NZIC

chemistry in new zealand

Vol 54 No. 1 February 1990

chemistry in new zealand

Vol 54 No 1 February 1990

Branch Editors:
Auckland: Dr Robyn Somervile, Mt. Albert Research Centre DSIR, Private Bag Auckland.
Waikato: Nick Robinson, c/- Chemistry Dept, University of Waikato, Private Bag Hamilton.
Manawatu: Dr Daryl Rowan, Biotechnology Division, DSIR, Private Bag, Palmerston North.
Wellington: Adrian Bennett, BRANZ, Private Bag, Porirua.
Canterbury: Dr Selwyn Maister, Christchurch Polytechnic, P.O.Box 22-095, Christchurch.
Otago: Dr George Emerson, Biochemistry Department, University of Otago, P.O. Box 56 Dunedin.

Published on behalf of the New Zealand Institute of Chemistry (Inc).
PO Box 12-347, Wellington.
Ph (04) 739-444,
Fax (04) 732-324
President: Dr. J. Waters, Hon.Gen.Secretary: Alan A Turner, Hon. Treasurer D.P. Karl.

CONTENTS

CATHEDRAL PRESS LTD, PO Box 9072, Newmarket. Phone 733- 902, Facsimile: 371-572
Advertising Manager Carl Roze. Phone Auckland 547-244.

NEWS

Distinction For Horticultural Scientist

Dr Grattan Roughan, a Fellow of the New Zealand Institute of Chemistry, has been awarded a Doctorate of Science from the University of Otago. This distinction marks his success in elucidating the biosynthetic mechanisms involved in the formation of the different glycerolipids within plant membranes. Dr Roughan is a senior scientist with the Division of Horticulture and Processing, Auckland.

Dr Roughan's early work showed that fatty acid desaturation and glycerolipid synthesis are different in animals and plants. Then he developed the theory that there are two pathways of glycerolipid synthesis in plant cells, one localised in the chloroplasts and the other in the endoplasmic reticulum. The specificity of acy transfer to glycerol-3-phosphate means that different molecular species of glycerolipids are synthesized at the different sites. Thus in plant cells there are two separate pools of glycerolipid precursor, each with a distinctive fatty acid disposition. A particular glycerolipid may be synthesized either in the chloroplast or in the endoplasmic reticulum or it may be synthesized from a mixture of both types of precursor. The operation of these two biosynthetic pathways is sufficient to account for the known fatty acid compositions and distributions within plant glycerolipids.

Dr Roughan's work has been important in that it has lead to convincing accounts of lipid synthesis in plants, and explains, for the first time, the very complicated fatty acid compositions of plant lipids. The impetus behind his work has been the hope that an understanding of the formation of glycerolipids in plant cell membranes could help solve the problem of chilling sensitivity in plants. The productivity of many of our most important agricultural plants and the storage of horticultural products such as fruit is limited by breakdown or "chilling damage" at low temperatures.

Dr Roughan was educated at Otago and Massey Universities. He joined DSIR in 1956 and for many years worked at Plant Physiology Division, Palmerston North, often in cooperation with Dr Roger Slack. In 1983 he moved to the Division of Horticulture and Processing, Auckland. In 1988 he was elected Fellow of the Royal Society of New Zealand and received a Ministerial Award for Excellence in Science for his work on lipid sythesis.

Auckland Branch News

The AGM of the Auckland Branch was held on the 8th November. The meeting was well attended and heard outgoing chairman Tony Herd talk about a successful year. The branch committee made a conscious effort during 1989 to provide a programme of general topics for branch meetings as well as catering for more specialised interests. The year began with Dr Barry Axon from the DSIR talking on the **Forensic analysis of explosives**, and was followed by a successful public discussion meeting on **Atmospheric Pollution — the Greenhouse effect and Ozone depletion** by Assoc. Prof. J Hay (AU), Dr. Steve de Mora (AU), Mr Lindsay Roke (Fisher & Paykel), and Mr. John Sherlock from the Aerosol Association. A joint address for the RSC/NZIC by Professor Warren Roper (AU), was presented at the April meeting and this was followed by our second public discussion meeting on the **Abuse of Drugs in Sport**, given by Mrs Sue Nolan (DSIR) and Dr. Tony Edwards (GP). In May a one day Industrial Safety seminar on **Working with Chemicals** was held at the Continuing Education Dept (AU), and the branch meeting consisted of an enjoyable visit and winetasting at the Villa Maria vineyard. In June Dr. Don Lewellyn visited us and gave his presidential address, followed in July with three meetings, firstly a joint meeting with IPENZ on **Cold Fusion-Hot Science,** by Dr. Gordon Miskelly (Caltech) then a **Perfume Workshop** run by Bush Boake and Allen, and Dr. Murray Nichols from the Cosmetics Manufacturers Ltd., and the final meeting of the month on **Enzymic Catalysis** given by Dr. A.J. Kirby from Cambridge. In August we held a joint meeting with the A.U. Dept. of Psychiatry and Behavioural Science given by Prof G Johnson of Sydney, and in September Mr. Fred Holland Managing Director of Revertex and Immediate Past President of the New Zealand Chemical Industry Council addressed the branch on the **Effects of changing Government policies,** both financial and environmental on the chemical industry, and discussed the public image of chemistry, and the response of the Chemical Industry Council to this. Our annual dinner was a dine and dance, held at the New Orient restaurant, and was a roaring success. Our 1989 year was completed in December with an address by Mr. Pat Fox of the Institute of Sport and Corporate Health, on the Chemistry of Running, wherein terms like 'carbohydrate loading' and 'hitting the wall' were explained to both the runners and non-runners present. The committee was very active in the area of promotion of chemistry at the intermediate and secondary school levels. An educational page in the NZ Herald on 'Chemistry Day' was devoted to chemistry, a good response was received to the poster and essay competition, and a crystal growing competition was organised with the copper sulphate (kindly donated by Copper Sulphate Ltd.) and over fifty crystals duly arrived through the mail (in fact!) An open day for seventh form students was held at AU and ATI and concurrent with this, the scholar of the year competition which was won by Ellen Carter of Epsom Girls Grammar.

At the AGM the new committee for 1990 was elected. It consists of Rodney Norris (DSIR), chairman, Dianne Webster (National Testing Centre), secretary Jan Coddington (AU), treasurer, Frans Komen (NZ. Steel), John Rogers, Neil Debenham (Oregon Paints), Neil Edmonds (ATI), Penny Brothers (AU), Robyn Somerville (DSIR), Sharielle Alexander (AU), Tony Betts (AIDD), and Tony Herd (ATI).

At this meeting Professor R E F Mathews talked about current issues in NZ Science Policy following through earlier events to the Beattie Committee Report and the recently created Ministry of Research Science and Technology which is to be headed by Dr. Basil Walker as chief executive. An increasing proportion of Government science money will be competed for by state and private organisations with funding to be allocated by the independent Foundation of Research Science and Technology.

Manawatu Branch News

New Zealand Dairy Research Institute

Dr Wayne Sanderson, Assistant Director, resigned at the end of September and moved to Melbourne to take up a Senior Management position with the Murray Goulburn Co-operative (Dairy) Company.

Dr Jeff Plowman, formerly with the DSIR in Christchurch, has joined the Protein Chemistry Section.

Dr Chris Bloore, Head of the Milk Powders and Drying Section, resigned in early February to move to Dunedin with his wife who has been accepted as a student for the Presbyterian Ministry at Knox Theological College.

Cont. next page

EDITORIAL

"When they met a chemistry was set up between them" This quote from a television interview refers to an attraction between two people, and although quite dreadful, in misusing a technical term, it could well refer to what unites the membership of the Institute of Chemistry. It is rather nice to see the word 'chemistry' used as a term implying light, sweetness, and friendly cooperation between people attracted to each other by their interest and ability. This is how we would see the Institute of Chemistry, and indeed is how it functions, although arguably not with total perfection. The Institute exists as a band of people interested in the subject of Chemistry, and wishing to promote it and their own importance.

The journal, which has six issues a year does not aim to supplant technical publications, but as one of its functions tries to give news about people whose work is in the field of chemistry. For the collection of material we are indebted, and give thanks to the Branch Editors. One who retires this year writes 'I have thoroughly enjoyed my association with Chemistry in NZ over the past twelve years. It has given me the excuse to attend many meetings I've found to be most interesting. Also it has forced me to attend branch meetings, many of which I've found to be more interesting than their advertising would suggest. A few I have found deadly.'

Since membership of the Institute is a Professional qualification, entry standards are guarded over by a membership committee. It is hoped this year that Branches will recruit to student membership, a large fraction of students completing tertiary chemistry courses.

If the deadly parts can be suitably neutralized the Institute will be strong. Can you envisage a hydrogen sulphide person 'setting up a chemistry' with a sulphur dioxide person, or if that is too abstruse, a sodium person meeting a chlorine person? A methane person could well spark it off with an oxygen person, although the ozone layer might well take offence. Who says chemistry is dull and boring?

B.E.S.

LETTER FROM AUSTRALIA

There are certain authors who accompany us through our lives. The successive editions of their books form part of the cultural literacy of our particular society — think of Benjamin Spock, Mrs (did she have a given name?) Beeton, Linus Pauling, Dorothy L. Sayers and A.I. Vogel — his given name was Arthur, but I had to look it up even though I have owned three of his books for over thirty years. In earlier times it was Jean Marcet and Henry Roscoe whose seminal books were found on chemical shelves. Grander works like the *Encyclopaedia Brittanica* might be beyond our individual purses but they occupy important places in institutional libraries where their wisdom nurtures not just generations but whole centuries of scholars.

The ninth edition of *EB* immediately comes to mind. Dubbed the 'scholars edition', it appeared in 24 volumes (plus index) between 1875 and 1889 and the contributors included such luminaries as Thomas Henry Huxley on biology and P.G. Tait who penned 74 pages on mechanics. The entry on Chemistry was largely the work of Raphael Meldola, but specific substances and the lives of great chemists were mainly covered by contributions from Scots — John Ferguson and William Dittmar of Glasgow and A. Crum Brown of Edinburgh.

Producing the *EB* has ben a more-or-less continuous activity since 1769 William Smellie edited Volume 1 (Aa-to-Bzo), following it over the next two years with Caaba-to-Lythrum and Macao-to-Zyglophyllum making a total of 2659 pages. Smellie wrote thus of the British language: 'like a healthy oak planted in rich and fertile soil, it has sprung up with vigour.' He might well write the same thing about the *EB* if he could see it today, even though constant editorial pruning has managed to keep its growth in check this century. The latest edition, the fifteenth, comprises 32 volumes and was produced between 1974 and 1986.

Although it is a pillar of the English speaking world, the *EB* owes something to a French predecessor of the early 1750s, Diderot's *Encyclopedie*, which in turn followed Ephraim Chambers' *Universal Dictionary of Arts and Sciences* (1728). It wasn't all plain sailing for the *Brittanica*, either, for many purchasers of the first Vol 3 objected to the explicit illustrations which accompanied the article on Midwifery, some tearing the offending pages from their copies and others threatening legal action.

I own a number of books for which I have collected successive editions but none so fascinating as Ben Selinger's *Chemistry in the Marketplace* (Harcourt Brace Jovanovich) of which the fourth edition has recently appeared. It still has the same catchy chapter titles, like 'Chemistry in the Boudoir', and its presentation is strictly product first, chemistry later — in good Science-Technology-Society fashion. Selinger's book is subtitled 'A Consumer Guide' but it is also an encyclopaedia, reference work and textbook. For student use Selinger thoughtfully includes a large selection of consumer experiments, eclectic enough to include determination of lead in petrol (using dithizone), properties of concrete, and calculation of the thickness of polyethylene films from the spacing of the interference fringes which muck up the baseline in their infrared spectra.

Ben Selinger is head of Chemistry at the Australian National University in Canberra. You can guess from the sort of book he writes that he's just about the most interesting chemist you would ever want to meet, a quality which has brought about his popularity as a speaker and participant at many a conference. He has also had a long-time interest in the nature of statistical evidence, as it might apply to questions of safety and health, and in the assessment of scientific evidence presented in the courts.

Much of the product-specific information in the book and the commentary on legal and legislative matters is of Australian origin but clearly has international application. Don't be put off by the Aussie flavour: there's nothing about prawns or barbecues but maybe Ben will respond to your pleas by including them in the fifth edition.

In reviewing the third edition of *Chemistry in the Marketplace* I noted Selinger's flair for the inclusion of offbeat material, like the triple pun — he claims it's unique — about the place where the sun's rays meet. I was unable to find it in the latest edition despite the assistance of 14 appendixes (shouldn't they be appendices, Ben?) and a superb 24 page index, which make this 600 page chemical supermarket a delight to visit.

Ian D. Rae

MORE NEWS

Manawatu News Cont.

The Aseptic Processing Section, formerly headed by **Dr David Newstead**, has been combined with the Milk Powder and Drying Section.

Drs Lawrie Creamer, Steve Haylock and **Rex Humphrey**, and **Mr Ramsey Southward** attended the 1989 International Chemical Congress of Pacific Basin Societies (Pacifichem '89) in Honolulu, held just prior to Christmas. Over 7000 were registered for the Conference which consisted of 100 Symposia. Approximately 4500 papers were presented there.

Dr Owen Mills leaves shortly with his family to spend 12 months' study leave at the Southern Regional Regional Research Centre, US Department of Agriculture, New Orleans to study the flavour of peptide and protein materials.

In the Printpac-UEB Food Awards, presented in November, Institute staff gained awards in the following: New Zealand Trade Development Board Award — for development of a new dispersible calcium caseinate **Miss Diane O'Carroll** — (New Zealand Dairy Research Institute); **D. Gerald O'Meara** (New Zealand Dairy Board), **Mr Max Scott** (Bay Milk Products).

Industrial Products Category Award for the Alaco range of speciality butterfat products: **Dr Lawrence Eyres** and **M. Craig Galloway** (New Zealand Dairy Board), **Dr Robert Norris**, Messrs **David Illingworth and Rowland Cocup** - (New Zealand Dairy Research Institute); **Messrs David Munro and Geoff Wheeldon** (Bay Milk Products).

