


August 1983, Volume 47 No. 4



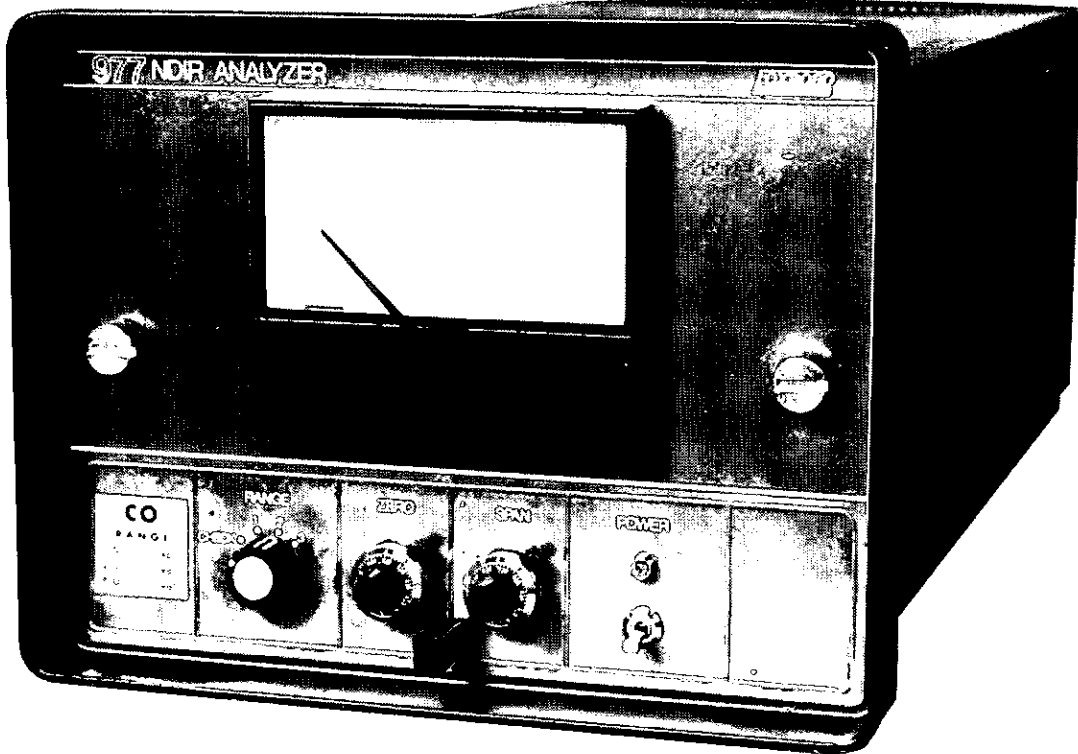
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NZIC Annual Conference

with the NZ Biochemical Society and the NZ Soil Science Society
August 23-26, 1983, University of Waikato

REGISTRATION:

3-8 p.m. Monday, 8-9 a.m. Tuesday-Friday. Student Union Building (Gate 1, Knighton Rd).
For further details on registration, accommodation, or transport contact Dr C. Devine, M.I.R.I.N.Z. Ham. 56-159.

PROGRAMME:

Tuesday Aug. 23 — Morning Sessions

- 9 a.m. Opening by the Minister for Science, Dr Ian Shearer.
11 a.m. Tilden Lecture by Prof. Robin Clark, University College London.
"Resonance Raman Spectroscopy — A New Technique of Wide Application in Chemistry."
11.45 a.m. Plenary Lecture by Prof. Kenneth Rinehart, University of Illinois.
"Applications of Mass Spectrometry to Bio-organic Chemistry."

Tuesday Aug. 23 — Afternoon Sessions

- 1.30-4.30 SYMPOSIUM ON CALCIUM AND CELLULAR CONTROL.
The Role of Calcium as a Second Messenger — Mary P. Thompson, University of Otago.
Calmodulin — Prof. J. G. T. Sneyd, University of Otago.
Calcium Regulation in Vertebrate Skeletal Muscle — David A. D. Parry, Massey University.
Control of Sperm Motility — Ian Forrester, University of Otago.
Fertilisation of the Ovum by the Spermatozoa — D. Green, University of Otago.
1.30-3.10 SPECIALIST SESSIONS — Industrial, Chromatography (GC), Inorganic, Organic (NMR).
3.40-5.00 SPECIALIST SESSIONS — Industrial, Mass-Spectrometry, Inorganic, Organic (Synthesis).
5.00 p.m. Annual General Meetings — Biochemical Society, Inorganic and Organometallic Group, Massspectrometry Group.

Wednesday Aug. 24 — Morning Sessions

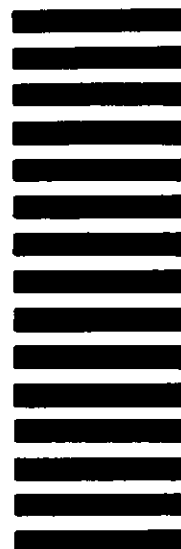
- 9.00 a.m. Plenary Lecture by Dr Ted Baker, Massey University.
"Structural Studies on Azurin, a Blue Copper Protein."
9.45 a.m. Plenary Lecture by Dr Claude Culvenor, C.S.I.R.O., Melbourne.
"Studies on Plant and Microbial Toxins Affecting Livestock."
11-12.30 ANALYTICAL SYMPOSIUM
A1 — New Procedures for Purification of Proteins by HPLC and Affinity Chromatography.
W. S. Hancock, D. R. K. Harding, D. R. Knighton and J. S. Ayers, Massey University.
A2 — Immunoassays in Biomedicine.
R. A. Richardson, Syntax Lab. (NZ) Ltd.
A3 — Gas Chromatography — Its Role in the Identification of Volatile Food Contaminants.
F. B. Whitfield, C.S.I.R.O. Food Research, North Ryde.
11-12.30 PLANT AND MICROBIAL TOXINS SYMPOSIUM
T1 — Lolitrem Neurotoxins from Perennial Ryegrass, *Lolium Perenne*
R. T. Gallagher, Ruakura Animal Research Station.
T2 — Isolation and Structural Studies on a Toxin from the Blue-Green Alga, *Nodularia Spumigena*.
J. W. Blunt, P. E. Mulligan and M. H. G. Munro, University of Canterbury.
T3 — Glucose Nitropropanoyl Esters as Insect Toxins and Feeding Deterrents from *Lotus Pedunculatus*.
R. F. N. Hutchins, O. R. W. Sutherland, C. Gnanasunderam, D. R. Greenwood, G. A. Lane and G. B. Russell, DSIR, Auckland and Palmerston North.
T4 — Effect of Sporidesmin Dosing on Biliary Changes of Sporidesmin, Lyolecithen and Bile Acids in Sheep.
R. J. Fairclough and B. L. Smith, Ruakura Animal Research Station.
11-12.20 SPECIALIST SESSIONS — Biochemistry, Inorganic.

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Wednesday Aug. 24 — Afternoon Sessions

FIELD TRIPS — Departing 12.30.

Thursday Aug. 25 — Morning Sessions

- 9 a.m. Plenary Lecture by Prof. Hugh McKenzie, ANU Canberra.
"Comparative Aspects of Milk Proteins of Different Species: Case Studies in Protein Chemistry."
- 9.45 a.m. Plenary Lecture by Prof. Keith Syers, Massey University.
"Chemistry of Soil Fertility."
- 11 a.m. SYMPOSIUM ON COMMERCIAL PROCESSING OF PROTEINS.
Commercial Extraction and Uses of Casien — C. R. Southward, NZ Dairy Research Institute.
Commercial Extraction and Uses of Whey Protein — W. J. Harper, NZ Dairy Research Institute.
Biomass Refining: Extraction of Protein from Lucerne and Grass — R. McDonald and P. Donnelly, Ruakura Agric. Res. Centre.
- 11-12.30 SPECIALIST SESSIONS. — Soil Chemistry — Physical, Analytical, Inorganic, Biochemistry, Organic (Sugars & Lignins).

Thursday Aug. 25 — Afternoon Sessions

- 1.30-5.00 Biochemistry (Proteins and Enzymes). Soil Chemistry — Mineralogy and Soil Solution
- 1.30-3.10 SPECIALIST SESSIONS — Analytical, Chromatography, Inorganic, Organic (Synthesis).
- 3.40-4.30 Easterfield Address by R. Newman, Chemistry Division, DSIR.
- 4.30-5.30 NZIC Annual General Meeting

Friday Aug. 26 — Morning Sessions

- 9 a.m. Plenary Lecture by Dr Don Weiss, C.S.I.R.O., Sydney.
"Processing with Magnetic Particles — Applications to Water Treatment."
- 9.45 a.m. Plenary Lecture by Prof. Peter Fensham, Monash University.
"Chemistry, Education, Society."
- 11-12.30 SYMPOSIUM ON WATER QUALITY AND POLLUTION CONTROL.
Under the auspices of the NZ Committee for Water Pollution Research and Control.
- 11-12.30 SYMPOSIUM ON CHEMICAL EDUCATION
Uses of Microcomputers.
- 11-12.30 SPECIALIST SESSIONS — Soil Chemistry — Organic Matter. Biochemistry, Chromatography (HPLC).

Friday Aug. 26 — Afternoon Sessions

- 1.30-4.30 Chemical Education — Curriculum and Teaching Methods.
- 1.30-3.00 Water Pollution.
- 1.30-3.00 Soil Science.

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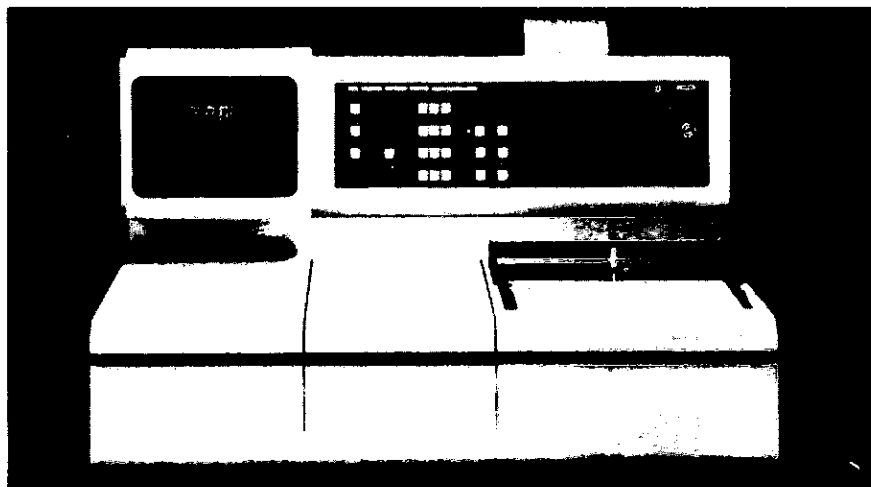
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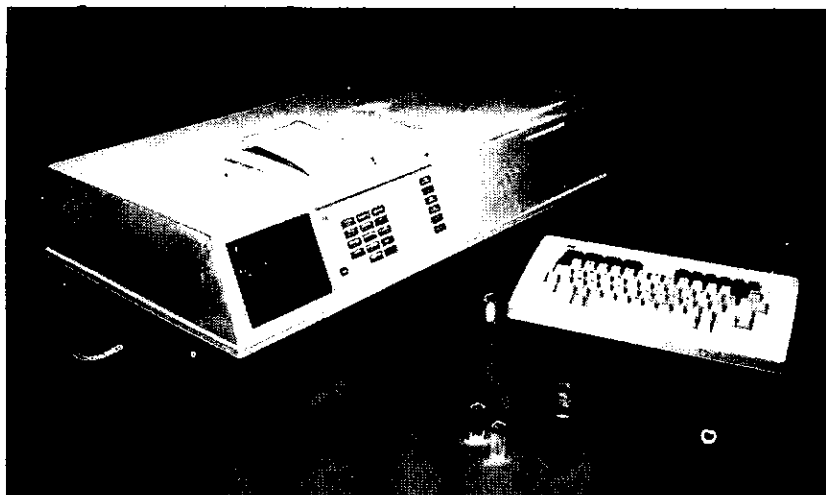
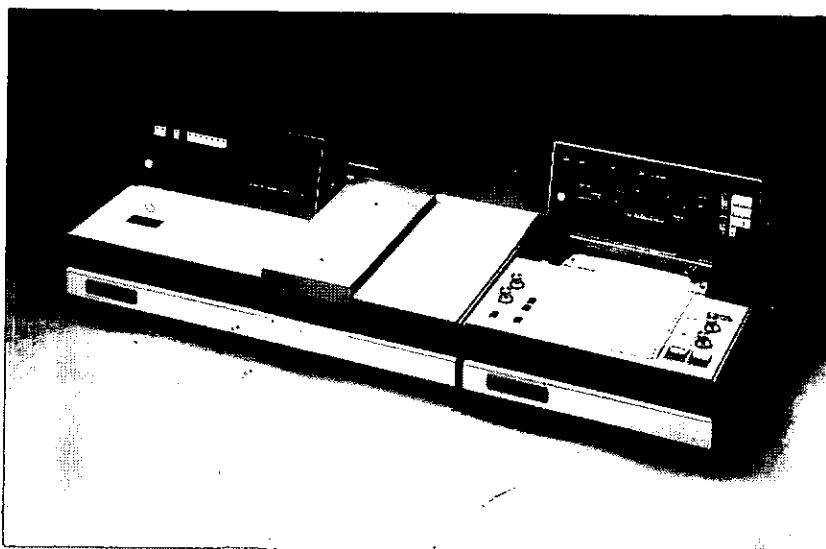
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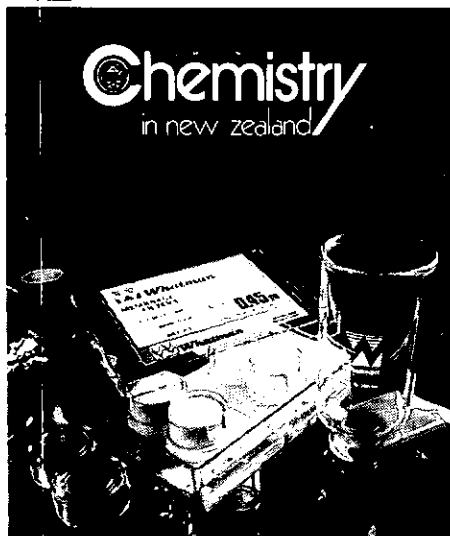
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Otago: Dr Derek Whyman, Chemistry Dept, University of Otago, P.O. Box 56, Dunedin.

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CONTENTS

Guest Editorial
 Pat Holland ponders the traps and treasures of analytical chemistry 78

Annual and Financial Reports 92

Conference Guests
 A brief look at plenary and invited speakers at this year's Annual Conference 79

Conference Programme
 The August Conference in Hamilton, programme details 73

Obituary
 Arthur C. Kennett 80

Letters to the Editor
 Further proof that someone reads The Sceptical Chemist 80

The Sceptical Chemist 99

Aspects of Chromatography in Agricultural Research
 Denis Lauren and Pat Holland discuss the applications of HPLC and GC to agricultural problems 81

Electron Spin Resonance Spectrometry and its Applications to Biochemistry
 Eric Ainscough and Andrew Brodie of Massey University discuss ESR spectroscopy and its application to biochemical research 86

Low Temperature Spectroscopy
 Applied Biochemistry Division Scientist R.V. Asmundson outlines the advantages of spectroscopy at liquid nitrogen temperatures 89

The Identification of Factors Affecting Sperm Stored for Artificial Insemination
 Peter Molan talks about the production of calves without a lot of bull 91

Branch News 97

General News
 Discount on DSIR publications 99

People 80

Integrated Systems for Automated Acquisition and Control 100

Conferences 85

DSIR and Research Institutions 98

GUEST EDITORIAL

ANALYTICAL CHEMISTRY — TRAPS AND TREASURES

The analyst is often Cinderella in the professional stakes of chemistry. However, a high percentage of practicing chemists in New Zealand, particularly in the industrial, agricultural and processing areas, have a strong involvement with analytical chemistry. Chemical and biochemical researchers are also increasingly dependent upon the results from complex analytical equipment. These facts are recognised by the Universities and Technical Institutes which are training our next generation of chemists. What often seems to be lacking is an emphasis on the creative side of modern analytical chemistry.

The stereotype of a routine job where one follows 'engraved on stone' methods which are being rendered even more sterile by automation, is quite inappropriate. Innovation is always needed to improve the accuracy or speed of particular analyses. Every analysis has the possibility to yield the treasure of an unexpected discovery to the attentive and enquiring analyst. Creative input from analytical chemists is often crucial to progress on particular research projects. The trend to automation of instruments is also emphasising the need for

questioning minds with a good understanding of chemical, physical and electronic principles.

The 'good old days' of simple colour reactions or titrations are rapidly disappearing. With the availability of much more sensitive and specific techniques such as chromatography, atomic or mass spectroscopy, and immunoassays, samples can now be closely characterised for the analytes of importance. This interspersing of an instrument between analyst and chemical 'reality' requires the analyst to have a good understanding of the chemical principles, instrumental parameters, and limitations of the particular technique being applied. Only then can the output be fully interpreted and problems with particular samples or the instrument itself be recognised and corrected.

The use of programmable digital controllers and data processors has allowed an at times bewildering versatility to be built into modern instruments. However, this increased sophistication has not always resulted in equipment that is easier to use or able to provide enhanced analytical performance over the previous generation of instruments. In the rush to automate, companies have often neglected R and D into improving the basic analytical technology. However, laboratory automation is becoming firmly established and has some obvious advantages, so railing against it can only condemn one as old-fashioned or perhaps uncharitable. It is some of the wider implications of automation in analytical chemistry that are of concern.

Automation, particularly in the area of data handling may relieve the analyst of many tedious operations such as plotting

calibrations and measuring charts. However, automation also carries with it the responsibility to fully understand the manipulations which the microcomputer is carrying out on the analysts' behalf. Many examples can be found of the dangers in uncritical acceptance of results printed out as numbers by devices such as chromatographic integrators. In routine analyses, some quality control can be maintained by well-designed check sample programmes. However, these checks are not easily incorporated into short run analyses.

Servicing of microprocessor controlled equipment is another problem. Certainly the more recent models incorporate useful self-testing routines. However, microprocessor circuitry can be extremely difficult to trouble-shoot on site when serious breakdowns occur. Circuit board substitution is then the best solution but the maintenance of local stocks is an additional cost which can be difficult to handle in the small and fragmented New Zealand instrument market.

Of the myriad of computer games Dungeons and Dragons has perhaps the greatest fascination as one grapples with everchanging and unseen forces behind the video screen. Chemists can now enjoy similar pleasures as they endeavour to operate modern microprocessor controlled analytical equipment. Adequate training, of a broad nature, is essential if such instrumentation is to be used to its potential and without the danger of producing erroneous results.

