier in this process has



Schematic Diagram of the Canterbury FA/SIFDT Instrument

Figure 1: The FA/SIFDT instrument—the common link between the disparate research areas of extraterrestrial chemistry and the detection of trace levels of volatile organic chemicals (VOCs) in ambient air.

been overcome, namely raising the necessary funds, there is seemingly unlimited potential for applications of the new technique.

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The 2001 Nobel Prize In Chemistry

The 2001 Nobel Prize in Chemistry, announced on October 10, has been awarded to. **Dr William S Knowles** (formerly of Monsanto, St. Louis, Missouri), **Professor Ryoji Noyori** (Nagoya University, Japan) and **Professor K Barry Sharpless** (The Scripps Research Institute, La Jolla, California). The Royal Swedish Academy of Sciences awarded the Prize for their development of catalytic asymmetric synthesis. The achievements of these three chemists are of great importance for academic research and for the development of new drugs and materials. Moreover the reactions are being used in many industrial syntheses of pharmaceutical products and other biologically active substances. The prize has been awarded in two parts, one half jointly between **Knowles** and **Noyori** for "their work on chirally catalysed hydrogenation reactions" and the other half to **Sharpless** for "his work on chirally catalysed oxidation reactions".

Now 84 years old, **Knowles** made the first chiral transition metal catalyst for hydrogenation reactions in the 1960s, thereby obtaining the desired enantiomer as the final product of reaction. In short order, his research led to an industrial process for the production of the L-DOPA drug that is used in the treatment of Parkinson's disease. Sixty-three years old, **Noyori** is Professor of Chemistry at Nagoya University in Japan. He has added further recent developments to the Knowles process to provide what are today's general chiral catalysts for hydrogenation. In contrast, 60-year-old **Sharpless** (formerly of MIT but now at Scripps Institute in California) gains his half of the Prize for developing chiral catalysts for oxidation reactions. In essence the 2001 Laureates have opened up a new field of research that has allowed for the results of their basic research to be used in a number of industrial syntheses of pharmaceutical products such as antibiotics, anti-inflammatory drugs and heart medicines.

It was Knowles' pioneer work of the early sixties that led to his 1968 breakthrough when he was working at Monsanto. Based upon earlier studies with the achiral rhodium catalyst $Rh(Ph_3P)_3Cl$, Knowles replaced the triphenylphosphine ligands by one of the enantiomers of a chiral phosphine. The initial phosphine was not enantiomerally pure but in the hydrogenation of a prochiral alkene it gave a product mixture in which there was 15% enantiomeric excess. Although modest and with little practical use, the result showed proved that catalytic asymmetric hydrogenation was possible. In short order, Knowles evolved the work into an industrial synthesis of the amino acid L-DOPA in high enantiomeric excess. The drug, useful in the treatment of Parkinson's disease, formed the basis for the award of the 2000 Nobel Prize in Physiology or Medicine to Carlsson. Subsequently Monsanto used the diphosphine ligand DiPAMP in a rhodium complex to give a 100% yield of DOPA enantiomers that contained 97.5% of the desired L-DOPA. This, the first catalytic asymmetric synthesis, has been succeeded now by many others.

Ryoji Noyori has led the development of better asymmetric hydrogenation catalysts not for alkenes as much as carbonyl compounds even in the presence of esters. In 1980 Noyori and his group synthesised of both enantiomers of the diphosphine ligand BINAP. Rhodium(I) complexes of BINAP catalyse the synthesis of certain amino acids with an enantiomeric excess of up to 100%. Exchanging the rhodium for ruthenium(II) gave a complex that hydrogenates many types of molecules with other functional groups present giving both high chemical yields and high enantiomeric excess. The Ru-BINAP is a catalyst used in the production of (*R*)-1,2-propandiol for the industrial synthesis of an antibiotic, levofloxacin. Noyori's catalysts have found wide application in the synthesis of fine chemicals, pharmaceutical products and new, advanced materials.

Alongside the advances in chirally catalysed hydrogenation reactions, Sharpless has developed corresponding chiral catalysts for oxidations. He recognised the great need for catalysts for asymmetric oxidations and has made several important discoveries that are exemplified by his chiral epoxidation. In 1980 he provided a practical method that led to the catalytic asymmetric oxidation of allylic alcohols to chiral epoxides by employing a chiral titanium complex that gives high enantiomeric excess. The catalyst results from reaction of $Ti(OPr\text{-}i)_4$ with diethyl D-tartarate. The metal simultaneously binds the chiral ligand, the hyperperoxide and the substrate and then effects the chiral epoxidation. The reaction has had very wide applications in both academic and industrial research such that many have identified the Sharpless epoxidation as the most important discovery in the field of synthesis during the past few decades.

Additional information is available from the Swedish Academy of Sciences: http://www.kva.se

Ed.

Report from ICBIC-10, 26-31 August 2001, Florence, Italy

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As part of a round-the-world trip, tending to collaborations in Paris; Washington DC; Portland, Oregon; and Vancouver, Canada, and checking out among other things how much greener the grass might be elsewhere, I attended the Tenth (neon) International Conference on Bioinorganic Chemistry in Florence, Italy, 26-31 August 2001. The trip was made possible by a generous inducement by the Conference Organisers of not only the opportunity to give a keynote lecture but cold hard cash.