Massey University

Drs Margaret Brimble, Eric Ainscough, Joyce Waters, Ian Watson and Neil Waters, along with a group from the DRI, attended the 1989 International Chemical Congress of the Pacific Basin Societies (Pacifichem '89) in Honolulu just prior to Christmas.

Massey University News

At about 6.45 am on the 11/12/89 the inorganic research laboratory was gutted by a fire that was thought to originate from a refregerator. Extensive damage to the laboratory, equipment, chemicals, apparatus, instruments, and vacuum lines was incurred and records were destroyed along with many chemical samples. Several research students lost many personal items and this will set them back in their studies.

Adjoining analytical and physical laboratories also suffered from some smoke and or fire damage. Chemicals and solvents stored in closed cupboards, and research records kept in filing cabinets escaped major damage and thus the usefulness of such storage systems was noticed. Nobody was present in the laboratory at the time of the fire.

HONOURS

Two chemists were honoured in the Queen's new year list: Professor Emeritus M F Robinson of Dunedin awarded a CBE for services to nutrition education and research, and Dr. A J Ellis of Lower Hutt, former Director-Gen-

OBITUARY

The death is reported on December 13 of Peter de la Mare, Emeritus Professor of Chemisty at Auckland. A full obituary notice will appear in a later issue of the journal.

CORRECTION

October issue p106 Yearbook, Entry No. 12 Allan Aspell and Associates Ltd.

Please delete "Telarc registered laboratory".

Inorganic Chemistry '91 Conference

The "Inorganic Chemistry 1991" Conference, run under the joint auspices of the Royal Australian Chemical Institute and the New Zealand Institute of Chemistry, will be held at the University of Waikato, Hamilton, New Zealand, during the week 28th January to 1st February 1991.

Speakers who have already agreed to present Plenary Lectures include:

T.J. Collins (Carnegie Mellon), G. Christou (Indiana), G. Huttner (Heidelberg), A. Nakamura (Osaka), P.P. Power (Davis), A. Sargeson (Australian National University), K. Wade (Durham), K. Weiss (Bayreuth). There will also be a Burrows Lecture and a full range of session lectures and poster presentations, together with a lively social programme.

Hamilton is centrally situated in the North Island, and is a convenient base for trips to Rotorua, Waitomo Caves, Taupo, the Coromandel Peninsula, and other scenic attractions, so that pre-or post-conference tours can be readily arranged.

Enquiries to: **Dr B.K. Nicholson**, Chemistry Department, University of Waikato, Hamilton, New Zealand.

PEOPLE, CONFERENCES & OTHER NEWS

D. Payne

David Payne has been appointed to manage the newly formed operation of ICI Instruments in Auckland. David brings with him over twelve years experience in the Scientific Industry and more importantly his reputable skill in supporting New Zealand users of analytical equipment.

4th EUROPEAN CONFERENCE ON THE SPECTROSCOPY OF BIOLOGICAL MOLECULES, ***University of York, England. 1-6 September 1991***
Contact: Prof R.E. Hester, Department of Chemistry, University of York, Heslington, YORK YO1 5DD, England.

This conference will follow in the general style of its predecessors, the last of which was held in Rimini, Italy, in September 1989. The focus will be on Raman and Infrared spectroscopies and their many applications in biochemistry, molecular biology, and in biomedical subject areas. A few of the plenary lectures and invited papers will, however, be based on other types of spectroscopy (NMR, CD, transient absorption, time-resolved fluorescence, etc.) and x-ray crystallography, to provide a critically comparative context. This is a major international event. The conference will include poster sessions and a technical exhibition and will take place on the attractive campus of the University of York. Sight-seeing and tours in and around the beautiful 2,000 year old city of York will be arranged in conjunction with the scientific programme.

WATER

A one day symposium on this vital subject is being arranged by the Auckland branch and the University Centre for Continuing Education. It will be of value to everyone concerned with water treatment, water analysis or water quality in general. The scale of water usage is immaterial — whatever is appropriate to the needs of one's organisation. The date has not yet been decided but will probably be in April.

Anyone interested, whether as a participant, speaker or supplier of equipment or chemicals, is invited to contact the Centre, the Auckland branch Chairman, or Lester Stonyer.

RSC Certificate in Applied Chemistry

The Auckland Technical Institute has been approved by the Royal Society of Chemistry (UK) to teach a course in analytical chemistry leading to a certificate that is issued by the RSC. Although each approved institution sets its own syllabus and examinations to allow emphasis on local requirements, the course is carefully moderated by the RSC to ensure a consistent standard and a Certificate with international recognition. The standard entry requirement is NZCS Chemistry with 5D1 (AAVA 5156) as a prerequisite but university chemistry graduates or others with analytical experience are welcome to apply.

Those interested in the course should contact Dr Tony Herd either at ATI, Private Bag, Auckland. or 51 Pencarrow Ave, Epsom, AK3 (ph 606017). The number of students will be limited to 12.

COVER STORY

ICI INSTRUMENTS - JUST ARRIVED. HERE TO STAY.

Following a rapid rise to success as a manufacturer and distributor of an internationally respected range of HPLC and Spectrophotometer instrumentation, ICI Instruments (Australia) are proud to announce the opening of an office in Auckland, New Zealand.

With the enviable benefit of having the resources and experience of ICI (one of the largest users of analytical instrumentation in the world), ICI Instruments has been able to quickly capitalize on the innovations from its own developments and those of the Australian and worldwide Scientific Community. The resources and the experience of ICI has enabled ICI Instruments to launch a comprehensive range of analytical equipment that addresses not only performance requirements, but also operational ease demanded by the user, which is often overlooked.

Take, for example, the ICI Instrument's LC1260 Electrochemical Detector, developed in conjunction with an Australian University and refined by ICI using the experience of its own analysts, production and service staff. The module was then beta tested by a number of key users whose suggestions were regarded during the final design stages. The end result is a highly sensitive Eletrochemical Detector that utilizes a unique wall jet design cell, enabling the electrode to be quickly and easily removed, and achieving rapid stabilization of the baseline. The microproccessor controlled ECD is easy to operate and incorporates a cleaning mode to extend electrode operating life. It has already received an extremely positive reception from users around Australia, Asia and Europe.

Through market research, ICI Instruments have identified that ease of use, reliability, and user serviceability are as important to the analyst as is performance. Accordingly, our design teams have used this information to develop instruments that address these user requirements. Typical example of ICI's approach to meet the needs of the analyst, is the LC 1100 pump which has a membrane to keep corrosive buffers completely seperate from the mechanical parts, and an Autosampler LC1600 that withdraws samples into the flow path avoiding the cumbersome need for a seperate wash cycle. All products have been deliberately designed to allow user serviceability for the many items which may require periodic replacement such as pump seals.

One of the major areas identified by our own analysts for improvement over existing designs was in software. Having investigated other systems currently available, we set about designing a whole new dimension of user flexibility and convenience into our data stations and instrument controls. The performance of the DP800 is designed to grow with the ability of the user, hence the newest lab assistant can run a routine test whilst maintaining the sophistication required to effectively handle demanding HPLC seperations and method development.

ICI Instruments also distribute the GBC range of spectrophotometers, manufactured in Melbourne by the GBC company, owned by ICI Instruments.

In the last twelve months, ICI/GBC have launched a superb range of instruments with full computer control and results processing. These products have surpassed former developments with innovative features such as:—

the most flexible and user friendly software available today.

multi-element systems with fully automated lamp changing and alignment available with the top of the range GBC 906.

the revolutionary Ultra-Pulse background correction which overcomes many of the traditional problems associated with background.

The GBC range is setting the pace for spectrophotometer developments around the world, and already has a significant user base in New Zealand.

To complement ICI Instruments comprehensive range of instrumentation, we also distribute and support an imported range of equipment. Equipment such as the Dani range of GC with some the most advanced sample injection techniques available, and a range of supporting equipment and accessories including columns, lamps and eletrochemistry meters.

In adressing the testing of physical and mechanical properties of materials, ICI Instruments has also assembled a range of products including:—

High temperature, high capacity, thermal analyzers from Setram (France) for DSC, DTA and TGA.

Rheology testing equipment from Bohlin (Sweden) including the compact and versitile Visco 88.

The Polymer Labs thermo-mechanical analyzer (DMTA).

The Lloyd range of tensile and comprehensive equipment.

ICI Instruments has a commitment to become one of the major suppliers of analytical instruments around the world. There are a large number of new instruments under development in our laboratories for release over the next couple of years, as well as some novel techniques for applying current technologies to analytical problems.

To aid us in our goal, we have appointed David Payne to manage our New Zealand operation. David brings with him many years of experience in the Scientific Community and more importantly his reputable skill in supporting New Zealand users of analytical equipment.

Our commitment to be a major supplier of analytical instruments is demonstrated by our superlative customer service and support that you can rely on, always.

Should you have an existing or imminent need, contact David Payne at our Auckland office on (09) 735-765.

NMR AS A CHEMICAL TOOL

Jan Coddington, University of Auckland

Nuclear magnetic resonance started life as a physicists' orphan, somewhat maligned and unappreciated. By the time of the first review article in this journal[1], it had become the favourite child of many spectroscopists and has continued to develop as an essential chemical tool. Its current growth is being driven by the demands of molecular biologists, biophysicists and geologists as well as by chemists.

This article discusses some of the current applications of NMR. The examples used are research projects involving the Bruker 400MHz instrument at the University of Auckland (Figure 1). Regular users of the instrument include the Chemistry, Biochemistry, Zoology, Botany departments and the Cancer Research Laboratory of the University of Auckland, and the Chemistry department of Waikato University. Occasional users have included researchers from the Pathology, Physiology, Cellular and Molecular Biology departments, DSIR and commercial consulting chemists.

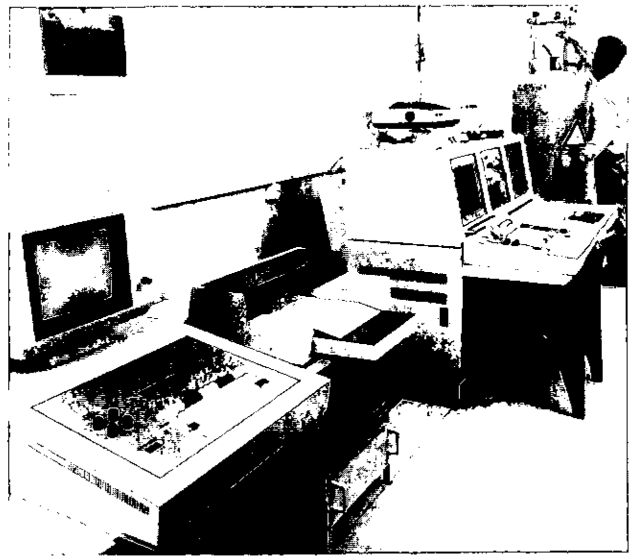
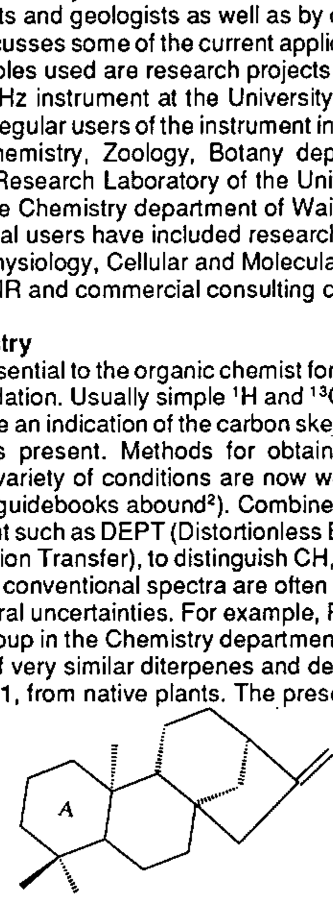


Figure 1 The Bruker AM400 NMR spectrometer installation in the Department of Chemistry, University of Auckland.

Organic Chemistry

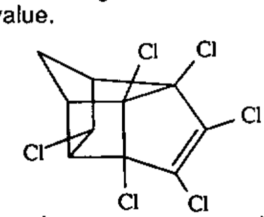
NMR is now essential to the organic chemist for any type of structure elucidation. Usually simple ^1H and ^{13}C spectra are enough to give an indication of the carbon skeleton and functional groups present. Methods for obtaining such spectra under a variety of conditions are now well developed. (Excellent guidebooks abound[2]). Combined with an editing experiment such as DEPT (Distortionless Enhancement by Polarisation Transfer), to distinguish CH, CH_2 and CH_3 groups such conventional spectra are often sufficient to resolve structural uncertainties. For example, Professor Con Cambie's group in the Chemistry department isolates a large number of very similar diterpenes and derivatives, such as kaurene 1, from native plants. The presence of a

1



keto or hydroxyl group in ring A is common and is easily determined from the ^{13}C chemical shifts: a C=O occurs about 210ppm and a CH-OH at about 75ppm. The position and stereochemistry of the substituent is assessed by the magnitude of the ^1H coupling constants: an equatorial OH will allow its geminal H to show a large diaxial coupling (*ca.* 12Hz) to any vicinal axial H, while an axial OH will permit a 1,4-W coupling (*ca.* 1.5Hz) to any suitable equatorial H. The rest of the molecule can be examined similarly since most signals are quite well resolved. A range of these compounds has now been investigated and the combined data set is of predictive value.

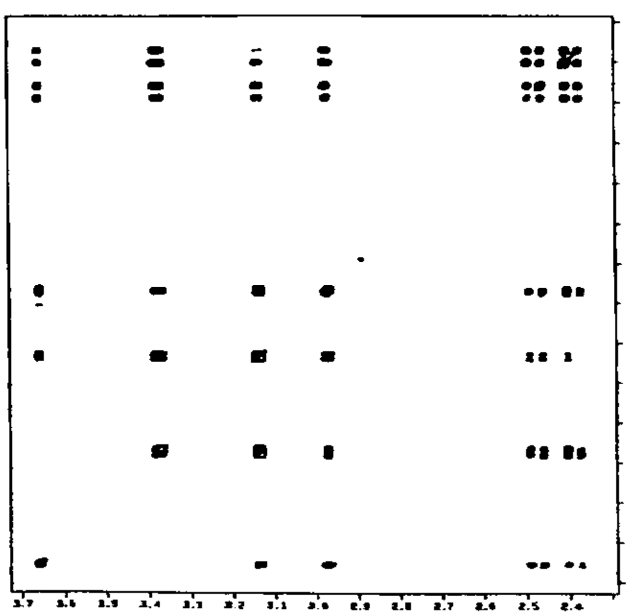
2



Sometimes, spectra have so many overlapping resonances and the coupling pattern is so complex that they appear hopelessly jumbled. New techniques *(new pulse sequences)* have helped enormously by spreading the information into two dimensions. It is possible, for example, to have just the chemical shift information in one dimension and the coupling network in the other. These methods are now the backbone of modern NMR analysis and application monographs are appearing[3].