Dr Patrick T. Holland
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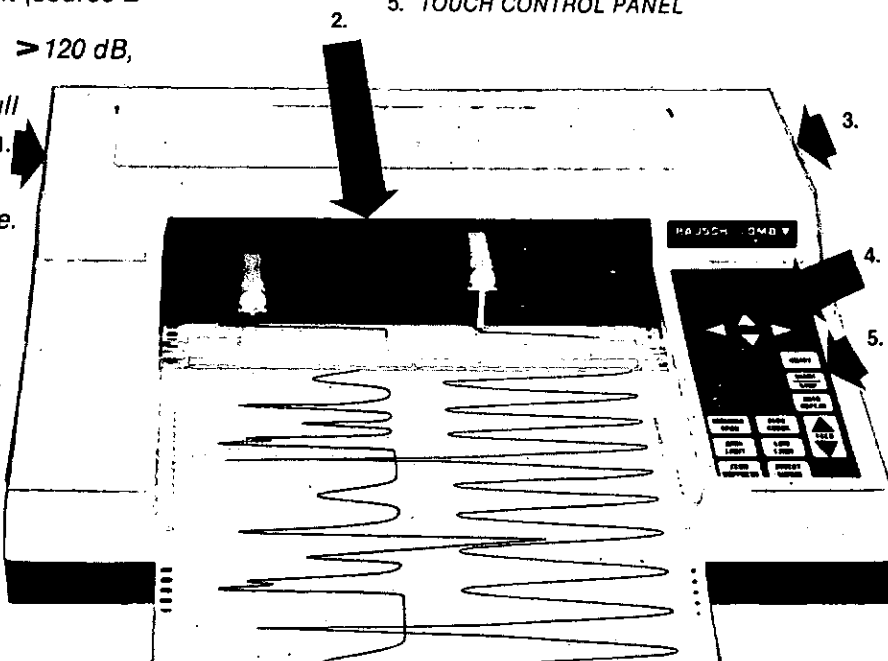
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CONFERENCE GUESTS

DR E.N. BAKER

Ted Baker is a graduate of Auckland University, having completed a Ph.D. there in 1967 under the supervision of Prof. Neil Waters. Following that, he spent three years at the University of Oxford working with Prof. Dorothy Hodgkin and Prof. David Phillips on X-ray crystallographic studies of proteins. During this period he was involved in the successful structure analysis of insulin. Since 1970 he has been on the staff of the Department of Chemistry, Biochemistry and Biophysics at Massey University, where he is now Reader. He has built up, at Massey, a programme of research into protein structure, by X-ray crystallography. One protein to have been extensively investigated has been actinidin, the proteolytic enzyme from kiwifruit, but he has not lost his original interest in copper coordination chemistry and bioinorganic chemistry, and recent structural studies on the copper protein azurin are a result of this.

PROF. R.J.H. CLARK

Robin Clark graduated from University of Canterbury with an M.Sc. in 1957 and went on to obtain his Ph.D. at University College, London, under Professors Lewis and Nyholm. He was awarded his D.Sc. and FRSC in 1969. He is currently Professor of Chemistry at University College and also has held a number of visiting Professorships at Universities in the USA, Europe and



New Zealand. He is the 1983/84 holder of the Royal Society of Chemistry Tilden Lectureship and Medal. His plenary address constitutes the Tilden Lecture to the NZIC. His wide-ranging research interests in inorganic chemistry have had an emphasis on the structural, energetic and bonding information obtainable from vibrational spectroscopy.

DR C.C.A. CULVENOR

After receiving a Ph.D. at the University of Melbourne in 1948 and a D.Phil. from Oxford University in 1950, Dr Culvenor joined CSIRO Division of Industrial Chemistry later to become the Division of Organic Chemistry and then Division of Applied Chemistry. There he engaged in studies on pyrrolizidine alkaloids of plants causing diseases of livestock and also Phalaris poisoning and perennial ryegrass staggers in sheep. In 1964, he was awarded a D.Sc. from the University of Melbourne. Dr Culvenor's group was transferred in 1972 to CSIRO Division of Animal Health where as a Chief Research Scientist, he has been Leader of the Biological Chemistry and Toxicology Section. Studies have continued in the above fields as well as isolation of the toxins causing lupinosis and annual ryegrass toxicity.

PROF. P.J. FENSHAM

Following academic training at Melbourne, Bristol and Cambridge Universities where he received M.Sc., Ph.D, Ph.D. respectively, Peter Fensham was appointed Lecturer in Chemistry at University of Melbourne in 1956. After promotion to Reader in Physical Chemistry he moved to Monash University as Professor of Science Education in 1967 and currently is Dean of Faculty of Education at Monash. He is a Fellow of Royal Australian Chemistry Institute and this year was Royal Society of Chemistry Nyholm Memorial Lecturer.

PROF. K.L. RINEHART JR

After graduating B.Sc. from Yale University and Ph.D. from University of California, Berkeley, he was appointed Instructor in Organic Chemistry at the University of Illinois in 1954 and subsequently rose to Professor of Organic Chemistry in 1964.

His research interests have included biosynthesis of antibiotics, structure determination and synthesis of natural products with special emphasis on peptides and polyene antibiotics and chemistry of compounds from marine sources with biological activity.

Major achievements recently have been the structural elucidation of peptides by new mass spectrometric techniques FDMS and FABMS; development of the technique of mutasynthesis; isolation and characterisation of depsi-peptides didemnin A, B, C, which have potent antiviral properties.

Prof. Rinehart is the current Erskine Fellow at the University of Canterbury.

PROF. J.K. SYERS

Professor J. Keith Syers was appointed to the Chair of Soil Science at Massey University in 1972. In the same year he was elected Fellow of the Chemical Society and of the New Zealand Institute of Chemistry. He was awarded a D.Sc. from Canterbury University in 1975 and elected Fellow of the Royal Society of New Zealand in 1981.

PROF. H.A. MCKENZIE

After receiving B.Sc.Hons, M.Sc. and Ph.D. from the University of Sydney, Dr McKenzie worked in CSIRO Food Research and Chemistry Department of Sydney Technical College on light absorption, magnetic properties and redox potentials of Group VIII metal complexes. For a period he was Visiting Fellow at Princeton University Chemistry Department where he worked on infra-red spectroscopy with Dr J. Turkwich. At this time he became interested in protein chemistry and his first research was on the nature of two forms of silk fibroin with the late Sir Hugh Taylor FRS.



In 1959 he helped set up the Department of Physical Biochemistry at the Australian National University in Canberra with Dr A.G. Ogston FRS. At present he is Professorial Fellow and leads the Protein Chemistry Group which has made comparative studies of secretory and blood proteins of a variety of species. With Professor Edsall of Harvard, he has used various approaches towards a classification of the state of water molecules in proteins.

DR D.A. WEISS O.B.E.

Dr Weiss, the current President of the RACI, is the inaugural RACI/NZIC exchange Fellow. He is at present Director, Planning and Evaluation Advisory Unit, CSIRO, responsible for strategic planning procedures in CSIRO.

DR FRANK B. WHITFIELD

CSIRO Division of Food Research, North Ryde, N.S.W. Invited speaker for Analytical and Chromatography sessions.

The North Ryde group, under Dr Keith Murray, pioneered many of the techniques that are now standard in trace volatiles research — polymer trap concentration, glass capillary column GC, peak trapping, reaction chromatography, and direct coupled capillary column GC/MS. Dr Whitfield's recent research has included detailed chemical studies on flavour compounds from passionfruit and avocado and on off-flavours in a variety of food products. He has recently visited food research laboratories in Europe and Scandinavia.

OBITUARY



ARTHUR KENNETT

Arthur Kennett, B.Sc.(Hons)(Lond.), F.N.Z.I.C., D.F.C., died on 5 June 1983. Arthur's career in chemistry began after service in the Royal Air Force from 1942-46 which saw him emerge as a Flight Lieutenant Air Navigator and with the Distinguished Flying Cross, which he was awarded in 1945 for his duties with the Pathfinders. He completed his B.Sc(Hons) in Chemistry in 1948 and was appointed as a Chemist with British Oxygen Co. in the same year. He became senior chemist with that company in 1953 and in the same year served on the British Standards Institute subcommittee on PVA adhesives. This association with standards committees was to continue until his death.

In 1964, Arthur emigrated to New Zealand to take up an appointment as Principal Scientific Officer with the Chemistry Division (Auckland Branch) DSIR. At Chemistry Division he specialised in industrial chemistry, in particular with plastics and rubbers and provided the major government consultancy on plastics usage and problems for the Auckland region. Outside of the laboratory, he was an enthusiastic sports follower, and was delighted to be able to attend the 1982 Wimbledon Final during a visit to the United Kingdom.

Arthur was very active on scientific bodies, joining the NZIC in 1964 and becoming a Fellow in 1973. He served on the Auckland branch committee from 1970, becoming Council Delegate from 1973-75 and Branch Chairman in 1974. He also

chaired the Polymer Chemistry Group of the Institute and organised many meetings in the area. The most recent, and perhaps the most successful, of these was an Adhesives Symposium run in April this year in Auckland. At the time of his death, Arthur was working towards the organisation of the Industrial Section at this year's conference in Hamilton. Another major contribution to the NZIC was his chairmanship of the Hazardous Chemicals Committee, which saw the transfer of executive responsibilities of this committee to Dunedin in 1982.

Arthur was also an active member of the Australasian Corrosion Association. He was Chairman of the New Zealand Branch in 1970-71 and Australasian President in 1976/77. He represented both the DSIR and the Institute on numerous SANZ committees on plastics and hazardous chemicals, and was frequently consulted on the suitability of many International Standards for the New Zealand market.

A scientist dedicated to his work, Arthur played an unobtrusive but extremely important role in New Zealand Chemistry. He will be remembered for his cheerful approach to his work, and his enthusiasm for imparting his knowledge. It is fitting that 1983 has seen the publication by ACA of his booklet "Degradation of Plastics (Causes and Mitigation)" as well as the staging of the Adhesives Symposium previously mentioned.

P.E.N.

PEOPLE

Dr Jim Sprott has recently been honoured by appointment as Honorary Consul for Canada in Auckland, the first time the Canadian Government has made such an appointment in an English-speaking country. Consular offices have been established at 61 Wakefield Street, and as well as providing general consular services will also be involved with trade promotions. Dr Sprott will also continue to operate as a consulting chemist from the same address.

Dr Adrian J. Sprott has recently been appointed agent in New Zealand and Australia for Corrosion Service Co. Ltd of Toronto, Canada. The agency involves anodic and electrochemical protection of industrial process equipment. CSCL has developed special methods applicable to the Pulp and Paper Industry to control both general corrosion and stress corrosion cracking. Dr Sprott has been overseas studying this process, and returned to New Zealand in July and has set up offices at 61 Wakefield Street, Auckland.

Anne Haines, Senior Product Development Officer for Unilever (NZ) Ltd is shortly leaving for Baltimore, Maryland, where her husband is doing post-doctoral studies. Her position at Unilever is being taken by Anne Chittenden.

Bob Foulkes has left WRONZ and is now Applications Chemist for Alphatech Systems Ltd in Auckland.

Dr Selwyn Maister of Christchurch Polytechnic is currently taking six weeks of Technical Refresher Leave at DSIR (Chemistry) in Christchurch. He is devoting most of his time to becoming acquainted with HPLC in anticipation of new equipment expected later in the year.



LETTERS TO THE EDITOR

Dear Sir,

Your highly entertaining but sceptical chemist questions (June 1983) the reliability of dioxin analyses at the ppb level. This very small amount of material is inevitably accompanied by larger quantities of other compounds and it would indeed be difficult to determine accurately quantities that were actually present at this level.

However, in the leachate in question, the final conclusion was that dioxin was NOT detected at a level above the assessed detection limit (40 ppt). The detection limit declared for our work was validated by the achievement of good recoveries from spiked samples. Bearing this in mind, the statement that dioxin was not present above 40 ppt would seem to be reasonably sound. As is often the case, the media give less publicity to a positively negative than to a tentatively positive finding.

Yours faithfully
Gordon Leary

Director DSIR Chemistry Division

Dear Sir

The article in the June 23 issue under the heading of "The Sceptical Chemist", on dioxin, deserves some comment.

It is acknowledged that analysis of very low levels of any compound inevitably raises the question of accuracy.

However, in the case of dioxin analysis we believe that results in the region of 1 ppb and indeed in the parts per trillion range in some instances, are quite significant.

Such values are widely reported by many analysts specializing in this area and their methods have been validated at these low levels.

Ability to test for pesticide residues does not necessarily indicate an ability to immediately carry out the complex clean-up and identification procedures required for the highly specialized dioxin analyses; considerable experience is required.

Our laboratory at Ivon Watkins-Dow has had many years of experience in dioxin analysis, having to date performed over 7000 analyses.

The leachate reported by another laboratory to contain 1 ppb dioxin (this claim was later retracted) was also analysed by the IWD laboratory and it was shown that dioxin was undetectable by a procedure capable of detecting 50 ppt dioxin. The IWD result was confirmed by the DSIR.

It is inferred in the article that dioxin residues were buried in the dump and it was queried whether this was the correct thing to do, as dioxin can be destroyed by photolysis.

In fact, dioxin containing residues from our 2,4,5-trichlorophenol plant were not buried in the dump, but stored in a secure area on site and later destroyed by incineration in a specially designed imported incinerator.

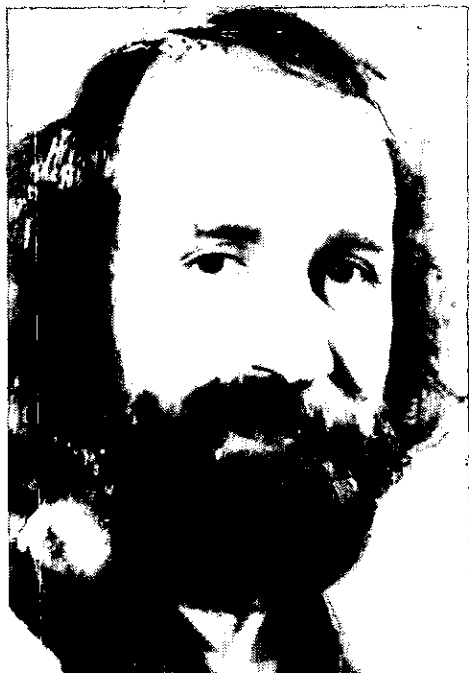
Traces of dioxin at the dump site arise from 2,4,5-trichlorophenoxyacetic acid (2,4,5-T) wastes and were present at the same low concentration as that present in 2,4,5-T products used by the farmers at that time.

Sincerely

E G Brooker
Chief Research Chemist
Ivon Watkins-Dow Ltd

ASPECTS OF CHROMATOGRAPHY IN AGRICULTURAL RESEARCH

D. R. LAUREN and P. T. HOLLAND



Ruakura Soil and Plant
Research Station,
Ministry of Agriculture
and Fisheries,
Hamilton



Denis Lauren graduated in Chemistry at Otago University, B.Sc. (Hons) in 1969 and Ph.D. in 1972. After working as a post doctoral fellow on peptide synthesis and the use of polymeric reagents with the National Research Council of Canada in Ottawa, he joined the staff at Ruakura in 1974. He has since worked with insect pheromones, in particular the sex attractant of the grass grub beetle, and also has a strong interest in HPLC analytical techniques.

Patrick Holland gained a Ph.D. in radiation chemistry at Queens University, Ontario in 1970. After working on data systems, high resolution mass spectrometry and lunar sample analysis at Berkeley California, he returned to New Zealand in 1972 to join MAF. He is currently in charge of the Ruakura mass spectrometry resource and also has responsibility for pesticide work on horticultural crops. He is Chairman for the 1983 NZIC Conference organising committee.

The techniques of high performance liquid chromatography (HPLC) and gas chromatography (GC) are ideally suited to several areas of agricultural research. In some instances HPLC and GC are simply alternative choices, each giving adequate sensitivity, selectivity and speed of analysis. For others, one technique is preferred over the other due to the chemical and physical properties of either analyte or substrate or to the complexity of the extract. In a few instances, the two techniques may be combined.

Both HPLC and GC are used extensively in many research projects at the Ruakura Agricultural Research Centre. Some analyses use standard published procedures, but in most cases, analytical and separation methods have been developed or improved upon to cope with specific areas of interest.

HPLC

An area in which HPLC is ideally suited involves studies on the efficacy and longevity of aquatic herbicides. One chemical under evaluation, fluridone, can be analysed by GC¹, but HPLC analysis can substantially reduce the workload.

For example, water samples may be injected directly into the HPLC after filtration². A UV detection limit of about 1 ng at the λ_{max} of 230 nm means that with 1000 μ l injections, down to 0.001 mg/litre can be detected. Since most commercial autosamplers are able to make injections of at least 250 μ l the potential for rapid analysis of samples at

levels above 0.005 mg/litre is obvious. In the case of the GC method, while solvent extraction can be avoided by concentration using reversed-phase mini-columns such as Sep-Pak or Bond-Elut, an unpleasant and time-consuming derivitisation step is required.

A similar situation exists for sediment samples. A complex extraction and clean-up procedure is required before both HPLC and GC analysis^{1,2}, but the ability of subsequent direct analysis without the need for derivitisation means HPLC is again preferred.

The fluridone analysis also allowed testing of alternative detection systems for HPLC analysis. Fluorescence detection is often quoted as advantageous over UV because of sensitivity and selectivity. Using a filter fluorimeter, UV detection at the λ_{max} was compared with fluorescence detection at the best available combination of 254 nm excitation/370 nm cutoff emission. Fluorescence was no more sensitive than UV, but it was hoped that the selectivity of fluorimetry might preclude the need for the arduous, two column clean-up of sediment samples. In fact, extracted sediment samples from the Aka. Aka peatlands showed less interference in the UV traces than in the fluorescence traces.

In the right situation, however, fluorescence does have a significant part to play in HPLC detection. For analysis of the tremorgenic mycotoxins, janthitrem. A, B, C and D, fluorescence detection was up to 10³ times more sensitive than UV detection at the λ_{max} ³, and has also proved to be more selective than UV for screening culture extracts.

The gain in sensitivity achievable between UV and fluorescence will obviously change between different instrument combinations. For example, the basic sensitivity of various makes of filter fluorimeters can vary by up to two orders of magnitude. In addition, two variable UV detectors are now available which have an inherent sensitivity of better than, or at least as good as, most fixed wavelength detectors, thus increasing the strength of UV detection.

Sensitivity and selectivity considerations aside, the combination of UV and fluorescence detection is a useful tool in peak characterisation^{3,4} and one available to users without access to sophisticated multiwavelength or rapid-scan spectrophotometric detectors. The ratio of UV absorbance to fluorescence response should remain constant for a pure component. Figure 1(a) shows the chromatogram of a janthitrem B (Jan B) standard, with an absorbance/fluorescence ratio for Jan B of 1:4. Figure 1(b) shows a culture extract. The peak at the retention time of Jan B showed an absorbance/fluorescence ratio of 1:16, suggesting either contamination or a different component. In fact, re-analysis of both mixed and pure samples with water-methanol (32:68) showed that the culture extract contained no Jan B.

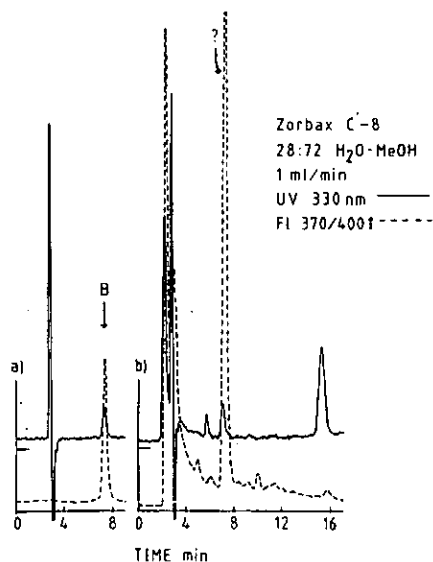


Fig. 1 Combined UV (upper trace) and fluorescent (lower trace) estimation of Jan B in a fungal culture extract. 1(a), Jan B standard; 1(b), extract.

Derivatisation plays a role in HPLC analysis just as in GC analysis. In the analysis of putrescine in plant tissue as an indicator of potassium nutritional status⁵, derivatisation is required to make the analyte detectable by UV. While methods of putrescine analysis were available using paper chromatography, thin-layer chromatography and GC, most of these had problems. The implementation of an HPLC analysis proved more difficult than originally thought. Although several methods had been published for standards or urine samples, most of these proved to be unsatisfactory of plant samples. A suitable analytical method was subsequently developed and adapted to automatic HPLC⁶. Figure 2 illustrates the isocratic analysis at two solvent compositions of the putrescine content of lucerne.

Derivatisation may be used in HPLC analysis not only to enhance detectability, but also to modify chromatography behaviour. For the HPLC analysis of carbamate insecticide, carbofuran, and its 3-hydroxy and 3-keto metabolites, the vastly different capacity factors made gradient, or prolonged isocratic, analyses a necessity⁷. Derivatisation with 1-fluoro-2,4-dinitrobenzene⁸ (FDNB) produces more strongly retained products which can be eluted more closely together by either isocratic or gradient analysis. An added advantage is that the FDNB derivatives may be analysed at equivalent levels by either HPLC or GC. This allows positive peak identification by two different separation and detection systems.

