



August 1979 Vol. 43 No. 4

Chemistry

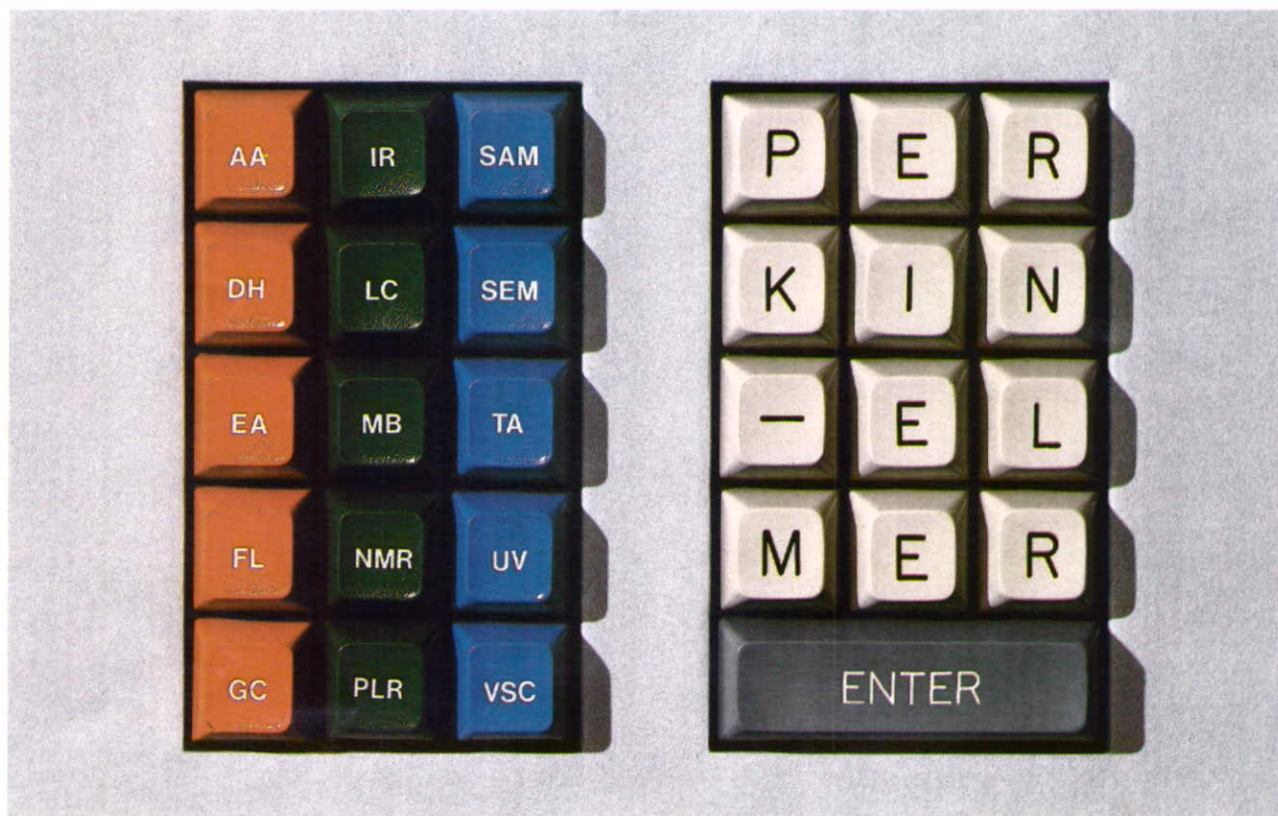
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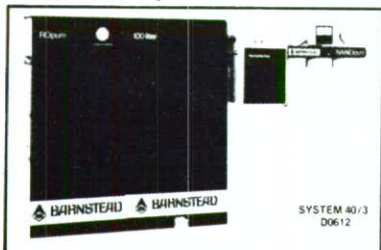
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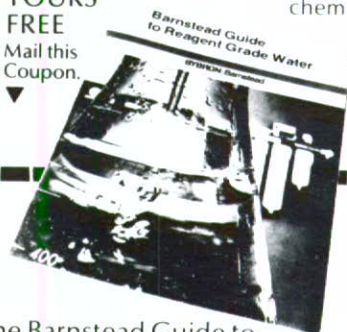
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STOP PRESS

The Industrial Specialist Group plans a half-day symposium on October 3 on "Agricultural Chemicals — Present & Future". Venue is the Auckland Leagues Club, Parnell, Auckland. For programme and details contact John Yolland (Box 9001, Auckland or Ph. 545-717)

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The organisers of the 1979 Institute conference have chosen to place the emphasis of the plenary lectures on NZ Chemical Industry. This was done for two reasons. One sometimes hears murmurs that conferences are "too academic" and have little to interest members from an industrial background. The plenary sessions this year are designed broadly to cover chemical industry in NZ, particularly those areas which look likely to become increasingly important to the economy in the future. It is hoped that the topics chosen will prove of interest to the industrial wing of the Institute (who could put their registrations where their moans had been) and also to the academic wing, who produce the one essential raw material of all chemical industry — competent graduates.

The second reason for choosing an industrially-based theme is that the conference provides an opportunity for publicising chemistry. Over recent years "chemistry" has taken quite a hammering in the media and in public esteem. The word "chemical" has taken on perjorative overtones. For example; "chemical" spills are "neutralized" in a blaze of publicity by the fire service, or "chemical" contaminations of our environment, our food or ourselves are always good for headlines. In the background there lurks the implication that the problem arose from "chemicals" and, by further implication, "chemistry" in general. Any compound which is regarded as beneficial is somehow not seen as a chemical, but as a drug, or a plastic or whatever, and favourable publicity by-passes chemistry. The fact that all "chemicals" are produced to meet a public demand and that problems generally arise from the follies of society at large do not seem to register. Nor does the fact that much of the current pollution bandwagon is simply a reflection of the greater sensitivity of modern analytical techniques. Of course spills, pollution etc. are undesirable, whatever their origin, but an attempt should be made to present chemists as the monitors, rather than causers of the problems.

Chemical industry has also received more than its share of negative publicity. Undoubtedly, many chemical industries in the past have proved to be bad neighbours — although the blame should often be placed at the accountants' door, rather than the chemists'. Currently, chemical industry is in the news, with the recognition that the continuation of the present level of personal mobility is dependent on the production of liquid fuels. This is a problem close to the public consciousness and provides an opportunity to refurbish the public image of chemistry.

We hope that the theme of the conference provides an opportunity for some positive publicity for chemistry, and that all members take any opportunities which come their way to present chemistry as beneficial to society. An improvement in the public image of chemistry must benefit us all — in terms of personal remuneration, diversion of restructuring axes, elevation of sinking lids, increased student enrolments or alleviation of whatever form of discomfort the current malaise causes.

Neil Curtis
Chairman, 1979 NZIC
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Polemics From The Pulpit

We were surprised to read the other day an announcement of a "Journal of Automatic Chemistry". Our first reaction was that it must be a joke, like laevo-rotatory ice. But No! We wrote away and sure enough a copy came back automatically. The editorial material could interest many of our readers who are concerned with automating analyses, which is a theme for this issue; they may be frightened at the price and the poor binding. However to us a Journal of Automatic Chemistry implies automatic chemists, all brains and no heart or spirit. We should hope that no members of the NZIC fall into this category: we find in our experience and reading of the literature that good chemists are men of wide vision and many talents. Our lasting impression of Wattie Whittlestone, whose exciting career is dealt with in another part of this issue, is seeing him some 30 years ago walking up and down Dunedin railway station playing his recorder while other Conference delegates waited for a train.

We came across in our reading a suggestion that every chemist is at heart a poet. Sir Humphrey Davy (1778-1829) is known inter alia for his experiments with laughing gas, which he said "made me dance about the laboratory and kept me in a glow ever since". It is recorded that a lady of the day had whitened her skin with a bismuth preparation, and then bathed in the sulphurous waters at Harrowgate, whereupon her skin turned jet black, which surprised her so much that, in keeping with the tradition of the day, she swooned. About this the poet-chemist wrote:-

We do not share her great surprise,
We know the law the underlies
This lady's change of hue:
For what she though was H₂O
Contained some H₂S, and so
She came down in Group II.

The idea of an automatic chemist takes no account of the Varieties of Chemical Experience which uplift us and our colleagues. We were moved by a recent article by Ronald Bentley of Pittsburgh about "prochirality". In 1948, there came to an Oxford chemist, A. G. Ogston, what he describes as "a gift, out of the blue" by which he saw that certain compounds, such as aminomalonic acid, were not chiral (asymmetric) in the accepted sense, but could still present two aspects to an attacking enzyme. The concept of prochirality is one which we, in the autumn of life, have not yet been able to fully grasp, but we were cheered by the experience of Vennesland, quoted in the same paper, who describes how he read Ogston's paper through several times, and used some stick and ball models to assist his thinking. He goes on, "While I was staring bleakly at the models, they suddenly told me the answer, but not in words, just in a picture. What happened in that moment of sudden insight seemed to be that I was suddenly graced with the ability to see the asymmetric carbon as van't Hoff had originally seen it. The feeling I experienced was a curious combination of exhilarating, sweet relief and total dismay: 'Oh you idiot, why haven't you realised that before'. There were quite a few of us who had experiences similar to mine after the appearance of Ogston's paper". Compared with the savants we have mentioned you will have gathered that we do not claim to be more than dim-witted, but we still get our exhilaration from chemistry and meeting chemists particularly in conference.