I had attended the first of these conferences in 1983, also held in Florence, but none of the intervening meetings. It was interesting to see how the field of bioinorganic chemistry had changed and redefined its own image of itself over 18 years. In 1983, then an assistant professor at Georgetown University, Washington DC, I presented a poster on model systems for non-heme proteins that contain the mu-oxo diiron(III) motif (Fe^{III}-O^{-II}-Fe^{III}). This time I presented a talk on the structure of manganese superoxide dismutase at a resolution of 0.90 Å, a resolution only slightly inferior to that of most small molecules.

Bioinorganic chemistry has changed massively since the early 1980s. At the 400-strong 1983 meeting, most papers were on model systems for one biological system or another, and except for hemoglobin and myoglobin, most metalloenzymes had not been structurally characterised. By 2001, the balance has shifted with the majority of papers being on materials of direct biological origin. A substantial amount of work is now being done not *in vitro* but *in vivo* – the realm of the new area of Chemical Biology. Even more striking is the number of women scientists not merely in the area but at the forefront of the area of bioinorganic chemistry. Woman speakers comprised nearly a quarter of the total number of speakers, and about the same fraction of the 1200 registrants. In 1983, there were only a handful of women present.

I presented my paper on Tuesday covering work begun by PhD graduate and The Royal Society of New Zealand Hatherton Awardee Ross Edwards and continued by Bryan Anderson of the Institute of Molecular BioSciences at Massey University, on the structural determinants of activity of iron and manganese superoxide dismutases. This work (in collaboration with Jim and Mei Whittaker of the Oregon Graduate Institute of Science and Technology, Irene Morgenstern-Badarau of the Université Paris-sud in Orsay and Ted Baker of the University of Auckland) included the structure of a mutant of manganese superoxide dismutase determined to 0.90 Å resolution. This trumped a prior presentation on Monday by a colleague who claimed that he had the biggest structure at this resolution, where all atoms including many hydrogen atoms can be individually resolved. Our ultra-high resolution structure proved to be a little bit bigger. This session also featured work on metal-ion transport systems for copper, which now has me thinking about what systems exist to transport manganese into proteins.

Highlights of the conference included:

· Valerie Culotta (Johns Hopkins University) on the mechanism of copper transport and transfer into CuZn superoxide dismutase.

· Tom O'Halloran (Northwestern University) on monitoring and control of Cu and Fe ions in cells (to levels such that there is at most one such ion running loose per cell!).

· Steve Lippard (MIT) on the neurochemistry of nitric oxide and zinc, monitored by fluorescent probes into Zn-rich vesicles of particular brain cell.

· Bob Williams (University of Oxford) on new mass spectrometric methods that allow subtle isotopic mass effects, which differentiate kinetic from (pseudo)-equilibrium processes, to be tracked when metal ions (e.g. iron and copper) move from external solution into cells and into proteins.

· Bob Scott (University of Georgia) on the subtle way by which redox potentials in simple electron transfer proteins (rubredoxin, FeS-$(cys)_4$ centre) are tuned (or not) by non-bonded effects.

· Maria Carrondo (UNL, Portugal) on the structure and properties of a multifunctional protein in which a non-heme diiron centre removes adventitious dioxygen, converting it to water (There are still no models for the binding of dioxygen to a non-heme diiron centre.

· Anne Marie Pyle (Columbia University) metal ion binding to RNA, especially to activate RNA molecules that function as enzymes (ribozymes).

· Gary Brudvig (Yale University) on models for water oxidation chemistry – interesting chemistry, but still no real insight into how water is oxidised in photosynthesis (nor has the structure of the oxygen-evolving complex helped demystify this complex chemistry). This is probably the remaining holy grail of bioinorganic chemistry.

· Larry Que (University of Minnesota) on synthetic high-valent diron-mu-oxo species that functionalise alkanes.

· Dennis Riley (MetaPhore Pharmaceuticals) on a very elegant computer-aided design of synthetic superoxide dismutatases to enhance cellular defences subjected to high oxidative stress and act as a tumour suppressor – spectacularly lucid presentation.

· Yoshihito Watanabe (Okazaki National Research) on changing the oxygen-storage protein myoglobin into an oxygenase.

· Shigetoshi Aono (Japan Advanced Institute of Science and Technology) on the structure and function of sensor hemoproteins that sense levels of dioxygen, nitric oxide and carbon monoxide in cells and then signal to other proteins which organise cellular responses.

· Mike Maroney (University of Massachussetts) on the active-site structure (beautiful EXAFS!) of a weird nickel-containing superoxide dismutase.

There were whole sessions on vanadium bioinorganic chemistry and metal-DNA and metal-RNA interactions, metals and cell signalling and bioinorganic therapeutics that I could not get to, as there were six parallel sessions, and even people from Massey University can not be in more than one place simultaneously.

Abstracts for the conference can be found in the *Journal of Inorganic Biochemistry*, **2001**, *86* (issue 1).