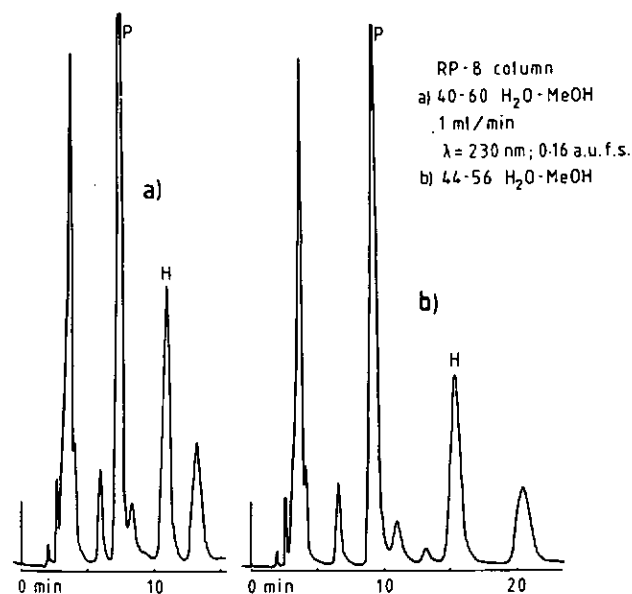


Fig. 2 Separation of the dibenzoyl derivatives of putrescine (P) and the internal standard, 1,6-diaminohexane (H), from lucerne extract.

GC AND GC/MS

GC has the advantages of speed of analysis plus the availability of a range of highly sensitive and selective detectors⁹. These have led to it being the preferred technique for pesticide residue analysis. Advances in column technology, including highly deactivated supports for packed columns and fused silica WCOT columns, now allow the majority of pesticides to be chromatographed intact at nanogram levels.

Horticultural diversification is proceeding rapidly with an increased volume and range of produce being exported. The strict and often conflicting quality control standards applied by the various markets have led to the need for much more detailed information on pesticides. A method¹⁰ has been developed at Ruakura to determine residues of a wide range of pesticides on fruit crops. It offers speed and cost savings over published multiresidue methods.

The key features of the method are the use of methanol as the extractant, cleanup by partitioning into toluene followed by activated carbon column cleanup and determination by GC with electron capture detection (ECD). Methanol provides an inexpensive yet highly efficient extraction of over 80%. Partitioning into toluene recovers the majority of pesticides while leaving behind highly polar co-extractives such as sugars. Activated carbon is particularly effective at removing chlorophyll pigments which have been found to have a deleterious effect on GLC columns.

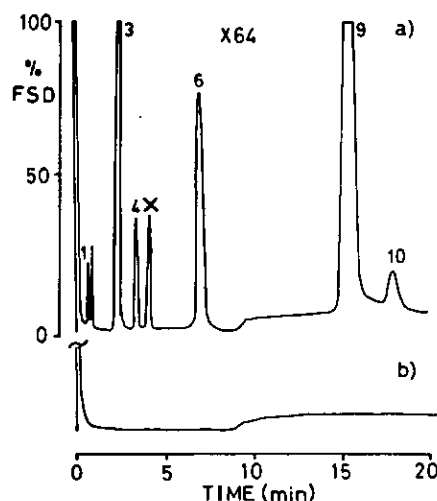


Fig. 3 ECD chromatogram of kiwifruit extracts. (a) field treated fruit, (b) untreated fruit. 1:diazinon, 3:vinclozolin, 4:dichlorofluanid, 6:captan, 9:phosmet, 10:aziphosmethyl.

Chromatograms of extracts of field sprayed and unsprayed kiwifruit are shown in Figure 3. The OV-225 column gave the better resolution and inertness for the pesticides studies than less polar packings. The electron capture detection does not exhibit uniformly high sensitivity to all pesticides but the large dynamic range of modern constant current designs means even compounds with only a moderate response, such as diazinon, can be measured. The detection limits for the method are less than 0.1 mg/kg for the pesticides studied.

Confirmation of unusual pesticides detected by this method can be carried out using detectors with different selectivities to the ECD. The alkali flame ionisation detector is very suitable for measuring pesticides containing P or N while the flame photometric detector is selective to P or S.

However, mass spectrometry (MS) provides the most definitive confirmation of chemical identity and is indispensable where complete unknowns are encountered or where no standards are available. The development of a data system for the Ruakura MS has made high sensitivity fast scan capillary GC/MS a routine technique for different identifications in the residue field^{11,12}.

A recent example is provided by unidentified peak X from the kiwifruit extract (Figure 3). Following silica gel "mini-column" chromatography a purified fraction was submitted to GC/MS. The total ion current chromatogram is shown in Figure 4(a), with peaks due to vinclozolin (V) and the unknown (X). The spectra of two of the main components (Figure 4(b)) show that the unknown is a degradation product of the fungicide vinclozolin, the result of loss of the vinyl side chain. The presence of this peak in the GLC trace from routine monitoring of kiwifruit can therefore be attributed to photolytic or metabolic breakdown of a registered pesticide, rather than to the use of another unacceptable chemical.

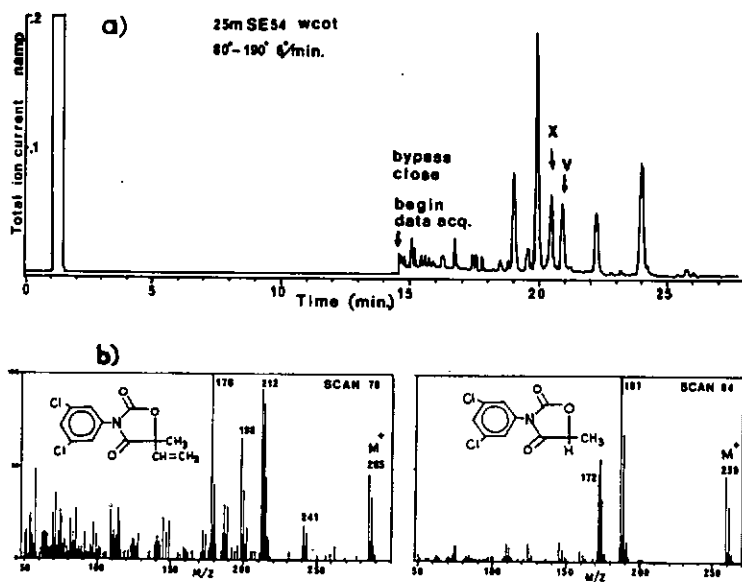


Fig. 4 GC/MS of kiwifruit residues. (a) total ion current chromatogram, (b) mass spectra of vinclozolin and desvinyl vinclozolin.

GC/MS has also been useful in residue problems involving dairy products. For example, routine monitoring by MAF Dairy Division revealed a small batch of butter which contained, in addition to the usual low level DDE residues, what appeared to be butyl esters of 2,4,5-T. With the emotional issue of this herbicide it was essential to have a confirmation. Figure 5(a) shows the chromatography reconstructed from computer stored MS data. Even with the resolving power of the capillary column, coextractives mask the area of interest. However, a much clearer picture is obtained (Figure 5(b)) by plotting the ion current as individual masses characteristic of 2,4,5-T. The peaks due to the isobutyl and n-butyl esters were clearly identified at levels of less than 0.1 mg/kg. The contamination was traced back to misuses of containers in a milking shed.

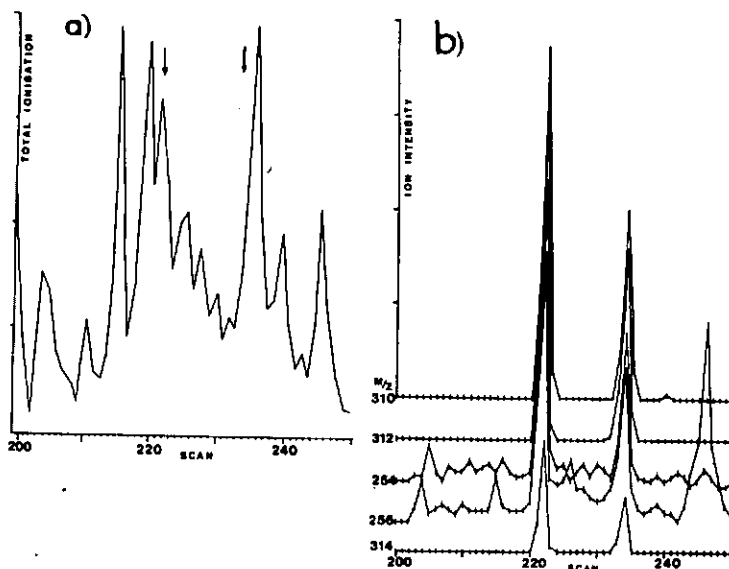


Fig. 5 GC/MS of butter extract containing 0.09 mg/kg 2,4,5-T. (a) reconstructed total ion chromatogram, (b) selected ion chromatogram.

The recent development of robust and highly deactivated fused silica WCOT columns has made capillary GC attractive for routine residue work. An accurate and sensitive assay has been developed for 2,4-D and 2,4,5-T residues on plant material suspected of being affected by herbicide spray drift. It uses on-column injection techniques with a 25 m by 0.32 mm i.d. OV 1701 bonded phase WCOT column, electron capture detection, and the 2,4,5-T isomer as internal standard. The overall analysis time was reduced from that for standard methods by elimination of a cleanup step. The high resolving power of the capillary column enabled the analytes to be separated from coextractives.

SUMMARY

Chromatographic techniques have been developed at Ruakura to carry out a range of low level analyses in agricultural chemistry. The emphasis has been to produce simple, direct procedures which allow high sample throughput and minimise time consuming evaporations and transfers. Use is made of minicolumn cleanup techniques followed by optimisation of the separation and detection power available in HPLC and GC. GC/MS has been developed as a confirmatory technique and for identification of metabolites.

ACKNOWLEDGEMENTS

This work has been greatly aided by the skilled technical assistance of M. P. Agnew, T. K. McGhie and D. A. McGaveston.

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LOW TEMPERATURE SPECTROSCOPY

R. V. Asmundson
Applied Biochemistry Division
Palmerston North

R. V. Asmundson is a scientist at the Applied Biochemistry Division of the DSIR, where his interests lie in the area of the biochemistry of anaerobic microbes. Originally from Davis, California, he completed a bachelors in biochemistry from U.C. Berkeley, and, after a stint in the US Navy, he came to New Zealand to study for an M.Sc. in Microbiology at Massey University. Since completing the M.S.c. he has married, completed a Ph.D. in biochemistry, and has three children.



Spectrophotometry of samples cooled to liquid nitrogen temperature is a technique which has been in use for the study of cytochromes for more than thirty years¹ during which time it has found applications in the study of electron transport and pharmacology². The advantages of the use of low temperature spectrophotometry over that at room temperature have been listed² as the following: 1) good spectra may be obtained from turbid samples, 2) the extinction co-efficient is increased 10 to 20 fold, thus allowing use of more dilute samples, 3) resolution of closely situated peaks is improved, and 4) transient states of a reaction or steady states may be frozen at the temperature of the refrigerant used and the absorption spectrum observed. The purpose of this short article is to give a brief description of apparatus which may be used for low temperature spectrophotometry and an application that we have made of it^{3,4}.

The apparatus shown in Figure 1 was designed to fit into a Carey 219 double beam spectrophotometer and consists of a cell, a Dewar flask and a mount to hold the cell and Dewar in the light beam of the spectrophotometer. The sides of the sample cuvette are formed by a U-shaped piece of brass with a tongue below it. The U-shaped portion may be 1.3mm thick (the thickness defining the length of the light path) and is sandwiched between two thin perspex sheets. These three pieces, forming the cuvette, are held together by brass plates on both sides with screws passing from front to back. The cuvette is held by a plastic handle from the top which has slots to allow accurate positioning. The cuvette fits into a holder containing the Dewar in which the silvering is absent from a window through which the spectrophotometer light beam passes. The Dewar holder fits into a mount which can be adjusted to position the window in the light beam.

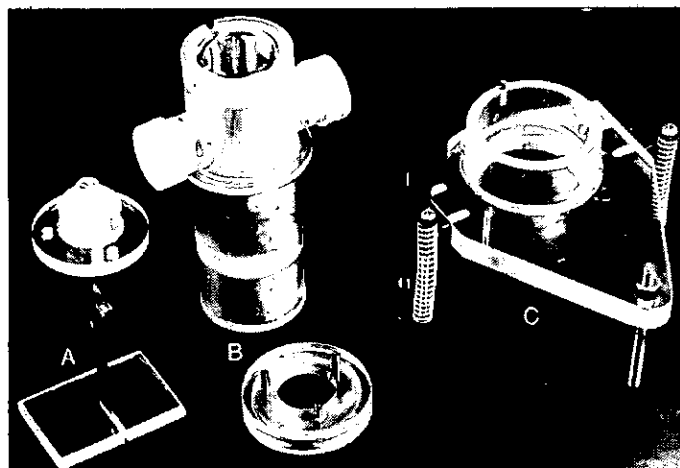


Figure 1: Apparatus for low temperature spectrophotometer. An apparatus designed to fit into a Carey 219 Spectrophotometer is shown. A. Low temperature cuvette. B. Dewar flask in perspex holder containing desiccant. C. Mount for Dewar flask holder.

Samples are prepared by placing them in the well of the cuvette and submerging the whole cuvette in liquid nitrogen (Keilin and Hartree¹ used liquid air and liquid oxygen without noticing any effect of oxygen on cytochrome spectra of their membranes). Liquid nitrogen is added to the Dewar to a level below the window, and, when the sample is frozen, the cuvette is quickly transferred to the Dewar. The tongue of the cuvette allows heat transfer from the cuvette to the liquid nitrogen, thus keeping the temperature of the sample low. A reference sample is prepared similarly and a difference spectrum may be recorded.

The peak height of spectra of samples prepared in this way is about ten-fold that of spectra observed at room temperature, as shown in Figure 2 for the α -absorption peak of cytochrome b.

A further amplification of peak height may be obtained by preparing samples in 50% aqueous glycerol. Samples are frozen in the cuvettes as described above and appear, when frozen, as a transparent glass. They are then allowed to warm at room temperature until they become microcrystalline, when they appear milky white by reflected light and smoky red by transmitted light. When they are evenly microcrystalline, they are recooled in liquid nitrogen and may be scanned in the spectrophotometer. This procedure amplifies the peak height about two-fold over that when only water is used. It is thought that this increase is due to an increase of the light path due to internal reflection through the microcrystalline sample. Besides problems due to the high viscosity of 50% glycerol, a problem with this procedure is that water, which crystallises in a fluff on the faces of the cell when it is being warmed, is difficult to remove evenly from both the reference and sample cells, thus giving a variable baseline. In general, the cells should be exposed as little as possible to air to avoid this condensation.

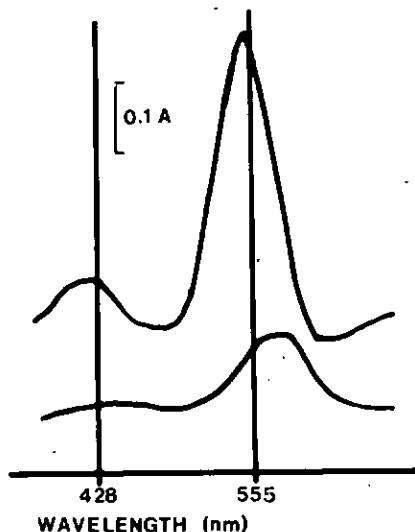


Fig. 2

Figure 2: Room and low temperature difference spectra of cytochrome b in membranes from *P. shermanii*. Protein was present at a concentration of 0.62 mg ml^{-1} . Membranes in the sample cuvette were reduced with a few grains of sodium dithionite and a difference spectrum was recorded against fully oxidised membranes. RT, room temperature; LT, low temperature.

We have used this method to examine the redox state of cytochromes in membranes prepared from *Propionibacterium shermanii*, a bacterium used in the manufacture of swiss cheese and interesting to us because of its anaerobic electron transport system. This method was particularly useful in our work in that it allowed us to distinguish the presence of four b type cytochromes in these membranes³. This was shown most clearly in difference spectra of membranes poised at known redox levels. Ten samples were prepared which were poised at redox potentials such that at the highest potential the cytochrome b was fully oxidised and at the lowest potential it was fully reduced. A selection of spectra from a single experiment is shown in Figure 3.

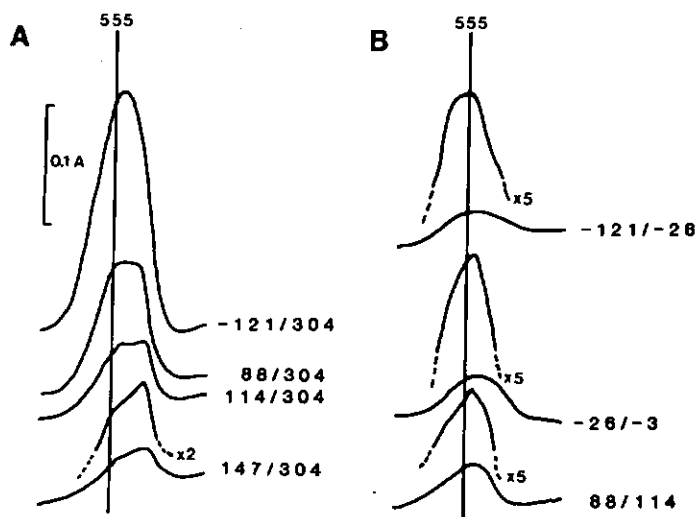


Figure 3: Low temperature difference spectra of redox poised membranes. Aqueous suspensions of membranes with a protein concentration of 0.65 mg ml^{-1} were prepared as described in the text, and difference spectra were recorded. The redox potentials in mV of membranes in the sample beam and reference beam, respectively, are shown to the right of the corresponding spectrum. Some spectra are repeated immediately above the original with a vertical scale expansion indicated by the factor to the right.

The first set of difference spectra (Figure 3A), in which the most oxidised sample was used as the reference, showed a cytochrome b peak which increased in size as the redox potential was lowered. The first b cytochrome to appear as the redox potential of the sample was lowered had an absorption peak at about 562 nm. As the redox potential of the sample was lowered further, a second b cytochrome peak appeared with an absorption maximum at about 557 nm. As the redox potential was further lowered, the α peak of cytochrome b became so large that little structure within the peak could be observed.

The absorbance contribution from a particular wavelength (or species of cytochrome b) could be better assessed from difference spectra of membranes poised at adjacent redox potentials in the series (Figure 3B), since only the absorption caused by the smaller incremental decrease in redox potential was observed. As the redox potentials of the pairs of samples observed were lowered, the b cytochromes with absorption peaks at 557 nm and 562 nm were no longer observed, since they were fully reduced in both the sample and reference beams. This permitted detection of two more b cytochromes with absorption peaks at 553 nm and 557 nm. These latter two b cytochromes would not have been clearly visible except by observation of the difference spectra at low temperature of redox poised membranes.

Hopefully this example of an application of low temperature spectrophotometer will indicate the utility of

the method. In circumstances where sample material is scarce, where resolution of complex absorption peaks is necessary or where a 'transient' state may be preserved by freezing, it offers distinct advantages over other available methods.

ACKNOWLEDGEMENTS

Perspex fittings shown in Figure 1 were designed and made by Mr P. van Dingenen of the Mechanical and Electrical Services Section at the Applied Biochemistry Division, DSIR. Dewars were made and silvered by Mr S. Oliver, formerly of the Massey University glassblowing shop.

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THE 1984 INTERNATIONAL CHEMICAL CONGRESS OF PACIFIC BASIN COUNTRIES

In 1982, the Chemical Institute of Canada, the Chemical Institute of Japan and the American Chemical Society agreed to sponsor the above Chemical Congress; these societies providing the substantial budget for planning and supporting the meeting.

The NZIC has accepted an invitation to participate in the Congress and has nominated the current President to be a member of the Congress Planning Committee. Dr Wright recently attended the first meeting in Tokyo of the Congress Executive and Programme Planning Committee.

The 3-day meeting, in mid-May, hosted and organised locally by the Chemical Society of Japan, had responsibility for agreeing on financial and congress management and development of a scientific programme.