The most useful of the new experiments is undoubtedly COSY *(Correlated Spectroscopy)* which gives a map of the coupling partners of every hydrogen in a molecule. This was used extensively by Dr. Alistair Wilkins at Waikato to determine the structure of 2, a constituent of commercial chlordane. The number of chlorine atoms present and their relative stereochemistry had to be established. The coupling interactions between the hydrogen nuclei were used to do this. Part of the COSY spectrum is shown in Figure 2.

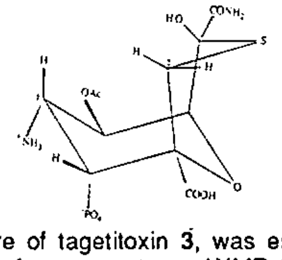
Figure 2 Part of the 2-D ^1H-^1H correlation spectrum (COSY) of compound 2.



A correlation between two hydrogens is indicated by a *cross peak* at a grid position corresponding to the chemical shift (one in each dimension) of the nuclei involved. In this way, the whole skeleton could be traced.

Biomolecules

The appearance of 2-D techniques has given renewed impetus to the study of biological molecules where materials may be unstable and of limited availability. At the Division of Horticulture and Plant Processing, DSIR, Dr. R. Mitchell has isolated and characterised a phytotoxin produced in liquid cultures of a pathogenic plant bacterium.



The structure of tagetitoxin 3, was established using a combination of mass spectra and NMR. Several 2-D heteronuclear NMR correlation methods were used to unequivocally connect carbonyl ^{13}C H nuclei to several bonds away. A critical piece of information was also supplied by the observation of a nuclear Overhauser effect *(NOE)* between the H at C7 and one of the H nuclei at C2. This effect is the result of dipolar couplings and is observed ony when H nuclei are within 0.4nm of each other.

Most biomolecules are immense by solution NMR standards and further complicate observation by being soluble only in water. Because their concentrations are usually not more than 1-2mM, such molecules can only be routinely observed using high-sensitivity ^1H spectra. Special methods are then needed to remove the massive H_2O peak that otherwise dominates the spectrum. Even in D_2O solution, the residual HOD peak is huge and must be suppressed. The overall result is that such spectra are collected over long periods to get useful results. Nevertheless, many proteins, carbohydrates and nucleic acids have been studied.

Some typical spectra of the relatively small protein, bovine parathyroid hormone, are shown in Figure 3. Many of the lines are broad and there is considerable overlap.

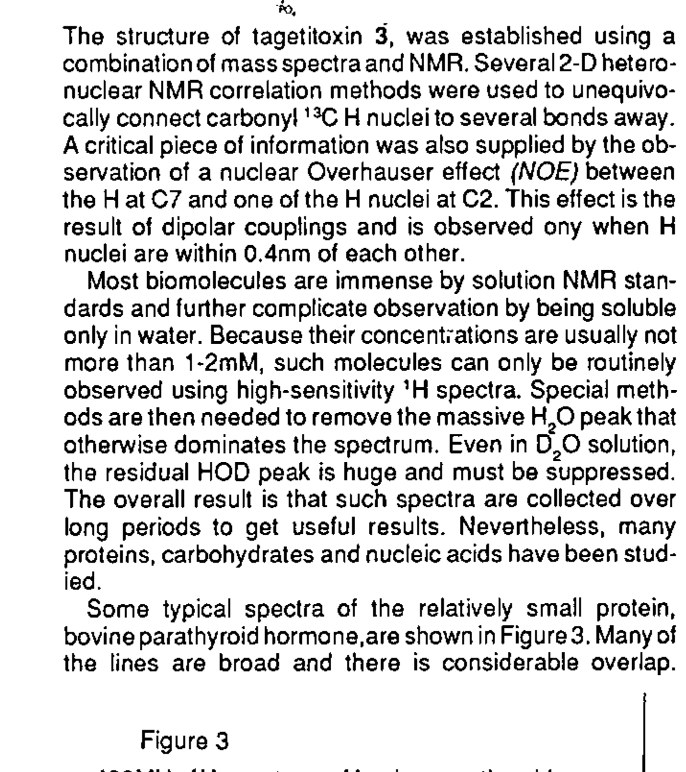


Figure 3

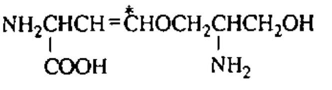
400MHz ^1H spectrum of bovine parathyroid hormone in D_2O at pH 6.3, residual solvent suppressed by pre-irradiation.

However, it is still possible to obtain information about the tertiary structure of the protein, for instance as the pH is changed. In particular, the aromatic region from 6-10ppm is quite well resolved. It can be used to determine the pK_a of individual histidine residues and indicate accessibility to solvent. Any specific conformational changes in the other aromatic amino acids are also easily observed. In water, the region also contains all the NH resonances whose behaviour is characteristic of specific amino acids and conformations of the global protein structure. Dr. Peter Barling in the Biochemistry department is using this information in the study of structure-activity relationships of the various domains of the protein.

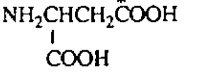
In an equally technically demanding project, a group led by Professor Alistair Renwick is investigating the carbohydrate sequences of several glycoprotein hormones, using primarily 2-D NMR methods.

All NMR studies of biomacromolecules depend on the exquisite sensitivity of the new spectrometers with high-field superconducting magnets. This sensitivity is also used to advantage in labelling and feeding studies. Metabolic pathways were originally determined by feeding radioactive ^{14}C-labelled precursors. Isolation of products was often very tedious and difficult. It is now routine to feed ^{13}C-labelled material which is NMR visible but not radioactive. Incorporation of the label can often be determined without isolation of individual products. A whole bacterial culture, for example, may be put in an NMR tube and, under ideal conditions, signals will only be detected from those compounds containing the label. (The problem of assigning the signals to specific compounds may not be trivial).

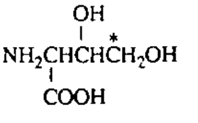
Part of the biosynthetic pathway of rhizobitoxine **4**, another toxin from a plant pathogen, has been determined in this way by Dr. Mitchell at DSIR. The pathogenic bacteria were fed aspartic acid **5**, which was specifically labelled with ^{13}C at the C4 carboxyl position. Enhanced ^{13}C NMR signals, indicating incorporation of label, were detected at the C1 and C4 positions of rhizobitoxine. Label was also detected at the C4 position of hydroxythreonine **6**, confirming a previous suggestion that it was an intermediate in the pathway. In this case, the compounds were extracted and partially purified before the NMR experiments were done.



4



5



6

In Vivo Studies

One of the most fascinating and challenging areas in NMR is the study of biologically viable samples. These can include cell cultures, perfused organs and even whole plants and animals. Dr. Alison Stewart of the Botany department and Dr. Alwyn Rees of the Marine Research Laboratory have been interested in the symbiotic relationship between the algal and fungal components of various New Zealand lichens. The major metabolite is one of several polyols, such as arabinitol, ribitol or mannitol, and is species specific. As such, the identification of the compound may serve as an aid to taxonomic classification. Intact lichens and their methanol extracts give good ^{13}C NMR spectra where the dominant peaks arise from the polyol present. Experiments to follow the path of the algal photosynthetic product to the major fungal metabolite are now in progress: the lichens are maintained in an atmosphere of $^{13}CO_2$ for 12 hours and then spectra are obtained after various times.

Some sea anemone species are also involved in a symbiotic relationship with algae. There is great interest in whether the alga supplies glycerol or lipids (fatty acid triesters of glycerol) to its host. Dr. Rees has identified an anemone that can be examined by NMR: it is small enough to fit comfortably inside a 10mm NMR tube. Figure 4 shows the ^{13}C spectrum of 50 of these live animals, surrounded by sea water. The major peaks can be assigned to lipid with resonances for both carboxyl and unsaturated bonds as well as the expected methylene envelope being observed. Also present are peaks corresponding to glycerol and several amino acids. The resolution of the spectrum is impressive since many *in vivo* samples give generalised blobs for spectra. The anemones did not appear to be under stress. A ^{31}P study showed normal energy metabolism with the expected levels of ATP and the animals resumed feeding when returned to a more spacious environment.

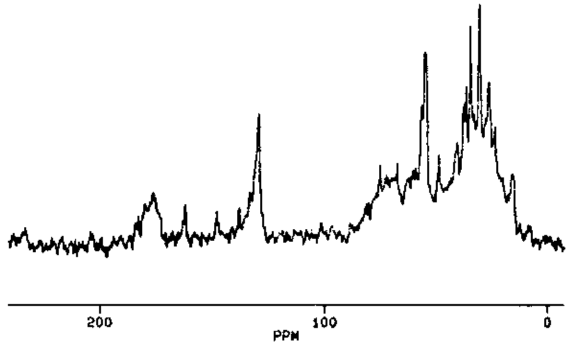


Figure 4 100MHz ^{13}C spectrum of sea anemones (genus *Anthopluera*) in sea water with 10% D_2O. Total acquisition time of 30 minutes.

Monitoring the health of a living system using ^{31}P NMR is becoming routine. Figure 5 shows the spectrum of an intact rat heart. In a healthy muscle such as this, high levels of phosphocreatine (-5ppm) and ATP (-8m -12, -22ppm) and low levels of inorganic phosphate (0ppm, but pH dependent) and ADP (-7, -12ppm) should be observed. Dr. Stuart Humphrey in the Pathology department is interested in the use of various buffer systems to extend the functional lifetime of hearts for use in transplants. An organ preparation is placed in the spectrometer, operating at 278 K, and spectra are obtained every 30 minutes until there is no phosphocreatine or ATP left. At that point, the pH of the organ has usually changed substantially, indicating pathological dysfunction. This is easily followed by the chemical shift changes of the inorganic phosphate peak.

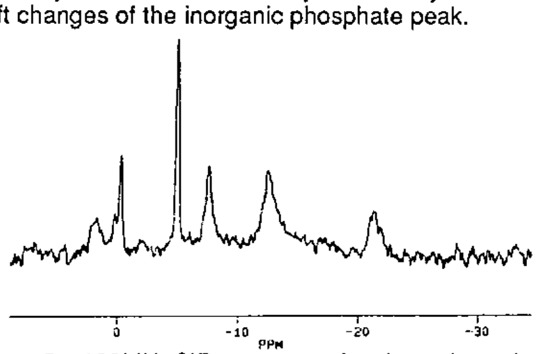


Figure 5 162MHz ^{31}P spectrum of an intact heart from a juvenile rat. The organ was suspended in buffer and cooled to 278 K. Total acquisition time of 8 minutes.

Inorganic Chemistry

These bio-organic applications have been driving much of the current wave of software development in NMR. Better hardware, such as frequency synthesisers and more powerful transmitters, has resulted from demands for easy observation of all the magnetically active nuclei. NMR is becoming an increasingly important technique in modern inorganic chemistry[4].

Most organometallic and coordination compounds bear ligands containing H and C atoms, which often give simple spectra. The presence of a metal atom at the centre of the coordination sphere can influence the ^{1}H and ^{13}C spectra in several ways however. Some metal centres, particularly transition metals with partially filled d shells, are paramagnetic and they have a dramatic effect on the spectra. The unpaired electron spins interact with the nuclear spins so that peaks are often broadened, sometimes to the point of disappearance, and the chemical shifts are significantly changed.

A metal centre can also behave as a heteroatom, affecting the chemical shift of nearby H and C atoms. For example, a hydride ligand (hydrogen bonded directly to a metal) usually has a resonance much further upfield than the 0-10ppm range typical of organic molecules. In the diamagnetic ruthenium complex $RuHCl(CO)(PPh_3)_3$ (prepared by Stage III undergraduate chemists at Auckland), the hydride ligand is observed at -7.2ppm in the ^{1}H spectrum. The presence of phosphorus atoms in the complex results in coupling to the hydride and the resonance appears as a doublet of triplets. This is good evidence for two of the PPh_3 ligands being equivalent, indicative of a specific geometry around the metal. Professor Warren Roper's group has synthesised many new ruthenium, osmium and iridium compounds containing both phosphine (PR_3) and fluorocarbon ligands. There is extensive coupling between ^{31}P, ^{19}F and ^{1}H nuclei, leading to very complex spectra.

Figure 6 shows the ^{31}P spectrum of a porphyrin complex prepared by Dr. Penny Brothers' group. Here, the central atom is phosphorus and it is coupled to eight chemically equivalent hydrogens on the porphyrin macrocycle and a further six equivalent hydrogens on the two methoxy ligands. The resonance appears as a nonet of septets.

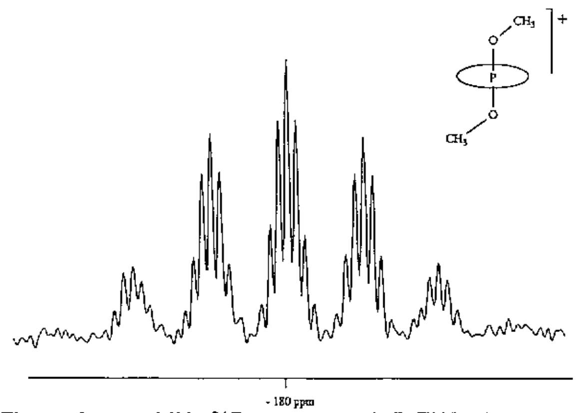
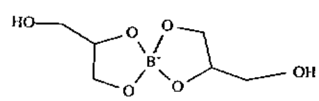


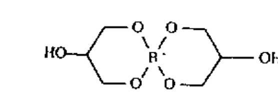
Figure 6 162MHz ^{31}P spectrum of $(P(TTP)(OCH_3)_2)^{+}Cl^{-}$ in $CDCl_3$ with no proton decoupling. $^{3}J_{PH}$=25.5Hz (coupling to 6 methoxy H), $^{4}J_{PH}$= 2.9Hz (coupling to 8 pyrollic H). TTP= *meso* tetra-*p*-tolylporphyrin.