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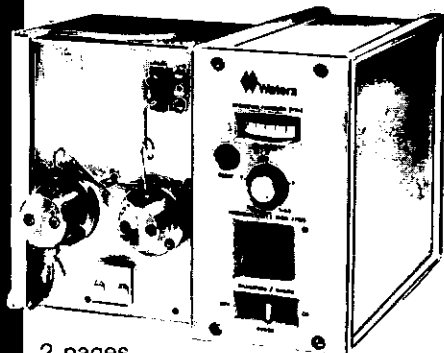
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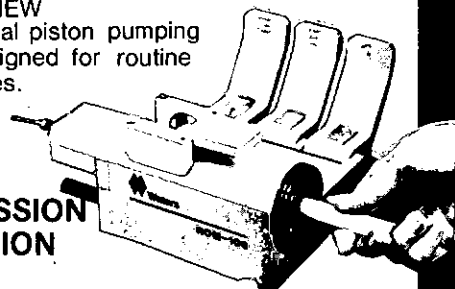
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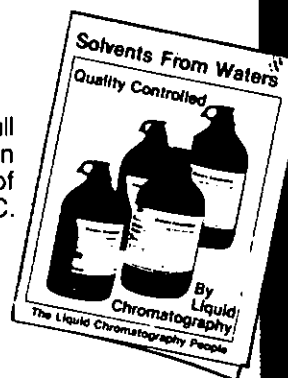
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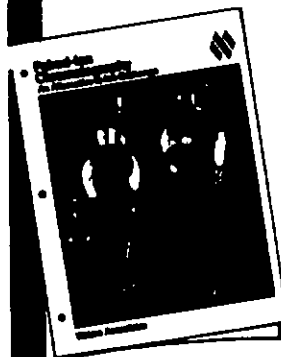
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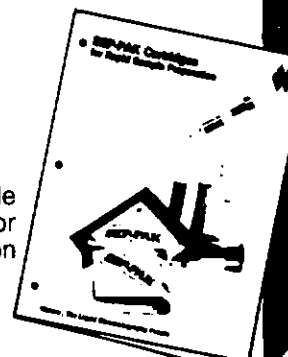
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What's Happening

Prof. G. B. Petersen, Biochemistry Dept., Otago University who has recently been appointed chairman of the Government's Advisory Committee on Novel Genetic Techniques, attended the COGENE Conference at Wye College, Kent, England, in April. (COGENE is an international Committee on Genetic Experimentation which is itself a subcommittee of the International Council of Scientific Unions). The conference was called jointly by COGENE and the British Royal Society specifically to discuss progress and problems in the field of genetic engineering and was attended by some 150 scientists from 30 countries. Invited speakers gave up-to-date accounts of the techniques available, of the achievements and of the prospects in this field.

Mr G. W. Broughton, general manager, McLeod Bros. has just completed a 2-year term as chairman, Otago/Southland branch, NZ Manufacturers Federation. McLeods are heavily involved in exporting soap products manufactured in their Dunedin plant.

NZ Pharmaceuticals Ltd recently commissioned a new laboratory for both research and development and quality control work. At the opening ceremony the company was presented with an Export Award in recognition of the successful international marketing of the company's refined bile acid products.

Dr. R. P. Garland has just returned from a technical marketing trip, visiting the company's customers and potential customers in America, Europe and Japan.

Prof. D L Trimm, School of Chemical Technology, University of NSW, is considering setting a "focus for catalysis" to cater for chemists and chemical engineers with interests in catalysts. Enquiries to Prof. Trimm, University of NSW, Box 1 Kensington, NSW, 2033 Australia.

We have received advice that **Dr. R A Robinson** who will be remembered by many for his excellent research work, particularly on the physical chemistry of solutions at Auckland prior to 1947, has died in Florida aged 75.

Our distinguished editorial predecessor **Prof. Emeritus Hugh Parton** has written a history of the "University of NZ" published jointly by Auckland and Oxford University Presses for the University Grants Committee. It records the history of a University which had "no students, no laboratories, no lecture halls, no academic staff merely a brass plate and an Act!" It was formed mainly as an examining body in 1970 and expired in 1961.

The Institute's archives are housed in the Chemistry Dept., Canterbury University, where they are cared for by **Mr B Cox**. He would be grateful for any copies of the Journal prior to 1959 and especially for Vols 1-4, of which he has no copies. Also sought are Vol 32, Nos 2 and 6 (1968) and any extra copies of Vols 32 and 33 would be welcome.

GAMBLING PAYS OFF

Researchers in NZ can thank the gambling instincts of the average Kiwi, for his devoted purchases of lottery tickets helps fund research equipment buying.

According to the Scientific Research Distribution Committee, which allocates lottery profits for research equipment, the following disbursements have been made during the period 1976-1978:

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- a. amount allocated by Lottery Board of Control \$250,000
- b. amount allocated for equipment \$198,900

1977

- a. amount allocated by Lottery Board of Control \$250,000
- b. amount allocated for equipment \$121,500

1978

- a. amount allocated by Lottery Board of Control \$300,000
- b. amount allocated for equipment \$236,800

Dr. Rob McKeown, Dept of Pharmacy, Otago University, has probably the most complete set of Institute publications in existence but needs the following to complete his collection: Fundamentals of Commercial Chemical Development, H. G. Woolman (1955); List of members NZIC and NZ section RIC (1947); Rules, regulations and code of ethics NZIC (1947 only and cyclostyled conference booklets with summaries of papers for 1950-55 inclusive. Can anyone help?

A urea plant in Indonesia, which recently became a urea exporter, is losing money even though it is using low cost natural gas as feedstock and enjoys a high operating rate. This from Kiyoshi Nakamaya, assistant manager, Mitsubishi Chemical Industries' market development research laboratory to the recent ACS/CSJ congress.

Fines totalling \$US24,400 have been levied against the American Cyanamid Co Willow Island pigment plant, where 5 women claimed they had to undergo sterilisation operations last year to keep their jobs. The company intends challenging the fines, imposed because of claimed overexposure to lead and to potentially cancer-causing chromates.

Starting late August, the Auckland Technical Institute in association with the NZIC Polymer Group will run a short course on the theory and application of modern polymers and associated materials under the title "Aspects of Polymer Science". Twelve 2hr sessions are planned starting August 29 plus a 3-day block course in November. Registrations should reach the head of the Applied Science Dept., ATI, Private Bag, Auckland, by August 10.

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BRANCH NEWS

Auckland

In May the branch held a joint meeting with the Chemistry Dept. of the University. The topic was high-field NMR, with special reference to the extension of the technique to nuclides other than protons and carbon-13. The speaker was **Prof. George Levy**, Professor of Chemistry, Florida State University, who gave a stimulating talk that was much appreciated by the large audience. Discussions continued over dinner between a group of keen members, Prof. Levy, and also **Prof. Pierre Lazlo**, from the University of Liege, Belgium, who had presented a lecture at the University earlier in the day on the development of sodium-23 NMR for the study of metal ion binding to biomolecules.

Speaker at the June meeting was **Dr. C. H. Hendy**, senior lecturer in chemistry, Waikato University. Dr. Hendy gave a superbly-illustrated talk on many aspects of geochemistry in Antarctica, particularly analytical studies of recent lake deposits.

Waikato:

The May meeting was addressed by the Institute President, **Dr. Ted Harvey**. Ted, who is Registrar, Victoria University, spoke on "*The Scientist in Administration*." In June, **Dr. Bruce Graham**, a former Waikato University graduate from Ken Mackay's group and now a chemist in the Health Dept's Environmental Laboratory, gave an instructive and entertaining lecture on "*Air Pollution Monitoring*."

Manawatu:

The May meeting took the form of a Symposium on "Energy Prospects for NZ". Many members of the audience of 42 were from beyond Palmerston North, some coming from Hawke's Bay. The symposium was opened by **Dr. Ian D. Watson** (Department of Chemistry, Biochemistry and Biophysics, Massey University) with some general remarks on the availability of various forms of energy. **Dr. J. H. Chemistry in New Zealand**

Troughton (Ministry of Agriculture and Fisheries, Wellington) then discussed the consumption of energy in NZ and **Mr P. A. Toynbee** (Coal Research Association of NZ) described the contribution of coal as a fuel and its conversion to other products. (We hope to publish this in our next issue — Ed.)

Mr John H. G. Milne (Shell Oil Co., Wellington) concluded the formal part of the symposium with a discussion on the role and availability of various petroleum products, both indigenous and imported. The symposium ended with a lively discussion.

Our next meeting, on September 18, will be addressed by **Dr. J. S. Ayres** (Department of Chemistry, Biochemistry and Biophysics, Massey University) on "Developments in NZ Cellulose Ion Exchangers." The branch's AGM and chairman's address (**Dr. Andrew M. Brodie**) will be held on October 15. Further details of these meetings can be obtained from **Dr. David R. Husbands**, Department of Chemistry, Biochemistry and Biophysics, Massey University.

A Science Fair, consisting of contributions from pupils of local high schools, will be held in the Queen Elizabeth College Hall, Palmerston North, September 6-8, 1979. The fair is funded by the public through the Kiwanis Club and is supported by various scientific organisations. The branch will donate a prize for the best entry in the Chemistry section. The winning entry will be on display at the October meeting.

Wellington:

Branch chairman **Dr. John Featherstone**, who spent June in Europe for a series of meetings and discussions in connection with his work on dental caries, is the recipient of the 1979 Hamilton Award of the Royal Society of NZ. The local meetings have included the Presidential address in early May, which was also delivered to our members in the Nelson area. Also in May, **Prof. R. Loehr** spoke to the branch on the "Eutrophication Caused by Agriculture." The June meeting, held jointly with the Wellington Potters' Association, attracted an audience of over 100 for **Dr. Harry Percival's** lecture "Earth & Fire: The Chemistry of Pottery." The lecture's popularity can be assessed from the fact that the lecturer was answering questions informally for an hour! We were pleased to welcome **Stan Brooker**, our Editor, to this meeting.