The Congress will be held in Honolulu from December 16-21, 1984. It is expected that attendance will be in excess of 2500 from about 20 Pacific Basin nations.

Symposia accepted for the Congress are: Agrochemistry, Analytical-Clinical-Environmental-Health, Applied, Biological-Pharmaceutical, Catalysis-Colloidal-Physical-Surface Economics-Management, Information Transfer, Inorganic-Nuclear-Geochemical, Macromolecular, Organic.

Within these ten broad areas, about 50 topics have been approved and identified by title, proposer and number of technical sessions. Consideration is being given to additional topics suggested at the Tokyo meeting. Members of NZIC will be asked if they are prepared to become involved in organising or contributing to these Symposia.

A first circular outlining the Congress is expected to be available shortly with a second circular in December 1983. Deadlines for abstracts will be in June 1984.

Seminar on Land Treatment of Wastes, 7-9 February 1984, University of Waikato, Hamilton. Contact: Dr R. J. Wilcock, Water Quality Control Centre, M.O.W.D., Private Bag, Hamilton.

OVERTASMAN

Ionizing Energy Treatment of Foods Symposium, 5-6 October 1983, Sydney. Contact: The Secretary, Ionizing Energy Treatment of Foods Symposium, P.O. Box 1384 North Sydney, N.S.W., 2060.

OVERSEAS

KEM TEK, 6th International Fair of Plant and Equipment for the Chemical Process Industries, 14-18 November 1983, Copenhagen. Contact: Danish Trade Office, C.P.O. Box 2154, Auckland.

Chemasia '83, 3rd Asian International Chemical and Process Engineering and Contracting Show and Conference, 7-10 December 1983, Singapore. Contact: Steven Seet, Singapore Exhibition Services Ltd, 11 Dhoby Ghaut No. 13-01 Cathay Building, Singapore 0922.

K'83, International Plastics and Rubber Fair, 5-12 October 1983, Dusseldorf. Contact: Fairs of Europe, P.O. Box 3076, Auckland.

ELECTRON SPIN RESONANCE SPECTROMETRY AND ITS APPLICATION TO BIOCHEMISTRY

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Biochemistry and Biophysics,
Massey University,
Palmerston North



Eric Ainscough (left) and Andrew Brodie are on the lecturing staff at Massey University. Their current research interests are in the field of co-ordination and metalloprotein chemistry.



Introduction

Electron spin resonance (ESR) spectroscopy is a technique for studying molecules having one or more *unpaired* electrons. The technique is extremely specific since there are unlikely to be many unpaired electrons in any one system.

The Electron Resonance Condition

Electron spins are quantized. In other words they can only take up certain allowed orientations in a magnetic field. In the absence of a magnetic field the electrons are randomly orientated, but in the presence of a large external magnetic field, they can align themselves either parallel or antiparallel to this field, with an energy separation dependent on that field strength. The lower energy, or parallel state becomes more populated. If a microfrequency, ν , is applied so that electrons parallel to the magnetic field absorb energy and become antiparallel then this is the condition known as paramagnetic resonance. The equation $h\nu = g\mu_B B$ describes this resonance condition where μ_B is the Bohr Magnetron for the electron, B is the magnetic field, h is Planck's constant and g is a proportionality constant which reflects the electronic environment of the unpaired electron in the molecule. If the electron spin is the only source of magnetism then the "spin-only" value for g is 2.0023, but deviations arise because of the presence of orbital magnetism that adds to, or subtracts from, the spin magnetism. For most radicals this mixing is induced by the applied magnetic field and is only a small perturbation on the spin magnetism, typical shifts being $\leq \pm 0.1$. The extent of mixing depends upon the magnitude of the spin-orbital coupling constant ξ , and since ξ increases with atomic number, the shift Δg , may be large for heavy atoms in a molecule. For a transition-metal complex the central metal atom is usually the major source of g shifts, but ligands containing heavy atoms may also make a contribution.

The value of g can depend upon the orientation of the applied magnetic field with respect to the molecule, hence the g value is said to be anisotropic and has a different value for each field alignment. For example tetragonal or

axial copper (II) structures give rise to g values of g_{\parallel} (or g_z) and g_{\perp} ($g_x = g_y$) depending on whether the magnetic field is directed along the tetragonal z axis or perpendicular to it (i.e. along the x and y axes). The g_{\parallel} values can range from 2.08 to 2.42 depending on the nature of the ligands, while g_{\perp} can be about 2.04. Other transition metal ions, e.g. Fe^{3+} , can have g values of 1.4-3.1 for low-spin and 2.0-9.7 for high-spin states^{1,2,3}.

Similarly, the di(tert-butyl)nitroxide radical which has the unpaired electron localized in the $p\pi$ orbital of the nitrogen atom (as opposed to being delocalized in an aromatic radical system) displays anisotropy in solid crystalline samples with $g_z = 2.0027$, $g_x = 2.0089$ and $g_y = 2.0061$ ⁴. If the unpaired electron is in a symmetrical molecular magnetic field the g value is constant for all applied magnetic orientations and is said to be isotropic. If the nitroxide molecules tumble in a random manner in a non-viscous solution then anisotropic effects are averaged out and an isotropic g_0 value near 2.006 is observed ($g_0 = \frac{1}{3}(g_z + g_x + g_y)$). (In the case of axial symmetry, e.g. tetragonal Cu^{2+} , $g_0 = \frac{1}{3}(g_{\parallel} + 2g_{\perp})$)^{1,2,3}.

Basic Instrumentation

A typical ESR spectrometer is shown in Figure 1. The sample is placed in a resonance cavity (see Figure 2) located between the faces of a magnet and this cavity is joined to a microwave energy source (klystron) and detector, by a hollow metal tube called a wave guide, which guides the microwave energy to the resonance cavity and the signal back to the detector. An attenuator varies the microwave power going to the cavity and a circulator insures that the microwave power is directed to the cavity and all resonance signals are directed to the detector. The magnetic field is varied by sweep coils located on the magnet while the klystron frequency is held constant. In a typical experiment, with this frequency, ν , about 9.1 GHz, the magnetic field, B , necessary for electron resonance is about 3200 gauss and g is near 2.0. The ESR signal is displayed on a recorder as the first derivative of the absorption resonance.



Figure 1. A Varian E-104A ESR spectrometer. Miss V. Ritchie is about to insert a sample into the sample cavity. Mrs J. Husbands examines a spectra.

Hyperfine Coupling

This is the term used to describe the magnetic coupling that can occur between the spin of the unpaired electron and those of nearby magnetic nuclei (i.e. those which have magnetic moments). This electron-nuclei coupling gives rise to additional spectral lines. For example, the ESR spectrum of the small spin-label molecule TEMPO (a nitroxide)³, gives three main lines arising from a single nitrogen hyperfine structure, while a single $^{63}\text{Cu}^{2+}$ nucleus, gives four allowed transitions. For nitrogen, the

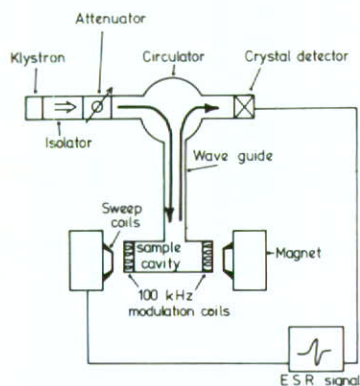


Figure 2: A simplified block diagram of an ESR spectrometer.

nuclear spin quantum number I is one, while for ^{63}Cu it is $\frac{1}{2}$. In general there are $2I + 1$ equally spaced hyperfine lines. The splitting (A) can vary from 6-32 gauss for spin-labels, to 180-200 gauss for A_{\parallel} and about 14-30 gauss for A_{\perp} for tetragonal $^{63}\text{Cu}^{2+}$.

If, as in the CH_3 radical, the unpaired electron couples with three equivalent proton nuclei, then there will be $2nI + 1$ lines ($n = \text{number of equivalent nuclei}$), and in this case four lines are seen ($I = \frac{1}{2}$ for ^1H) with relative intensity 1:3:3:1. The magnitude of A reflects the strength and type of bonding between (in this example) the carbon atom and proton and the spin-density on the protons can be calculated. (Information about the chemical structure of a free radical can also be obtained from the ESR technique).

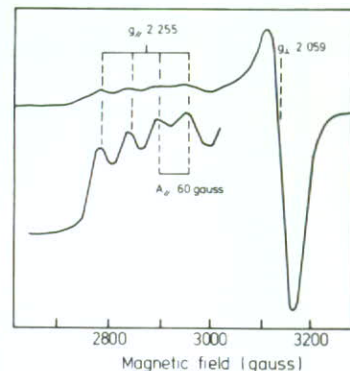
For non-axial isotropic systems $a_0 = \frac{1}{3}(A_z + A_x + A_y)$ while axial systems have $a_0 = \frac{1}{3}(A_{\parallel} + 2A_{\perp})$.

Some Biochemical Applications

ESR is a useful non-destructive technique which has been applied to a variety of biochemical problems. The following examples briefly illustrate its use in two different areas.

(1) The use of Cu^{2+} ions to probe metal protein interactions

Figure 3: Frozen solution ESR spectrum of the ^{65}Cu lactoferrin complex ($\text{Cu}^{2+} - \text{HCO}_3^-$)₂Lf.



Naturally occurring copper is a mixture of ^{63}Cu and ^{65}Cu . While it is not necessary to use isotopically pure copper (e.g. as either $^{63}\text{Cu}^{2+}$ or $^{65}\text{Cu}^{2+}$), its use does give rise to more highly resolved spectra.

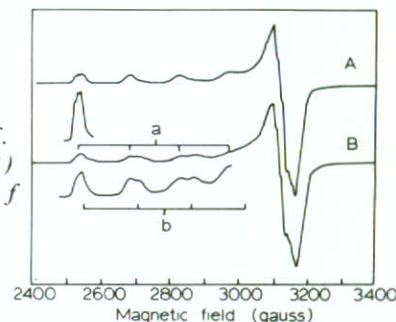
Human Lactoferrin

Human lactoferrin is a non-haem iron binding protein of molecular weight about 80,000 found in human milk and other bodily secretions. The protein binds specifically two Fe^{3+} ions and the observed ESR spectrum, with a strong resonance at $g = 4.29$ and a weak resonance at $g = 8.84$ is characteristic of the metal ion being high-spin in a distorted octahedral environment. However, further information about the specific metal binding site has been gained by replacing the Fe^{3+} ions with $^{65}\text{Cu}^{2+}$ ions⁵. The spectrum (Figure 3) with $g_{\parallel} (g_z) > g_{\perp} (g_x, g_y)$, is known as an axial type and suggests the Cu^{2+} ion to be in an approximately tetragonal environment. The four components of g_{\parallel} , which arise from ^{65}Cu hyperfine coupling, are clearly resolved with the splitting (A_{\parallel}) being 150 gauss. The lowest field component of g_{\parallel} shows a further splitting into three lines spaced 10 gauss apart. This arises from the interaction of a nitrogen donor ligand (probably histidine) with the $^{65}\text{Cu}^{2+}$, since as mentioned above for nitrogen, the nuclear spin $I = 1$, and hence $2I + 1 = 3$.

The specific binding of metal ions to human lactoferrin requires one anion (ordinarily bicarbonate) per metal ion to complete the co-ordination sphere. ESR spectroscopy has been used to show that there is a difference in these anion binding sites, in that only one of them will accept an oxalate ion. The addition of $^{65}\text{Cu}^{2+}$ ions to metal free lactoferrin in the presence of excess oxalate, yields copper (II)-lactoferrin-oxalate complexes. If the Cu^{2+} to protein molar ratio is 1:1, the monocopper(II)-lactoferrin-oxalate complex, $(\text{Cu}^{2+} - \text{C}_2\text{O}_4^{2-})\text{Lf}$ is formed. Its ESR spectrum (Figure 4), with $g_{\parallel} = 2.347$, $A_{\parallel} = 143$ gauss, and $g_{\perp} = 2.072$, is remarkably similar to the original dicopper(II)-lactoferrin complex, $(\text{Cu}^{2+} - \text{HCO}_3^-)_2\text{Lf}$ (Figure 3) and indicates the nature of the copper co-ordination sphere has not changed significantly. Addition of further Cu^{2+} ions to increase the Cu^{2+} to protein molar ratio to 2:1 produces a hybrid complex, formulated as $(\text{Cu}^{2+} - \text{HCO}_3^-)(\text{Cu}^{2+} - \text{C}_2\text{O}_4^{2-})\text{Lf}$ in which the second copper has bound to the vacant site utilizing HCO_3^- as the obligatory anion. As shown in Figure 4 (lower spectrum) a new set of resonances appears, virtually identical to those of $(\text{Cu}^{2+} - \text{HCO}_3^-)_2\text{Lf}$.

Figure 4: Frozen solution ESR spectra of ^{65}Cu lactoferrin oxalate complexes.

(A) $(\text{Cu}^{2+} - \text{C}_2\text{O}_4^{2-})\text{Lf}$.
 (B) $(\text{Cu}^{2+} - \text{C}_2\text{O}_4^{2-})(\text{Cu}^{2+} - \text{HCO}_3^-)\text{Lf}$
 (a) Cu^{2+} with $\text{C}_2\text{O}_4^{2-}$ as co-anion;
 (b) Cu^{2+} with HCO_3^- as co-anion.



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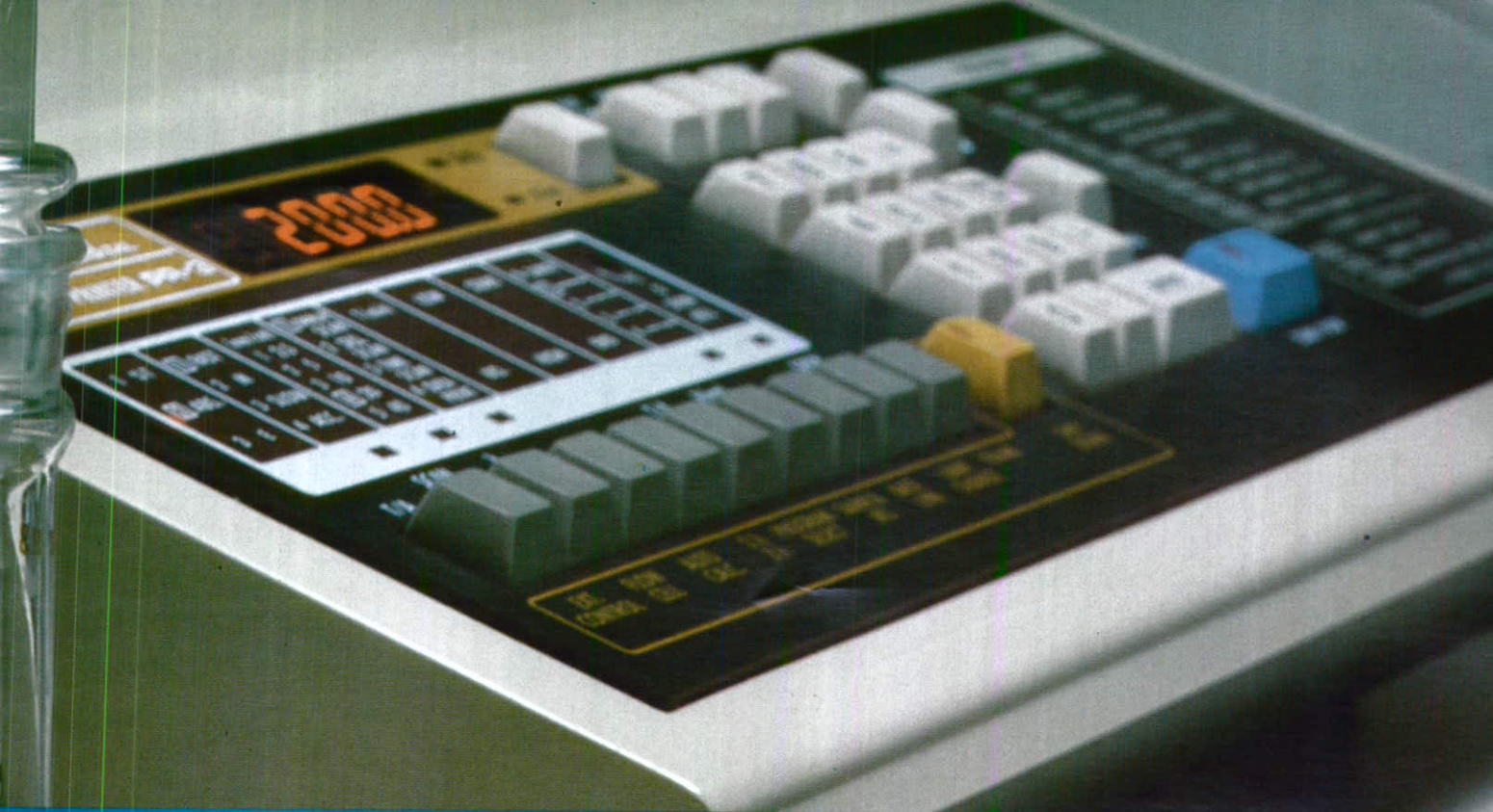
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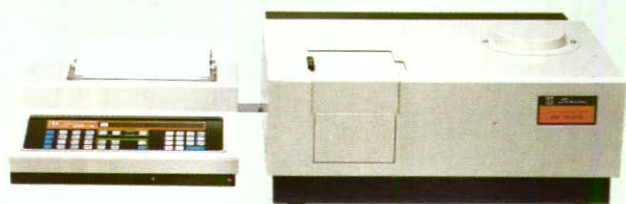
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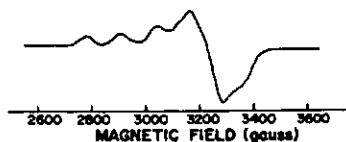


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Superoxide Dismutase

Bovine erythrocyte superoxide dismutase is a cuprozinc protein of molecular weight 31,200, containing two identical subunits with one Cu^{2+} and one Zn^{2+} ion per subunit. The Cu^{2+} ESR spectrum⁷ (Figure 5) does not show tetragonal symmetry, but displays rhombic character with a splitting of the g_{\perp} resonance into $g_x = 2.03$ and $g_y = 2.11$. The $g_{\parallel}(g_x)$ parameter is 2.26 and $A_{\parallel} = 130$ gauss. This spectrum is typical of a structure lying between a square pyramid and trigonal bipyramid⁸. The X-ray structure⁹ shows the copper to be bound to four imidazole rings from the sidechains of four histidines, in a tetrahedrally distorted square planar geometry. Electron density near one of the axial positions of the Cu^{2+} ion was probably water (the other position was blocked). The ESR spectrum confirms that water is bound to the copper to give a five-co-ordinate geometry and the structure in solution is similar to that in the crystal. ESR data also show that upon removal of the Zn^{2+} ion (which is bridged to the Cu^{2+} ion by an imidazolate ion from histidine 61) at pH 3.6, the copper site becomes more tetragonal with little rhombic distortion. A speculation for this behaviour is that this may be due to a pH-dependent conformational change in the zinc binding loop and this relaxes the Cu^{2+} ion geometry.

Figure 5: Frozen solution ESR spectrum of bovine superoxide dismutase.



Azurin

The blue copper protein azurin from *Alcaligenes denitrificans*, is an electron transport protein with a molecular weight of about 14,000 which binds one Cu^{2+} ion per molecule. The striking feature of its ESR spectrum is the low A_{\parallel} value of 60 gauss (Figure 6)¹⁰ which means the Cu^{2+} co-ordination environment is not of the usual tetragonal type and the bonding is more covalent. Indeed, the X-ray structure¹¹ shows the Cu^{2+} ions to be strongly bound to three ligands (two histidines and one cysteine) in a near trigonal plane. Two additional ligands may or may not be weakly bound above and below this plane.

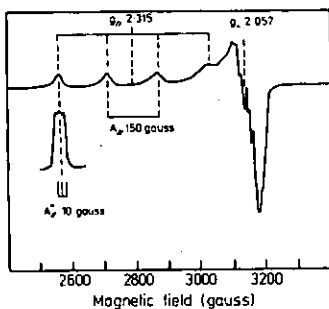


Figure 6: Frozen solution ESR spectrum of azurin from *Alcaligenes denitrificans*.