Chemical Exchange

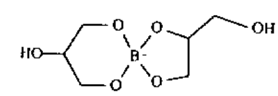
The advantage of a multinuclear spectrometer is the ability to chose which element in a molecule will give the most informative spectrum. Often this will be the atom at the centre of the complex. The spectra of these nuclei will be relatively simple since there will be only a few different chemical shifts present and the coupling patterns should be straightforward to interpret.



7



8



9

Dr. Michael Taylor has been interested in the formation of complexes between borate and polyhydroxy compounds. It has been established that the $B(OH)_4$ is complexed by diols to give both mono-chelated and bis-chelated anions. 1,2-Diols form five membered ring complexes and 1,3-diols form six-membered rings. Glycerol is a 1,2,3-triol, which may behave as a 1,2- or 1,3-diol in its interaction with borate. The ^{11}B NMR spectrum of a 1:3 mixture of $NaB(OH)_4$ and glycerol showed separate peaks for the monocyclic five- and six-membered rings as well as the bis-spirocyclic forms **7** and **8**. The mixed complex **9** is also present. The ^{11}B spectrum contains at least eight peaks, since the borate anion is participating in polyborate formation equilibria as well. The ^{13}C and ^{1}H spectra can be interpreted in terms of the major species observed but they are quite complex. This system is obviously most easily studies by starting with the less familiar NMR nucleus.

The most readily accessible nuclei are those which have a nuclear spin quantum number, I, equal to1/2. These include ^{1}H, ^{13}C, ^{19}F, ^{31}P and ^{119}Sn. The last of these has been used in another of Dr. Taylor's projects to study the behaviour of tin (II) halides in solution. The ^{119}Sn spectra of aqueous mixed halide solutions consist of single lines, the positions of which depend on the composition of the mixture and lie between those of the separate chloride, bromide or iodide systems. The signals are averages of the chemical shifts of the various species present: $(SnX_nY_{(3-n)})^-$ (X,Y =Cl, Br, I, n=0-3).

These are labile in water at room temperature on the NMR timescale. If these solutions are extracted with diethyl ether and the extracts cooled to 213 K, then the ^{119}Sn spectra show each of the individual species present (see Figure 7). The exchange rate has been slowed down by lowering the temperature in a less coordination solvent. Thus the chemical shifts of all ten trihalogenostannate(II) anions can be determined.

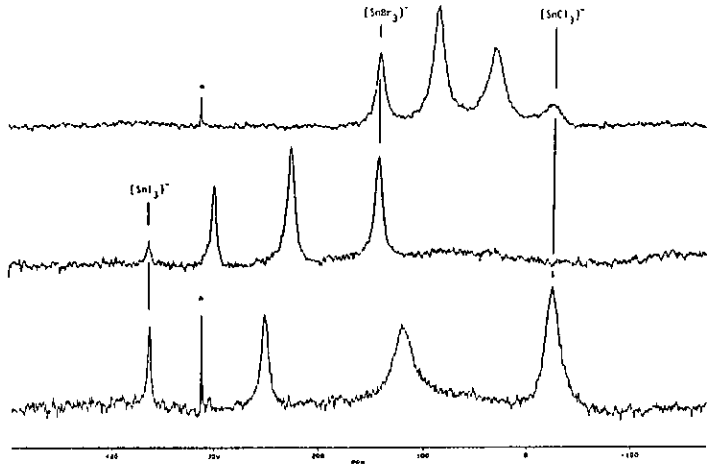


Figure 7 149MHz ^{119}Sn spectrum of tin(II) mixed halide systems at 213 K. Diethyl ether extracts with total (Sn) ca. 0.5M.* Denotes a "folded" signal from a small amount of tin(IV) species.

Physical Interactions

If a suitable probe nucleus can be found, NMR is also useful for looking at physically interacting systems as well as more orthodox chemical exchanges. ^{129}Xe is another nucleus with I= 1/2. Xenon gas is composed of large polarisable atoms whose chemical shift is very sensitive to the environment. Dr. Russell Howe has been using ^{129}Xe NMR to study the structure and composition of several zeolite catalysts which are important in hydrocarbon refining and synthetic petrol production. Most of the NMR protocols described here rely on liquid samples or at least on samples that approach homogeneity, contained in unsealed glass tubes (see figure 8). This is not the case for the zeolite experiments. The sample consists of solid zeolite material in the bottom of a tube which is then filled with a known amount of xenon gas and the whole sealed off from the atmosphere. The experiment works because the xenon atoms behave like a liquid inside the zeolite, interacting with each other and with the solid. The properties of the catalysts depend on the size, shape and coatings of their internal pores and these are exactly the variables to which the xenon nuclei are responsive. The results are spectra which give an indication of the size of the catalyst pores, their water content and the effects of a variety of heat treatments mimicing the operating conditons under which the zeolites are used.

The interaction between sweeteners and taste receptors is also amenable to interrogation by NMR. A surprisingly wide range of compounds elicit the same sweet taste on the human tongue. These include saccharin, aspartame *(Nutrasweet)*, potassium cyclamate, lead acetate and chloroform as well as sucrose and most of the monosaccharides. No structural similarities between these are obvious. The taste response may be triggered by a specific molecular conformation when interacting with the receptor. NMR can be used to determine the solution conformation of the molecules and monitor any changes when they meet the receptor. A major restriction is the unavailability of isolated functioning human taste buds. These are considered to be essentially lipid membranes and are modelled by unilamellar phospholipid vesicles. Changes in the ^{1}H and ^{13}C chemical shifts and parameters monitoring molecular constraints such as relaxation times, are being used to examine the effect of the liposomes on a selection of sweet compounds.

NMR Trends

These examples, while covering a wide range of research interests, simply indicate what is possible on one type of modern NMR spectrometer. The subject is much wider. Some other important areas under intense development are; experiments giving data in three dimensions with an inherent increase in available information, spectroscopy of solid materials using a range of nuclei, and magnetic resonance imaging (MRI) which can display NMR-edited maps of living systems as an alternative to CAT scanning. At the moment, these appear to be separate and disparate. Library classifications of books in these areas certainly finds them widely dispersed. This reflects the enormous range of applications rather than underlying fundamental techniques. It may be that NMR is really evolving as a discrete discipline.

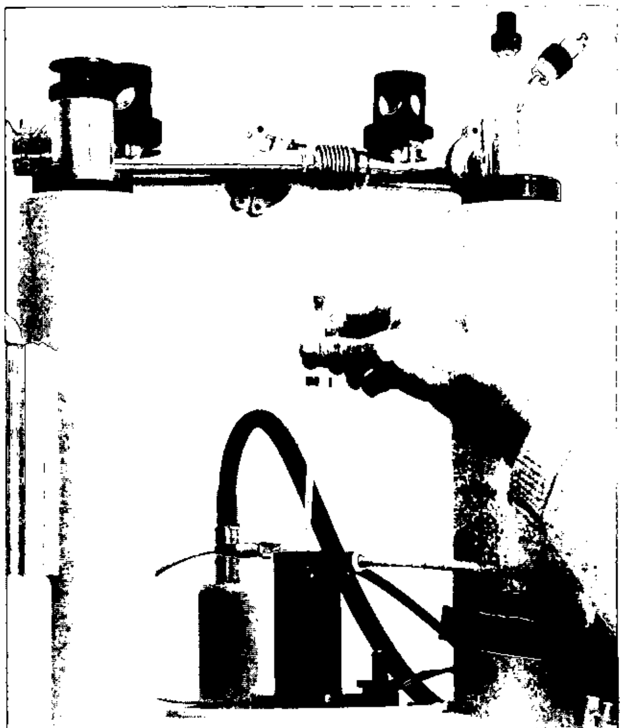


Figure 8 A normal liquid sample being inserted into the superconducting magnet of the AM400 spectrometer. The two high turrets with the connecting cross bar are the tops of the dewar holding liquid helium.

References

1. B.R. Davis, 1965, J. NZIC, 29, 7-13
2. (a) R.J. Abraham and P. Loftus, 1978, *Proton and Carbon-13 NMR spectroscopy*, Heyden & Son Ltd. London.
   (b) E. Breitmaier and W. Voelter, 1987, *Carbon-13 NMR Spectroscopy*, VCH, New York.
   (c) J.K.M. Sanders and B.K. Hunter, 1988, *Modern NMR Spectroscopy*, OUP, Oxford.
3. (a) W.R. Croasmun and R.M.K. Carlson, Eds., 1987, *Two-dimensional NMR Spectroscopy, Applications for Chemists and Biochemists*, VCH, New York.
   (b) G.E. Martin and A.S. Zektzer, 1988, *Two Dimensional NMR Methods for Establishing Connectivity*, VCH, New York.
4. J. Mason, Ed., 1987, *Multinuclear NMR*, Plenum Press, New York.

The N.Z. INSTITUTE OF CHEMISTRY
The N.Z. BIOCHEMICAL SOCIETY
And The N.Z. SOCIETY OF PLANT PHYSIOLOGISTS

1990 CONFERENCE

Chemistry - Resources and the Future

VICTORIA UNIVERSITY OF WELLINGTON

20-23 AUGUST

Preliminary Programme

and

Call for Papers

Conference Chairman - Dr Ken MacKenzie, Chemistry Division, DSIR, Private Bag, Petone. Tel. (04) 690-513, Fax (04) 694-500.

Conference Secretary - Dr Neville Tapp, Unilever Ltd, Private Bag 1, Petone. Tel. (04) 666-949, Fax (04) 683-338.

A REGISTERED SESQUI- CENTENARY EVENT

CONFERENCE PROGRAMME

The following is a preliminary programme. Minor modifications are expected on receipt of abstracts for the Specialist and Poster Sessions. Specialist Symposia will be arranged under the following broad themes:

- Analytical Chemistry and Chromatography
- Biochemistry and Plant Physiology (especially Plant Molecular Biology)
- Carbohydrate and Organic Chemistry
- Chemical Education
- Geochemistry and Industrial Chemistry
- Health and Environmental Chemistry
- Inorganic and Physical Chemistry
- Science Policy
- Spectroscopy (including a workshop session at DSIR)

Preliminary Programme

	Monday	Tuesday	Wednesday	Thursday
8.30-9.20		Belton	Lorimer	Hughes
9.20-10.10		Adam	Peacock	Rothbart
10.10-10.40		Tea	Tea	Tea
10.40-12.20		5 x 20 min Specialist Sessions	Poster I	Hodson Poster II (100 min)
12.20-1.30		Lunch	Lunch	Lunch
1.30-3.10	MS Workshop at Chem. Division DSIR	5 x 20 min Specialist Sessions	5 x 20 min Specialist Sessions	5 x 20 min Specialist Sessions
3.10-3.40		Tea	Tea	Tea
3.40-4.30		Devlin	Ferrier	Maddox (1 hour)
4.30-5.20		Gunston	Gravestock	Closing Ceremony (30 min)
5.20-7.00	Dinner	Dinner		
7.00-7.30	Opening Ceremony	Walker (1 hour)	Conference Dinner	
7.30-8.30	Maddox Public Lecture	Science Policy (1 hour)		
8.30-9.30	Trade's Mixer			

[All plenarys of 50 min]

NB) NZIC Annual General Meeting to be included. (Time yet to be finalised).

PLENARY SPEAKERS

The Conference committee has confirmed the participation of an unusually large number of quality plenary speakers from both within New Zealand and overseas. Photographs and biographical data will be published in the next issue of Chemistry in New Zealand.

ADAM, Dr Colin	Director, Institute of Industrial Technologies, CSIRO, Melbourne, Australia.
BELTON, Dr G G	Director, Central Research Laboratories, BHP, and Professor of Extractive Metallurgy, University of Newcastle, Australia.
DEVLIN, Dr John P	Research Director, Boehringer Ingelheim Pharmaceuticals Inc., Ridgefield, CT, USA.
FERRIER, Prof. Robin J	Professor of Organic Chemistry, Victoria University of Wellington, NZ.
GRAVESTOCK, Dr Mike	Research Director, ICI Carbohydrate Group, Jealotts Hill, UK.
GUNSTON, Mr Robin	Commercial Manager, NZ Refining Co., Whangarei, NZ.
HODSON, Dr Derek	Senior Lecturer, Education Department, University of Auckland, NZ.
HUGHES, Ms Helen	Parliamentary Commissioner for the Environment, Wellington, NZ.
LORIMER, Dr George	Central Research and Development Department, E I du Pont de Nemours, Wilmington, DE, USA.
MADDOX, Mr John	The Editor, Nature, London, UK.
PEACOCK, Dr Jim	Chief, Division of Plant Industry, CSIRO, Canberra, Australia.
ROTHBART, Dr Herb L	Director, North Atlantic Area, Agricultural Research Service, USDA, Philadelphia, PA, USA.
WALKER, Dr Basil	Chief Executive Officer, Ministry of Research, Science and Technology, Wellington, NZ.

CONFERENCE FEES

Registration forms will be sent out in April/May. To enable budgeting, the likely fees are given below.

Full Registration

Society Member	**$230** reduced to **$180** if received by 1 June
Non-Member	**$270** reduced to **$220** if received by 1 June
Student	**$50**

One-Day Registration

Society Member	**$115** reduced to **$90** if received by 1 June
Non-Member	**$135** reduced to **$110** if received by 1 June

Chemical Education Symposium only **$50**

ACCOMMODATION will be available at the University Halls of Residence (cost approximately $40/day for full board), or at nearby Hotels.

CALL FOR PAPERS

Papers are invited in the specialist areas listed previously, or in any other related area of chemistry, biochemistry or plant physiology.

Papers offered for oral presentation should be of 20 minutes duration (including time for questions). The alternative is to present a poster. As a result of the large number of plenary speakers, a limited number of oral presentations will be available. These will be distributed on a **first-come, first-served** basis.