Developing A Survey Instrument To Evaluate Tertiary Chemistry Students' Attitudes And Learning Experiences†

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Introduction

New Zealand tertiary institutions, like others worldwide, have experienced a decline in science and chemistry enrolments in recent times as students seek other career paths that they perceive to be more lucrative. In a previous article we described a qualitative study of the learning experiences of students enrolled in a first year chemistry course at a New Zealand tertiary institution.[1] Researchers in education and science education have two choices of methodology, a qualitative or a quantitative approach, and each possesses advantages and disadvantages. Qualitative studies typically use resource intensive data gathering techniques such as interviews. These studies are useful in that they allow researchers to study issues of interest in great depth and, for example, allow investigators to probe for underlying reasons about students' views for abstract scientific concepts.[2] However, because qualitative studies are more labour intensive, they typically involve only small numbers of participants, which in the minds of many researchers and teachers results in a lack of generalisability. In other words, it is not necessarily clear what implications the findings hold in other contexts. In contrast, quantitative studies involve larger numbers of participants. By the judicious use of statistical analysis, researchers can investigate changes and trends, and extrapolate their findings to a large (or target) population. However, whilst the results from quantitative studies are more generalisable, they are often less detailed. Hence researchers are confronted with a trade-off situation in which they must choose between the depth of understanding provided from qualitative studies, versus the generalisability of a quantitative approach: because of this dilemma, increasingly researchers employ a mixed methodology approach.[3]

In this paper we describe a quantitative study that complements previous qualitative work.[1] We report on the development of a questionnaire that investigates tertiary level learning experiences of chemistry students, along with their attitude toward chemistry and chemistry self-efficacy.

Measuring Student "Attitude-Towards-Science" and "Attitude-Towards-Chemistry"

Students' attitudes towards science as reported in the science education literature are usually measured using purpose-designed questionnaires (more commonly referred to as instruments). The two most widely used instruments employed to measure attitude-toward-science are the *Scientific Attitudes Inventory II* (SAI II)[4] and the *Test of Science Related Attitudes* (TOSRA).[5] However, SAI II measures scientific attitude, which is different from attitude-toward-science. Scientific attitude is a response to statements such as: "Scientists discover laws that tell us exactly what is going on in nature." In contrast, attitude-towards-science is a response to statements such as: "Working in a science job would be fun." The SAI II has been criticised extensively in the literature for its lack of theoretical grounding and lack of validity, *i.e.*, an indication of how effective a method is in answering the questions asked.[6,7] The TOSRA instrument is considered to possess better validity than SAI II, but is based on a secondary school context. Hence it is not appropriate for a tertiary environment. For example, statements in TOSRA regarding the enjoyment of science 'lessons' are inappropriate for undergraduate students, because the term 'lesson' could be taken to mean lecture, laboratory, or tutorial in the university environment. Thus for a tertiary level study TOSRA requires major revision.[8]

There has been much less research into students' science self-efficacy, *viz.* a student's perception of his/her ability to undertake (a) specific scientific task(s). Although there has been some recent interest in the measurement of science self-efficacy,[9,10] most self-efficacy research has been concerned with mathematics students.[11] Self-efficacy is task specific and so an instrument that measures science self-efficacy of, for example nursing students, is not appropriate to measure the science self-efficacy of first year chemistry students.[9]

Research into student learning experiences, like studies of science self-efficacy, is limited. There is a considerable body of literature on the measurement of student perceptions of their learning environment,[12] and the relationship between student attitude and self-efficacy, and their learning environment.[13] However, research into student learning experiences is different from learning environment research, in that the former also incorporates experiences and work required outside structured classes. White *et al.*[14] developed an instrument to measure the learning experiences of first-year tertiary physics students. However, based upon anecdotal evidence, the instrument possesses no theoretical framework and is specific to the educational context in which it was developed.

Instrument design is a complex task, particularly for holistic concepts such as attitude toward science or chemistry. Research in this area has been extensively criticised for lack of *construct validity*, which examines the question:[15] Are we really measuring what we think and say we are measuring? For example, consider the question: "Are your chemistry classes presented in an interesting manner?" This may seem like a straightforward enough question. However, a first-year chemistry student attempting to answer such a question in a survey instrument may think, "What do they mean? Are they talking about my lectures, tutorials or maybe my laboratory classes?" Such ambiguity about the term 'classes' means that the question has low construct validity, in that the researchers may believe they are measuring students experiences in a lecture environment. However, the students involved in the study may consider the term 'classes' to mean lectures, tutorials, or practical classes, and answer the question accordingly.

There are a number of ways to maximise construct validity. Firstly, the instrument structure must be based on a well-defined theoretical framework. Secondly, instruments must be subjected to a pilot study using a sample that is similar in demographics to that of the target group. Whilst it is inappropriate to rely solely on expert opinion, such a panel can contribute to clarity ensuring, for example, that scientific terminology is used appropriately.[7,16,17]

Development of the Chemistry Attitudes and Experiences Questionnaire (CAEQ)

An examination of the literature indicated that to understand students' attitude-towards-chemistry, chemistry self-efficacy and perceptions of their learning experiences (in tutorials, lectures, and practical classes), it would be necessary to develop a new instrument. Moreover, the instrument needed to be soundly grounded theoretically, and appropriately trialed with a group similar to that of the target population. Because we wished to measure what influence students' learning experiences might have upon their attitude towards chemistry and chemistry self-efficacy, we developed the *Chemistry Attitudes and Experiences Questionnaire* (CAEQ). The final version of the CAEQ consists of three scales, each containing a number of subscales as shown in Table 1. The attitude-toward-chemistry scale contains a total of 22 questions across the five subscales: *attitude toward chemists*, *skills of chemists*, *attitude toward chemistry in society*, *leisure interests in chemistry*, and *career interest in chemistry*. The self-efficacy scale, containing 17 questions, consists of one scale with students not appearing to have different efficacious beliefs for the different tasks in chemistry.[18a] The learning experiences scale, consisting of 35 questions, has four subscales: *demonstrator learning experiences*, *i.e.*, graduate assistants, that supervise practical classes, *laboratory class learning experiences*, *lecture learning experiences*, and *tutorial learning experiences*.