(2) The use of spin-labels

Many biomolecules have no paramagnetic centres, but ESR spectroscopy can give useful information about these molecules if a spin-label is attached³. The nitroxide spin-label moiety can be introduced on to a coenzyme, inhibitor, or spin-labelled lipid and the ESR spectra can provide information about the molecular mobility and structure of the binding site. The same spin-label can also be directly attached to a protein (or another macromolecule) and the spectra can give information about the structure of the macromolecule and its conformational changes. As seen before, the interaction of the free electron with the nitrogen nuclear spin gives rise to a three-line hyperfine structure of the spin-label spectrum, and it is the anisotropy of this hyperfine splitting with respect to a magnetic field direction which gives the structural and motional sensitivity of


the spin-label method. For example, in water, the nitroxide group rotates rapidly and the ESR signal consists of three narrow lines of equal height, but near immobilization of the spin-label occurs when it is buried in a protein (which moves slowly in aqueous solution on the 'ESR time scale') and this results in a differential line broadening in the spectrum. If the spin-label is attached to a biopolymer by a chain, the nitroxide group will rotate, but if it is attached to the surface directly it may restrict N-O rotation, so very different states of spin-label immobilization can be obtained. Also different conformations of a protein may have different spin-label mobilities.

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THE IDENTIFICATION OF FACTORS AFFECTING SPERM STORED FOR INSEMINATION

P. C. Molan
University of Waikato

Dr Peter Molan is Senior Lecturer in Biochemistry at the University of Waikato. He has just commenced a year's sabbatical leave working at the NZ Dairy Board's Artificial Breeding Centre at Newstead, near Hamilton.

Artificial insemination is used extensively in the New Zealand dairy industry, with 1½ million inseminations being performed annually. It is the economic advantages of the service that have led to its adoption on such a scale. Because such highly selected sires are used, the improvement in herds using the service is substantial. Cows from herds that have used artificial insemination since 1960 are now producing 38% more milk-fat. Nationally this increase in production is currently worth \$150 million per annum. Another important economic factor has been the low cost of the service.

Two things that have contributed greatly to the efficiency of the artificial insemination service have been the extension of semen by dilution, and advances in the technology of sperm storage. The dilution of semen allows up to 100,000 calves to be produced from a single bull. The diluents used have been developed to maintain the fertility of the semen by protecting the sperm from damage and by prolonging the period for which the motility of the sperm is maintained. The development has been empirical, and a large part has come from the work of Pat Shannon at the NZ Dairy Board Artificial Breeding Centre at Newstead. Semen that is stored frozen in liquid nitrogen is diluted with a buffer containing a glycerol, egg yolk, antibiotics, glucose, and citrate or skim milk powder. The same constituents are used in the diluent for semen that is distributed in a liquid state, but in addition glycine, caproic acid and catalase are included. The catalase is added to break down hydrogen peroxide formed by the amino acid oxidase activity of dead sperm. Damage by the hydrogen peroxide was found to be a major cause of loss of fertility. However, there are other as yet unidentified causes of loss of fertility: each insemination still requires two million sperm, and if the semen is frozen twenty-five million are required.

The cause of the damage to the sperm that occurs on freezing, preventing further dilution of the semen, is currently under investigation because of the interest in reducing the damage. The breeding season for most of New Zealand's dairy herds is spread over no more than three months of the year, yet it is not feasible to replace the less conveniently distributed liquid semen with frozen semen collected over the whole year. Because of the loss on freezing, far fewer inseminations can be performed from a bull if the semen collected over a whole year is frozen, compared with the number that can be performed with non-frozen semen collected over just the breeding season. The damage on freezing appears to result from destabilisation of the sperm membrane by a component of the seminal plasma. Sperm collected surgically from the epididymis are very resistant to damage by freezing, but are rendered susceptible by contact with the secretion. It has been found by Joan Baas, a doctoral student from the University

of Waikato, working with Pat Shannon at Newstead, that the susceptibility to damage by freezing is caused by the non-dialysable fraction of seminal plasma. To determine this, fractions were tested against sperm that had been washed free of the destabilising effect of the seminal plasma by centrifuging into Ficoll.

It was observations made working with the washed sperm that led to the discovery of other factors in seminal plasma that affect fertility. The sperm were found to be inactivated by washing away the seminal plasma but motility could be restored by replacing the seminal plasma or by adding various proteins such as bovine serum albumin. However, it was noticed that seminal plasma gave a shorter period of reactivation, the period varying inversely with the concentration of seminal plasma added. This suggested that there was an inactivating factor present as well as an activator. Also it was found that there were two different types of activation. When the motility resulting from the addition of protein ceased it could be restored by addition of seminal plasma or the phosphodiesterase inhibitor theophylline. If the sperm were dialysed overnight then almost no motility at all resulted from the addition of protein alone, indicating that the other factor is bound reversibly by the sperm.

Research is now being focused on the identification of these three factors that affect fertility, as well as on the factor causing loss of resistance to damage in freezing. A method has been developed to assay each factor independently¹. Fractionation of seminal plasma has shown that the factor causing irreversible inactivation is non-dialysable, like the motility-stimulating factor for which proteins can be substituted. The other stimulating factor, for which theophylline can be substituted. The other stimulating factor, for which theophylline can be substituted, has been found to be a small molecule, of less than 500 daltons. Isolation and identification of these factors would allow another aspect to be investigated, that is whether they are involved in some types of male infertility where sperm is present in semen but is non-motile. However, identification has yet to be achieved.

A major limitation to progress has been the quantity of the factors that can be isolated. Despite the impression given by the size of the source, this work is far from "bucket chemistry." Although many research projects on natural products involve difficulty in collecting the starting material, few can rival requiring a technician to step in with expert timing under 1 tonne of aroused bull to collect each 5ml lot of material that is mostly water anyway.

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NZIC ANNUAL REPORT 1982-1983

On behalf of the Council we have pleasure in presenting the Annual Report for 1982-83.

The policy of annual increases in subscription adopted in 1980/81 has allowed Council, despite inflation, to provide financial backing for more activities of members.

However the rate of growth of membership declined this year. Council is concerned to attract more members from chemists qualified to become so in industry and amongst students and graduates of the tertiary education system. There are many more chemists being trained than recruited to the Institute.

This year has been notable for considerable development of the Institute's contacts with sister societies overseas — in particular the decision by the NZIC and RACI Councils to establish a Visiting Speaker programme, a CER for chemistry, beginning in August 1983.

PRIZES

Institute prizes were awarded as follows: *Easterfield Award*: Dr R.H. Newman, Chemistry Division, DSIR, Petone.

ICI Prize: Assoc. Professor D.J. McLennan, Chemistry Department, Auckland University.

Shell Industrial Chemistry Prize: Dr D.H. Buisson, Fish Processing Research Group, DSIR, Auckland.

Chemical Essay Prize: A.R. Whyte, Chemistry Department, University of Canterbury.

Student Paper Prize: K.R. Sharrock, Waikato University.

Chemistry V AAVA Prize: 1981, Miss D.J. Siegers, Chemistry Division, DSIR, Auckland. 1982, Miss C.M. Kahukura, Chemistry Division, DSIR, Auckland.

MEMBERSHIP

The NZIC has 1527 members, an increase of only 12 this year. Council are anxious for Branches to promote more actively the Institute and to attract more members, particularly students and new graduates. The President has written an invitation to last year's chemistry and biochemistry graduates to join and has addressed classes of senior students in the universities so that they become more aware of the services and benefits provided by the Institute.

Some particularly notable members died during the year, including five Honorary Fellows, Mr M.S. Carrie (a former President), Dr H.C. Holland, Sir T.H. McCombs (former Cabinet Minister and High Commissioner), Prof. A.D. Munro and Mr D.F. Waters.

The Council was pleased to note the award of CBE and an Honorary D.Sc. (Auckland University) to Dr E.G. Bollard, Hon. FNZIC, who is current President of the Royal Society of New Zealand.

The President of the Royal Australian Chemical Institute, Dr D.E. Weiss, was elected an Honorary Fellow during his term of office and our President, Dr D.E. Wright, has been similarly honoured by the RACI.

CONFERENCES

1982 Annual Conference. The Institute thanks Prof. M. Shepherd (Chairman), Dr Joan McKenzie (Secretary) and the Committee for a successful Conference with the NZ Biochemical Society in Dunedin. The Conference theme was "Chemistry in the Life Sciences" and proved a popular and appropriate title for the region.

A successful innovation, which other Branches will find hard to copy, was a Mayoral Reception in the Dunedin Civic Centre.

Two major Symposia were held — one to honour the retirement of Prof. R.E. Corbett from the University of Otago, the other describing research on lignite which is a substantial energy resource in the Otago/Southland region.

Despite competing chemical and biochemical conferences in Australia the Otago Conference was highly successful, being attended by 180 delegates and producing a profit in excess of \$2000.

A Post Conference Symposium on the Regulation of Carbohydrate and Lipid Metabolism attracted 90 delegates for two days.

INTERNATIONAL CONFERENCE ON OILS, FATS AND WAXES

This conference "Fats for the Future", sponsored by the RSNZ, IUPAC and NZIC and organised by a local committee headed by Mr S.G. Brooker, was held in Auckland in February. It featured many distinguished chemists and biochemists including Nobel Prize Winner Prof. S. Bergstrom. It was a great success, being attended by 45 overseas and 90 New Zealand participants. Council's loan of \$3000 was returned with interest.

ADHESIVES SYMPOSIUM

This meeting, organised by the Polymer Chemistry Group, was held over two days during April in Auckland. It was attended by representatives from more than 30 companies and was so popular applications had to be declined. The late Mr A.C. Kennett was the organiser of this Symposium, which will increase Institute funds by more than \$1000.

CHEMEX 82

"Chemex 82", trade display and exhibition, was organised by Trade Publications Ltd and held in December 1982 in Auckland. The NZIC participated with the Auckland Branch providing an NZIC stand. This gave information on the Institute and in collaboration with Chemistry Division, DSIR, an opportunity to test blends of fruit juice.

INTERNATIONAL CHEMICAL CONGRESS OF PACIFIC BASIN SOCIETIES

This Conference, scheduled to be held in Hawaii in December 1984, aims to bring together formally for the first time members of the chemical societies in the Pacific region.

The Chemical Institute of Canada, the

Chemical Society of Japan and the American Chemical Society have provided funds for the Congress budget. In addition to these societies, the RACI, FACS, NZIC, Peoples Republic of China, and the Federation of Latin American Chemical Associations have become involved in planning and organising the Congress.

INTERNATIONAL CHEMISTRY

The Council has agreed that NZIC should have increased formal collaboration with sister institutes overseas.

The most important decision has been to establish with the Royal Australian Chemical Institute a Visiting Speaker Award programme on an annual basis with NZIC and RACI providing speakers alternately. The first award has been made to Dr D.E. Weiss, OBE, FAA, FTS, FRACI, who is Director of CSIRO's Planning and Evaluation Advisory Unit and President of RACI. He will visit New Zealand for our 1983 Conference and will address Branches.

The Honorary General Secretary called on the RACI, South African Chemical Institute, Gesellschaft Deutscher Chemiker, Royal Society of Chemistry and the Singapore National Institute of Chemistry to offer them personally the NZIC's thanks for their contributions to our Golden Jubilee, during April — July 1982. In addition to personal links with officers of these bodies these visits by Dr Rogers have resulted in useful information on the way RSC provides MP's with material about issues involving chemistry and legislation and on registration of chemists in South Africa for example.

Another significant event has been exchange of views between NZIC and representatives of the American Chemical Society and the Chemical Institute of Canada. In October 1982 Dr R.W. Parry and Dr R.P. Mariella, President and Executive Secretary, American Chemical Society respectively, visited Auckland, Wellington and Christchurch. With the President, General Secretary and Dr Percival they called on the Minister for Science and Technology, Dr Ian Shearer, in the Beehive. Dr Parry spoke on "Chemistry — Hope for the 80's". This first visit to New Zealand by an ACS President is to be followed in June by the 1983 President of ACS, Prof. F. Basolo, Morrison Professor of Chemistry at Northwestern University, Illinois.

Two Presidents-elect of the Chemical Institute of Canada also had contact with NZIC during 1983. Prof. R.U. Lemieux, FRS, of the University of Alberta, worked at the Victoria University of Wellington for three months and visited Branches. Prof. H.C. Clark, a graduate of the University of Auckland and now at the University of Guelph, visited Auckland for the University's Centenary.

Other visitors have been: Prof. R.G. Bates, University of Florida, who spoke in Hamilton, Palmerston North, Wellington and Dunedin in June; Profs F.G.A. Stone (Bristol) and H. Werner (Wurzburg) who came in September after the RACI 7th National Convention in Canberra.

NZIC BALANCE SHEET AS AT 30TH APRIL, 1983

1982		1982		1982	
\$		\$		\$	
	CURRENT LIABILITIES:				CURRENT ASSETS:
1,549	Sundry Creditors	3,935.30		3,191	Bank of New Zealand
197	Subscriptions in Advance	388.42		72	Air New Zealand: Deposit Account
-	Symposium Registrations Advance	2,660.00		3,208	Prepayments: Re Future Conferences, etc.
			6,983.72	1,110	Sundry Debtors
(1,746)				2,985	Stock of Publications on Hand
	SPECIAL ACCOUNTS:				15,098.65
2,054	Overseas Visitors Travelling		(13,721)		
567	Easterfield	566.86			INVESTMENTS:
(2,621)					Royal Society of New Zealand - Unsecured
	ACCUMULATED FUNDS:				Deposit (15%, 30.11.85)
23,330	Balance, 1.5.82	35,785.61		1,000	North Canterbury Hospital Stock
12,455	Add: Excess of Income over				(5.25%, 1.11.84)
	Expenditure for Year	2,235.90		500	Lyttelton Harbour Board Stock
					(6.25%, 1.7.98)
(35,785)	BALANCE, 30.4.83		38,021.51	3,000	U.D.C. Group Holdings Ltd
					(17.0%, 19.5.84)
				4,000	B.N.Z. Term Deposits - Various Terms
				3,000	Marac Holdings Ltd (16.75%, 19.5.83)
				14,035	Marac Holdings Ltd (13.69%, 4.11.83)
					Fletcher Challenge Ltd
					(18%, 30.11.86)
				(25,535)	3,000.00
					29,277.84
					FIXED ASSETS: at cost
					Office Equipment
					1,100.41
					Less: Accumulated Depreciation
					685.41
					415.00
					Films
					822.08
					Less: Depreciation
					308.08
					Presidential Chain
					514.00
					266.00
					1,195.60
					(896)
					\$45,572.09
					\$40,152
					\$45,572.09
					\$40,152

AUDITOR'S REPORT:

We have audited the financial statements of the New Zealand Institute of Chemistry (Inc) in accordance with accepted auditing standards, and have carried out such procedures as we considered necessary. Financial statements of the 1982 Otago Conference Committee had not been subject to audit at balance date. Subject to the foregoing, in our opinion the financial statements give a true and fair view of:

(a) The state of the Institute's affairs as at 30th April, 1983.

(b) Its income and expenditure for the year ended 30th April, 1983.

CHRISTCHURCH:

SHANAHAN, WINDER, TOMLIN & CO.

21st June, 1983.

Chartered Accountants

Per: A.J. Tomlin

Prof. M. Kasha, University of Florida, spoke during November in the Chemistry Departments in Auckland, Wellington and Christchurch on large molecule spectroscopy and photochemistry. Prof. J.W. Robinson, Louisiana State University, discussed atomic absorption spectroscopy in January - February.

Prof. M.B. Rubin, Technion, Haifa, in February - March lectured on aspects of ketone chemistry at all six University Chemistry Departments and Chemistry Divison, DSIR, in Wellington.

OVERSEAS VISITORS' FUND

Council has a fund to support visits to Branches by distinguished overseas chemists and has circulated guidelines designed to ensure Branches can most effectively use it. Recommendations on transferring this fund to Branches and how visits can best be organised so that Branch members will have an opportunity to hear visiting speakers are being considered by Council. It is hoped to have a new procedure operating in 1984.

FINANCE

Although Council budgeted for a deficit of \$2,500, the balance sheet shows an excess of income over expenditure of \$2,235. This very satisfactory turn around is due in part to the Conference profit achieved by the Otago Branch. Expenditure was generally close to budget with several items under forecast contributing to the excess of income. Income exceeded target. Although it is disappointing to note a further substantial increase in subscription in arrears, the Institute is in a sound financial position.

Requests for assistance from Branches and groups of members have increased

considerably. Council has acceded to them with grants or loans, some of them quite substantial. This "risk" capital has been well used. So far all advances have been returned and Council is thereby encouraged to continue this support, examples of which are noted elsewhere in this report.

Capitation grants to Branches have been increased and a special grant was made to subsidise student travel to Conference.

The Journal required thirty per cent of Council's expenditure. Further escalation of these costs will need to be carefully watched.

International contacts have increased markedly in the last two years and are likely to be at the least maintained at their present level. These contacts are important to the community of New Zealand chemists and will require funding.

For these reasons and to allow for steadily increasing costs a modest but regular increase in subscriptions is necessary. To be effective a professional body must maintain a realistic subscription and it is worth repeating that the NZIC subscription is less than those of sister organisations overseas and of other major New Zealand professional societies like the engineers.

PUBLICATIONS

Council is indebted to Dr Herd and the Journal Editorial Committee who have produced issues of "Chemistry in New Zealand" of increasing quality. The Magazine Factory relinquished the publishing contract after the February issue. Advertising revenue had declined as a result of economic conditions.

The new publisher is providing a more attractive publication and is obtaining

more advertising. Publication of a Yearbook early in 1984 to include the 1983 List of Members is under consideration. The 1982 edition of the List was in a similar format to 1981's Golden Jubilee one.

Dr Powell arranged for revision and re-printing of "Careers in Chemistry", which is distributed by Branches, and of the brochure about the Institute sent to applicants for membership.

Council expresses its appreciation to Dr J.E. Fergusson and the Editorial Committee who since May 1978 have produced 19 issues of Chem NZ on behalf of the Chemical Education Group of the Institute. Council has contributed to the cost of this publication in recognition of the valuable links it has developed with chemistry teachers throughout New Zealand. Dr A.M. Brodie and a group of members of the Manawatu Branch have assumed responsibility for Chem NZ.

NZIC TIE AND SCARF

At the suggestion of Dr Wright a search was begun for a design suitable for use on a tie and scarf for members.

COUNCIL COMMITTEES AND REPRESENTATIVES

Following talks with members of several of Council's Committees Dr Wright tabled a paper which resulted in Council appointing a sub-committee to draft for its consideration guidelines for Council Committees.