PLEASE INDICATE YOUR PREFERENCE FOR AN ORAL OR POSTER PRESENTATION

THE DEADLINE FOR PAPERS AND ABSTRACTS IS 1 MAY, 1990

INSTRUCTIONS FOR ABSTRACTS

The ORIGINAL and ONE copy are required.

1. **Size and presentation** - Abstracts must be typed in camera-ready form and within an area of maximum typing width 160mm and maximum typing depth of 180mm on A4 paper. Please ensure that the abstract is free of typographical and grammatical errors and of good quality for reproduction. Dot matrix imaging is not suitable.

2. **Title** - In upper case.

3. **Authors** - Lower case except for first letters and initials. Place an asterisk after the author who will present the paper or poster.

4. **Affiliation** - Lower case, starting with the affiliation of the presenting author followed by the other authors.

5. **Text** - This should be as informative as possible and should contain relevant information or methods and results. Conclusions drawn should be clearly outlined. Statements such as "The results will be discussed" should be avoided. Do NOT indent. Leave one line space between paragraphs.

6. **Acknowledgements** - If necessary to appear one space below the text.

7. **References** - In the text the citation should be numerical in order of use. References to be listed, no heading, one space below the text (or acknowledgements) and given in numerical order, citing the authors, the year of publication, the title of the journal, volume number and the first page number. References to books should also contain the year and place of publication, and the publishers.

8. The Conference Committee reserves the right to make the final selection of papers in accordance with the requirements of the programme. Unless asked to the contrary, any oral presentation that cannot be given a time slot will be slotted into the poster programme and the authors notified as soon as possible.

Do not fold abstract - mail it flat.

Send abstracts by 1 **May** to:

Dr Neville Tapp
NZIC/NZBS/NZSPP Conference Secretary
Development Department
Unilever (NZ) Ltd
Private Bag 1
Petone
NEW ZEALAND FAX (04) 683-338

FLAVOUR COMPONENTS OF COFFEE, TEA, MILO AND BRANDIES

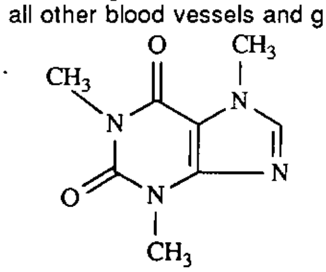
J.J. Rustenhoven

As an innovation, an essay produced as an assignment by a student in a second year chemistry university course "Perspectives in Chemistry" is printed below. The author's opinions are his own and are not endorsed by the editor or the Institute of Chemistry.

My ninth edition of the Encyclopaedia Britannica ascribes the flavour of coffee as being due to caffeone, the essential oil produced when the coffee bean is roasted. Not the most in depth answer but not a bad attempt for 1897. At the other extreme, the science library has to offer a lovely doctoral thesis expounding in great depth the many hundreds of complicated structures that the humble coffee bean has to offer. In French.

The distinctive coffee aroma is due to a bewildering array of compounds, numbering at least 500. Those compounds identified as contributing to the coffee aroma differ in flavour from "mushroom-like" to "nutty" to "sweet burnt caramel", to "roasted nutty" to name a few[1]. Many of these compounds are carbonyls, both aliphatic and aromatic, there are also numerous alicyclic and several heterocyclic compounds involved. The most common aromatics are polyphenolic compounds. The amino acids (green coffee beans contain at least 17) when roasted with sucrose also give distinctive tastes. Most notable is the result of roasting a 1:1 molar ratio of proline (≈7% of the amino acid content of roasted coffee beans)[2] and sucrose which produces an intensely bitter taste. Not only must all these components be present in the correct ratios (for any given coffee type of course), but the pH of the coffee solution is also important. Above a pH of ≈5.2 the coffee becomes excessively bitter, at low pH (below ≈4.8) it is sour. At a pH of 5.7 it is actually described as having a cigar taste![3]

Caffeine also contributes to the bitter taste, but can hardly be described as a major flavour component. After all, neither tea, cacao, maté, guruana nor the African kola nut taste of coffee. It is however responsible for most of the physiological effects of coffee. These include greater ability to concentrate, narrowing of the cranial blood vessels, enlargement of all other blood vessels and greater alertness.



caffeine

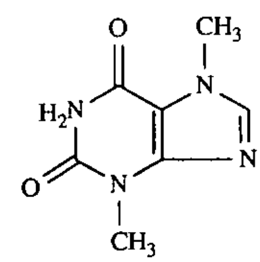
How then are these flavours produced (if not from a bottle of Kahlua or Delcafé)? None of the aromas is present in the green beans. During roasting the beans are heated to between 200 and 250°C. Browning reactions as well as the formation of aromas take place mainly during this step. In particular the carbohydrates fragment to give the many carbonyl compounds, the combination of sucrose and amino acids has already been mentioned. The structures formed from this combination have not yet been elucidated.

Clearly the longer the roasting, the more reaction occurs and the fuller the coffee flavour. It must also be remembered, however, that many of these compounds are volatile and will be lost during excessive roasting. Lightly roasted coffees reveal more delicate, individual tastes but are also more acidic as the acids have not had a chance to evaporate or break down.

Tea too is not of itself a very flavoursome substance. Usually it undergoes a series of steps to create its characteristic flavour, again the product of a range of aromatics, phenolics and caffeine. The tips of the tea bush (if it is a good tea) are picked and dried until they are limp ("withering"). They are then "rolled" in which the different cells are crushed so that their contents become mixed and are able to react on subsequent heating.

Next, the tea is "fermented" during which process polyphenolics, in the presence of oxygen, are converted by a polyphenoloxidase enzyme to the pigments (tannins) that give the tea its colour. Tannins also give tea body. They bind proteins, including those in the mouth which causes a sense of constriction associated with a full-bodied drink. Accordingly, if the fermenting is carried on too long, the tannins will tend to bind to themselves giving a dull, flat tea. Those who adulterate their tea with milk effectively remove the tannins by binding them preferentially to the excess milk proteins.

theobromine



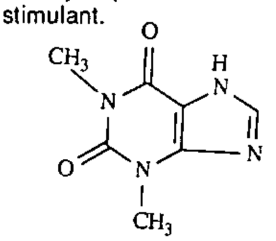
Again the list of flavour components for black (processed) tea is a long one, but the descriptions are very different[4].

They are predominantly of "leafy", "floral" and "woody", with fewer described as "earthy", "smoky" or "burnt" flavours. Caffeine is also important to the taste of tea. More so than in coffee because of the lack of other bitter compounds such as the generally bitter polyphenolics which are the subject of fermentation. Again caffeine dominates the physiological effects of tea, although two closely related alkaloids, theobromine and theophylline, are also present but in very much smaller quantities.

Milo is a horrid concoction made for those who cannot hold down their hot chocolate. If an unhealthy amount of this debilitated substance is used per cup the predominant taste is, it could be argued, that of chocolate. This, obviously, is the work of cocoa. Cocoa in itself however is quite bitter and large amounts of sugar are added. In fact Milo contains 6% more sugar than cocoa, so that sucrose may certainly be termed a major flavour component. The other flavours are due to the "malt and other cereal extracts" (which impart that unmistakeable "it's nearly bed-time" flavour) and of course the elusive "flavouring substance" on which Nestlé neglect to elaborate.

As for tea and coffee, raw cocoa (cacao) beans are devoid of the aroma for which we know them. The fresh cacao bean is described as tasting of vinegar. To create the chocolate flavour careful attention is paid to the time of harvesting, fermentation and roasting. In these last two, adequate aeration is of particular importance. The roasting serves to create the desirable aroma, and to remove the undesirable ones, as well as to kill the larvae and eggs of pests. Acetic acid (produced by oxidation of ethanol from fermentation) evaporates, and some undesirable esters and the bitter phenolics partially decompose. Amongst at least 400 aroma contributing compounds are 2-methylpropanal and 2-methylbutanal which together with a methylphenylhexanal impart various chocolate tastes. Many other aromas are variously characterised as "nutty" some as "fruity" or "floral", others "burnt" and "roasted" and one as "caramel"5. The major alkaloid in cacao is theobromine (a compound quite devoid of bromine, but fit to stimulate the Gods) Whilst not very important as flavouring it is, like caffeine, a mild stimulant.

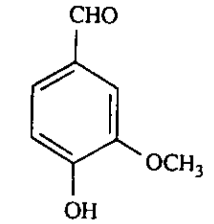
theophylline



On a more stimulating note still, a brief discussion on **Brandy**. The greatest physiological effect in this delightful beverage is naturally that of ethanol. This is but one, and not the most important flavour component of Brandy. A Brandy's taste may be partially traced to the wine from which it was distilled. Brandies in general are higher in poisonous methanol than many other distilled liquors[6] (plum and pear brandies contain well over 1000mg of methanol per 100 ml of ethanol). They also contain, Cognac in particular, many higher alcohols which contribute to the flavour. Some of these may be implicated in the physiological phenomenon known as the hangover.

The wine used for Cognac must be new. It will contain some organic acids which during the distillation can react with alcohols to produce a variety of esters which may contribute to the aroma. (The alcohols also oxidize to some extent to aldehydes, particularly acetaldehyde). As Cognac is aged for anything up to 50 years, but at least 15 years in oak, there is ample time for flavour from the oak to be imparted to the brandy.

vanillin



Particularly important as regards flavour of Cognac are about eight aromatic aldehydes originating from the oak. These include p-hydroxybenzaldehyde and vanillin[7] — which clearly is important in vanilla flavours. Interestingly, if wines that have been treated with sulfur dioxide are used then this may end up as sulfuric acid in the brandy. Some brandies will dissolve iron (and other metal) pipes, pumps and containers. Such brandies, it is considered, are best not kept in metal vessels!

REFERENCES

1. a fuller list is found in *Food Chemistry*, p 688 table 21.7a
2. " " " " " " " " ; p 685 table 21.4
3. see *Food Chemistry*, p 690 figure 21.3
4. a fuller list is found in *Food Chemistry*; p 698 table 21.16a
5. " " " " " " " " ; p 707 table 21.2a
6. see *Food Chemistry*, p 677 table 20.18
7. see *Technology of Wine Making*, p 613

BIBLIOGRAPHY

Amerine, Berg and Cruess	The Technology of Wine Making Avi publishing 1972
Belitz and Grosch	Food Chemistry Springer-Verlag 1987
McGee	On Food and Cooking

"How are we failing Maori Students of Chemistry"

By Pauline McPherson Waiti - Te Timatanga Hou, University of Waikato

A lecture given in the Chemical Education Symposium 'Chemistry in a time of change' NZIC Conference August 1989

The asking of this question allows me, in my attempt to answer it, to focus on the accessibility of Education to Maori people.

A glance at official statistics, namely early school leavers, state exam results, tertiary education graduates, crime, unemployment, homeownership, and health will confirm my view that Education has largely been inaccessible to a majority of the Maori population for the last 100 years.

Why has this been so?

I am unaware of any cognitive disadvantage that "being Maori" bestows on our race. Could it possibly be that the structure of the Education system set up in colonial New Zealand is at fault and has slowly produced a race of people who are lost in their own land?

I would have to say "yes" to this.

This process began with the establishment of the 1867 Native Schools Act and its assimilation policy. One of the functions of Education, I believe, is to "help develop a student's full potential in his or her future social, economic and cultural life"(1). It is obvious from the statistics that this simply has not occurred for the majority of the Maori population and whereas assimilation has reaped positive results for the colonials, this process has definitely become the death knell for the Maori people.

The definition of the word assimilate is "to make like, absorb into the system"(2), so for the Maori, assimilation produces brown-skinned pakehas, and surely it is becoming painfully obvious that this is no longer acceptable. Maori people have the right to be recognised as Maori.

Now we as educators must look at alternatives for Maori Education, in terms of what Maori people want for their Maori children. Maori people are dissatisfied and have been for a number of years and I am sure you are well aware of initiatives such as the Kohanga Reo Movement at preschool level, Bilingual, Total Immersion and Kura Kaupapa Maori Schools at primary level, and Bilingual Units at Secondary level.

Let us refocus on our starter question: **How are we failing Maori students of Chemistry?** With specific reference to the body of knowledge loosely defined by the term Chemistry and more broadly called Science, I would have to say that the Educative process begins to fail Maori students at the Form 3 level, the time when a formal Science Education begins. In actual fact I believe the the majority of Maori children begin to fail from the day they enrol at Primary School at 5 years of age. However that could well be the topic of another address.

I can see 3 areas which need to be discussed:

1. **Teacher attitudes and expectations**
2. **How Maori students feel**
3. **The curriculum.**

Teacher attitudes and expectations form part of the Hidden Curriculum and there is no doubt that this may, more than anything else, determine the relative educative disadvantages experienced by both girls and Maoris. The majority of teachers are middle-class, monocultural and monolingual. They have little knowledge of "things Maori" and often consider pakeha culture to be superior to Maori culture. They have low expectations for Maori pupils and hold, what has been termed "deficit" views regarding Maori children's intelligence and competence especially in "real" subjects like Science and Maths. As stated in the Department of Education's recent publication "Countering Sexism in Education", "Expectations are very powerful" "Expectations affect learning" and "Often our expectations are unconsciously held and not readily identified by us". Richard Ennis has pointed out ". . . most teachers are blithely unaware that they are unwitting collaborators in a system that is so manifestly unfair and unjust to a large section of our New Zealand population . . . it is rarely their children, or those of their closest relatives, friends and neighbours who fail . . . "(3).

Now, couple this group of people with a group of students who have come through 7 or 8 years of being educated in a system that perpetuates the myth that Maori are inferior, useless, dumb and lazy and I am sure you can see the start of failure. Many children have come through all their school life having basic indignities committed against them like name mispronounciation. The message anyone receives in such a situation is one that lowers their self-esteem and makes them feel ashamed of what having that name stands for. This group of students is not going to be confident in a system that has already labelled them as failures. They will not be forthcoming and willing in a classroom where they feel that they have nothing worthwhile to contribute because they aren't worthwhile as people. What are **these** students going to learn in this Form 3 Science class?