Canterbury:

The June meeting was organised by the Chemical Education Group and considered "The role of analytical chemistry in schools". Several speakers took part during the evening — **Dr. Jack Fergusson** (University Chemistry Department), **Dr. John Cretney** (Christchurch Technical Institute), **Alan Wooff** (Christchurch Boys' High School) and **Denis Hogan** (Chemistry Division, DSIR). The extent to which modern analytical chemistry should be introduced into the school syllabus was discussed and a number of suitably simple but relevant experiments were demonstrated.

The July meeting took the form of a mid-winter dinner, the after-dinner speaker being none other than **Prof. Ted Harvey**, the Institute President, who spoke on "Chemists in Administration".

Otago:

The President visited the branch on June 14 for a combined meeting/social evening. On May 10 **Prof. Leon Phillips**, University of Canterbury, gave an address titled "Lasers on Chemistry".

PEOPLE

Former TELARC director **John Gilmour**, who came to NZ in 1973 from NATA, TELARC'S Australian counterpart, has returned to NATA to become Registrar.

Dr. M J Taylor (Chemistry Dept., Auckland University), **Dr. John Rogers** (Fertiliser Research) and **Stan Brooker** (Journal Editor) have been re-elected for further 3-year terms on the Council of the Auckland Institute and Museum.

Mr W D Holloway has left Auckland Hospital's gastroenterology laboratory and joined ABD, DSIR, Palmerston North.

Mr Y W O'Callaghan has resigned from Fibremakers (NZ) Ltd and is now with House of York Wallpapers, Levin.

Mr R T Bell has been named general manager, Watty Ltd.

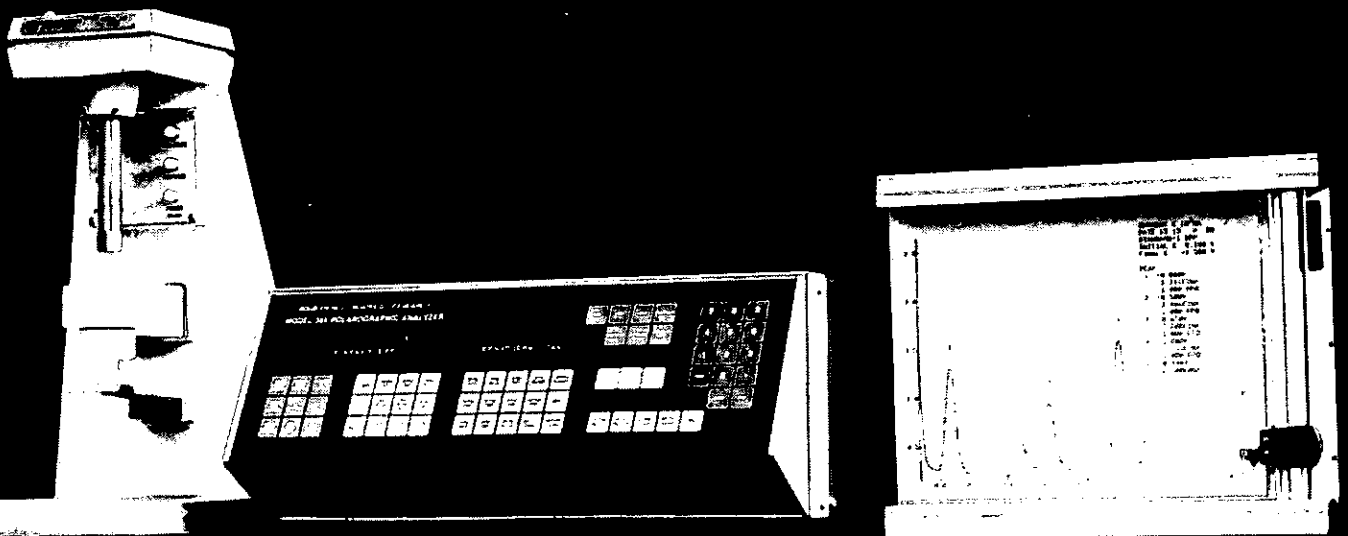
Mr Warren Hutchinson has moved from the NZ Sugar Refining Co. to a new position with the Honey Marketing Board.

Mr. A. J. Kettle (B Sc. Hon., Otago) has been appointed by Abels Ltd. as a research assistant. He will be working with **Dr. L. Eyres** on research and development in the field of edible fats and oils.

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METHANOL, AMMONIA AND UREA PRODUCTION

E.R. Palmer,
Industrial Processing Division,
DSIR

Methanol and ammonia may both be produced from natural gas by closely related processes. Ammonia may subsequently be further reacted to yield urea for fertilizer or chemical use.

The natural gas wellstream is first subjected to various treatment and separation processes by the gas production authority to remove heavier hydrocarbons and leave a feed-gas stream consisting predominantly of methane. For both methanol and ammonia production, the methane is decomposed by steam over a nickel catalyst at high temperatures and about 30 bar pressure yielding carbon monoxide and hydrogen.



In ammonia production these gases and the remaining unconverted hydrocarbons pass to a secondary reformer where air is introduced providing oxygen and nitrogen. The remaining hydrocarbons are converted to hydrogen, carbon monoxide and carbon dioxide. Further reaction with steam over an iron catalyst converts much of the remaining carbon monoxide to carbon dioxide and produces additional hydrogen. The carbon dioxide is removed by absorption in monoethanolamine or hot carbonate solution and, to avoid poisoning the ammonia synthesis catalyst, the gases are normally passed to a methanation reactor in which any remaining carbon oxides are converted to methane.

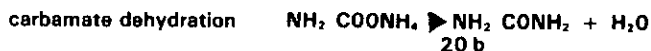
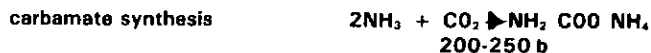


The synthesis gas stream, now consisting essentially of nitrogen and hydrogen, is compressed to between 200 and 300 bar and fed to the ammonia synthesis reactor. Reaction takes place at about 500°C over an iron oxide catalyst. The synthesis pressure used varies with the size of plant, but the tendency nowadays is for large plants with high pressures, 300 bar or greater, using centrifugal compressors. By suitable heat exchange with the incoming gases, the product ammonia is produced as a liquid.



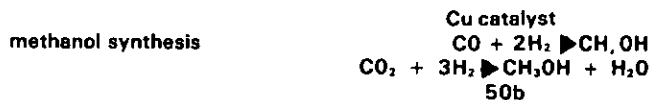
Urea is produced in a two-stage process. Firstly, ammonia and carbon dioxide are reacted to ammonium carbamate by reaction in an autoclave at 20 to 30 bar in the liquid phase with excess ammonia and with a high carbamate recycle. The carbamate is subsequently decomposed to form urea and water. There are many process variants, mainly related to methods of recovery and recycle of ammonia, carbamate and carbon dioxide. Urea is crystallised or prilled from the concentrated product solution. The co-produced impurity biuret must be closely controlled as it is toxic to some plants.

Chemistry in New Zealand



The carbon dioxide required for the urea synthesis is obtained from the steam reforming of the original natural gas. In the case of the Kapuni plant it is expected that this will be supplemented by additional carbon dioxide recovered from the natural gas treatment plant, if production of urea is to be maximised.

In the production of methanol, the mixture of carbon monoxide, carbon dioxide and hydrogen from the natural gas reformer is compressed to the synthesis reactor pressure, without any intermediate processing. The synthesis pressure required depends on the catalyst system used. A number of proprietary designs are available for the methanol synthesis reactor. The ICI process operates at 50 to 100 bar and 250 to 270°C with a copper-based catalyst; alternative processes use higher pressures and temperatures (300 - 350 bar, 370° - 380°C) with zinc chromite-based catalysts. The reaction is usually carried out with a slightly hydrogen-rich feed, purge gases being used for in-plant fuel. CO/CO₂ molar ratios between 20 to 1 and 1 to 2 may be used; the preferred range is between 3 to 2 and 4 to 3. Methanol is condensed from the reactor product stream; a portion of the gases are purged to eliminate any build-up of the methane or nitrogen and the remainder recycled to the reactor. The crude methanol is purified to remove water and higher alcohols and esters formed in the reactor. The extent of purification depends on the product grade required — fuel grade or one of the chemical grades.



Synthetic gasoline may also be produced from natural gas via synthesis gas processes. The traditional Fischer-Tropsch synthesis process may be used to produce a wide range of hydrocarbons, or alternatively synthetic gasoline may be produced by the Mobil process from methanol. The economics of these processes are generally most favourable for large plants, in excess of 500 tonne/day output. Developments in recent years have markedly increased the energy efficiency of synthesis gas processes but necessarily at some increased capital cost.

Ethane and other higher hydrocarbons could be fed to a steam reformer for methanol or ammonia production, but the reverse is not true. Ethylene, a precursor for many plastics and other petrochemicals, can be produced by cracking ethane and higher hydrocarbons, but methane is not a suitable feed for this process. Synthesis gas-based products and petrochemicals are not therefore necessarily competing for the same feed stock and if suitable economic markets existed ammonia, urea, methanol and petrochemical plastics could all be produced from Kapuni and Maui natural gases.

Chemical And Biochemical Research In Facial Eczema In NZ

D.E. Wright,
Agricultural Research Division
Ministry of Agriculture & Fisheries.

Facial eczema is the popular name for the disease pithomycotoxicosis which was first seen in farm animals in NZ early this century. Its occurrence is largely restricted to the North Island, but outbreaks have been reported in Australia, South Africa and USA. Economic estimates of the annual cost of the disease in NZ range up to \$25 million, depending upon the severity of the outbreaks.