The Chemistry Syllabus Committee as a result of discussion with officers of the Department of Education has suggested that the Institute can best help schools to illustrate the importance of chemistry in the community by:

1. Listing chemists prepared to speak to schools and teacher colleges on their

INCOME AND EXPENDITURE ACCOUNT FOR YEAR ENDED 30TH APRIL 1983

1982	EXPENDITURE:	1982	INCOME:
\$	ADMINISTRATION & SUNDRY EXPENSES:	\$	
6,955	Honoraria	7,684.95	(39,814) Subscriptions
5,232	Travelling Expenses - Internal	6,240.26	49,433.51
	- Overseas	500.00	Interest - Bank of New Zealand
5,497	Printing, Stationery, Postages, Tolls etc.	7,874.13	1,059.00
1,500	Branch Expense Grants - re Subscriptions Rec'd	7,116.00	- Local Body Stock
			83.76
			- U.D.C. Group Holdings Ltd
			508.55
			- Marac Holdings Ltd
			1,743.44
			- Fletcher Challenge
			190.85
4,684	- Special	75.00	- Fats Conference
410	Computing, Address Labels, etc.	714.51	200.00
	- Overseas Visitors Expenses	2,322.65	(5,650) Conference Surplus (Otago)
2,119	Conference Expenses Paid by Institute	-	2,338.04
998	Audit Fee	975.00	Overseas Visitors Account, 1.5.82
	- Specialist Group Expenses	48.88	(transferred to General Funds)
	- Promotion - Chemex Display	724.00	
200	Prizes	150.00	
300	Grant - Re Chemistry Teaching Project	-	
70	Subscriptions - Royal Society of New Zealand	383.00	
14	- Common Concern	-	
125	- S.A.N.Z.	125.00	
	- N.Z.C.W.P.R.	50.00	
194	- F.A.C.S. (2 years)	455.53	
100	- N.Z.I.E. Water Research Group	-	
	- N.Z. Futures Society	50.00	
218	Depreciation	320.68	
(23,932)		35,809.59	
	PUBLICATIONS:		
	Journal - Publisher	15,266.03	
	- Editor Honorarium	1,200.00	
	Careers Booklet & Sundry Publicity	1,721.00	
	Chemistry in a Young Country	2,985.72	
	Chem, N.Z.	460.47	
	Lists of Members	690.00	
	Sundry Publications	1,215.36	
25,741		23,538.58	
	Less: Publication Sales	1,757.82	
	Sales 'Chemistry in a Young Country'	1,136.96	
	Stock on Hand	1,048.00	
11,980		3,942.78	
(13,761)		19,595.80	
37,693	TOTAL EXPENSES	\$55,405.39	
12,455	EXCESS OF INCOME OVER EXPENDITURE	2,235.90	
<u>\$50,148</u>		<u>\$57,641.29</u>	<u>\$50,148</u>

Particular Accounting Principles
Depreciation has been charged using the straightline method based on the estimated 5 year economic life of the assets concerned.

STATEMENT OF ACCOUNTING POLICIES:
General Accounting Principles
The general accounting principles appropriate for measuring and reporting of profit under the historical cost method have been used by the Institute.

speciality.

2. Listing, by consultation with members in industry, chemical and related plants prepared to show school groups chemical processes in action.

Finally, it is a pleasure to record our thanks to Branch, Council and Conference Committees and to the Council officers and representatives. Notable among the important contributions these members make to the work of the Institute is that of Stan Brooker who has stepped down as Honorary Librarian after 30 years service.

D.E. Wright, President

J. Rogers Honorary General Secretary
2 July 1983

Elected Officers:

President - Dr D.E. Wright
1st Vice-President - Prof R.D. Batt
2nd Vice President - Mr A.W. Mackney
General Secretary -

Branch Delegates to Council:

Auckland - Mr N.G. Thom
Waikato - Dr R.M. Daniel
Manawatu - Dr E.N. Baker
Wellington - Dr H.J. Percival

Canterbury - Dr H.K.J. Powell
Otago - Dr J.M. McKenzie

Officers Appointed by Council:

Registrar - D.J. Hogan (31/12/84)
Administrative Secretary - Mrs N.E. Wignall (31/12/84)

Journal Editor - Dr A.C. Herd (31/12/83)
Hon. Librarian - Dr L. Eyres (31/12/83)

Committees Appointed by Council:

Membership Committee - Dr T.A. Rafter (31/12/83)
Dr A.F. Wilson (31/12/84)
Dr H.K.J. Powell (31/12/85)

Pending a review of NZIC Council Committees in August, the following have been held over from last year:

Publications - Dr H.K.J. Powell
Dr J.R. Cretney

Energy & Materials resources -
Dr A. Metcalfe
Dr K.L. Mackie
Dr I.D. Watson

Public Affairs - Dr D.M. Bibby
Dr S.I. Smedley
G.R.G. Wright

Hazardous Chemicals - Dr W.A. Temple
Prof. A.D. Campbell
Assoc. Prof. M.R. Grimmett
A.M. Scrymgeour

Environment - Dr R. Lavery
Dr P.W. Larking
Dr W.A. Temple
Prof. A.D. Campbell

Archives - Dr R.F.C. Claridge
Registrar - Admin. Secretary

Chemistry Syllabus Committee:
J.B. Butchers

W. Freitag

Dr D.C. Weatherburn
Dr L.P. Aldridge
Dr H.J. Percival

Representatives to other bodies:

UNESCO - Dr G.R. Burns (31/12/83)
AAVA C'tee for Science - W. Freitag (31/3/86)
AAVA (Deputy) - N.R. Edmonds (31/3/86)
SAANZ - J.G. Fletcher (31/3/85)
Dr H.J. Percival (31/3/84)
RSNZ Member Bodies Council - Dr D.E. Wright (31/12/83)
M.B. Management C'tee - Dr H.J. Percival
Prof. R.D. Batt
Dr D.E. Wright

Membership:

During the year the following changes in membership have taken place:

Members elected to Fellowship	6
New Members	26
Member reinstated	1
Assoc. M. elected to Membership	2
Grad. M. elected to Membership	20
New Associate Members	7
Grad. M. elected to Assoc. M.	1
Tech. M. elected to Assoc. M.	3
New Graduate Members	20
Tech. M. elected to Grad. M.	1
Student M. elected to Grad. M.	1
New Technician Members	3
New Student Members	7
Deaths	13
Resignations	24
Struck Off	17

NZIC Annual General Meeting

The Annual General Meeting of the New Zealand Institute of Chemistry will be held at 3.30 p.m. on Thursday 25th August 1983 in the Main Lecture Theatre at the University of Waikato, Hamilton.

Agenda

1. Welcome by the President, Dr D.E. Wright.
 2. Presentation of 1982 Easterfield Medal to Dr R.H. Newman.
 3. Easterfield Address.
 4. Apologies.
 5. Minutes of 1982 AGM to be confirmed.
 6. Matters arising.
Prince and Princess of Wales Travel Awards.
 7. Annual Report: see this issue.
 8. Finance - 1982/83 Statement of Income and Expenditure.
- 1982/83 Balance Sheet - see this issue.
 9. Election of officers: President, First Vice-President, Second Vice-President, General Secretary.
 10. Awards and Prizes: ICI Prize, Shell Industrial Chemistry Prize, Essay Prize, Student Paper Prize.
 11. General Business.
- J. Rogers
Honorary General Secretary.

Branch Membership:

	1980	June 1981	April 30 1982	April 30 1983
Auckland:	368	382	397	401
Waikato:	113	116	123	122
Manawatu:	134	141	148	138
Wellington:	319	319	334	345
Canterbury:	177	180	201	199
Otago:	111	115	119	131
Overseas:	182	187	193	191
	1406	1440	1515	1527

Specialist Groups:

Group:	Secretary:	NZIC	Non-IC	Total
Analytical	D.J. Hogan	45	3	48
Biochemistry	Dr A.M. Robertson	43	81	144 (incomplete)
Chemical Education	D.T. Howarth	159	301	460
Chemical Engineers	E.R. Palmer	no records		
Chromatography	Dr J.A. Zabkiewicz	111	102	213
Electrochemistry	Dr A.J. Eastaerl	39	27	66
Geochemistry	Dr G.J. Churchman	32	103	135* bulk mailings not recorded
Organic Chemistry	Dr K.E. Richards	86	5	91
Polymer Chemistry	A.C. Kennett	49	17	66
Thermodynamics	Dr D.V. Fenby	no records		
X-Ray Crystallography	Dr W.T. Robinson	24	2	26
Trace El. & Health	Dr T.E. Kjellstrom	no records		
Industrial Chemistry	J.R. Yolland	19		19
Inorg. & Org-Metallic	Dr J. Simpson	62	21	83

Obituary

We record with regret the deaths during the year of the following members:

R. Hicks, H.G. Woolman, N.L. Wright (Auckland).

Dr H.C. Holland Hon. Fellow (Waikato),

D.F. Waters Hon. Fellow, (Waikato).

J.G. Fraser (Manawatu).

Professor A.D. Monro Hon. Fellow, H.J. Wood, (Wellington).

M.S. Carrie Hon. Fellow, Sir Terence

McCombs Hon. Fellow, C. Mooyman,

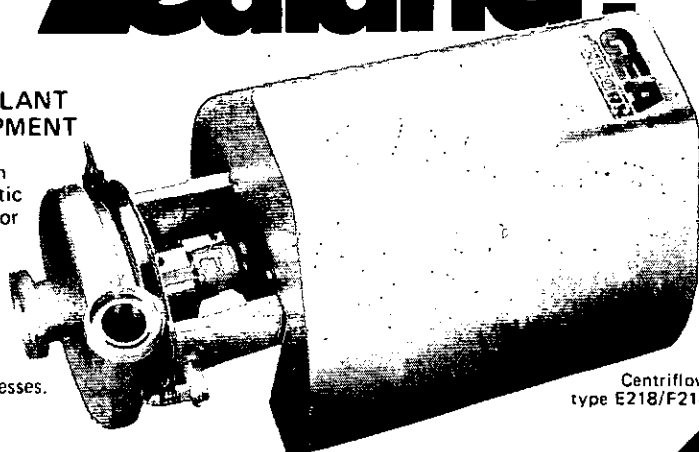
C.B. Radcliffe, (Canterbury).

J.W. McChesney (Otago).

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BRANCH NEWS

AUCKLAND

During May the Auckland Branch Committee had the pleasure of a visit from *Prof. Howard Clark*, President of the Canadian Chemical Society, who was in Auckland for the University Centennial celebrations. *Prof. Clark* conveyed his best wishes to the Institute, and took part in a lively discussion on several matters of mutual concern. In particular, attendance at branch meetings was discussed. It appears that in Canada most branches have moved to only a few general meetings a year, because of poor attendances. Instead there is a much greater effort put into the area of continuing education, on both a local and national scale.

Prof. Clark also described his Society's Old Goats' Club, a system well worth consideration for the NZIC. On two occasions each year the incumbent President meets up with the OGC whose role it is to comment on current administrative policy and issues of concern to the Society. Membership of the OGC is open to all previous office holders. Suitable candidates for such a group in the NZIC immediately came to mind, though it was felt that the criteria for membership might possibly be broadened, to include any of our more senior members with an overwhelming urge to contribute to the proceedings.

The June branch meeting was held at the Professional Club with lunch followed by an address from *Prof. Fred Basolo*, President ACS. Both during his address and in discussions over lunch, Fred talked about the activities of the ACS and some of the matters of current concern to its members. Details will be reported in a separate feature in a later issue. The main part of the talk was about chemistry in China and featured numerous colour slides and Fred's personal impressions from his two visits to that country.

WELLINGTON

Dr Robin Fenwick and *Mr Terry Childs* of the Whey Division of the NZ Dairy Board gave a combined talk at the June meeting on "Proteins as Food Ingredients." Using examples from the Dairy Industry the speakers discussed how the functional properties of food proteins can be enhanced to assist in food formulation.

WAIKATO

Two branch meetings were held in June. At the first of these *Dr David Plackett*, Forest Research Institute, Rotorua, gave a well-presented talk on the "Chemistry of wood preservation in Canada," which led to some interesting comparisons with developments in New Zealand. At the second very well attended meeting, *Prof. Fred Basolo* gave an overview of research on "Synthetic oxygen carriers of biological interest," including some comments on the importance of developing artificial blood.

MANAWATU

At a meeting on 3 May, *Dr Doug E. Wright* presented book tokens to *Miss Erin M.*

O'Donoghue and *Miss Debra J. Baker*, Branch prize winners from the 1982 Massey University 300 level chemistry and biochemistry courses respectively. *Dr Wright* then delivered the Branch's Presidential Address on "Biomass as a Source of Energy." Fuels from the biomass must meet a number of important criteria namely, they must be cheaper than existing fuels and use local material with well-tested technology in processes that are strategically, socially and environmentally acceptable. New fuels need to have a similar energy density and be miscible with presently-used fuels so that they will fit into the current distribution system with a minimum of modification to the engines they power. *Dr Wright* described the production of ethanol from a number of sources such as sugar cane, wheat, maize, sweet sorghum, sugar beet and wood. Many problems arise in the production of these materials, their conversion to alcohol and the disposal of waste materials. Biogas (approx. 70% methane and 30% carbon dioxide) produced by the fermentation of waste materials is an important energy source in many countries. It could be introduced soon to New Zealand. Possible alternatives to diesel were also described by *Dr Wright*. Unfortunately, large areas of land would be required to produce economically significant amounts of fuel materials and this could interfere with food production, unless extensive break-crop agricultural practices are utilised.

Alternative fuels were discussed further by *Dr Molly Melhuish*, Editor of "Energywatch," when she addressed a Branch Meeting (7 June) on "Chemical and Strategic Information Related to CNG and Other Energy Resources." Although government planners hope for a single replacement for each type of fuel that is currently being used, *Dr Melhuish* claimed that a more realistic approach would be the production of a diversity of fuels from numerous sources. In the latter situation, if one source of material becomes unavailable, then the overall supply of fuel will not be seriously affected and the ready substitution of other materials is feasible. A greater research effort is required to develop alternative uses for CNG (e.g. as a diesel fuel extender — see "Energywatch" No. 1 1983) and to develop new technology for gas storage (e.g. adsorption or absorption onto solids). Biogas, unlike ethanol, is chemically stable and, because it doesn't need an expensive distillation process for its recovery, it is easy to refine. The development of alternative uses for the carbon dioxide byproduct would also be most desirable. The fact that the time for questions was as long as *Dr Melhuish's* initial presentation, is a good indication of the intense interest in the subject shown by the audience.

In a brief visit to Palmerston North on 27 June, *Prof. Fred Basolo*, President of the American Chemical Society and Morrison Professor at the North Western University in Evanston (near Chicago), Illinois, discussed aspects of inorganic chemistry with staff of the Department of Chemistry, Biochemistry and Biophysics at Massey University, addressed an Advanced Inorganic Chemistry group at the University, attended a Press Interview and addressed an evening meeting of the Institute's Manawatu Branch. At the group meeting *Professor Basolo* discussed his contributions to inorganic chemistry, the graduate employment situation in the United States and various aspects of ACS publications. In his address to the Branch, entitled "Synthetic Oxygen Carriers of Biological In-

terest," he described a variety of synthetic organometallic compounds of the transition elements that react reversibly with oxygen and some with carbon monoxide.

CANTERBURY

During June the Canterbury Branch "Chemistry in Action" programme was taken to Timaru. Over 100 students from Timaru secondary schools heard *Dr Peter Ingham* (WRONZ) discuss the chemistry of natural and synthetic fibres, then saw some very vivid demonstrations of the effectiveness of flame proofing techniques which have been developed at WRONZ. *Dr Selwyn Maister* (Christchurch Polytechnic) then outlined the training opportunities and career prospects in chemistry at both technician and graduate level.

The June meeting of the Branch was a dinner meeting held in conjunction with the Canterbury Branch of the NZ Institute of Food Science and Technology. Local dieticians and nutritionists were invited to attend. The dinner was held in the Cloisters Restaurant and the Student Union, University of Canterbury, and the guest speaker was *Dr Joan McKenzie*, Nutrition Department, University of Otago. In a well illustrated address, *Dr McKenzie*, an expert in trace elements in human nutrition, dealt with New Zealand's unique trace element environment, the effect of food processing on trace element availability and aspects of chemical properties and bio-transformation.

At the end of June a special branch meeting held with the Association of Clinical Biochemists was addressed by *Prof. Fred Basolo*. In a well attended meeting with over 50 people present, *Prof. Basolo* spoke on "Synthetic Oxygen Carriers of Biological Interest." He outlined the discovery of the metal-complex dioxygen carriers and the work at Northwestern University (Illinois) on these materials, in particular Cobalt complexes such as $\text{Co}(\text{acac})_2(\text{en})$. The extension of this work into more "natural" systems involving iron complexes and Cobalt-globin complexes was an excellent example of the development and sophistication of a chemical model. *Dr Basolo* also spoke briefly on the role of the ACS and its information services.

OTAGO

The Branch Dinner was held in May. This was a successful social event during which Associate *Prof. I. Ralph Edwards*, of the Pharmacology Department, related amusing incidents connected with his activities in the Poisons Centre.

Dr Doug Wright visited the South in June and gave his Presidential Address, entitled "Biomass for Energy," to Southland members on the 15th and to Otago members on the following day. It is only recently that Presidents have been prevailed upon to include Southland in their itinerary and *Dr Wright's* visit was much appreciated both there and in Dunedin.

On 30th June, the President of the American Chemical Society and eminent inorganic chemist, *Prof. Fred Basolo*, visited the Branch and University Chemistry Department. His stay was brief, but started with a special morning tea at the University Staff Club where he met members and other invited guests. After this, he gave a lecture to students and staff on the history of complex chemistry. A Branch lecture followed entitled "Contributions of Chemistry to Societal Needs."

DSIR AND RESEARCH INSTITUTIONS

CHEMISTRY DIVISION, GRACEFIELD

Dr L.J. Wright has returned to the Inorganic Materials Section after a period of study leave in the United States.

Dr D. Sheppard is visiting the U.S. Geological Survey at the Portland Oregon Cascades Volcanic Observatory to work on the analysis of volcanic gases.

Mr W. Kitt retired recently from Chemistry Division. Mr Kitt spent most of his career in the Geochemistry Section, but for the last two years has been part of the Forensic Section.

SOIL BUREAU (DSIR)

Dr Kevin Tate is attending a joint meeting of International Society of Soil Science (ISSS) Commissions III (Soil Biology) and IV (Soil Fertility and Plant Nutrition), and the British Society of Soil Science, being held at Reading University, England on 4-8 July. At the meeting Kevin will be giving an invited lecture on "Biological Transformation of Phosphorous in Soils" and also co-presenting a poster outlining current work at Soil Bureau on the P cycle in soils. While in the UK Dr Tate is visiting various research institutions including Rothamsted, Letcombe Laboratories, Glasshouse Crops Research, and the Institute for Terrestrial Ecology.

BUILDING RESEARCH ASSN OF NZ

Dr Peter Foster has been appointed to the Board of the National Library of New Zealand.

Dr John Duncan presented a paper on "Approaches to Corrosion Awareness" to

an Australasian Corrosion Assn Symposium in Christchurch.

Dr Hugh Baber has been appointed to serve on the TELARC Applied Physics Registration Advisory Council.

WATER QUALITY CENTRE (HAMILTON)

Dr Bob Wilcock has recently returned from a visit to the USA and Canada, where he visited several research laboratories and presented a paper at the International Symposium on Gas Transfer at Water Surfaces at Cornell University.

RUAKURA AGRICULTURAL RESEARCH CENTRE

Mike Lowe has resigned from his position as Senior Technical Officer in the Ruakura Soil and Plant Research Station, after spending six years working with *Dr Ron Henzell* in the Organic Chemistry Section and ten years with *Dr Max Sutton* in the Spectrochemistry/Plant Analysis Section. Mike has set up a private analytical laboratory in partnership with well-known local veterinarian Harry Dewes.

Dr David Sheat has retired after spending the last thirteen years working as a Scientist in the Ruakura Soil and Plant Research Station.

Dr Chris Clark has returned to the Ruakura Soil and Plant Research Station after studying for his doctorate in the Department of Agronomy, Cornell University, Ithaca.

Dr Bob Hutchinson has been appointed Superintendent of the National Dairy Laboratory.

WHEAT RESEARCH INSTITUTE

A number of new staff have recently joined W.R.I.

Alistair Marris, a Canterbury M.Sc graduate in chemistry is working on quality evaluation. He was previously with NZ Forest Products working on research into packaging.

Bryan Laughland, an Auckland M.Sc graduation in Physics is also working on quality evaluation.

The third new staff member is *Peter Cressey*, who completed a B.Sc(Hons) in Chemistry at Canterbury in 1982. He is working on a joint project on wheat quality with *Dr W.B. (Bill) Campbell* from the C.S.I.R.O. Wheat Research Unit who is spending several months at Wheat Research Institute.

CHEMISTRY DIVISION, CHRISTCHURCH

The impending formation of a National Water Centre to be based in the new DSIR building at Ilam has elicited the following from a Wellington colleague:

T'was said to a section called water,
Go south 'cos we think you oughta,
There's a cosy wee place,
With lashings of space,
Once we lay a few bricks and some mortar.