Generally, curricula on the whole have been monocultural and based in the European Tradition. A Maori child sits in a class with a wide range of experiences which are never relevant, never discussed and may sometimes even be trivialized. What is being taught is often out of context with the students world — when you look through a Junior Science book and see nothing that relates to you or your culture, it can turn you off. A student I teach this year has said to me that she thought atoms were a pakeha thing and that Maori's didn't have them!

But good news, as a response to the report of the Curriculum Review Committee in 1987, The F1-5 Science Draft Syllabus for Schools has been produced. A document which actually addresses the fact that two groups of students, Girls and Maori's are currently under-represented in Science. Compulsory reading would have to be page 8, the section entitled "Making Science Accessible" and along with the frameworks that have been provided to allow a teacher to teach from a context relevant to his/her students, I am sure you will all agree that a major mindshift has occurred in the one area that even most liberalists would never have dreamed of it happening. But the fact is, when something is not working for a large proportion of people you should have to change it and at least, question it.

Now with positive changes occurring in the Science Curriculum, and hopefully in other curriculum areas, I would now like to look at a way that would allow Maori students to have better feelings about School and of course, Science and Chemistry.

I believe Bilingual Education will help to ensure that Maori people are educated according to the stated functions of Education earlier mentioned, that is, to help develop a student's full potential in his or her future social, economic and cultural life.

The aims of Bilingual Education in New Zealand are to produce bilingual individuals in both the English and Maori Languages, to maintain the Maori Language as a living communicative language and to improve the educational outcomes of Maori children. The role of the Maori Language is unquestionable central to a Bilingual Education Programme in New Zealand. If the status of the Maori Language is raised then so too is the status of the Maori students. Teachers within a Bilingual Education Programme would ideally be Maori Language users and be supportive, sympathetic and sincere. Curriculum areas taught in a Bilingual Education Programme would acknowledge and value both cultures in this country.

Currently in New Zealand Secondary Schools attempts at Bilingual Education are occurring in Bilingual Units. If a school community believes that current educational provisions are not meeting the needs of their Maori students then I believe a Bilingual Unit needs to be set up. This Unit would attempt to create an atmosphere conducive to cultural sensitivity, self-esteem, self-confidence and pride to ensure and develop social, academic and cultural understanding and competence. In the long term, Bilingual Education will produce students who are able to operate efficiently in both cultures and languages of this country. If Maori students are more confident of themselves as Maori, they will be more able and willing to aquire properly the skills of another (Pakeha) culture. Moreover, their acquisition and development of Maori skills will, I believe, actually enhance their acquisition and development of Pakeha skills.

The process of setting up a Bilingual Unit is crucial — consultation with the Maori community must occur and legitimization of the Unit must come from the hierarchy within the school. Anything smacking of tokenism (which can easily happen to a minority culture) has to be avoided. Inherent in any successful Bilingual Unit I believe is a certain amount of separatism, in terms of one structure existing alongside another structure, to ensure the aims of the Unit are achieved. For afterall, the only alternative to separatism when you are a minority is assimilation and we are all too well aware of the effects of that.

The reality of Bilingual Units presently in operation is that there is a major lack of resources — people resources and curriculum material resources. More Maori people with the language need to be infront of our young as positive role models, more caring and sincere people need to be there as well. Here we can challenge places like Teachers' Colleges to increase their intake of Maori trainees and to provide adequate courses to allow people to teach effectively in bilingual Units. Equity courses such as Te Timatanga Hou are important in the process of empowering Maori people so that more Maori people are in front of more Maori people in a positive way. More money must be directed to producing resources that can be used by Billingual teachers, with such limited resources for Bilingual Education you may say it is unrealistic to expect all subjects to be taught in the Maori Language in a Bilingual Unit. However, positive attempts can be made — the simplest requirement for a teacher in a Unit surely would be the willingness and ability to correctly pronounce names and then the next step would be a commitment to learn the language.

Let us now return to our hypothetical Form 3 Science class of Maori students. By now they should be part of a Bilingual Unit — they should be starting to learn their language and they should be begining to feel confident and safe in their environment. They should be seeing positive role models and also they should be coming into contact with teachers who value them as Maori people. One advantage my students have in having me as their Science teacher is that I am like them, I know what it is like to be a Maori because I am one — there are certain experiences we share simply because we are Maori, that is with regard to a teacher student relationship we have a base on which we can build a learning relationship.

The Science Teacher will be attempting to devise a programme that will allow the students in front of her/him to think that Science is a part of their world. With reference to the frameworks set out in the Form 1-5 Draft Syllabus the teacher could begin the year teaching a unit call "Science and Me" or "Ahau' — the first topic could be called "Whakapapa" (genealogy) which for Maori students would serve as positive reinforcement (the message given would be along the lines of 'this person acknowledges the importance of my past to my existence today'). I have never felt entirely comfortable, although I always did it, starting off F3 Science with a list of Laboratory Rules — all those Don'ts — is there any wonder many students thought of Science as a negative thing.

The Science that follows on from an initial look at one's past and then to one's existence in the present world is overwhelming — the body, growth and development, health and disease, digestion, levers and machines, inheritance and variation to name but a few areas. Move oneself sideways into the kitchen and more Science — cooking, freezing, microwaves, cleaning substances, food — then a step outside — plants and animals, conservation, telecommunications, local industry. You see the Science is the same, what we have to do is teach it in a more appropriate manner.

I would like to mention at this point however, a warning: we have to be careful that in contextualizing content we do so sensitively and accurately and we must make sure that all the necessary information is made available and is passed on — afterall we do not want to 'ghettoize' Maori Education. Laboratory Rules are important but perhaps they are more relevant once the student feels that they themselves belong in the lab in the first place.

Our class of students will learn through the year that Science is an integral part of every person's everyday life — and hopefully that Science isn't only a Pakeha thing! They will learn that atoms are part of being Maori, Pakeha, Jewish, Gentile, Male, Female, White, Black — with apologies to Professor Dodd who on the one hand arrogantly says that the new Syllabus is "pretty depressing stuff written by people who clearly do not understand what Science is about" and on the other hand says that "Science is Universal" (4). Funny isn't it, I know alot of people who were educated by 'real' scientists like Professor Dodd, who still think that Science only occurs in the Science Lab and is only done by white, middleclass males — hardly universal!

In conclusion, I hope I have been able to provide some ideas to promote some discussion on the question asked at the begining of this address. I am aware that I have not addressed many issues that follow on and lead up to the one discussed here such as 'How are the Secondary Schools going to cope with the influx of Kohanga and Total Immersion Primary School children in a few years?' 'When is the energy, time and money going to go into developing the necessary resources needed for Bilingual Education?' 'What is the particular fate of the Maori woman in Education?' 'What is the role of courses such as Te Timatanga Hou?'. However, rest assured, there is much discussion going on in Maoridom on these and many other issues pertinent to them and their children.

I would like to acknowledge the people whose recorded work on Bilingual Education provides a basis for addresses such as this, the people who tirelessly work in all the areas to do with Maori Education and all the people in this land who actually believe that this country can be truly Bicultural. Finally, to everyone who believes in the Principles of The National Common Curriculum — that the curriculum be common to all schools, accessible to all students, non-racist, non-sexist, whole, balanced, planned, co-operatively designed, responsive, inclusive, enabling and that it allows students to enjoy significant success, that it provides Education that is of the highest quality, that it reflects the fact that Education is a lifelong process and that it provides learning that is enjoyable for all students, a hearty greeting — Kiaora. Sounds like the perfect Bilingual Unit to me!

FOOTNOTES

(1) Taken from an unpublished paper written by Tame Kuka, Wiremu Mathews, Karaitiana Tamatea and Uenuku Fairhall on the Philosophy, Aims and Desired Outcomes of the Tauranga Boys College Bilingual Programme.

(2) 'The Pocket Oxford Dictionary of Current English' sixth Edition, Edited by J.B. Sykes.

Cont on page 14

THE STATE OF THE CHEMICAL INDUSTRY IN NEW ZEALAND

A talk by Fred Holland — Managing Director of Revertex Industries and Immediate Past-President of the New Zealand Chemical Industry Council.

New Zealand has been in a ferment of change for the past five years but political trends never happen in isolation. Throughout the western world we are seeing trends in public opinion and public policy in two key areas which are so strong that none can stand in their way. Woe betide the King Canute who tries for now to bring back socialism to Maggie Thatcher's England. Or the chemical company who ignores the fact that the Emperor's clothes are now green. For the two dominant themes of modern political debate are a balanced budget and a concern for the environment.

On the economic front we have seen the new willingness of electorates to accept tough medicine in order for their governments to pay their way. Monetarism, user-pays and a reliance on market forces to solve our economic ills are all symptoms of 1980s economic thinking. We have seen treasury storm troopers lay waste to government department, local bodies and quangos in the name of financial efficiency. Trade barriers have come down, government trading departments are being forced to turn a profit and those of us in export have had to cope with an exchange rate which has been a tool of monetary policy. Having set all this in motion, the government is now responding to the beat of a new political drum, the one sounded by the environmental movement.

Resource Management

This may sound an unusual cause in a country like New Zealand where environmental problems are not nearly as great as in Western Europe or North America, — but for a labour government which has put 150,000 out of work and is seen by many as uncaring, the green trend in politics is a potential life saver. There is nothing like a good dose of ozone depletion, greenhouse effect, or closer to home, the Manukau Harbour, to take the headlines off our economic woes.The challenge for the government is to find a way of embracing pro-environmental policies without setting up a raft of new quangos or more important, without costing itself a lot of money. The challenge for the chemical industry is to identify the risks and opportunities which these trends pose and to develop strategies which will allow us to stay in business until they have run their course.

The resource management law reform process now underway envisages the enforcement of new green legislation being handled by regional councils, which is why industry self regulation is a theme which is finding a lot of favour at present both in New Zealand and overseas. Both are ways for government getting its way on green issues without having to pick up the tab for costs.

Resource management is a businesslike phrase, but it's one which has been coined by the Ministry for the Environment to cover a grab bag full of environmental issues from pollution control and soil erosion, through to the logging of Beech forests and the regulation of mining. The management of hazardous substances — in manufacture, packing, transport, storage, use and eventual disposal — is a key part of the RMLR process. It's one where the NZCIC has had deep involvement in the last 18 months.

Green Issues

As the public focus on green issues grows in the lead-up to the 1990 elections, chemical companies will need to be seen to be squeaky clean. If there are major accidents which reveal that the industry is not obeying its own voluntary standards, the concept of industry self regulation will be tossed out the back door. For a vote-concious government, a balanced budget is one thing. To be seen to be throwing the book at the chemical industry is another. Already, the government has announced its intention to create a new policy-making quango with responsibility for environmental protection. The precise nature of this body's functions and the manner in which they will be implemented are now the topic of political and bureaucratic debate. The extent to which it will be a standard-making body and the extent to which it will be policeman has yet to be determined. The rigidity of its standards and the extent to which industry self-regulation will be permitted is all in the melting pot right now.

Turning our attention to the NZ chemical industry the twin issues of market forces and environmental concern are tailormade to have maximum impact. We see an industry which had been built up during the 50s and 60s when support for local manufacture and full employment were the major planks of government policy, while the bouyant farming economy ensured that we could afford the cost. These policies had led to the development of a very fragmented industry servicing an already very small market by world standards so that each individual unit had insufficient throughput to show an adequate return without unreasonably high levels of protection.

Balancing the books

The government's objective of balancing the books and reducing inflation resulting in a policy of reduction in protection coupled with a high valued NZ dollar has had a dramatic effect on the section of the industry I am familiar with and I suspect other areas of the chemical industry have faced similar major restructuring. Of the twelve significant surface coating companies which were trading in the early 80s only six remain, and by an amazing coincidence the same numbers apply to the change in the resin and polymer industry. I do not think there is any one brave enough to say that the rationalisation is yet complete. The restructuring has resulted in the establishment of much more soundly based companies which at least have a chance of survival in the open economic environment with throughputs getting closer to volumes experienced overseas. The increased volumes have enabled the survivors to upgrade their operations with more efficient bulk handling systems thus further enhancing their chances of survival. The argument often brought up when industry rationalisation is occuring is the potential for price hikes in the face of reduced internal competition. In today's climate this is not happening and will not happen because to survive we must not only ensure that we are competitive against imports but we must also make sure that the industries which consume our outputs are also able to survive against imported competition.

CER with Australia is having its impact on the chemical industry with most companies in the industry having very close trans Tasman ties enabling us to view the two countries as one market with both industry and product rationalisation occuring again leading to economy of scale and efficiency. With free trade between the two countries virtually in place the only inhibition preventing a full flowering of this trade is restrictive shipping practices. Freight travelling between Australia and New Zealand must make it the second next most expensive strip of water in the world after Cook Strait.

NZ Chemical Industry Council

On the environmental front the chemical industry is right in the firing line as we represent an easily identified and targeted entity. The industry recognised this trend five years ago and formed the NZ Chemical Industry Council to tackle the issue along with the associated matters of Health and Safety.

Two key issues were identified, industry credibility and public understanding and these have formed the basis of our approach since then.

First and foremost came industry credibility. Several high profile incidents both off-shore such as Bhopal and Seveso and locally, the Parnell fume case and several spectacular fires, triggered a high level of public concern and raised the very real issue of whether the advantages of the output of the chemical industry were worth the apparently inherent risks.

The industry knew that to survive it had to reduce or, if possible, eliminate the risks. In the western world, and New Zealand was included, chemical industry chief executives took on the role of chief environmentalist and no issue has higher priority for them.

The NZCIC executive, comprised of chief executives of leading chemical manufacturers and importers, identified areas of immediate concern and pooled resources through working sub-committees to establish codes of practice which have been published and circulated to members and other interested parties. These form the minimum standard which members must meet. This programme has led to a reduction in incidents and because of the improved communication with the emergency services those incidents which have occurred have been handled quickly and efficiently with the minimum of fuss or risk.

These codes of practice also form the basis of our case to government for a self regulatory process. It is a concept which many politicians and agencies want to endorse. But for this policy to win, we are going to have to make sure that it is working on the ground; that the standards are in place throughout the industry and that they are being enforced by management. As with all things the performance of the weakest player will determine the success of the team. So the challenge for the council is to broaden membership and to get every one on side. Having made a start on getting our own house in order the NZCIC has now embarked on a programme geared to lift the image of chemistry and the chemical industry in the eyes of the general public.