Research was initiated in the late 1930s and has progressed through several phases. This article describes current knowledge and research into future control methods.

Isolation of the causative fungus *Pithomyces chartarum*; extraction, purification and chemical characterisation of the epidithiodioxopiperazine based sporidesmin toxins in the late 1950s (1,2) and the discovery in the early 1960s that some fungicides will control field outbreaks of the disease were notable achievements. Preparation of gram quantities of sporidesmin allowed experimental production of facial eczema and facilitated studies on the pathology of the disease and has provided biochemical data on the biological events resulting in toxicity and provided the means to test alternative methods for control of the disease.

Clinically, the disease is characterised by photosensitivity and is accompanied by loss of weight and productivity (e.g. lowered milk production) and possibly death. Bile duct occlusion is an important factor in the pathogenesis of the disease.

Using serum levels of the enzyme γ -glutamyl-transferase which is leaked from damaged liver tissue, Towers (3) has demonstrated that the incidence of sub-clinical disease can be substantial. In a survey of 1357 milking cows in Waikato, 9.4% had clinical facial eczema, whereas elevated enzyme levels were found in 39% of the cows. While this enzyme has proved useful in identifying cows and sheep with liver damage, no prognostic value has yet been demonstrated in relation to other animal health problems such as metabolic diseases or calving problems.

The biochemistry of sporidesmin toxicity is not understood. Swelling of mitochondria and decreased respiratory control are known biochemical responses *in vitro*. Middleton (4,5) has suggested that sporidesmin as a lipid-soluble uncharged disulphide may react with thio groups — possibly specific thiols — in membranes. Evidence for a disulphide interchange has been obtained by reacting sporidesmin with dithiothreitol and by chromatography demonstrating the formation of new products of the reaction. The most significant biological effect of its action on membranes is inflammation most obviously causing changes in bile canalicular membranes.

Understandably research effort has emphasised the importance of achieving an economic, reliable and practical form of disease control. The use of fungicidal sprays, in

conjunction with a knowledge of climatic conditions favouring the growth of *P. chartarum*, and spore counting of pasture samples, is now the basis for field control (6). However, the economic worth of the method does depend upon reliable forecasting of toxicity and is not cheap, particularly in hill country where aerial spraying is necessary. Considerable research effort is now directed towards alternative methods of control.

In 1975 the use of zinc salts in preventing facial eczema in sheep and cows was reported (7). In a series of papers the effectiveness of zinc in preventing liver damage in laboratory animals or in farm animals has been demonstrated.

Despite its effectiveness, no recommendations to farmers to use zinc have been made. Because of the high dose rate required — the effective dose is 10-20 times greater than the normal intake from pasture — zinc toxicity can be a hazard (8,9).

Dosing trials have shown that toxicity is related to dose rate, period of dosing and method of dosing. For example, oral doses cause oesophageal groove closure in ruminants (10) the dose being directed into the abomasum, thereby causing inflammation and abomasal lesions. Possible methods for providing zinc include spraying insoluble zinc salts onto pasture, dissolving zinc salts in drinking water (11) or individual doses. The latter has the advantage of dose monitoring, but on a daily basis would be labour intensive and not practical for sheep farmers.

Ramberg (12) using zinc-65 found very low absorption of zinc and the process of oral dosing is inefficient with respect to the amount absorbed. Safe and long acting dosing of parenteral zinc has yet to be perfected.

Control over absorption of zinc from the gut is very effective. A 70-fold increase in zinc intake increases absorption by only 70%. Over 98% of ingested zinc is not absorbed from the gut.

The mode and site of action of zinc in protecting animals is not known. If it acts in the gut then poor absorption is presumably advantageous. If it acts within target organs such as the liver or kidney, then low absorption is undesirable. Little evidence is available on this point.

The question why does zinc protect against sporidesmin is unanswered. When this is known a more rational system of using zinc or other metals, if they have similar protective properties, may result.

Genetic Studies

Different animal species vary greatly in their response to sporidesmin. As well, variable responses amongst sheep in flocks with clinical outbreaks of facial eczema are known. Campbell (13) *et al.* have demonstrated the possibility of breeding for resistance to the disease. From the results of two trials in 1974 and 1975 in which lambs were on toxic pasture or individually dosed with toxin, he concluded that there is a wide range of susceptibility to the toxin with an estimated heritability of resistance between 0.4-0.6 indicating the good possibility of selecting resistant animals.

This work has continued with the aim of building up flocks of resistant or susceptible animals to further determine heritability, to develop biochemical tests, to simplify selection which currently is wasteful, being based on animal responses (loss of weight, serum enzyme levels, photosensitivity, death) to doses of toxin, and to provide animals for research on understanding the mechanisms of resistance.

Many factors may be involved in determining the susceptibility of an animal to a toxin. Lowered susceptibility of the target site or reduced concentration of the toxin at the target site will provide increased resistance.

The concentration of sporidesmin in the liver of an animal will depend upon the amount dosed or ingested with pasture, on the efficiency of absorption from the gut, on its metabolism to more or less toxic metabolites, and on its

August 1979

rate of excretion. There is good evidence that metabolism of sporidesmin is an important factor in determining resistance.

In 1978, Fairclough *et al.* (14) using ^3H -, ^{14}C - or ^{35}S -labelled sporidesmin incubated with liver microsomes from sheep treated with hexachlorobenzene to induce mixed function oxidases, formed at least 8 different metabolites and assigned tentative structures to two of these.

They also described an assay for the rate of sporidesmin metabolism in which ^{35}S -sporidesmin was incubated with the 10,000 g supernatant fraction prepared from liver biopsy sampled from Romney and Merino sheep. Two to three-fold differences in metabolism rate were found amongst sheep, the Merino sheep having higher rates than the Romneys. Since Merino sheep are considerably more resistant to facial eczema than Romneys, these results support the hypothesis that metabolism of sporidesmin is involved in resistance.

Further evidence for the role of detoxification has been obtained by Mortimer, Manns and Coe (15) in sheep treated with the inducing chemical hexachlorobenzene. After dosing with sporidesmin, serum γ -glutamyl transferase levels, the number of clinical cases and mean liver damage scores were all higher in control compared with induced animals. Protection was also achieved in sheep grazing toxic pasture.

Little is known about the enzymes responsible for sporidesmin metabolism. Considerable research effort is directed towards developing a valid assay for sporidesmin metabolism, to understand the genetics of detoxification, to identify marker enzymes for genetic selection and to establish methods for inducing detoxification to enhance sporidesmin metabolism. With this knowledge it should be possible to select resistant animals on a large scale and to include cattle, as current work is restricted to sheep.

Immunisation Against Sporidesmin

Sporidesmin is a small molecule and unlikely to induce antibody responses. Since the early 1970s attempts have been made to couple sporidesmin or analogues to proteins and use these complexes to study antibodies to the toxin.

Initial experiments have tested sporidesmin — poly-L-lysine which when injected into rabbits resulted in a weak antibody response (16). This complex was made by opening the disulphide bridge with sodium borohydride, the sulphhydryl groups were then alkylated and reacted with

poly-L-lysine, resulting in about 28% of the lysine residues being substituted with sporidesmin.

More recently Fairclough, Mortimer and Ronaldson (17) have coupled sporidesmin with bovine thyroglobulin and surprisingly found that immunisation with this material increased sporidesmin toxicity.

In conclusion, new methods to control facial eczema can confidently be expected in the 1980s. Prospects for developing immune systems by raising antibodies to sporidesmin do not appear bright.

As our knowledge of the mechanism of zinc protection becomes greater the development of practical systems using zinc should be possible. In the long term, the selection of resistant animals offers an attractive solution to the problem. Progress will depend on establishing how persistent is resistance and identifying resistant animals and using these for extensive breeding. The induction of detoxification enzymes at present is only a useful experimental tool and its practical significance will depend upon identifying safe, effective and cheap inducers and development methods to use inducers.

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Automation Of Flame Spectroscopy For Agricultural Analysis

O. E. Clinton
Ruakura Soil and Plant Research Station
Hamilton

This article describes the evolution of two automated spectroscopic flame instruments at Ruakura and their use for the analysis of specific sample solutions associated with agricultural research and advisory work. One of these instruments, a 4 channel system, has recently been implemented and can determine Mg, Ca, Na and K in soil leachates and plant digests at the rate of 200 samples/hr.

Chemistry in New Zealand

A spectrochemical laboratory was set up in 1950 by the late Mr J. E. Allan, FNZIC, at the laboratories of the then Rukuhia Soil Fertility Research Station, Hamilton. Extensive studies in plant nutrition and the fertility status of NZ soils were projected at this time and the requirement for a reliable and efficient analytical service for plants and soil extracts was considered essential.

The development of spectrochemical methods of analysis was pursued with some vigour by Mr Allan and progress was quite rapid. The application of techniques involving arc, spark and flame spectrography enabled relatively large numbers of samples to be processed routinely for many nutritional elements of interest in soil fertility research. Extensive use was made of the Lundegardh flame spectrographic method for the determination of Mg, Ca, Na, K, Mn, Cu and Fe in solution. For this method, a few millilitres of solution were introduced into a spray chamber and the finer particles fed into an air-acetylene flame. Radiation from the flame passed through a spectrograph and an exposure time of 1 min. was required to produce line spectra of adequate intensity on a photographic plate. Up to 60 spectra could be recorded on a plate.

Flame Spectroscopy (Cont)

With an ever increasing demand for such analyses, at a time when "staff ceilings" and finance were very restricted, it was considered that the automation of this procedure would almost completely eliminate operator time and allow a greater number of samples to be analysed in a working day. An automatic apparatus was eventually built around a Hilger medium quartz spectrograph. Details of this apparatus, including the construction of all units from inexpensive materials and components, were subsequently published. (1).