The development of the CAEQ entailed comprehensive statistical analyses. A detailed description of this process has been reported elsewhere.[18a] In this paper, we focus on two aspects of the development of the CAEQ that we believe have been neglected in instrument development in the past: a well-defined theoretical framework, and techniques designed to ensure high construct validity. We conclude with an illustration of the utility of the CAEQ, using data gathered at two different tertiary institutions in New Zealand.

Developing a Theoretical Framework for the CAEQ

The theoretical framework for the development of the CAEQ is based on current thinking in behavioural theory and has been adapted from the *Theory of Planned Behaviour* (TPB) (Figure 1). The TBP is an all-encompassing theory that maintains behaviour is determined by many influences including significant individuals in one's life. According to the TBP, the behaviour of an individual is influenced by his/her attitude toward that particular behaviour, the attitude of associates, *e.g.*, peers, family and mentors, toward the behaviour, and the perceived control of the individual over the behaviour.[19] The focus of the CAEQ is on the *antecedents* of attitude toward enrolling in chemistry, namely their learning experiences, attitude-toward-chemistry and chemistry self-efficacy (in other words the concepts detailed on the left side of Figure 1). The influence associates' attitude and perceived behavioural control has also may influence students' attitude towards enrolling in chemistry. This influence is not addressed by the CAEQ, but has been investigated by us previously in a qualitative study.[1,18b]

As a first step in developing a theoretical framework for the CAEQ, we defined chemistry, attitude-toward-chemistry and chemistry self-efficacy. Chemistry is defined as the learned patterns for thinking, feeling and acting, that are transmitted via the acquisition of chemistry theory, skills and values. We used Allport's definition of attitude,[20] namely "a mental and neutral state of readiness, organised through experience, exerting a directive and dynamic influence upon the individuals' response to all objects and situations with which it is related", and Bandura's definition of self-efficacy,[21] as "people's judgements of their capabilities to organize and execute courses of action required to attain designated types of performance". Learning experiences were considered to be any experience resulting in a belief formation about chemistry (where that belief is attitudinal, knowledge, or skill based).

Maximising Construct Validity for the CAEQ

As mentioned above we sought to maximise the construct validity of the CAEQ during its development. Firstly, we employed the 'panel of expert's' technique. This involved subjecting the instrument to analysis by experts in the field that the instrument examines; in the case of this study, three chemistry academics.[17,22] The experts read the questions and provided detailed feedback about items addressed in the questionnaire. We then checked the readability of the instrument for participant comprehension by asking 19 participants to complete the instrument; the participants were subsequently interviewed. We also employed the skills of an experienced teacher of students from a non-English speaking background to examine the items for comprehension by non-English speaking

students. Next, the instrument was piloted in a first-year chemistry course (n=129). The data from the pilot study were subject to statistical analyses that enabled us to assign group questions under specific concepts or constructs, resulting in the formation of subscales, *i.e.*, the subscales of Table 1. After the pilot, we administered the CAEQ to students in first-year chemistry courses at the beginning and at the end of the first semester at two different New Zealand tertiary institutions. In the first administration, the participants completed only the attitude-toward-chemistry and chemistry self-efficacy components (n=469). The presumption was that these students had not experienced any tertiary chemistry learning experiences at this point, and hence it was inappropriate to ask them about their learning experiences. At the end of the semester the participants completed all three scales (n=337) and about one half had completed both versions of the questionnaire (n=177). After statistical analyses (factor analysis, reliability, and discriminant validity) two other tests of construct validity were undertaken. The first was predictive validity, which examines whether the instrument predicts something that it is expected to predict. The second was concurrent validity, which examines whether the instrument differentiates between two groups it is expected to differentiate between.

Evaluation of Predictive Validity for the CAEQ

An instrument has predictive validity if it successfully predicts something it is expected to.[23] To determine predictive validity for the CAEQ, the learning experiences subscales were correlated with the attitude and self-efficacy subscales from the data collected at the end of the semester using Pearson's correlation (Table 2).

The correlations are not particularly strong as the closer the correlation is to 1.0, the closer to linear is the relationship between the variables. However, all correlations were statistically significant ($p<0.01$), suggesting, for example, that perceptions of practical chemistry classes exert some influence on the participants' ability to recognise the required skills of chemists. Hence, according to the data obtained from the CAEQ as administered here, students' learning experiences are influenced by both their attitude and self-efficacy and *vice-versa* , as one might expect. In other words, the CAEQ predicts a result that it was designed to do, and hence it possesses high predictive validity.

Evaluation of the Concurrent Validity of the CAEQ

An instrument has concurrent validity if it differentiates two groups that it is expected to differentiate between such as subject majors and non-majors.[24] The theoretical framework used here, *i.e.*, the modified TPB, suggests that students intending to enrol in a second chemistry paper after completing their initial chemistry course would likely have a more positive attitude-toward-chemistry, a higher chemistry self-efficacy, and be more positive about their learning experiences, than those who do not intend to take chemistry beyond first year. We examined the data from our administrations of the CAEQ for concurrent validity from the data collected at the beginning of the year and found this to be the case. All of the subscale differences were found to be statistically significant ($p<0.01$), suggesting that the CAEQ also possess high concurrent validity (Table 3). Hence, overall the CAEQ possesses high construct validity, as measured by predictive and concurrent validity. This suggests then that the conclusions drawn from the theoretical constructs of the subscales will be valid.

Using the CAEQ to Develop an Understanding of Tertiary Chemistry Students' Learning Experiences

To illustrate the usefulness of the CAEQ, we used data obtained from administration at two New Zealand universities to investigate student perceptions of their tertiary chemistry learning experiences. This serves to illustrate how tertiary chemistry teachers and researchers can use the CAEQ to gain an understanding of the learning experiences of chemistry students at the first-year tertiary level.