Image of Chemistry

It is of concern to us that at a time when the public, Government and media attention is focussing on chemicals we have an educational system which appears to have an anti-chemistry bias. Whether we have enough specialists to meet our needs is one thing, but of even greater concern is whether the journalist moulding opinion, the government employee drafting legislation or the local body official, has ever had any exposure to chemistry during their educational programme. Accordingly the NZCIC is embarking on an ambitious 2 year public relations programme aimed at achieving a more balanced coverage of the industry in the media, a better informed political and bureaucratic process and a more positive attitude from the educational system. The media and political approaches are fairly standard stuff but the desire to get alongside schools and teachers at all levels is exercising our minds as to the best way to proceed. We know that we have a good story to tell but how best to get it across is the concern.

Research is not needed to tell us the importance of schools in attitude formation. Young adults choose careers and base many of their attitudes on experiences and ideas they come into contact with while at school. Unfortunately for the chemical industry teachers, even science teachers have had little or no contact with industry. They also teach in an educational environment in which extreme attitudes tend to hold sway. In the primary curricula topics like conservation and pollution are heavily emphasised while science tends to get only fleeting and theoretical attention. At secondary schools many students cease to have any contact with science topics after spending time in the third and fourth forms looking at basic scientific principles as part of a general science course. Vogue issues such as those raised by anti-vivisectionists and extreme environmentalists are key topics of discussion in liberal arts subjects such as English and Social Studies etc without the benefit of balancing information from industry, agriculture or science.

Several pilot programmes have been run in Wellington, Palmerston North and Auckland with leading chemical company speakers talking to science teachers, sixth form students and primary school children and the results have been extremely positive with the general comment being that this was the first time they had seen that there is another aspect to these topics and that their attitudes had been fixed by getting just one side of the story from the media. We believe that by balancing the information children get in schools and tertiary institutions we will improve the image of science based industry as potential career choices for school leavers. Longer term we will also influence the course of public debate. We are not looking to put across the story that pollution or undue risk is good for you but rather presenting the real picture of our industry which is one which sees its future inextricably tied to its ability to present society will all the benefits of chemical and scientific development managed in such a way that we present no short or long term threat to the life on this planet.

To some extent the two pressures on the industry are working against each other with additional investment to increase environmental protection being demanded at the very time when income is being hit by the tight economic policies. Fortunately industry rationalisation is helping in this area with improved facilities being justified by higher volume throughput but increased environmental protection does have a cost and in the end our whole community will have to bear that cost.

I have every confidence in our more streamlined chemical industry being able to compete at the highest standards and I know that the New Zealand society is willing to pay the cost of a better environment but just one little thought gives me concern. In our free and open economy how do we compete against those countries which choose to ignore the environment. Are we as a society going to insist on enjoying low cost imports and accept the lower environmental standards of the countries of origin? If that is to be the case then our society will need to review its ethics.

Cont from page 12

(3) Benton, Richard. 1987. 'If it's worth doing, is it worth doing badly?' (Paper presented at the First AARE/NZARE Joint Conference, University of Canterbury, Christchurch. December 3-6 1987.) NZCER.

(4) Taken from article written by Bob Jones in the NZ Herald Monday August 21 1989 entitled 'Sums, not silliness, should be school core curriculum'.

BIBLIOGRAPHY

Draft Syllabus for Schools, Forms 1-5 Science. Department of Education, Wellington, 1989.

'Maori-English Bilingual Education: Tauranga Boys College' H. Wagemaker Research Report Series No 51, Research and Statistics Division, Department of Education, Wellington.

'Getting It Right — Aspects of Ethnicity and Equity in New Zealand Education'. Edited by Walter Hirsh and Raymond Scott. Published by Office of the Race Relations Conciliator, 1988.

'Countering Sexism in Education' Department of Education. 1989.

A PROPOSED NICKEL SMELTER

R.M. Carr, Chemistry Department, University of Otago

Early in 1989 a representative of New Zealand Nickel Smelters Ltd visited several localities in the South Island presenting local authorities with plans for a nickel smelter. At a time of contracting economic activity with resultant high unemployment any suggestion of the establishment of new industry will undoubtedly receive serious attention. Several sites are under consideration and it is possible that one of them may have all the features required for the new industry.

The proposed smelter will be used to process an ore from New Caledonia believed to contain about 1.6% nickel. The ore is a lateritic type formed by weathering of rocks rich in magnesium and iron (ultrabasics — peridotite) of garnierite, a clay mineral similar to serpentine with idealised composition $(Ni, Mg)_6Si_4O_{10}(OH)_8$ and in limonite of composition $(Fe, Ni)O(OH)nH_2O$.

Detailed information concerning the ore composition has not been made available but it is probable that the laterite ore contains predominantly saprolite (silicate) together with a little limonite (oxide).

Mass% Compositions of Some New Caledonia Saprolites and Limonite

	Saprolites			Limonite
Fe	13.34	11.06	6.53	54.8
Ni	2.53	0.92	2.47	1.38
Cr	0.85	0.17	0.33	3.58
MgO	23.7	34.0	29.17	0.36
MnO		0.18	0.09	1.57
Al_2O3	1.07	1.74	3.16	1.26
SiO_2	42.1	49.5	37.3	0.30

The nickeliferous minerals are not amenable to physical separation, and hence an extremely large quantity of ore must be processed to yield a small quantity of product. The New Zealand smelter proposal suggests an output of about 42,000 tonnes per annum of ferronickel (75% Fe — 25% Ni) from 760,000 tonnes of ore. Ferronickel is utilised mainly in the production of alloys.

The proposed extraction procedure contains four stages viz. reduction, melting, slagging and fabrication. The ore will be shipped in bulk carriers to New Zealand at fortnightly intervals in 30,000 tonne lots.

Reduction to a nickel-iron sponge will take place in rotary kilns fired with limited quantities of coal and oil. The principal nickel ore, garnierite, dehydroxylates at about 550°C to form a very disordered, almost amorphous and hence very reactive oxide phase which crystallises to form the minerals olivine and enstatite at about 800°C. The kiln temperature which is maintained by the combustion of fuel oil must be held below 800°C to allow the nickel and iron oxides both to remain amorphous and to undergo reduction in the presence of coal. The overall chemical changes may be summarised thus:

$$(Ni, Mg)_6Si_4O_{10}(OH)_8 \xrightarrow{550°C} 6(Ni, Mg)0.4SiO_2(s) + 4H_2O(g)$$

$$NiO + C \longrightarrow Ni(s) + CO(g)$$

$$Fe_2O_3 + 3C \longrightarrow 2Fe(s) + 3CO(g)$$

$$(CH_2)n + 1.5nO_2 \longrightarrow nCO(g) + nH_2O(g)$$

Thermodynamic data indicate that carbon will reduce NiO at 500°C whereas a temperature above 700°C is required for the reduction of FeO. hence it is possible, under carefully controlled conditions, to selectively reduce the ore to obtain particular compositions eg 75-25 ferronickel. Controlled oxidation and thermal cracking of both oil and coal will yield carbon and carbon monoxide. The carbon will reduce the metal oxides in the amorphous condition while carbon in a limited air supply provides the thermal energy.

In the second stage the ferronickel sponge together with the huge bulk of worthless material is fed into an arc furnace where the ferronickel is melted to effect separation of the product. This process is conducted in an inert atmosphere of nitrogen to prevent oxidation of the alloy. During the solid state reduction and melting a significant amount of carbon (up to about 4%) is incorporated in the alloy, and is removed by an oxygen blow in the arc furnace. At the same time a little lime is added to ensure that all of the worthless material forms a slag which is removed. Thus conversion of the alloy to the required composition and slagging off constitutes the third stage of the process.

Finally the ferronickel alloy is either cast into billets or fabricated into granules and despatched to appropriate alloy manufacturers.

A smelter as described will have a significant environmental impact and could be a source of several hazardous materials. Of greatest concern is the annual production of about 600,000 tonnes of slag. Both the ore and the slag contain apreciable amounts of chromium which is toxic to plant and marine life. Hence careful management of ore and slag stockpiles to ensure total dust suppression will be mandatory. The disposal of such large quantities of slag constitutes a major problem. Slags have been used for land fill, roading and agricultural fertiliser but there are limits to the amounts which can be used in South Island localities. The presence of chromium in the slag could limit its usefulness as a fertiliser. Atmospheric emissions from the smelter would contain dus, carbon dioxide, carbon monoxide, water, and a minor amount of sulphur dioxide (from any sulphur present in the coal and fuel oil). These emissions may be reduced to acceptable levels by means of electrostatic precipitators and scrubbers. Within the smelter effective dust and emission control will be required to minimise any long-term hazards which could include lung cancer, nickel asthma and dermatitis.

From an economic viewpoint a nickel smelter of this size would provide initially 300 construction jobs followed by 130 at the smelter and a further 100 downstream. Deep water port facilities would receive more use and service industries of many kinds would be utilised. Electricity consumption is estimated to be 300 million units per annum equivalent to the output of a 34.25 MW generator. Other local inputs include significant quantities of agricultural lime, coal, liquid oxygen and liquid nitrogen, together with some refractories. The ore, fuel oil, some refractories and electrode paste would be imported.

References

1. Otago Daily Times, 3 February. 1989
2. Maquet M., B.D. Cervelle and G. Gouet (1981) Signatures of Ni^{2+} and Fe^{3+} in the optical spectra of limonitic ore from New Caledonia; Application to the determination of nickel content. Mineralia Deposita 16, 357-373.
3. Canterford J.H., (1975) The treatment of nickeliferous laterites. Mins. Sci. Eng. 7, 3-17.
4. Encyclopedia Britannica 15th Edn., 1978. v13
5. Kirk-Othmer Encyclopedia of Chemical Technology 2nd Edn, 1963. v13.
6. Minerals Yearbook (1984) U.S. Department of the Interior.
7. Mineral Facts and Problems (1980) U.S. Department of the Interior.
8. Nickel Smelting — Some Facts. Pamphlet compiled by Save Aramoana Campaign.

PRODUCT NEWS

NEW 3-PLACE DIGITAL DENSITY METER.

Anton PARR USA's new DMA 38 digital meter provides simple density measurement without a waterbath. The instrument's internal peltier effect thermostat operates from 15° to 45°C, yeilding densities precise to $\pm 1\times10^{3}$g/cm^{3} in minutes. It can be used with the SP3 sample changer to provide automatic measurement of up to 24 samples without operator attention.

The DMA 38 can display density, plus a related value such as °Brix, API gravity, or % alcohol. Displayed units can be changed via the standard RS232C port, using an IBM-compatible PC.

Also available are the Anton PARR DMA 48 and DMA 58 meters with four-and five-place precision respectively.

For further information please circle no. 10 on reader reply card.

Next generation detector for LC — Spectra Focus.

SPECTRA-PHYSICS' introduces Spectra FOCUS, the new real-time scanning UV-Vis detector for liquid chromatography. The "forward optics" design of Spectra FOCUS offers advantages over current diode array detectors such as high sensitivity for trace analysis. The versatile Spectra FOCUS detector can be used for either single or multi-wavelength operations. Any LC application can be performed by using easy-to-change flowcells — for analytical, micro, biotech, prep LC capillary electrophoresis.

Spectra FOCUS Chromatography Software which runs on the IBM PS/2 computer turns Spectra FOCUS into a powerful chromatography and spectroscopy LC data system that is compatible with standard applications programmes. The true multi-tasking operating system features: data acquisition, quantitation/reintergration, LC instrument control, 3-D plotting, peak purity, overlays of spectra, derivatives and multi-wavelength chromatograms.

For further information please circle no. 11 on reader reply card.

New low-cost, high reliability gas analyser from ADC

For measuring carbon dioxide (CO_2) concentrations in laboratory applications and plant physiology studies, the Analytical Development Company (ADC) Limited has introduced the low-cost EGA CO_2 analyser.

Designed with no moving parts, the manufacturers claim the unit is capable of providing reliable CO_2 measurements for many years with only minimal maintenance.

Based on the principle of infrared gas analysis, the EGA is not subject to poisoning or interference by other gases. CO_2 concentration is measured from 1 — 1999 ppm and displayed on the front panel digital display window. An analogue linear output facility is also provided.

Incorporated into the unit are a drier which removes water vapour and a soda lime cell for removing CO^2 for calibration purposes. A built in sample pump is also included which can be used or bypassed as required. Gas flow through the unit can be set from 40 — 400 ml/min.

The EGA is mains powered , weighs just 3.5 Kg and measures 160 x 305 x 155mm.

For further information contact Wilton Instruments, P.O. Box 31-044 Lower Hutt, Phone (04) 697-099, Fax (04) 697-240.

For further information please circle no. 12 on reader reply card.

THE UNIQUE DSC121

ICI Instruments are pleased to announce the new model DSC121 Thermal Analyser from Setaram. Derived from an earlier model the new unit continues the unique capabilities of very large temperature range, -120°C to 830°C, and exceptionally high sensitivity. The DSC121 has the ability to run particularly large and very small samples in ways not possible on other DSC systems. This includes ballistic heating (or cooling) to the starting temperature, and running samples under controlled pressure up to 100 bars.

The DSC121 is extremely easy to operate as all aspects of the instrument are under computer control, including gas switching. Setaram's unique sample enveloping transducer (Calvet) system, which measures heat flux and not temperature changes, gives the DSC121 many advantages. It provides exceptional accuracy especially when there are very weak heat flows, and ensures that sensitivity is not affected by gas flow rate during gas sweeping.

The unique features of the DSC121 allows all general applications that can be performed on other DSC's. However, the instrument is especially suited to polymer cure studies, metallurgy, combustion, explosives and specific heat measurements. It has the unique capability for measuring thermal conductivity of polymers and other solid materails with similarly low conductivity coefficients.

For further information please circle no. 14 on reader reply card.

Catalogue detailsHach simplified systems.

A new catalogue explains simplified, economical procedures and instrumentation for fertilizer and plant tissue and sap. Each section contains a flow chart showing steps of the analytical method(s), and example of typical procedures and information for ordering.

Hach's extensive analytical systems are characterize by easy-to-use instruments; single-dose pre-measured reagents; proven methods, and comprehensive, illustrated procedure manuals.