Many of its mechanical and electromechanical components utilised parts of aircraft dismantled after the war. Affectionately known as "George", this apparatus clattered away, unattended for periods of 1½ hours, had considerable "visitor appeal" and handled many thousands of samples over a period of about six years. However, considerable time was spent in the subsequent rather laborious reading of spectrographic plates and calculation of results, and eventually the advantages of the "direct reading" aspect of flame photometry became obvious. The sample changer itself continued to be used for some time with flame photometry.

Demands for the determination of the "major" elements, P, N, Mg, Ca, Na and K in ever increasing numbers was of primary concern and, of these, Ca, Na and K were ideally suited to flame photometry. For this reason, considerable research into all aspects of flame photometry was undertaken. This resulted in the design and construction of a three channel filter flame photometer for Ca, Na, and K by means of which simultaneous measurements of emission intensities could be obtained simply and quickly. All other elements (other than N and P) continued to be determined quantitatively by a porous cup spark spectrographic method.

With a growing realisation of the importance of magnesium in both plant and animal nutrition studies, the absence of a reliable and quick analytical method for this element was recognised as a severe limitation to further field research in this area. The potential of atomic absorption spectrometry as an analytical technique (2) was immediately recognised and exploited by Mr Allan. Theoretically, it appeared to be "tailor made" for an element such as Mg and indeed, the first published application of this technique related specifically to the determination of magnesium (3).

Fig. 2. Components of an automated 4-Channel flame photometer.

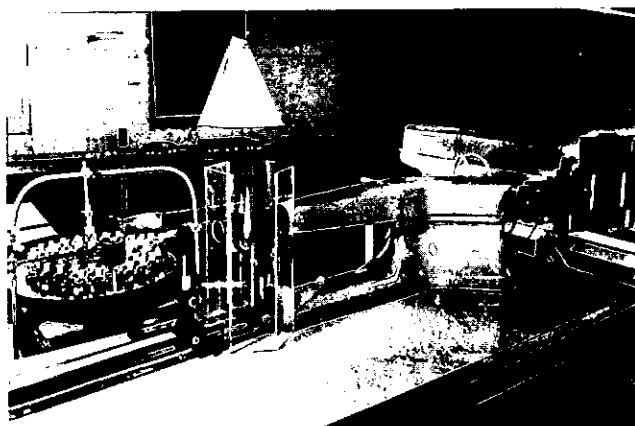
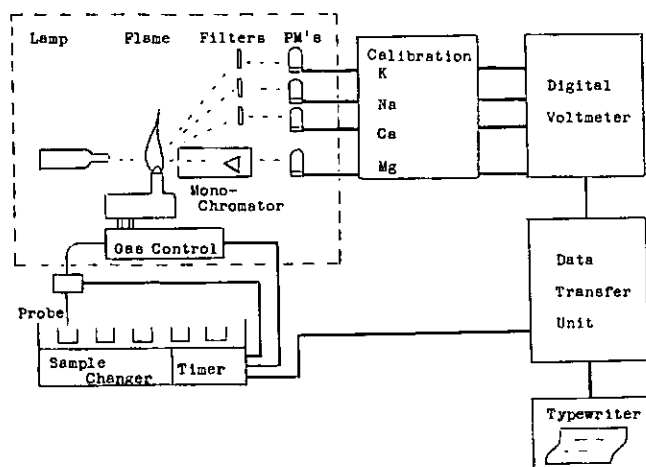


Fig. 1. "George" — an automated apparatus for Lundegardh flame spectrography — 1956.

Since the flame apparatus required for the atomic absorption method was similar to that employed in flame photometry, it was not long before the existing 3 channel flame photometer was rebuilt to incorporate a channel for Mg by atomic absorption. Designed to be used exclusively for the analysis of plant digests and soil base exchange leachates at Ruakura this 4 channel flame photometer has been in daily use as a dedicated instrument since 1962. In the 1977-78 year, it was used for the analysis of over 24,000 sample solutions for Mg, Ca, Na and K. This represents a current annual total of about 100,000 elemental determinations.

Although limited to the determination of these elements in specific concentration ranges and solution matrices, this instrument evoked considerable interest and not a little envy by visitors to the laboratory, especially those concerned with soil and plant analysis. The simplicity of operation, the simultaneous readout on galvanometers permanently calibrated in concentration units for both soil leachates and plant digests, together with the overall speed of sample throughput were impressive. In practice, 200 solutions could be analysed in about 80 min. by an unhurried but experienced technician. The design details for this instrument are basically similar to those of a 3 channel flame photometer built specifically for the analysis of soil extracts for K, Ca and Mg (4).

To cope with the requirement for even greater numbers of such analyses in the future and in recognition of the fact that there is a practical limit to the number of meter readings per sitting which any technician could be expected to make, this 4 channel flame photometer has now been fully automated.

A diagram of the component parts is shown in Fig. 2. The flame photometer utilises interference filters for wavelength selection for the emission channels Ca, Na and K, and a small monochromator to isolate the Mg resonance line for the absorption channel. For each channel, the radiation is detected with a photomultiplier tube and the signal is fed to an analogue calibration unit. This custom built unit contains relatively simple analogue circuitry to enable the calibration of each channel in concentration units to be affected while aspirating standard solutions of known element concentrations. At the same time, curve correction, which is necessary to linearise the calibration curves for Mg, Na and K, can be made. The electronic circuitry is based on active function generation (5).

Push-button flame ignition and extinction have been added to the original instrument. For safety reasons, the automatic shut-down of gas flows to the flame is controlled by a light sensitive diode located adjacent to

the flame. This was considered essential for a flame instrument which was required to be left unattended while operating in the automatic mode.

During the early development of this flame photometer, much effort was devoted to the attainment of a high degree of stability and reproducibility of the emission signals. Long term stability was achieved by ensuring adequate regulation of the air and acetylene supplies, the careful selection of materials for the construction of the nebulizer, chamber and burner components and the use of simple DC regulated power supplies.

The sample changer selected was that from the ISCO Fraction Collector Model 327. The mechanism is delightfully simple, and the plastic tube carriers eliminate corrosion problems. A simple solenoid-operated probe attached to the sample changer enables solutions to be aspirated sequentially. Its operation is controlled by an electronic timing facility of the fraction collector. This electronic unit also provides a trigger signal to initiate the channel scan of the Data Transfer Unit.



Fig. 3. Automated 4-Channel Instrument.

The Data Transfer Unit (Solartron) sequentially samples the signals from each channel, and with the associated Digital Voltmeter (Solartron Model 1426) converts these analogue signals to digital form. It also contains an output driver interface by which the final concentration data are transferred to an electronic typewriter (Adler).

In operation, and after a warm up period of about 10 min., each channel is calibrated using the manual scan mode and aspirating known standard solutions into the flame. When each channel has been calibrated, the equipment is switched to "AUTO" and the instrument can be left unattended to process up to 200 solutions. The last position on the sample changer can be used to trip a switch which immobilises the equipment and extinguishes the flame. For more continuous operation, tube holders containing those samples which have already been processed can be removed from the sample changer from time to time and further samples added.

The stability of the flame photometer was such that minimal signal integration was found to be necessary for automation. The total aspiration time for each solution has therefore been limited to 18 sec. which results in solutions being analysed for the 4 elements at the rate of 200/hr. Preliminary runs with this automated instrument have shown an overall variation of concentration values of less than $\pm 2\%$ of the mean.

It is anticipated that the addition of an interface for a punched tape or magnetic tape cassette for the storage of results or for further computer processing, should present few difficulties.



O. E. Clinton is a Senior Technical Officer with the Ruakura Soil and Plant Research Station, Hamilton. He has worked for many years in the field of spectrochemical analysis applied to agricultural materials at Ruakura, and was closely associated with the late Mr. J. E. Allan FZIC a recognised pioneer in atomic absorption spectroscopy.

He was elected a member of the NZIC in 1976 and is currently the Waikato Branch Treasurer. He was elected Fellow of the NZ Institute of Science Technicians in 1978. He is married with 3 children.

The analogue circuitry for concentration setting and curve correction was designed by Mr. D. Hamblyn whose assistance is gratefully acknowledged.

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The table on page 95 of our June issue contains a number of errors, below is a corrected version.

POLYACETYLENES IN ARALIACEAE
(Ref. Bohlmann et al. Chem. Ber. 1961, 94; 958)

FALCARINOL
 $\text{CH}_2\text{:CH.CH(OH).C:C:C:C.CH}_2\text{:CH:CH.C,H}_{16}$
Panax ginseng

FALCARINONE
 $\text{CH}_2\text{:CH.CO.C:C:C:C.CH}_2\text{:CH:CH.C,H}_{16}$
Hedera helix (Ivy)
Aralia elata
A. racemosa

Polyscias fructicosa
Panax ginseng

FALCARINDIOL
 $\text{CH}_2\text{:CH.CH(OH).C:C:C:C.CH(OH).CH:CH.C,H}_{16}$
Schefflera digitata (Seven finger)
Falcaria vulgaris.

FALCARINDIONE
 $\text{CH}_2\text{:CH.CO.C:C:C:C.CO.CH:CH.C,H}_{16}$
A. californica

FALCARINOLONE
 $\text{CH}_2\text{:CH.CO.C:C:C:C.CH(OH).CH:CH.C,H}_{16}$
A. nudicaulis
A. californica

A. mandshurica
A. racemosa.

Development Of Steroid Synthesis From Natural Products

J. Kloosterman, Solanum Extraction Industries Ltd., Waitara.

During the 1930's, scientists developed an understanding of the group of substances known as the steroid hormones, contained in human and animal bodies. Isolation and synthesis of these biologically active compounds began. The starting materials for isolation were the urine, adrenal glands, ovaries etc. from animals but the low yields of product obtained and the poor sources of supply could not keep pace with the growing demand.