It is important to note that the classes from the two institutions involved in the study have significantly different demographic compositions. The first institution, *University A*, had approximately 200 students enrolled in the first year-first semester chemistry class, of whom the majority were of New Zealand European decent. Over half of these students were enrolled in applied science degrees. The second institution, *University B*, had a larger first year-first semester chemistry class with over 600 enrolments. In the chemistry paper at University B a large number of the students were studying medicine or pharmacy and the university also had a wide ethnic diversity with, for example, a large proportion of participants identifying themselves as being of Asian ethnicity.

Each lecturer has a distinct personal style of teaching chemistry and the CAEQ can be used to investigate the impressions students have of different teaching styles. The two first-year chemistry courses offered at the universities represent the first encounter the participants have with tertiary chemistry learning. Despite having similar overall objectives and the same three learning experiences, *i.e.*, lectures, practical, and tutorial classes, the classes at the two universities are structured quite differently and cover different content. University A teaches basic chemical concepts, solution chemistry, and atomic theory while University B teaches organic chemistry and kinetics. The practical classes at University A are of three hours duration each. These are assessed on the basis of the completion of worksheets that are handed in at the end of the class for the first six weeks, with a write up in a laboratory book completed outside the practical classes for the second six weeks. All the experimental information and some theory are presented in a separate laboratory manual. In University B the practicals are of two hours duration each and are assessed purely on worksheets handed in at the end of the class. These worksheets include details of experimental procedure along with some background theory about the experiment. University A provides regular tutorial classes in which all students are formally enrolled, whereas University B offers weekly tutorials that are voluntary.

Table 1. Scales, subscales and sample questions for the *Chemistry Attitude and Experience Questionnaire* (CAEQ).

Scale Name/Subscale	Sample Item					
Attitude-toward-chemistry						
Attitude-toward-chemists	Chemists:	athletic	_ _ _ _ _ _ _	unfit		
Skills of chemists	Chemists:	inquisitive	_ _ _ _ _ _ _	indifferent		
Attitude-toward-chemistry in society	Chemistry research:	solves problems	_ _ _ _ _ _ _	creates problems		
Leisure interest in chemistry	Science fiction movies:	exciting	_ _ _ _ _ _ _	tedious		
Career interest in chemistry	Chemistry jobs:	interesting	_ _ _ _ _ _ _	boring		
Chemistry Self-efficacy	*Please indicate how confident you feel about:*					
	Achieving a passing grade in a chemical hazards course	Totally confident _ _ _ _ _ _ _ Not confident				
	Applying a set of chemistry rules to different elements of the periodic table	Totally confident _ _ _ _ _ _ _ Not confident				
	Ensuring the data obtained from an experiment is accurate	Totally confident _ _ _ _ _ _ _ Not confident				
	Propose a meaningful question that could be answered experimentally	Totally confident _ _ _ _ _ _ _ Not confident				
Chemistry Learning Experiences						
Lecture Learning Experiences	The lecture notes were interesting	SA	A	N	D	SD
Tutorial Learning Experiences	My tutors have encouraged me to study more chemistry	SA	A	N	D	SD
Practical Learning Experiences	The practical experiments were related to the lectures	SA	A	N	D	SD
Demonstrator Learning Experiences	It is easy to find a demonstrator to discuss a problem with	SA	A	N	D	SD

Table 2. Predictive Validity for *Chemistry Attitudes and Experiences Questionnaire* (CAEQ) as evaluated from Pearson's Correlation[a] between learning experiences subscales with attitude-toward-chemistry and chemistry self-efficacy subscales.

	Lectures	Tutorials	Practicals	Demonstrators
Attitude toward Chemists	0.43	0.30	0.39	0.38
Skills of Chemists	0.43	0.27	0.45	0.38
Attitude toward Chemistry in Society	0.34	0.24	0.39	0.35
Career Interest in Chemistry	0.41	0.25	0.38	0.32
Leisure Interest in Chemistry	0.42	0.24	0.38	0.37
Self-efficacy	0.38	0.29	0.47	0.34

[a]All correlations are statistically significant ($p<0.01$)

Table 3. Estimated means for subscales for the *Chemistry Attitudes and Experiences Questionnaire* (CAEQ).[a]

	Mean[b]	
Subscale	Planning to enrol in second-year chemistry	Not planning to enrol in second-year chemistry
Attitude Toward Chemists	4.5	4.2
Skills of Chemists	5.2	4.9
Attitude Toward Chemistry in Society	5.8	5.5
Leisure Interest in Chemistry	4.4	3.9
Career Interest in Chemistry	5.3	4.5
Self-efficacy	4.8	4.3
Lecture Learning Experiences	3.5	3.2
Tutorial Learning Experiences	3.6	3.3
Practical Learning Experiences	3.8	3.6
Demonstrator Learning Experiences	3.7	3.4

[a]Attitudinal and self-efficacy responses were measured using a seven point semantic differential scale (1=negative, 7=positive) whereas and learning experiences used the five point Likert scale (1=negative, 5=positive).
[b]All differences in estimated means are statistically significant ($p<0.01$)