Available through Wilton Instruments.

For further information please circle no. 13 on reader reply card.

Commonwealth Games — Drug Testing in Sport.

As over 2,000 atheletes competed in the XIV Commonwealth Games in Auckland New Zealand in January 1990, the Australian Government Analytical Labs (AGAL) in Sydney, were also preparing for the drug testing which has become a standard part of every major sporting event around the world.

Hewlett-Packard has traditionally been the major supplier of instrumentation since the introduction of drug testing in 1972 at the Munich Olympic Games. The XIVth Commonwealth Games in New Zealand were no exception, in that over $800,000 worth of HP equipment was running 24 hours a day to analyse the samples. HP also committed around-the-clock support to ensure the smooth running of the testing.

AGAL had on hand 6 mass selective detectors, 2 gas chromatographs, 2 liquid chromatographs, all automated. Three MSD's dedicated to steriod testing only. One MSD dedicated to confirmation of positives.

Approximately 40-50 samples were sent through for testing each day for the duration of the Games. Samples were flown over from New Zealand via couriers. Security was at a premium with all samples being checked to ensure seals secure and not tampered with.

For further information please circle no. 18 on reader reply card.

ADVANCED CENTRIFUGE WARE

NALGE COMPANY introduces **Nalgene UltraPlus™ Centrifuge Ware**, an advanced system of tubes, bottles and sealers for simpler ultracentrifugation. Safe and convient to use, Nalgene UltraPlus Centrifuge Ware is interchangable with other manufacturers' ultracentrifuge tubes and bottles — but costs less. The line includes Nalgene UltraLok™ Tube System, UltraBottle Assemblies and open-top UltraTubes, all designed to fit most commonly-used ultracentrifuge rotors; UltraTube Racks support tubes and bottles on the benchtops.

Each Nalgene UltraBottle Assembly consists of a transparent, polycarbonate Nalgene UltraBottle and screw closure with O-ring and plug for leakproof service at ultra speeds. UltraBottles are autoclavable and reusable.

Nalgene UltraTubes includes disposable thin-wall and reusable thick-wall, open-top tubes in four sizes. A choice of polyallomer tubes, which exhibit low protein binding and good chemical resistance, or polycarbonate tubes which are transparent are available. Thin-wall tubes are easy to pierce or slice , while autoclavable thick-wall tubes accomodate most commonly used ultracenttrifuge tube caps.

Nalgene UltraTube Racks provide stable support for Nalgene UltraPlus Tubes and Bottles during filling, capping and sealing procedures on the benchtop. These low-cost, transparent, acrylic rack hold tubes firmly without movement during manipulation. They also accomodate other tubes with similar diameters. Each tube location is numbered for easy sample identification.

For further information please circle no. 19 on reader reply card.

NEW PRODUCT RELEASE

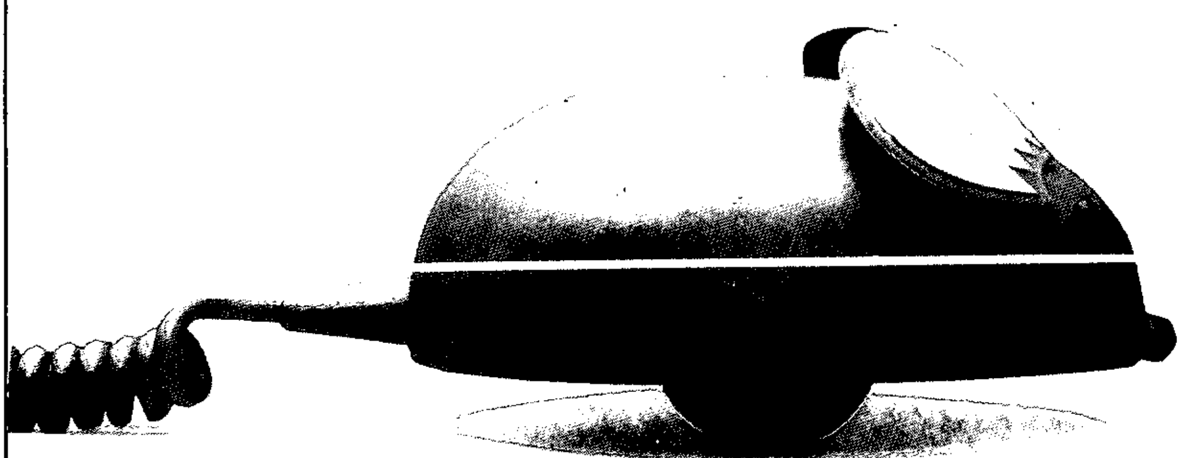
ICI Instruments has introduced the new LC1260 Electrochemical Detector to it's range of HPLC detectors. The highly sensitive and selective LC 1260 utilises a unique wall jet design cell, that enables the electrode to be quickly and easily removed. The microprocessor controlled ECD is easy to operate and incorporates a cleaning mode to extend electrode operating life. The LC1260 has a working potential range of +/- 2.0V in 1mV increments with the latest low noise electronics that incorporates a 1Hz active filter and averaging digital filter. The range of working electrodes include 1mm and 3mm Glassey Carbon, Au, Ag, Pt, set-in Kel-F.

For further information please circle no. 20 on reader reply card.

Reminder

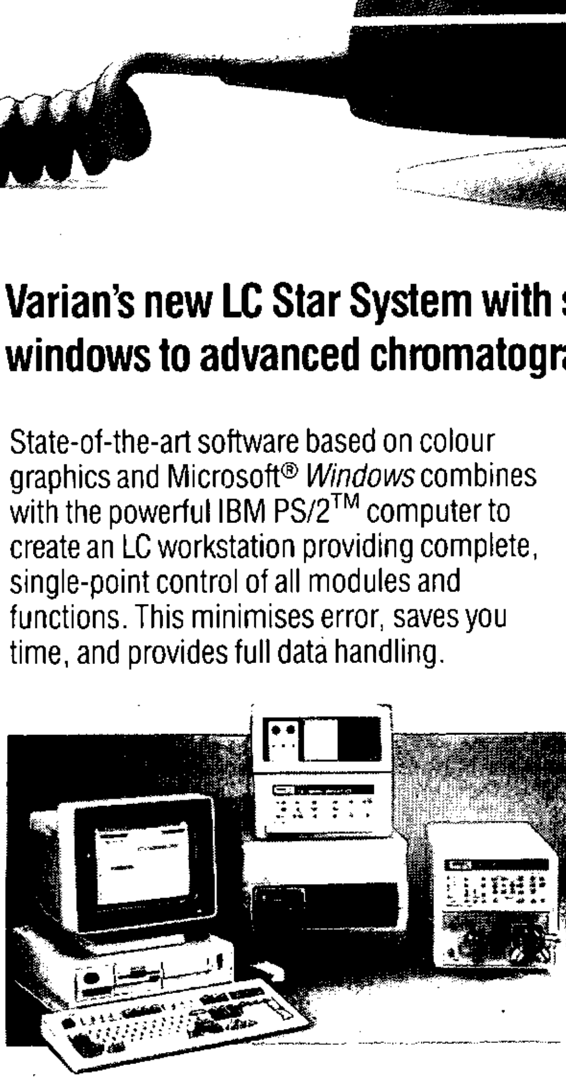
Entries for NZIC Prizes are due on 30th April Potential entrants are reminded to send entries to Alan Turner in Wellington.

Presenting our new window opener...



Varian's new LC Star System with single point mouse control opens windows to advanced chromatography and improved user productivity.

State-of-the-art software based on colour graphics and Microsoft® *Windows* combines with the powerful IBM PS/2™ computer to create an LC workstation providing complete, single-point control of all modules and functions. This minimises error, saves you time, and provides full data handling.



All Star System modules – gradient pump, programmable autosampler, diode array and UV-Vis detectors – are independently intelligent. This unique feature allows modules to operate as powerful, stand-alone components without the need for computer control.

Real HPLC flexibility and versatility gives you rapid throughput, methods diversity and reliable, continuous automation. Raise your productivity with unattended sample preparation.

Varian's LC Star System is designed for maximum reliability and easy maintenance.

Open the window now on top chromatographic results and call us today for further information.

varian

Marketed by:

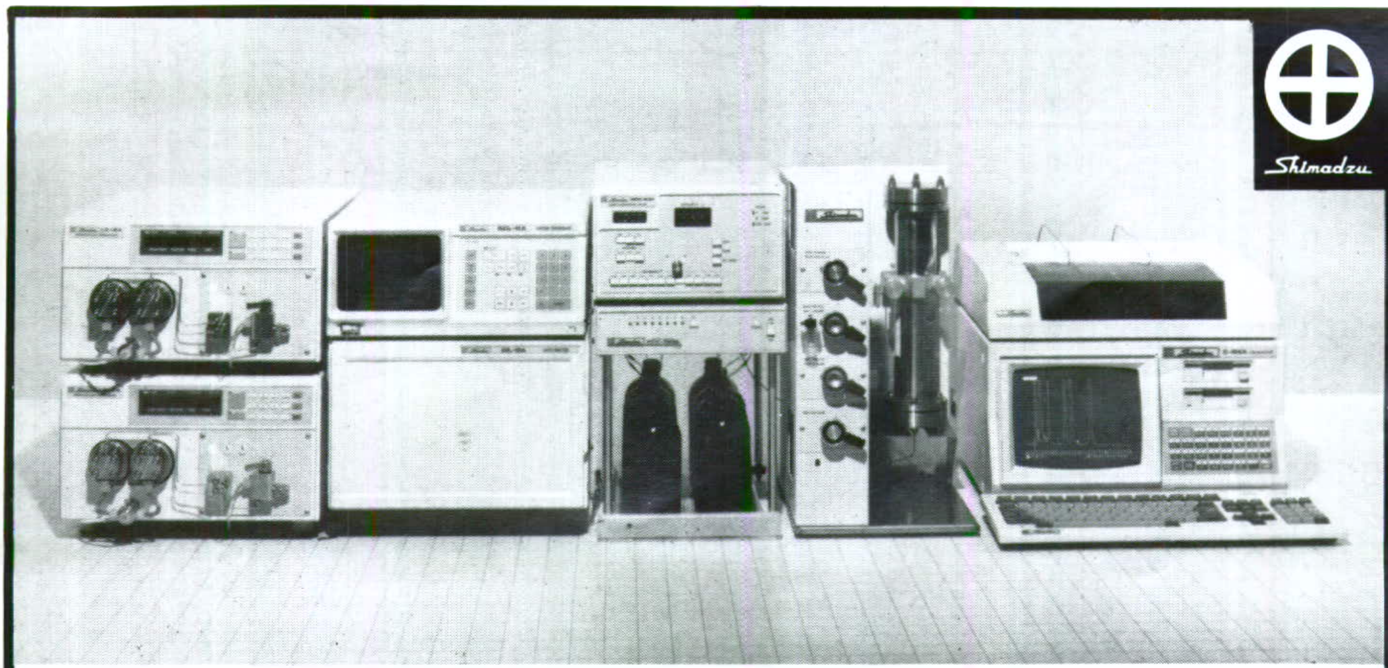
WILTON INSTRUMENTS

People you can count on

Auckland, Private Bag Northcote 9. Tel 418.3039
Lower Hutt, Box 31-044. Tel 697.099
Christchurch, Box 1813. Tel 663.663

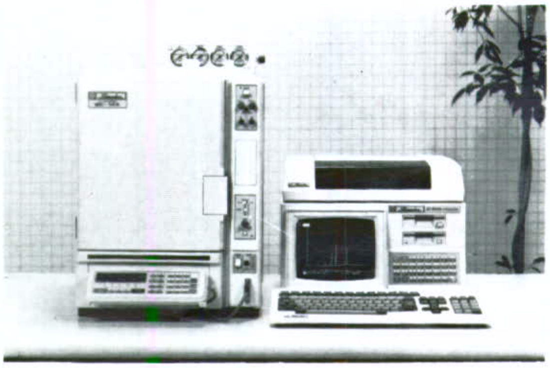
Microsoft is a registered trademark of Microsoft Corporation.
IBM PS/2 is a trademark of International Business Machines Corporation.

A member of the Salmond Smith Biolab group.

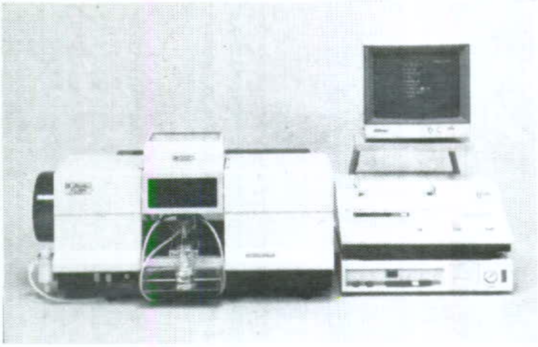


SHIMADZU — THE BRAND OF RELIABILITY

For a variety of needs . . .
Shimadzu analytical and measuring instruments



Automated analytical and measuring instruments of higher performance are the result of research and development in advanced technologies, quality control and laboratory automation.
Shimadzu has been a top manufacturer of analytical and measuring instruments since 1875. Advanced technologies in electronics, biotechnology and other fields are incorporated into the development of new products and applications technologies from a world-wide viewpoint.



AWA with twelve years experience marketing Shimadzu x-ray equipment are now proud to bring you the Shimadzu range of Scientific Instruments.

MAIN PRODUCT LINES —
ANALYTICAL & MEASURING INSTRUMENTS

- Spectroscopic Apparatus
- Electromagnetic Analytical Apparatus
- Chromatographs
- Thermal Analysis Instruments
- Environmental Pollution Analyzers
- Balances and Balance Appliances
- Powder and Particle Property Analyzers
- Magnetometers
- Biotechnology Instruments
- Other Analytical and Measuring Instruments

AWA Scientific + Medical

A division of • AWA New Zealand Limited

• Auckland	• Porirua	• Christchurch
P.O. Box 1636	Private Bag	P.O. Box 8421
Fax: (09) 763-214	**Fax:** (04) 379-412	**Fax:** (03) 481-727
Tel: (09) 760-129	**Tel:** (04) 370-159	**Tel:** (03) 481-171

Shimadzu