Synthetic studies began using cholesterol, obtained from wool grease or the spinal cords of cattle. Degradation of the sidechain was necessary to provide suitable precursors for the preparation of active compounds such as progesterone or testosterone. The sidechain was removed by oxidation, after protection of the 3-hydroxyl group by acetylation and the double bond by bromination, leading to the important intermediate DHA (androst-5-ene-3-ol-17-one 3 acetate). The yield of this step was very low and further purification was very laborious. Modern methods remove the sidechain by microbiological hydroxylation, which is very specific and gives good yields. In later years other important sources were the bile acids cholic and desoxycholic acid. These starting materials already contain an oxygen in the C ring and this makes the transformation into such 11-oxygenated products as cortisone, hydrocortisone, prednisone etc. much easier.

The discovery by US chemist Russel Marker that steroids could be made from diosgenin (Fig. II, 1a), a sapogenin extracted from yams of certain dioscorea species growing wild in Mexico, made this material the most important starting material for the fast growing steroid market and in 1965 about 75% of the world steroid consumption was obtained from diosgenin. The side chain degradation also developed by Marker gave much better yields and led to the same key-compounds as cholesterol.

In the past 10-15 years new starting materials and chemical processes have been developed and are threatening the supremacy of diosgenin. These sources can be classified into three main groups:

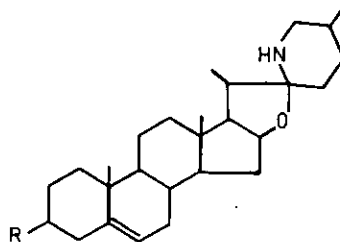
1. Coming from animals: To this group belong the above mentioned bile-acids and cholesterol.
2. Coming from plants: The most important ones in this group after diosgenin are: Hecogenin from sisal, sitosterol and stigmasterol from soya.
3. Total synthesis: After the structures of most steroids were elucidated, an ongoing effort was put in by many scientists into the total synthesis of steroid compounds. Many of these syntheses are

elegant exercises in pure chemistry but have only academic interest. However a few are in use for the production of specific compounds and are also economically competitive with the other sources.

It will be clear that the advantage of using starting materials of group one and two is the fact that the basic molecular structure, the perhydrocyclopentanophenanthrene is already present in the right stereo-modification.

Solasodine, although known for quite a long time, is one of the new alternatives for diosgenin. Leading to the same key intermediates, it is as versatile as diosgenin and so it can be used to produce a wide variety of finished products.

Fig. 1. Glycoalkaloids of *Solanum aviculare* and *S. laciniatum*



R = OH solasodine (aglycone)

R = D-galactose—D-glucose—D-rhamnose solasonine

R = D-glucose—D-rhamnose—D-rhamnose solamargine

Solasodine

During the 1940's, Prof. L. H. Briggs and his collaborators studied the extractives of *Solanum* species and described the structure of solasodine (Fig. II, 1b). Since then interest has been growing in the use of solasodine as a steroid precursor, as shown by reports coming from Hungary, Russia, Yugoslavia, India and other countries.

In general, solasodine is not present in the plant as a free steroid-alkaloid but as glycosides with various sugar residues. The sugar residues are attached to the C-3 oxygen of the steroid and are mostly trisaccharides. (Fig. I). In most *Solanum* species the highest solasodine contents are found in the leaves and the fruit and depending on the species this varies from 0.01 - 5% based on dry plant-matter.

Although processing (drying, extraction, etc.) is easier for berries than leaves, the expensive hand picking or

On March 9 1979, the Prime Minister, Mr R. D. Muldoon, officially opened Solanum Extraction Industries Ltd. in Waitara. The company is jointly owned by Fletcher Holdings Ltd. and Diosynth BV a subsidiary of AKZOPHARMA, the pharmaceutical division of AKZO NV and was formed to grow and process the NZ native weed poro poro into solasodine, a precursor for steroid hormone-synthesis.

Poro poro or bulli-bulli as it was called by the early settlers, belongs to the nightshade family of which the potato and tomato are more well known species.

In his opening speech Mr Muldoon said: "In many respects the Waitara factory is a model industry, bringing with it capital, technology, a market which we would not have without the Netherlands partner and a promising contribution to regional development. It may pave the way for other resource-based partnership projects, utilising NZ plant and other raw materials."

complicated mechanical harvesting of the berries has ensured that most studies have concentrated on leaf harvesting. In NZ, DSIR scientists (Smith, Mann, Davies etc.) and the IWD development group (Mason, Fawcner) have selected two native species; *Solanum aviculare* and *Solanum laciniatum* for further evaluation.

Based on this agricultural know-how, a new company, Solanum Extraction Industries Ltd, was formed by Diosynth Netherlands BV, and Fletcher Holdings Ltd. Diosynth is a subsidiary of the pharmaceutical division of AKZO and is basically a bulk-pharmaceutical supplier of alkaloids, biochemicals and steroid-hormones. The NZ partner, Fletcher Holdings Ltd, has experience in industrial agriculture via its linseed, rapeseed and lucerne activities.

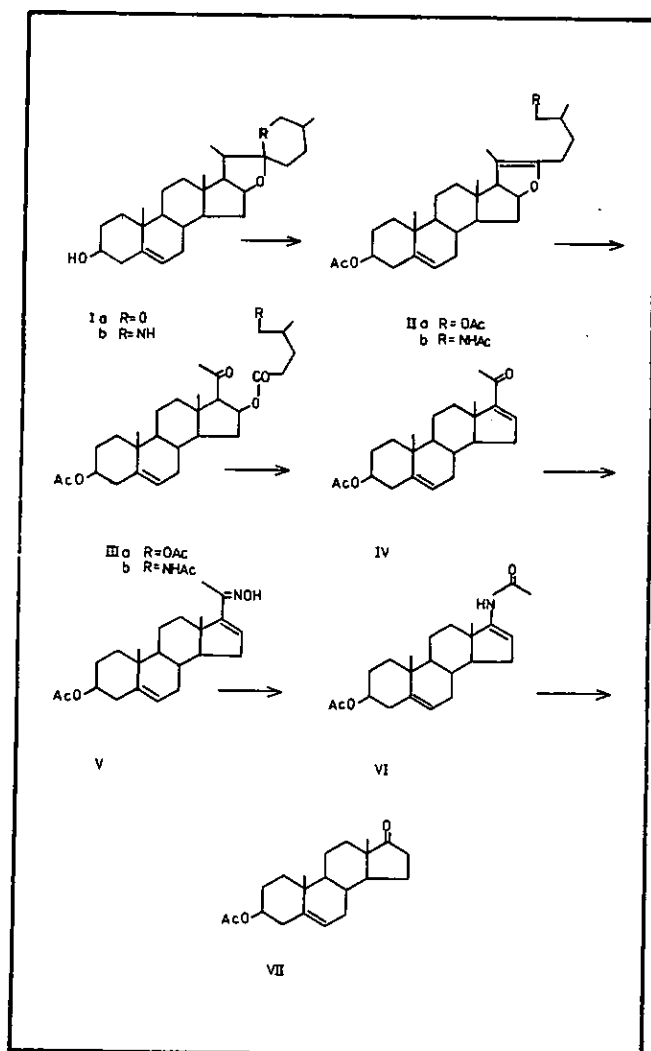


Fig. II. Sidechain degradation of solasodine and diosgenin

- | | |
|--|---|
| Ia diosgenin | IIa pseudoisomerization product |
| Ib solasodine | IIb pseudoisomerization product |
| IIIa oxidation product | IV 16-dehydropregnenolone acetate (DPA) |
| IIIb oxidation product | |
| V 16-D oxime | VI rearrangement product |
| VII dehydroisoandrosterone acetate (DHA) | |

Chemistry in New Zealand

Jan Kloosterman was born in the Netherlands in 1930 and completed his studies in chemical engineering in 1955. He has previously worked in the oil and fatty acid industry and was employed by Organon NV, which later became the pharmaceutical division of AKZO. Mr. Kloosterman spent the first 10 years in production management of various steroid manufacturing departments, finally as the manager of a pilot plant responsible for steroid and biochemical process development and raw materials supply.



He was appointed project manager of the NZ solasodine project in 1976 and managing director of Solanum Extraction Industries Ltd. in 1978. He moved with his family to NZ in 1978, where a son and a daughter attend Massey University, while his eldest son completes law studies in Holland.

Both major activities, agriculture and the first processing steps, were evaluated in 1977. For this purpose 20 ha were planted and a pilot plant was built to obtain the necessary processing data. At the end of 1977 the "go" decision was taken and in November 1978 commissioning started. Meantime, the agricultural operation was expanded to provide raw material for the new plant. As the crop was completely new it was impossible to go for contract-growing so the company leases the land from farmers and performs all the agricultural activities — growing transplants, planting, cultivation, crop maintenance and harvesting itself. As soon as enough data are collected to provide farmers with a growing-instruction manual, complete or partial contract growing will be offered. Considering the high capital costs involved in harvesters, plant and spraying equipment, the partial deal will be the most obvious one but it is not expected in a significant form before 1981.