W. Edgley
Water Section
Gracefield

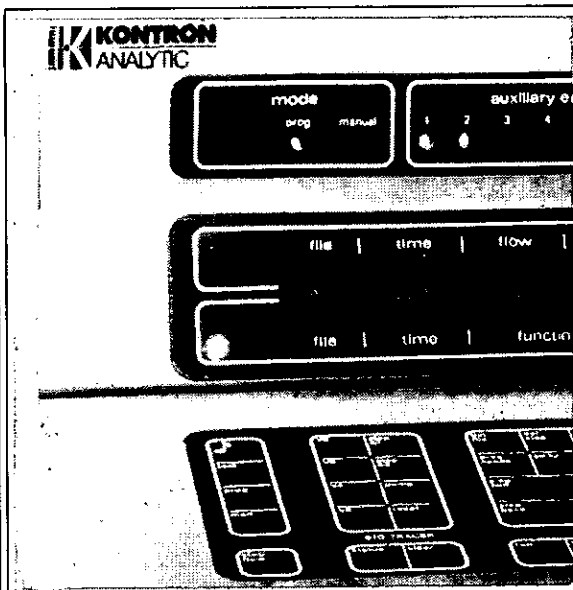
NZ AGRICULTURAL ENGINEERING INSTITUTE

The pilot scale beet ethanol plant is working again for its final season and will close down early in December. The ethanol produced is being sent to the Liquid Fuels Trust Board, Wellington for evaluation.

Studies into disposal of the waste products from the extraction process are continuing.

Update with Roche/Kontron diagnostic and analytical equipment

In an age when latest technology is constantly being overtaken, Roche/Kontron continues to lead the way in fields of analysis, with the highest quality manual and automated testing equipment. Roche/Kontron, open up new possibilities in medical and industrial analysis.



- Reagents for biochemistry
- Biological tests for human and animal health
- Centrifugal analysis machines
- Nuclear counters
- Spectrophotometers
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- Preparative and refrigerated centrifuges
- Disposables and ancillaries for a wide range of laboratory equipment

Confidence
inspired by
experience



Roche Products (New Zealand) Ltd
P.O. Box 12-492
Penrose, Auckland

For further information circle 7 on Reader Reply Card.

THE SCEPTICAL CHEMIST

... but better for who?

The Dairy Board, represented by their advertising agency, appears to have a particular and persistent contempt for chemists.

For over a year, the television, radio and magazine media have presented a near constant barrage of Dairy Board advertisements which seem aimed at insulting the integrity of the Chemistry Profession, and far less at reducing N.Z.'s contribution to a world butter mountain.

This style of "knocking" advertising hardly seems fitting for the ethics of a government-backed organisation which prides itself on the "pure," "healthy" and "wholesome" image of its "natural" pro-

duct. Much of this self-image is questionable, since butter is no more a natural product of cows than omeletes are of hens!

Butter, like its competing bread-spread products, is a compounded material, requiring expertise in its manufacture, and technical assurance of quality. Production of a 500g block of butter is a result of considerable expenditure of time, thought and money from several scientific disciplines — some remarkably related to Chemistry, but possibly better known as Dairy or Food Science.

Surely the Dairy Board cannot hope to gain patronage from the Chemistry Profession, nor impress the general public, by

presenting chemistry teachers as ridiculous people, pompous in their knowledge and estranged from popular thought, or by portraying practising Chemists as from an order with a scant disregard for the nation's health.

When a slogan bounces over the airwaves claiming "I want my sandwiches spread with butter — not something made by a Chemist!" one wonders whether comment will be raised by the N.Z.I.C., representing the professional interests of N.Z. Chemists. Perhaps the general public should be reassured of the true merits and abilities of N.Z. Chemists.

Anon.

(Contributions to this column should be sent to Dr A. C. Herd, Auckland Technical Institute, Private Bag, Auckland.)

GENERAL NEWS

DISCOUNT ON DSIR PUBLICATIONS

NZ Journal of Agricultural Research
NZ Journal of Experimental Agriculture
NZ Journal of Botany
NZ Journal of Geology and Geophysics
NZ Journal of Marine and Freshwater Research
NZ Journal of Science
NZ Journal of Zoology

The DSIR have recently offered to supply any of the above Journals to members of RSNZ Member Bodies at an annual subscription rate of \$18 plus \$2 postage, as against the current full rate of \$40 plus \$2 postage.

The names and addresses of NZIC members wishing to take advantage of this offer must reach the Registrar, Denis Hogan, by September 3, together with a cheque for the appropriate amount.

PRINCE AND PRINCESS OF WALES SCIENCE AWARDS SCHEME

The scheme is primarily designed to support New Zealand scientists or science technicians to travel overseas to develop their expertise, to use facilities not locally available or to promote locally developed technology. Grants for New Zealand based projects and visits by overseas scientists for developing New Zealand science and technology will also be considered.

Depending upon the finance available grants will support travel and living expenses for short term visits. It is hoped that in time up to about 15 awards will be made each year.

Firm details of the Awards will shortly be available with applications closing on September 30 with the Executive Officer, RSNZ, 4 Murphy Street, Wellington.

OCCA WELLINGTON SECTION

The AGM of the Oil and Colour Chemists Association (Wellington Section) elected Mr A. Thorburn as chairman and NZIC member David Holey as secretary. The postal address of the Wellington Section is P.O. Box 5019, Wellington.

ONTARIO SCIENCE CENTRE

Mr David Spence of the Ontario Science Centre visited Auckland and Christchurch recently, promoting the Science Centre concept. At a cocktail party, in the offices of Canadian Consul Dr T.J. Sprott, he described a Science Centre as a museum that moves, displays are designed to involve people to a greater depth than simple button-pushing and to impart scientific and technological ideas.

A scaled down mobile version known as a Science Circus is tentatively scheduled to visit Australia in the second half of 1984 and Mr Spence was interested in ascertaining potential support for a visit to New Zealand.



PRODUCT

HPLC
CENTRIFUGATION
ELECTRON MICROSCOPY
RADIOISOTOPES
NUCLEAR / X-RAY
HEALTH PHYSICS

GAMMA/RIA/LS COUNTERS
CLINICAL ANALYSIS
SPECTROSCOPY
PHOTOMETRY / RADIOMETRY
PH, ELECTROCHEMISTRY
HV POWER SUPPLIES, ELECTROSTATICS
REAGENTS /CHEMICALS

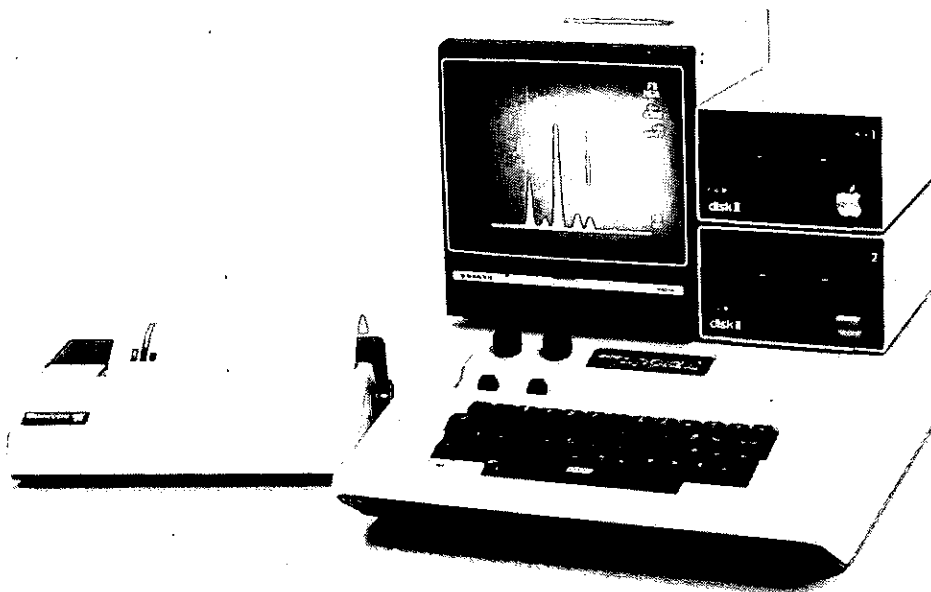
PRINCIPAL

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46 Gamma Street, Dunedin. Telephone: 774-716

Integrated systems for automated acquisition and control

John O'Neill, Alphatech Systems Limited



ISAAC is a new breed of instrument/micro-computer interface based on the philosophy of providing the hardware, software, language and support necessary to allow a speedy and flexible set-up of experiments with a variety of control parameters and sophisticated data acquisition and handling.

Micro-computers have been adopted enthusiastically by some scientists as an economical method of data acquisition from unsophisticated instruments such as basic chromatographs, spectrophotometers and electrochemical analyzers. They had not been adopted universally because of an understandable nervousness on the part of many potential users with regard to:—

1. the rapid shifts in micro-computer technology
2. reported delays experienced by colleagues in achieving the electronic interface.
3. dissatisfaction with various versions of Basic language for their purposes.

It appears that commercial concerns, such as CYBORG Corporation, USA, have recognised these problems and found solutions. The CYBORG ISAAC system comes in many configurations ranging from a multiplexed network of sensing and

control lines for process control to a dual channel analogue — to digital converter with CHROMATEXT software for immediate use in chromatography.

A number of benefits flow through to the scientist who adopts the philosophy of using a basic instrument/transducer/sensor with an ISAAC data/control system.

1. Prolonging the economic life of existing instruments.
2. Making best use of available funds by using basic instruments rather than sophisticated systems.
3. Obtaining personal control of data acquisition routines and data reduction programmes.
4. Having a data system which is independent of any one instrument and adaptable to various uses such as word-processing, income tax calculations, space invaders etc.
5. Adopting a data system which is wide-based.

An analytical instrument has a market of hundreds rather than thousands. Costs of development, documentation and support are lower per instrument when the production numbers increase. These factors related to scale are evident in the quality of information supplied with ISAAC/APPLE.

Repairs are largely within the ability of the local microcomputer agent. Replacement boards and sub-assemblies are the norm rather than the exception.

Recently, a new system has been introduced to interface to the IBM PC personal computer. In this case, distributed intelligence is employed in which —

1. ISAAC operates independently of the computer, once programmed.

2. High speed data acquisition is possible — (up to 200 KHA).

All options plug into an APPLE computer and allow the APPLE to run the experiment or process.

Programs allow APPLE to

- capture data
- recall data from memory
- display raw or processed data
- integrate
- expand peaks
- ratio wavelengths
- subtract baselines

If the standard program package is not suitable, the user can readily write his/her own program in LABSOFT BASIC. LABSOFT is an extension of APPLESOFT and incorporates 60 new commands which are called up in BASIC but executed in assembly language. These commands make LABSOFT easy, efficient and fast.

ISAAC hardware unit accepts multiple inputs of analogue or binary digital information. It also produces output through multiple binary signals or in analogue form through digital-to-analogue converters. A counter and day/time clock is included and Schmitt triggers are provided to monitor input signal levels. These functions in combination provide powerful programming facilities to stepping motor drives, voltage controlled oscillators, programmable power supplies, solenoids, valves etc. Voltage levels of input/output are selectable over a wide range and preamplifiers are available for low level signals.

3. Large memory capacity is provided — (up to 2 Megabytes).

4. True simultaneous data acquisition is allowed with negligible skew, from a number of channels.

With the IBM based instrumentation, applications such as transient analysis, vibration analysis, spectroscopy, failure analysis, high-speed physiological measurements are all possible.

In addition to the applications outlined above a further family of interfaces allow the APPLE micro-computer to function as a multichannel pulse analyzer. A fast analog-to-digital converter develops a spectrum of energies or pulse-heights for x-ray or gamma-spectrometry. Programs are available to allow quantitative analysis of samples by this means.

Plotting counts against time is easy for such a system and again programs exist for x-ray diffraction and fluorescence with automatic control of the spectrometer.

Image analysis and enhancement is another area of application with systems now available for inputs from video cameras, electron beam instruments or graphic tablets.

The future seems full of change in the world of instrumentation. As usual, the changes will be adopted widely, only when the supplier meets the requirements of the purchaser. The time for adoption of the micro-computer appears to be now.

For further information, circle on the Reader Reply Card.

"SQUIRREL" METER/LOGGER



Grant Instruments of the U.K. have used microprocessor technology to develop an economical combination digital meter/data logger.

The Squirrel will accept direct input from a wide range of temperature and humidity sensors, as well as processed signals from pH electrodes, D.O. electrodes, anemometers, flow meters, etc. The built-in Liquid Crystal display indicates the reading, the units being measured, and the function mode of the microprocessor.

The data logger function can have capacity for 2000 or 8000 readings, and reads to an accuracy of $\pm 0.4\%$ full scale with a linear sensor. Recording interval is adjustable from 1 second to 100 minutes to allow for varying rates of change in the measured parameter.

Recorded data can be loaded into certain computers such as Apple II, Epson, and Hewlett Packard for subsequent mathematical analysis, graphical results, and data storage. Grant have software available for the above three computers.

Early next year, a second series will be released which incorporates event-initiated reading, threshold-initiated reading, and alarm output facilities.

New Zealand Agents: Smith-Biolab Ltd. For further information, circle 9 on the Reader Reply Card.

ALLTECH HPLC COLUMNS

Alltech/Applied Science have introduced a range of low cost high quality HPLC columns packed with spherical media.

Alltech 'Econosphere' HPLC columns are packed with the highest quality spherical 5 micron media. Bonded phases are prepared with high coverage monomeric chemistry to assure maximum efficiency and reproducibility. Reverse phase materials (C18 and C8) are end-capped to provide maximum reverse phase interaction with minimum silanol activity.

At the same time, Alltech/Applied Science have introduced a new range of zero dead volume fittings for liquid chromatography. Fittings are available for all makes of HPLC, and, in conjunction, a new range of mirror finished empty HPLC tubing is also made available.

New Zealand agents: Alltech Associates N.Z. For further information circle 10 on Reader Reply Card.

PRODUCT NEWS

HPLC FROM GOW-MAC

GOW-MAC Instrument Co, now offer new High Performance Liquid Chromatography (HPLC) systems featuring reliable solvent delivery systems, 254nm fixed wavelength stable UV detectors using a Hg source, and at 'affordable' prices.

There are two models to choose from. Both models are complete liquid chromatographs combining a solvent delivery system, and UV detector in a single cabinet. They are designed with a minimum of controls to ensure ease of operation, quick adaptability for the user, leading to greater productivity.

The GOW-MAC High Performance Liquid Chromatographs are intended for dedicated use in analytical service labs, quality control labs, educational applications, or anywhere a precise, compact, easy to use liquid chromatograph is required.

New Zealand Agents: Alltech Associates NZ. For Further information circle 11 on the Reader Reply Card.

NEW DIODE-ARRAY SPECTROPHOTOMETER WITH INTERACTIVE BASIC PROGRAMMING FROM HEWLETT-PACKARD

Offering high sample throughput and accurate quantitative results, Hewlett-Packard's new HP 8451A diode-array spectrophotometer is a computer-controlled system capable of generating spectra over a wavelength range of 190 to 820 nano meters in as little as 0.1 second.

Tailored for productivity, the HP 8451A combines high photometric performance and interactive keyboard control. Its BASIC programming is designed for research or general-purpose applications in chemical markets where high-volume sample analysis is of prime importance.

An optional sipper system and automatic sampler permit fast, routine sample analysis (unattended) for several hundred measurements per hour. In addition, hardcopy output reports are generated for each analysis measurement.

Useful in time-based analyses such as kinetics experiments and liquid-chromatography detection, the HP 8451A is able to measure repetitively 25 single wavelengths every 0.1 second. This capability, along with flexible data manipulation, e.g., calculation of wavelength ratios, permits the HP 8451A to produce answers not possible on traditional scanning instruments.

Other features that enhance the analyst's measurement capability include:

- five concentration routines for quantitative results
- matrix multi-component analysis for quantitation of mixtures.

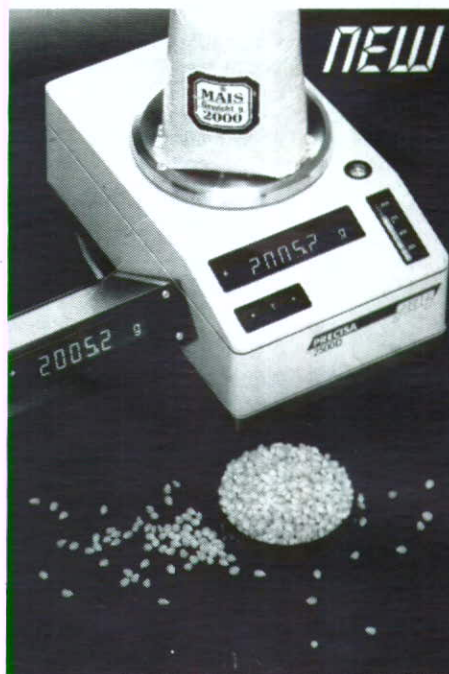
Designed for flexibility, the HP 8451A has two levels of data-handling capability. The first, accessed from the standard functional keyboard with simple key-stroke commands, performs a wide range of spectrophotometric functions such as concentration routines, peak annotations,

measurement cycles and spectral overlay functions.

From mid 1983, the 8451A Spectrophotometer will be available in New Zealand and HP factory specialists will be available during New Zealand wide demonstrations.

New Zealand agents: Northrop Instruments and Systems Ltd. For further information, circle 12 on the Reader Reply Card.

NEW PRECISION BALANCES FROM PRECISA



An enlargement of the range of precision balances has been announced by the Swiss balance manufacturer PRECISA. The two new balances offer the enduser an attractive range of 2500g with an accuracy of 0.1g, or a total capacity of 250g with a resolution of 0.01g. Although these balances are being offered at a very attractive price, they include different outstanding features, such as floating display, (indispensable when filling in) automatic calibration and adjustable integration time and stability. All PRECISA balances can be hooked up to computers, printers or calculators and can also be supplied with a multifunction box (different programs available) and a remote display. The range from PRECISA precision and analytical balances starts from 0.1mg up to 30kg, with two more new models with 500g/0.001g and 3000g/1g accuracy.

New Zealand agents: Kempthorne Medical Supplies Ltd. For further information circle 13 on the Reader Reply Card.

KONTRON TRACER MCS670 FOR AUTOMATIC VALVE SWITCHING TECHNIQUES

In general, valve switching is a means of re-routing chromatographic eluents using valves. When combined with the automatic switching of pumps, samples, detectors etc. valve switching allows the automation of those areas of chromatography, that are generally taken for granted as being time, solvent and man-power consuming.

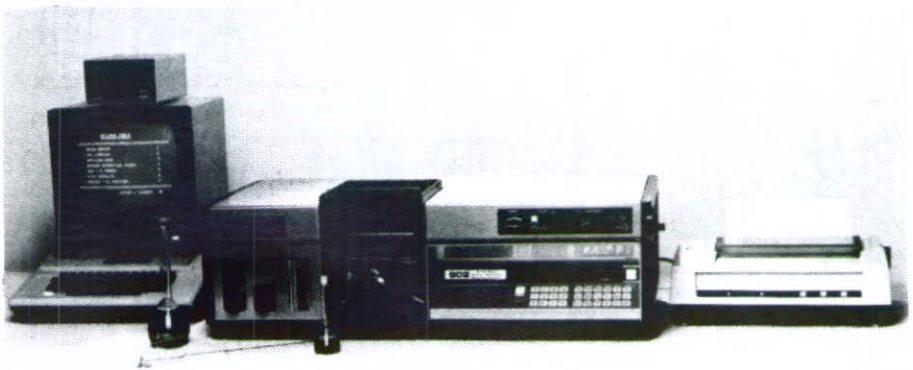
PRODUCT NEWS

The KONTRON TRACER makes all valve switching techniques possible. Techniques such as automatic sample clean-up; trace and residue analysis using on-line enrichment and sample clean-up; multi-column chromatography (e.g. boxcar chromatography) for improved resolution or for separation of complex matrices such as natural products and biological samples; method development — which involves selection of correct solvent and column; selection of isocratic or gradient conditions and selection of detection methods; automatic method selection for routine analysis over night or weekend. Also sample identification using wavelength scanning is possible.