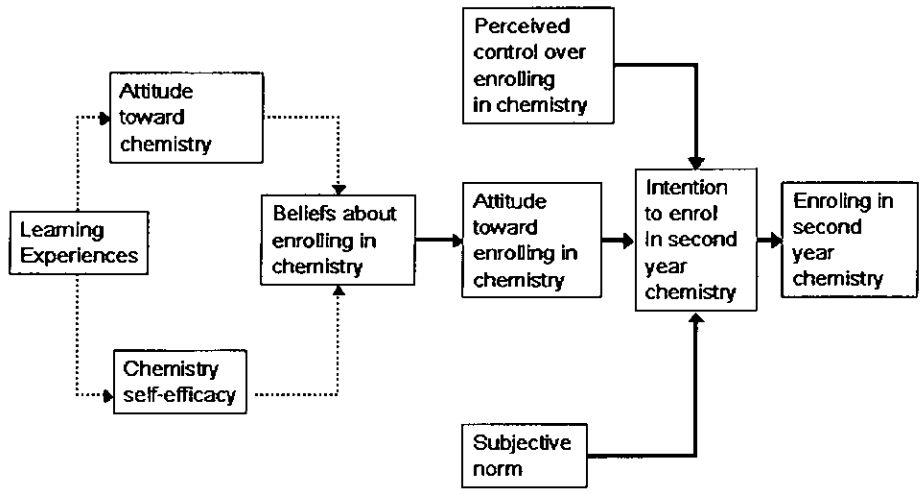

Figure 1. Theoretical framework used in developing the *Chemistry Attitudes and Experiences Questionnaire* (CAEQ). The focus in instrument development is on antecedents of enrolling in second year chemistry.

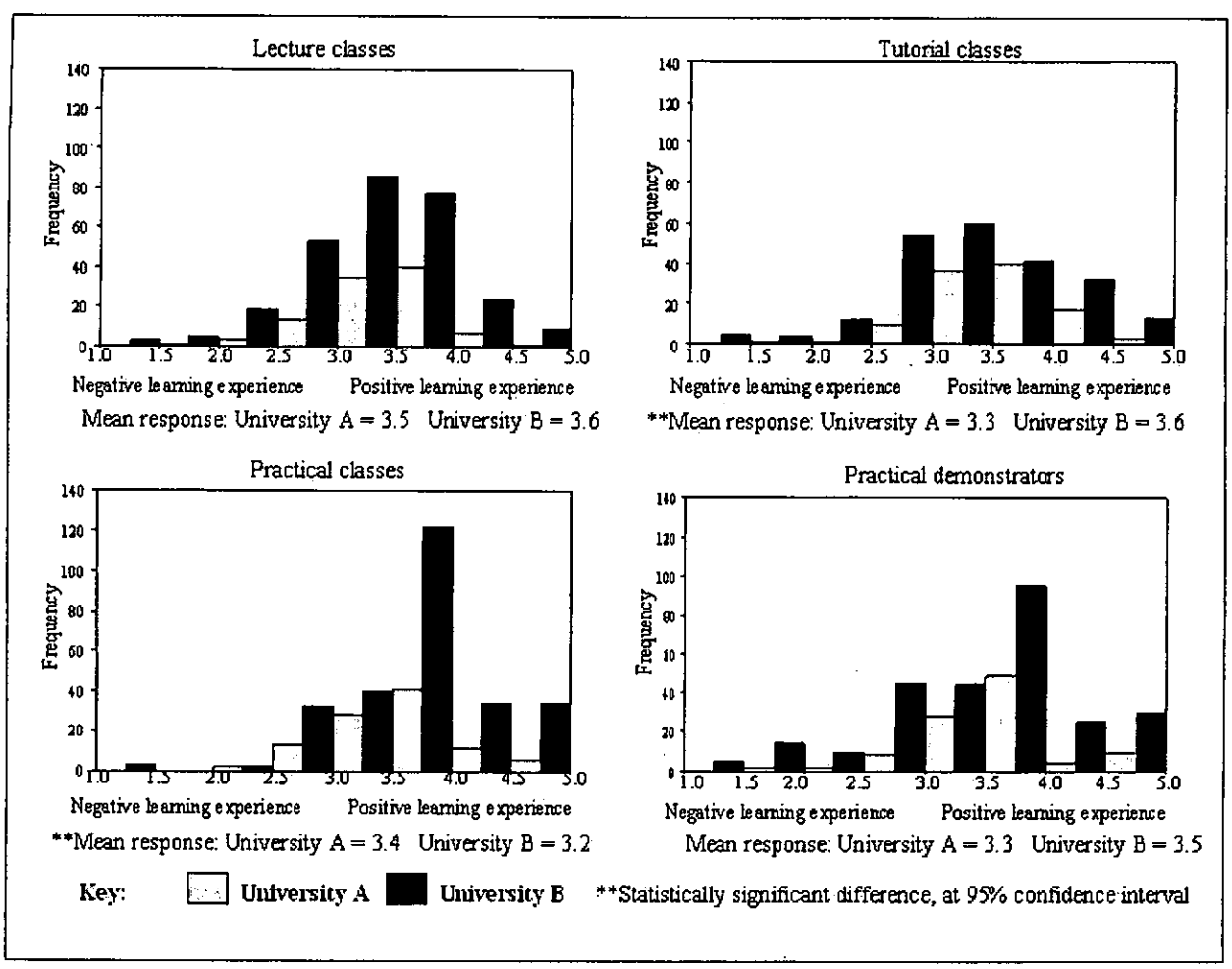

Figure 2. Student perceptions of their first-year chemistry learning experiences (n=337) as measured using the *Chemistry Attitudes and Experiences Questionnaire* (CAEQ).