The processing of the raw material into solasodine (Fig. II, 1b) and subsequently to DPA (16-dehydropregnenolone acetate, IV), one of the most important intermediates for steroid hormones, is a multistep degradation of the glycoalkaloids present in the plant and is shown schematically in Fig. II. Further transformation leads to DHA (VII), an intermediate for androgen and estrogen synthesis. In Fig. II the processing scheme for both solasodine (1b) and diosgenin (1a) into DHA (VII) is given to illustrate the similarity of both sets of intermediates until the DPA stage. After that there is no difference between the two processes, which produce products of 90-100% purity from which all the major classes of steroid products can be produced (androgens, anabolics, diuretics, progestins, estrogens, corticoids, and the oral contraceptives).

It can be seen readily that long multi-step syntheses are required to modify DPA (VII) into end products and pathways of 20 steps are not uncommon. The purity of final products is required to be greater than 99%, necessitating the use of complicated purification methods like counter-current extraction and molecular distillation. In the beginning, end products were sold on the basis of biological activity, but now the various pharmacopoeia contain very specific release specifications based on chemical and physical analysis.

NZIC ANNUAL REPORT 1978-79

ELECTED OFFICERS

President:	Dr W. E. Harvey
First Vice President:	Prof. A. D. Campbell
Second Vice President:	Dr A. J. Ellis
Secretary	J. G. Fletcher

BRANCH DELEGATES TO COUNCIL

Auckland:	Dr L. Eyres
Waikato:	Dr E. Payne
Manawatu:	Dr A. Brodie
Wellington:	Dr B. Halton
Canterbury:	Dr. R. F. C. Claridge
Otago:	Dr P. K. Grant

OFFICERS APPOINTED BY COUNCIL

(These appointments continue until the date shown, but are renewable. Appointments are made at the November meeting of Council).

Registrar:	Mr D. J. Hogan	(31.12.81)
Administrative Secretary:	Mrs N. E. Wignall	(31.12.79)
Journal Editor:	Mr S. G. Brooker	(31.12.80)
Hon. Librarian:	Mr S. G. Brooker	(31.12.79)

COMMITTEES APPOINTED BY COUNCIL

Membership Committee:	Mr J. S. Pollaard Prof. A. D. Campbell Dr J. Rogers	(31.12.79) (31.12.80) (31.12.81)
Publications Committee:	Dr R. F. Claridge Dr L. Eyres Mr S. Gray	(31.12.79) (31.12.80) (31.12.81)
Energy and Chemical Materials Resources Committee:	Prof. A. G. Williamson Dr G. J. Wright Dr A. Metcalfe	(31.12.79) (31.12.80) (31.12.81)
Hazardous Chemicals Committee:	A. C. Kennett R. H. Hopgood D. J. Olgivie One corresponding member from each branch	

REPRESENTATIVES ON OTHER BODIES

Technician Certification Authority Committee for Science:	Dr W. E. Harvey	(31.3.81)
Standards Assn. of N.Z.:	Mr J. A. Gilmour (resigned) Mr J. G. Fletcher	(31.3.80) (31.3.80)
UNESCO in NZ:	Dr G. R. Burns	(31.12.79)
Royal Society Member Bodies Ctte:	Dr I. D. Watson	(31.12.81)

MEMBERSHIP

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

Members elected to Fellowships:	34
New Members:	23
Reinstated:	2
Graduate Members elected to membership	17
New Associate Members:	8
New Graduate Members:	28
New Technician Members	6
Resignations	23
Deaths	9
Deleted	28

Consolidated membership figures for the last four years are as follows:

	1976	1977	1978	1979
Auckland	343	339	367	345
Waikato	97	94	110	114
Manawatu	128	124	123	126
Wellington	310	306	313	309
Canterbury	180	174	176	183
Otago	104	105	109	110
Overseas	140	138	150	168
	1302	1280	1348	1355

Council has expressed concern at the static nature of the membership growth of the Institute and membership opportunities must be brought to the attention of more potential members.

Obituary:

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

V. I. Beros, Mrs P. Broad, G. Chamberlain, A. C. Holmes, B. O. Jones, H. L. Longbottom, Mrs M. Lonska, G. M. Moir, Prof. S. N. Slater.

Specialist Groups:

GROUP	SECRETARY	MEMBERS	NON MEMBERS	TOTAL
Analytical:	D. J. Hogan	35	5	40
Biochemistry:	Dr M. Smith	.		
Chemical Education:	D. T. Howarth	383	244	627
Chemical Engineers:	Dr E. R. Palmer	.		
Chromatography:	Dr J. Zabkiewicz	181	72	253
Electrochemistry:	Dr A. J. Eastal	69	28	97
Geochemistry:	Dr J.B. Finlayson	147	111	258
Organic Chemistry:	Dr K. E. Richards	93		
Polymer Chemistry:	N. C. Cochrane	77	19	96
Thermodynamics:	Dr D. V. Fenby	.		
X-ray Crystallography:	Dr W.T. Robinson	26		
Trace Elements and Health:	Dr T. E. Kjellstrom	.		
Industrial Consultants:	J. R. Yolland	.		

* Total not available

PRIZES

Prize winners in 1978 were as follows:
Easterfield Medal for 1978:

Dr R. E. Mitchell

ICI Prize: Dr R. P. Garland

Chemical Essay Prize: C. J. Nokes

There were no student papers for 1978.

CONFERENCES

The annual conference for 1978 was held at Canterbury University in Christchurch, August. This conference was styled a "uni-conference" but still attracted many members and guests. These attending agreed that it was most successful.

The 49th ANZAAS Congress was held in Auckland January 22-26, 1979, during which Sections 2, 17, 18, A37 (Chemistry, Biochemistry, Food Science, and Trace Metal Research) held meetings. Approximately 180 members attended the Congress which attracted over 4,000 delegates and gave members the opportunity of part-taking in symposia and other sectional activities.

The Chairman of the Energy and Materials Resources Committee, Prof. A. Williamson, was financially assisted to attend two overseas conferences related to Energy Savings.

His report was published in *Chemistry in New Zealand* 43 (3) 1979.

The President represented the Institute at the ACS/CSJ joint meeting in Honolulu April 6, 1979.

OVERSEAS VISITORS

Mr Bob Schoenfeld, Editor, RACI Journal visited branches during 1979.

Dr Magnus Pike and Prof. D. Bryce-Smith were invited speakers to the 49th ANZAAS Congress and spoke to some branch meetings afterwards.

Dr E. Parker, Secretary, Royal Institute of Chemistry, visited NZ in November 1978 when he visited most branches and attended the November Council Meeting.

PUBLICATIONS

During the year the Institute entered into an agreement with Trade and Industrial Communications Ltd giving that company publishing rights to the Journal for two years from January 1, 1979.

This ended the long period during which members have voluntarily produced the Journal. Dr L. Creamer, the retiring editor, had maintained a high editorial standard. The Institute is greatly indebted to Dr Creamer and the retiring advertising manager, Mr T. R. Johnson, for their efforts during 1977 and 1978.

Due to financial difficulties Trade and Industrial Communications Ltd ceased its publishing operations on June 30. The Institute through its Publications Committee reached **Chemistry in New Zealand**

agreement with Mr J. A. Breckell who had offered to take over publishing responsibility. Mr P. Reaves is to continue as Managing Editor. A new agreement has been negotiated.

During the year a pamphlet describing the Institute was published and consideration was given to reprinting "Careers in Chemistry". A Journal Editorial Committee was established consisting of Mr S. G. Brooker, Drs A. Herd, W. Denny, T. Brittain.

HAZARDOUS CHEMICALS

The long established Auckland Branch Hazardous Chemicals Committee was recognised as the Institute's Committee and expanded to include corresponding members from other Branches.

Several Bills were considered and commented on by the Committee. Mr A. C. Kennett represented the Institute on S.A.N.Z. Committees studying draft standards for labelling and containerisation of Hazardous Materials.

PUBLIC AFFAIRS

During 1977 a working party chaired by Dr M. Kingsford reported. A special general meeting held during the 49th ANZAAS Congress considered the report and urged Council to be more active in public affairs. The Institute has joined the organisation "Common Concern" - which reviews Parliamentary activities. This link with the legislature has proved very useful.

INDUSTRIAL CHEMISTRY GROUP

As a result of a remit at the 1978 Annual General Meeting Council established an Industrial Chemistry Group. The Chairman, Mr J. Yolland, and Committee held two meetings and one plant visit during the year.

N.Z. BIOCHEMICAL SOCIETY

Council has expressed concern that the Institute must do more for the interests of members who are also members of the N.Z. Biochemical Society. A bio-chemist (Dr T. Brittain) has been appointed to the Journal Editorial Committee.

FINANCE

The Annual Statement of Income and Expenditure shows that the Institute again had an excess of income over expenditure. Council has exercised considerable restraint on expenditure and although no projects were delayed it is expected that the forthcoming Golden Jubilee Celebrations will require a considerable injection of funds. Unless there is an increase in membership it is expected that another subscription increase will be inevitable.

Branches accepted a Council

recommendation for the introduction of an centralized subscription collecting service to be operated by the Administrative Secretary. Early indications are that its introduction in May 1979 has been widely accepted and has been very useful in updating the official mailing list of the Institute.

CHEMICAL EDUCATION GROUP

This Group continues to produce a very useful publication — Chem NZ.

ENERGY AND MATERIALS RESOURCES

During the year a submission was prepared by the Energy and Materials Resources Committee for the Institute on the Government's publication "Goals and Guidelines". The submission was forwarded to the Minister of Energy. It is gratifying to note that several points made were accepted by the Ministry.

1981 GOLDEN JUBILEE

Arrangements have been initiated on various projects to celebrate the Golden Jubilee of the Institute in 1981. The Second Vice President, Dr A. J. Ellis, has agreed to be co-ordinator and Mr A. Mackney has established a 1981 Conference Committee in Auckland.