All these approaches have been described in the past but have not become popular due to lack of instrumentation. KONTRON has now made available the tremendous power of column switching with the introduction of the TRACER MCS 670.

New Zealand agents: Roche Products (N.Z.) Ltd. for further information, circle 14 on the Reader Reply Card.

NEW ATOMIC ABSORPTION SPECTROPHOTOMETER



The 902 double beam Atomic Absorption Spectrophotometer released by GBC Scientific Equipment Pty. Ltd., contains several novel features.

Operation of the instrument has been greatly simplified by incorporating an alpha numeric display effectively allowing

the instrument to inform the operator what actions are required.

The 902 also has a new 'time expanded' operation which takes a digital "snapshot" of absorbance data over a ten second period. This snapshot is replayed in slow motion enabling ordinary chart recorders to capture transient signals occurring in

graphite furnace atomizers. With this system it is possible to time resolve the lead peak from the non-atomic peak when analysing lead in 1% sodium chloride.

In addition the 902 makes more efficient use of the time available for sample beam theoretically improving signal/noise ratio by 40%.

New Zealand agents: Advanced Electronics Ltd. For further information circle 15 on the Reader Reply Card.

ALLTECH

For **ALL** your Gas & Liquid
CHROMATOGRAPHY
needs — the New Zealand location of the
world's largest chromatography supplier

ALLTECH/APPLIED SCIENCE

SS & Glass Columns
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Phases

Capillary
Gas Filters
Syringes
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And many more — over 10,000 lines
dedicated to Chromatography!

For further information circle 18 on Reader Reply Card.

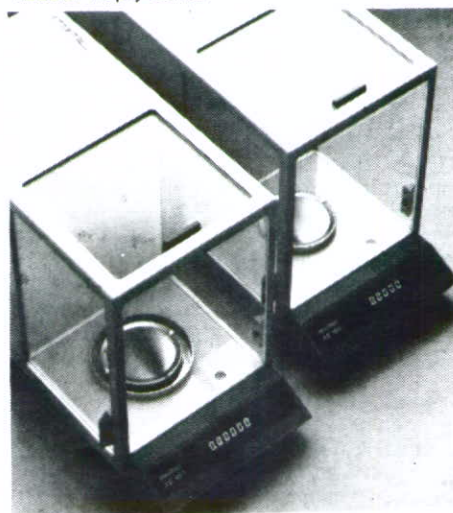
ALLTECH ASSOCIATES N.Z.

P.O. BOX 33527 TAKAPUNA AUCKLAND 9 NEW ZEALAND

NEW ELECTRONIC ANALYTICAL BALANCES FROM METTLER

Mettler is claiming a unique price/performance ratio for their new AE Top Loading Electronic Balances. Fast and easy to operate, the total operational functions are all operated with a single control bar.

New Zealand agents: Watson Victor Ltd. For further information circle 16 on the Reader Reply Card.

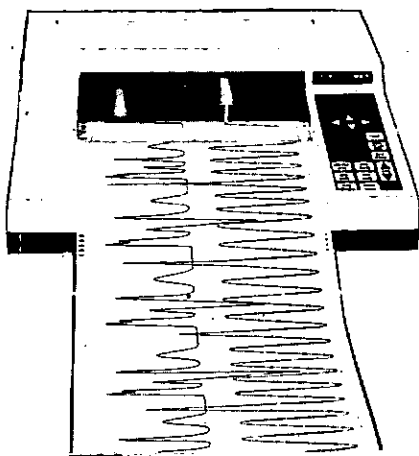


BIOLUMINESCENCE FOR ANALYTICAL MEASUREMENTS

Analytical Luminescence Laboratory have used research into bioluminescence (the light originating in living creatures) to develop a number of analytical instruments. It is claimed that bioluminescence testing has applications in such fields as soil analysis, milk testing, sewage treatment, and ATP determinations.

New Zealand agents: Watson Victor Ltd. For further information, circle 17 on the Reader Reply Card.

NEW RECORDER FROM HOUSTON INSTRUMENT



Houston Instrument, a division of Bausch and Lomb, have released the Microscribe chart recorder to follow their deservedly popular Omniscribe series.

The Microscribe recorder combines intelligent control and a classical servo pen recorder to provide increased capabilities at lower cost than a basic strip-chart recorder. This results from the use of microprocessor control and large scale integrated circuits. Dependability inherent in microprocessor control and LSI chip architecture is further joined with the time-proven non-contact capacitance servo rebalance system to assure reliability.

All parameters (chart-speed set, span set, zero check, chart repeat, chart start/stop, pen up/down and event mark) are addressable through a combined RS-232/standard parallel printer port for remote control. This option lets your system do all the "set up."

Automatic continuous self test function monitors critical system parameters including absence of chart paper. Typically this function will pick up a fault before it is serious enough to compromise performance. It also helps reduce cost of servicing since the fault is already isolated to a specific circuit or parameter.

Electrical power may be from 115/230 vac mains (50/60 Hz) or 12 vdc external battery. Average 12 volt drain during operation is 0.5 amperes. Internal standby battery provides "keep alive" power to the microprocessor memory, which stores parameters in effect at the time of power interruptions or voltage fluctuations.

Despite these features the Omniscribe is not superceded as the Microscribe does not have integration facilities.

New Zealand agents: S.D. Mandeno Electronic Equipment Co. For further information circle 19 on Reader Reply Card.

NEW TYPE OF GC DETECTOR

The ITD or Ion Trap Detector combines an ion source and mass filter in a single device without the need for ion focussing lenses.

Scanning at any of four sampling rates between 0.5 and 4s, or in a compound selective mode, it allows the chromatographer to obtain positive identification of compounds in complex mixtures. In many

PRODUCT NEWS

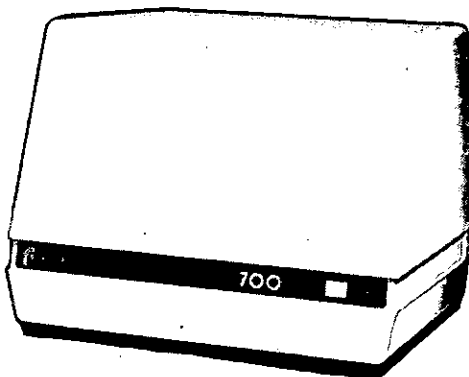
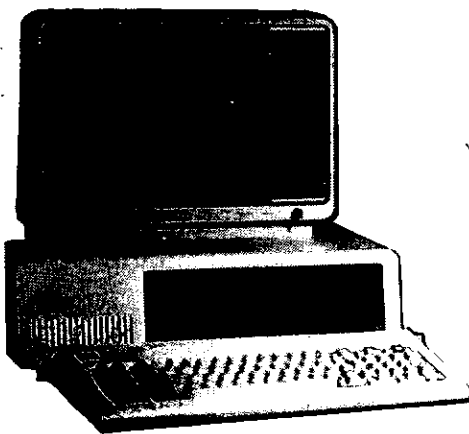
cases this can be done with only a single analysis. This contrasts with the usual procedure of performing several analyses employing conventional GC detectors, such as FID, ECD, or NPD.

The ITD delivers data in several easy-to-use familiar forms. In addition to chromatograms, specific mass chromatograms, mass spectra and quantitation reports are also provided.

The ITD is operated in conjunction with a user-friendly IBM Personal Computer. Simple one-letter commands initiate most of its operations from data acquisition to plotting complex chromatograms. The computer accepts all standard IBM software programs and peripherals. The powerful IBM Personal Computer controls data acquisition and processing and is also available to serve as a general purpose lab computer.

The ITD is installable on most capillary gas chromatographs. Installation is easy, without altering the thermal characteristics of the oven. A heated fused silica transfer line ensures that sample integrity is achievable by the use of an open split interface.

The ITD consists of one benchtop unit containing the detector, a turbomolecular vacuum pumping system, and the detector electronics. The software and cable necessary to interface it to an IBM Personal Computer are also included. The only interface required with its host GC is



a heated transfer line, furnished with the ITD.

Typical uses for the ITD include unknown mixture analysis, methods development for routine analysis, and quantitative analysis. Applications range from industrial hygiene and environmental analyses to clinical-biomedical use in monitoring drug and metabolite levels.

Mass range: 10 to 650 μ

Typical Sensitivity: < 1ng, universal, full scan mode; < 100 pg, specific, selected ion monitoring mode

Dynamic Range: 10⁴

Scan modes: Full scan or multiple ion detection

Scan speeds: 0.5, 1.0, 2.0 and 4.0 sec

Data System Required: IBM Personal Computer with 64 K memory, monochrome display, graphics printer and 320 KB floppy disk drive.

New Zealand Agents: Sci-Med (N.Z.) Ltd. For further information circle 20 on the Reader Reply Card.

INFRARED PROCESS GAS ANALYZER

The 977 Infrared Process Gas Analyzer, which continuously monitors the concentration of a given component in a gaseous process stream, was recently introduced by The Foxboro Company. The 977 is a competitively priced, precision analyzer for carbon monoxide, carbon dioxide, or methane. Typical applications are monitoring of gaseous process streams and ambient air, CO in parking garages, and experimental environments used in agricultural studies.

The 977 Infrared Process Gas Analyzer operates on the principle of non-dispersive infrared (NDIR) technology. It continuously determines the concentration of the component of interest in a gaseous stream by the measurement of infrared absorption by that component. The 977 combines in a single compact package an analyzer, sample and reference cells, and the electronics. The specially designed gas filled detector, along with other features, makes the 977 a highly reliable analyzer.

Plug-in options include 4 to 20 mA output, linearization, mechanical span checker, and three range calibration.

New Zealand agents: W. Arthur Fisher Ltd. For further information, circle 21 on the Reader Reply Card.



DEVELOPMENT CHEMIST

Our client is implementing a major new technology expansion in the paper coating and laminating field.

They seek a Development Chemist to carry out full R&D responsibilities, develop QC procedures and production trouble shoot to maintain quality standards and market leadership both in New Zealand and overseas.

This autonomous position is an attractive opportunity for a Chemist with a strong development flair in this field.

Confidential enquiries to:

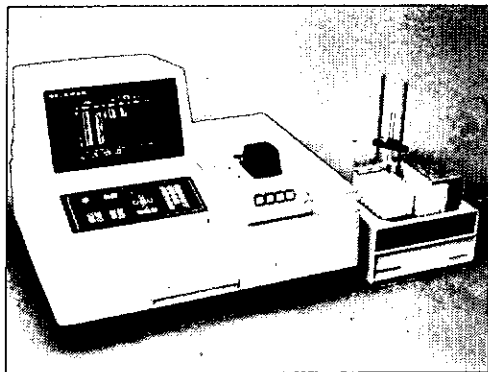
John Laurent
Ph: 790-200 Auckland

PRODUCT NEWS

RAPID SCANNING COMPUTING SPECTROPHOTOMETER

Beckman Instruments has released the DU6 UV/VIS Spectrophotometer.

The DU6 has a powerful microprocessor for computation of final answers; video display for set-up of parameters and monitoring instrument status and results; stabilized beam technology.



Single-beam optics have inherent advantages over double-beam instruments, provided that drift is reduced to 0.0005A per hour as in the DU-6. These advantages include —

- Point-by-point spectral subtraction
- Elimination of cell mis-match problems
- Fast response and low tracking error
- High optical energy and signal-to-noise ratio

A full range of options is available including sipper systems, batch sampler, Kinetics package, gel scanning. Six Kinetic runs can be handled simultaneously including rate calculations.

Three "QUANT" packages are available. "PEAK PICK" programmes select the peaks of interest, lists them with appropriate absorbance values.

The DU6 performs a systems self-test each time it is switched on. A Calibration Test Accessory provides automatic performance checkout of accuracy, noise, stray light.

New Zealand Agents: Alphatech Systems Ltd, "Beckman Product Specialists." For further information circle 22 on the Reader Reply Card.

VARIAN SPECTROPHOTOMETERS

Varian Associates USA have announced the introduction of new models of Cary Spectrophotometers claimed to represent the current state-of-the-art in UV/Visible spectrophotometric analysis.

The decision has also been made to transfer Cary Instrument Production to the Springvale Australian facilities of Varian Techtron which is the manufacturing plant for Varian's range of Atomic Absorption and routine UV/Visible Spectrophotometers.

Also new from Varian Techtron is the DMS100 Computerised Double Beam Scan-

ning UV/Visible Spectrophotometer with optional video display and printer plotter.

New Zealand Agents: Wilton Instruments (a division of Smith-Biolab Ltd). For further information, circle 23 on the Reader Reply Card.

ORION INDUSTRIAL MONITORS

An on-line analyzer that measures calcium hardness down to less than 0.0005 ppm is manufactured by Orion research. Designed to help prevent calcium scaling and optimize chelate therapy in industrial steam generating plants, the Orion 1520 Monitor detects calcium hardness in boiler tubes and other parts of the steam/water circuit before scaling can ruin the equipment in the circuit. Concentration is read visually or connected to an alarm and recording system. Calibration can be performed anywhere in the operating range. There are no pumps, solenoid valves or moving parts.

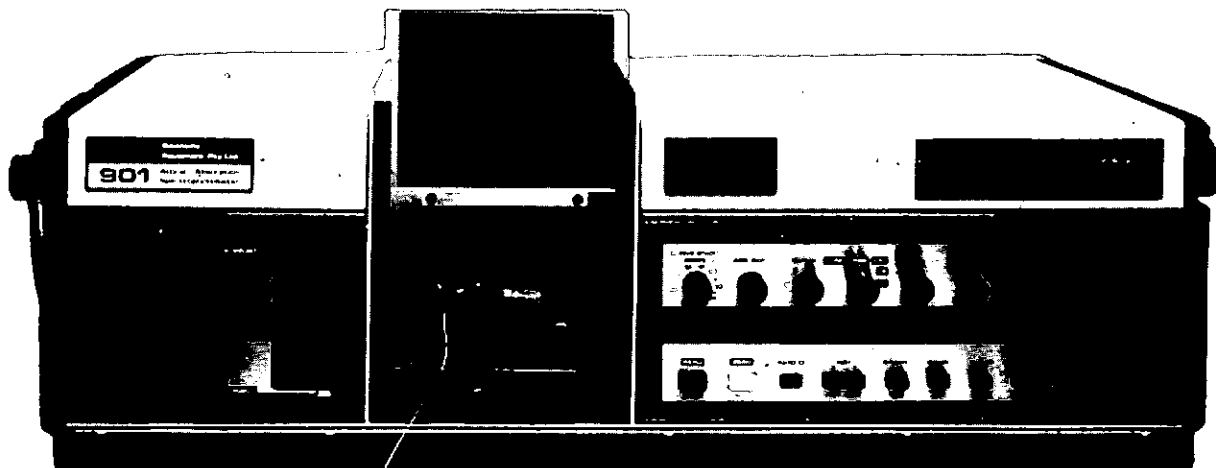
The Model 1520 is also suitable for potable water blending processes, reverse osmosis, and brewery water treatment systems.

Orion's ion selective electrode Model 1518 is claimed to measure hydrazine to as low as 0.0001 ppm.

The real on-line monitoring, unaffected by sample colour, turbidity and temperature allows for effective monitoring of hydrazine residuals in steam or water circuits.

New Zealand Agents: Watson Victor Ltd. For further information, circle 24 on the Reader Reply Card.

ATOMIC ABSORPTION SPECTROPHOTOMETER



G.B.C. Model SB901 Atomic Absorption Spectrophotometer

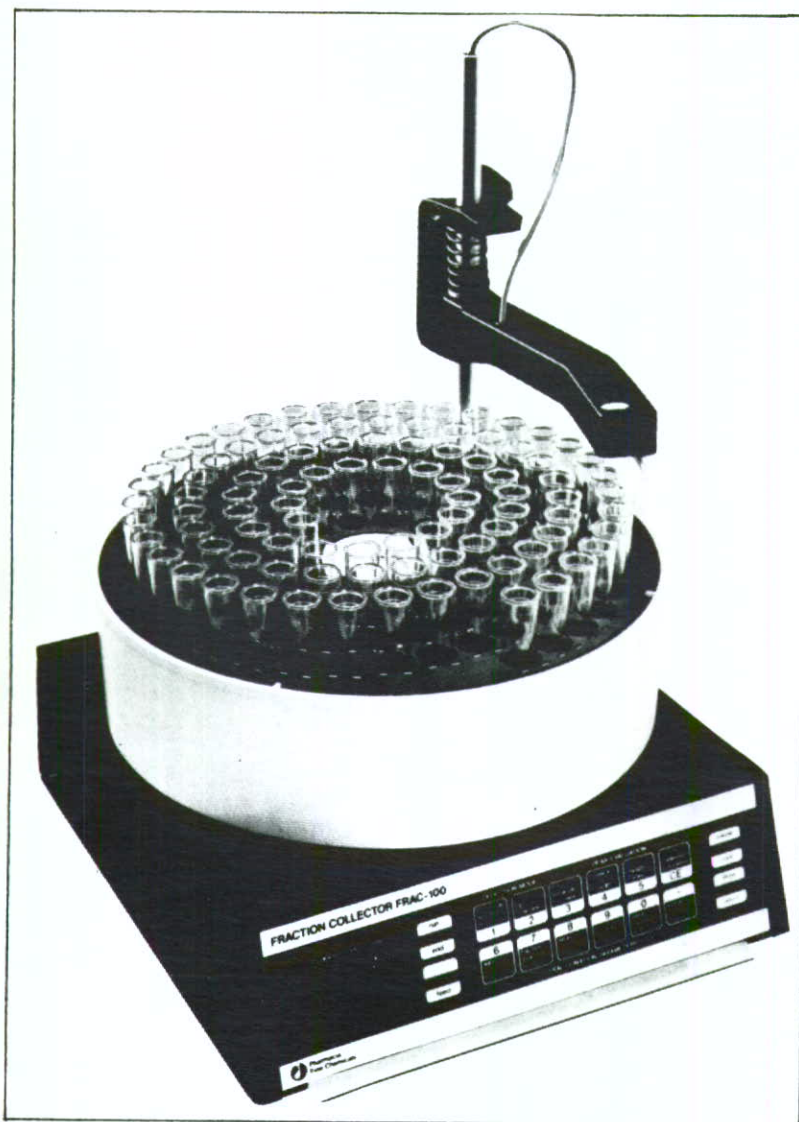
- | | | | |
|-------------------------|---|----------------|---|
| • Monochromator: | • 3 meter, range 185 to 900nm.
Bandpass 0.00 to 2nm. | • Sensitivity: | Minimum .7 ABS for 5ppm Cu soln., air/acetylene flame. |
| • Digital Readout: | Absorbance range 0.1 to 2.0
Concentration ± 2000 .
Peak height. Flame emission. | • Options: | Graphite Furnace, Hydride generator. Interface to Apple II computer. Interface to HP97S calculator. |
| • Background Corrector: | Operating frequency 285Hz
Range 0-2.0 ABS. | • Price: | About \$10,000. |

CONTACT: ADVANCED ELECTRONICS LTD, P.O. BOX 32-076 AUCKLAND 9. Ph: 451-305. Telex: 60048.
(This product is being displayed at the A.G.M.)

For further information circle 25 on Reader Reply Card.

FRAC-100

The essential fraction collector



The Pharmacia Fraction Collector FRAC-100 is the essential fraction collector for your laboratory.

Capacity: The FRAC-100 collects up to 95 fractions in standard tubes of any diameter between 10-18mm. An inexpensive accessory converts the rack to take up to 45 scintillation vials, 28 mm diameter. All tube positions are clearly identified by number.

Versatile: Fractions are collected on the basis of time or, together with the peristaltic pump P-1, volume.

Reliable: The Frac-100 has only a handful of moving parts and operates completely reliably in your lab, or cold room.

Automatic end of run: The end of the run can be controlled by time, by volume or by tube number.

Event marker: The start of the run and each tube change are marked by a TTL-compatible or contact closure signal to your recorder.

Fast: Tube change time is less than 0.7 sec.

Chemically resistant: The rack is resistant to most eluents used in modern liquid chromatography. In the event of spillage, the rack will hold 2 litres of liquid.

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