A comparison of the participants' perceptions of their learning experiences at the end of their first semester courses is given in Figure 2. Participants were generally positive about their learning experiences with very few students identifying their learning experiences to be very negative in all four subscales (Table 1). There were, however, statistically significant differences in the participants' perceptions of tutorial and practical classes. Fewer participants attended at least one tutorial class at University B (82%) than at University A (96%). Participants at University A were more positive about their tutorial classes, suggesting that they found the more structured nature beneficial. The participants likewise preferred more structure in their practical classes. It is interesting to consider this apparent preference for more structured learning opportunities. As mentioned above, the first year chemistry classes represent the participants first encounter with tertiary chemistry. Having come to university directly from high school, it seems likely that their school experiences may influence their expectation of appropriate pedagogy. Hence, as their most recent learning experience, *i.e.*, their high school learning, was relatively structured it is perhaps not surprising that, as reported elsewhere, these participants are happier in a more directive environment.[24]

Conclusions

The CAEQ was developed to measure first-year chemistry students' attitude-toward-chemistry, chemistry self-efficacy, and tertiary level learning experiences. Instrument development, as well as using the conventional statistical evaluation tools such as factor analysis, sought to address the validity issues that have adversely affected other attitudinal survey instruments. Construct validity was addressed by means of predictive and concurrent validity. Predictive validity was established by the development of a sound theoretical framework, derived from modern behavioural theory, specifically the TPB, along with definitions of chemistry, attitude and self-efficacy. Concurrent validity was evaluated by investigation of the instruments' ability to distinguish between two different cohorts of participants, intending majors and non-majors. These analyses revealed that the CAEQ possesses both high predictive and concurrent validity, and this, along with other statistical analyses,[18a] suggests that the CAEQ will prove to be a useful probe for tertiary chemistry teachers and institutions that wish to investigate the learning experiences of first year chemistry students. An investigation of student learning experiences illustrates the utility of the instrument and revealed that students investigated here prefer more structure in their teaching style than they currently experience. Given the broad scope of the CAEQ as evidenced by the subscales, there are many aspects of student attitude-toward-chemistry, self-efficacy, and learning experiences that are open to investigation. It is up to tertiary education researchers and teachers to decide if this instrument will be useful in gaining an understanding of their classroom practice and the perception students have.

The instrument is available from the authors in electronic form upon request.

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New Zealand Chemistry Olympiad – 2001

As a result of the training group selection examination in November 2000, offers were made to 33 of the 89 students (from 40 schools) to join the training group. During the first term of 2001 the group received training material, fortnightly assignments and sat two tests. It was decided to again hold a combined training/selection camp in Auckland but because of funding difficulties invitations to attend were made to only sixteen members of the training group; seven of the sixteen were females and nine were males, the most even distribution ever for such a camp. Non-Auckland students (from Dunedin, Wellington, and Havelock North) were provided with motel accommodation and evening meals consisted mainly of takeaways.

The training camp had what is now a usual format of 2 lectures, 2-3 problem sessions and a laboratory session each day. The camp was run by Drs Sheila Woodgate (Chemistry Department, University of Auckland), Robert Maclagan (Chemistry Department, University of Canterbury), and Jan Giffney (St Cuthbert's College, Auckland) with the assistance of other University of Auckland staff. At the end of the week a three-hour selection examination was sat. As expected from the quality of this year's group, the examination did not distinguish clearly the needed four students, so a group of six was chosen to receive additional training material and take another examination two weeks later.

The second examination allowed the choice of Irene Ballagh (Otago Girls' High School), Albert Bollard (Wellington College), Jack Chen (Auckland Grammar School), and Rosalind Phillips Havelock North High School) as the 2001 New Zealand Chemistry Olympiad Team – the tenth from New Zealand. The non-travelling reserve was Shawna Huang (St Cuthbert's College, Auckland). The remaining student in the final selection procedure was Jason Du of Takapuna Grammar School, Auckland.

The team gathered in Auckland on July 1 for a day of training and they attended a talk by, and reception for, the New Zealand born 2000 Nobel Prize winner, Professor Alan McDiarmid, before departing for Mumbai on 4 July. Robert Maclagan and Shiela Woodgate accompanied the team that stopped enroute for a day in Singapore.

In the Olympiad competition Irene Ballagh was awarded a Bronze Medal and Albert Bollard an Honourable Mention. Albert was unfortunately so ill on the day of the practical examination that he was unable to sit it. While the result was disappointing, the mentors were impressed with the diligence of the team.

Once again the mentors from other delegations expressed amazement at the lack of support of the Chemistry Olympiad by the New Zealand Government. Sheila Woodgate was re-elected to the Olympiad Steering Committee and plans to attend a meeting later in the year in Cambridge, UK.

Financial support for the team has been received from Faculty of Science, The University of Auckland, Unilever, Thermoplastic Engineering, Biolab Scientific, Crescendo Enterprises, New House Publishers and School Supplies. The New Zealand Institute of Chemistry has again acted as "banker" for the Chemistry Olympiad.

R Maclagan
University of Canterbury

Obituary: Frank Hurst, FNZIC (1920-2001)

Frank Hurst was born in 1920 in Nelson and educated at Nelson College. He commenced a science course at Canterbury University College in the late 1930s, but his studies were interrupted by war service, which largely involved meteorological work in Fiji. After the war, Frank took up studies again and completed a MSc in chemistry in the late 1940s. He then joined the scientific staff of the Christchurch Government Analyst, a branch of the Dominion Laboratory, where he worked on water and food testing.

In accordance with DSIR policy at the time, he was transferred around 1950 to the Dominion Laboratory in Wellington to gain further experience, and took up work in the Pesticides Section under Percy Clark. He worked on DDT, selenium, and mercury residues in fruit. Along with Percy, Frank developed an interest and aptitude in applying scientific techniques to assist the police in criminal investigation. In 1961, Dominion Laboratory completed its re-establishment in new laboratories at Gracefield, and the old laboratory building was vacated. Frank gradually moved into full-time work as a forensic scientist, and when Percy Clark retired in 1969, he was made Section Head of a new Forensic Section. Forensic work was expanding, and with new staff appointments, forensic biology was added to the wide range of criminalistic work in which Frank and his staff were already involved.

Frank Hurst was widely respected by his staff, and the police and courts, for his integrity, high standards, and attention to detail necessary in this type of work. He made a major contribution to criminal investigation in the course of his career. Frank was an avid reader, a source of information both in his work and with his knowledge on many subjects, and a spirited advocate in defence of his principles.

As a young man, he was a keen tramper and played senior hockey until in his forties. In more recent times he was a regular golfer. After retirement in 1982, he underwent a number of hip operations, and it was from the last of these that he failed to recover.

His wife Erna died in 1992. A son (Tony), a daughter (Julia), and grandchildren survive them.

Harry Stone, FNZIC.

NEW ZEALAND PHARMACEUTICALS LTD CELEBRATES 30 YEARS IN BUSINESS

Selwyn Yorke
Market Development Manager, New Zealand Pharmaceuticals Limited, P O Box 1869, Palmerston North

New Zealand Pharmaceuticals Ltd has now been in business for 30 years.

Last December, the Directors announced to the staff that to celebrate the occasion, the entire company would be invited to a party out of town over a long weekend. In February, the destination was revealed as the Australian Gold Coast! Yes, the staff were stunned! Early on Saturday 20th October, more than 60 of the 70 members able to make the trip, climbed aboard the Freedom Air flight to Coollangatta, returning *very* early on Tuesday morning.

A little earlier, in fact on the 16th of October, the team at NZP had another reason to celebrate. In the Manawatu Business Awards 2001, they were recognised as Manawatu's best manufacturer and production business and subsequently landed the Manawatu Supreme Business Award against some tough competition from the finalists in the other business categories.

Richard Garland went directly from completing his PhD under Professors Hartshorn and Coxon (University of Canterbury) into borrowed laboratory space at Massey University to work on the bile acid process. Now he is the Managing Director and on the occasion said, "We've put in a big effort to motivate our staff and our success has been because of the team effort. We're a stand-alone company relying on nearly 100 percent exports. We have to be able to create our own future."

How did NZP and the staff get to be in this position? Over the last 30 years, NZP has exported nearly $300 million worth of biochemicals, which they extracted and purified from animal and plant raw materials, to countries all over the world. Over $100 million of this has been achieved in the last five years.

The company was founded by TVL and the New Zealand meat industry, and later owned by ICI. In late 1997, the management negotiated a buy-out of the company and now 40 of the staff own shares in the business.

The company's first products were pharmaceutical intermediates extracted from sheep and cattle bile. In recent years, development has focused on a wider range of biochemicals and extracts from plant and marine materials. NZP also manufactures a variety of different biochemicals and extracts for the health food, cosmetic, biotechnology and aquaculture markets.

A key factor in securing strong export receipts into the high value biochemical industry is the various licenses held by NZP. They include a MAF Byproducts (Biological) Processing Licence and a Medicines Licence to manufacture specific medicines. NZP is also certified to manufacture active pharmaceutical ingredients according to the New Zealand code of Good Manufacturing Practice (GMP), which is equivalent to the European Pharmaceutical Inspection Code (PIC).

The company fosters innovation throughout its operations and in particular, places a high importance on product development. NZP has a Product Development team of 10 scientists to develop new product opportunities and a Quality Assurance team to measure and assure the quality of the products. To assist them, the company has well equipped laboratories and two pilot plants.

The mix of product development staff has changed over the years. The Company was built on a foundation of organic chemistry and chemical engineering. With expansion from steroids into polysaccharides and proteins there has been a move to broaden NZP's capabilities by employing people with degrees in the biological sciences. The graduates and technicians employed at NZP number about 24, including six PhDs, a chemical engineer, three technologists and 14 science graduates and technicians.

NZP staff and management see a strong future for the company in the area of bioactives. The building of relationships with the CRIs and universities is an integral part of the strategy for NZP to continue to grow but to also add value here in New Zealand.

Dr Garland summarised why NZP is successful, "We are a business built on integrity, good science, and an international network of close relationships".

And a comment about the trip to the Gold Coast, as summarised by one young employee, "absolutely awesome!"

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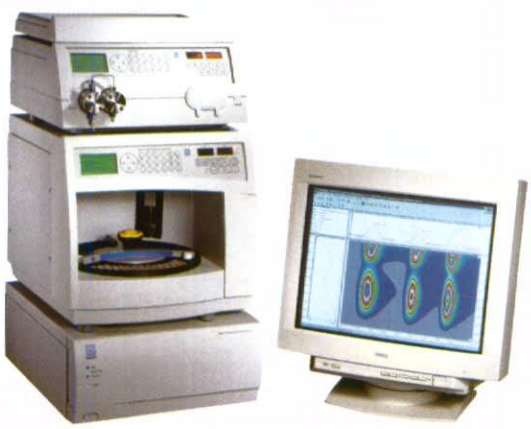

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