SALARY SURVEY

Dr G. Gainsford conducted a salary survey of members during the year. The number of respondents was 57.3% and the results were published in the November 1978 issue of the Journal.

The next salary survey will be held on 1st April, 1980.

ARCHIVES CENTRE

Council established an Archives Centre in Christchurch. A Committee chaired by Dr R. F. C. Claridge assisted by the Administrative Secretary has been collecting and collating records of the Institute into one catalogued file.

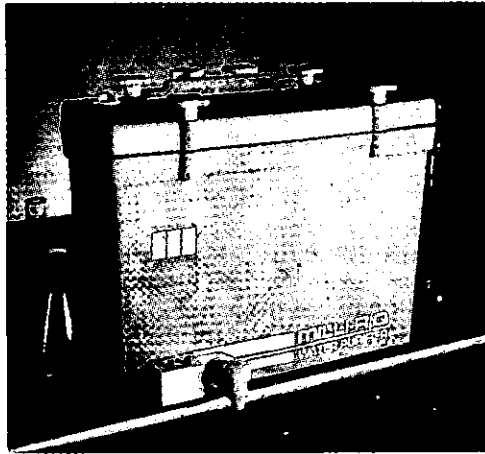
ACKNOWLEDGEMENTS

The activities of the Institute continue to be dependent upon the voluntary service of its members — especially in Branches. Without their enthusiasm and sacrifice the professional and other activities would not be serviced.

Special acknowledgement is made of the efforts of the Journal Editor, Mr S. G. Brooker who has taken this task on with typical enthusiasm far beyond the call of duty. The Institute is greatly indebted to his sacrifice, hard work and interest.

(Note. The annual accounts and balance sheet will be available at Conference.)

SMALL STILLS JUST BECAME OBSOLETE.



The Milli-R/Q™ Water Purifier.

Consistently Better water.

The Milli-R/Q Water Purifier from Millipore will give you purer water than even double distillation. For a lot less than the cost of a single-stage still.

But better water and lower cost aren't the only reasons the Milli-R/Q Water Purifier will make small stills obsolete. For example, compare the maintenance requirements. A still needs weekly acid cleaning. Without it water quality deteriorates due to the increased carry-over of entrained boiler deposits. But with a Milli-R/Q you simply replace cartridges a few times a year (typically, every 3-4 months).

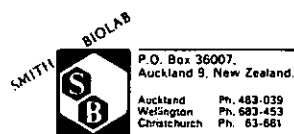
**The Milli-R/Q Water Purifier.
Better quality water than
even double-distilled.**

Smaller and more Economical

It takes up so little space, you can put it practically anywhere, on a shelf or counter top. And all installation consists of is connecting it to your faucet. The Milli-R/Q runs on tap pressure.

A comparably equipped still takes up to 3 times as much space and is almost double the price. Distillation also costs 2 to 3 times as much to operate. And it's extremely wasteful of heat energy and cooling water.

The Milli-R/Q Water Purifier.
The system that makes small stills obsolete.



WITH RESIDENT REPRESENTATIVES IN HAMILTON, PALMERSTON NORTH AND DUNEDIN.

15040D

A Minicomputer-Based Mass-Spectrometry Data System

P. T. Holland

Ruakura Soil and Plant Research Station, M.A.F., Hamilton

A mass-spectrometer being used for organic compound analysis produces a formidable amount of information. A typical mass-spectrum contains several hundred peaks with relative intensities ranging from 1000 to 1 and many spectra may need to be taken at intervals of only a few seconds, for example, in coupled gas chromatography (GC/MS). Using the traditional oscillographic recorder, the analyst quickly becomes overwhelmed by charts of the raw analog output which are uncalibrated in the mass or intensity scales. Before interpretation can proceed, tedious manual mass counting and peak height measurements must be made and comparison of spectra with those of standards is difficult. As background peaks in the spectra may occur at many masses it is not possible to correct spectra by analog means.

High resolution spectra, where the masses are determined accurate to 3 decimal places to allow assignments of elemental composition are another important area of mass-spectrometry. Many tedious measurements are involved and it is impractical to manually obtain accurate masses for more than a few peaks in a spectrum. Our work at Ruakura on pesticides, mycotoxins, plant lipids, amino acids and steroid hormones using these techniques was being seriously hampered by the problems in manual spectral interpretation and it was apparent that a data systems was required. Minicomputer based commercial systems are available with extensive program packages but their cost is very high. As several approaches have been documented in some details (1,2) and we had some knowledge of the algorithms involved, it was decided to develop our own system.

The configuration of the magnetic sector mass-spectrometer (Varian-MAT CH5) and data system is outlined in Fig. 1. Samples are introduced to the ion source using a direct insertion probe or via the gas chromatograph. The latter is especially suitable for complex mixtures as spectra can be obtained for each of the separated components as they emerge from the chromatograph. The primary function of the data system is to acquire spectra for storage and processing by digitising the output of the electron multiplier amplifier as the spectrometer is scanned. Typical mass-spectral peaks are about 1 msec wide and as 10-20 samples are required to adequately represent a peak (3,4), a digitisation rate of 50 μ sec/sample i.e. 20kHz is needed. As the computer memory would quickly become filled at this rate incoming samples must be discarded unless they are greater than some preset threshold level. As most microcomputers are not sufficiently fast to meet these requirements a Data General NOVA 3 16 bit minicomputer with 32K words of memory was chosen. Dual magnetic diskette drives provide an economical solution to the problems of program and data storage (160 K words per diskette). The well

Chemistry in New Zealand

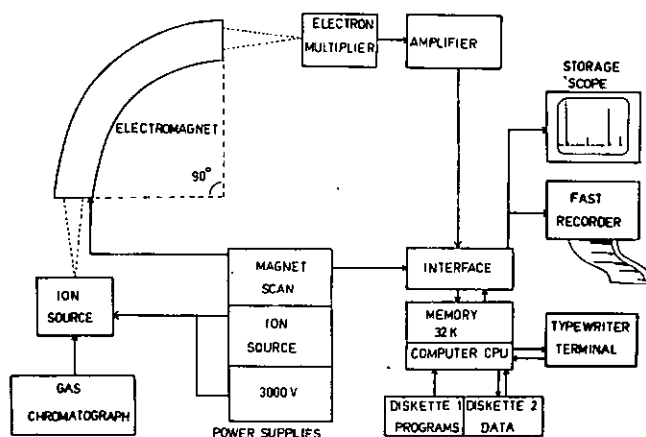


Fig. 1. Schematic of GC/MS data system

developed operating system greatly speeded program development by providing sophisticated file handling and supporting the programming tools of editors, assembler, FORTRAN compiler and relocatable loader. A 30 characters/second typewriter terminal is used for program entry and communication.

The interface between spectrometer and computer is a key element and rather than purchase a standard unit the design outlined in Fig. 2. was implemented at Ruakura to provide some additional useful features. A differential instrumentation amplifier provides good isolation of common mode noise from the spectrometer. The measurement of the weak ion currents is improved by using integration of the signal over the clock period (usually 50 μ sec) rather than the more usual sample-and-hold (0.1 μ sec aperture time). The integrator output is digitised by a 12 bit analog-digital converter (A/D) with a 8 μ sec conversion time. While one integrator is measuring the signal the other is read by the A/D and then reset. Mass-spectrometer peaks have a wide intensity range so the dynamic range of the interface is extended from 4095:1 (12 bits) to 32767:1 (15 bits) by autorange changing. The data from the A/D is sent to the computer memory in blocks using direct memory access which allows the central processing unit to process the data in parallel with acquisition.

The interface is driven by an assembler subroutine which forms part of a versatile FORTRAN based mass-spectrometry program. Programs are kept on one diskette together with the operating system. The other

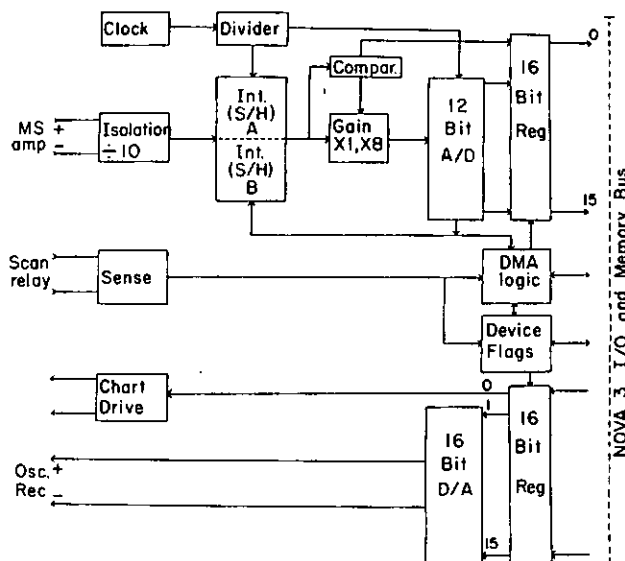


Fig. 2. GC/MS computer interface

Data System (Cont)

diskette is reserved for mass spectral data files, each diskette containing up to 560 spectra. The main program operates between parameter setting, command setting and command execution modes. In the parameter mode sample labels are accepted, disk files organised and a list of default values set for the various parameters controlling data acquisition, processing, storage and display. The operator can then initiate changes to any of the parameter by typing 2 letter cues. This selective parameters setting minimizes unnecessary dialogue with the computer, a fault of many interactive programs. When the parameters are set the operator shifts the program to the command mode where further 2 letter cues determine the operation(s) to be carried out on spectral data which have been placed in memory either from the A/D interface or from a diskette data file. The commands are implemented as subroutines or overlays with those requiring the fastest execution being written in assembly language. The command list is terminated with one of three codes which determines the number of scans to be processed and then the chosen subroutines are executed sequentially the required number of times.

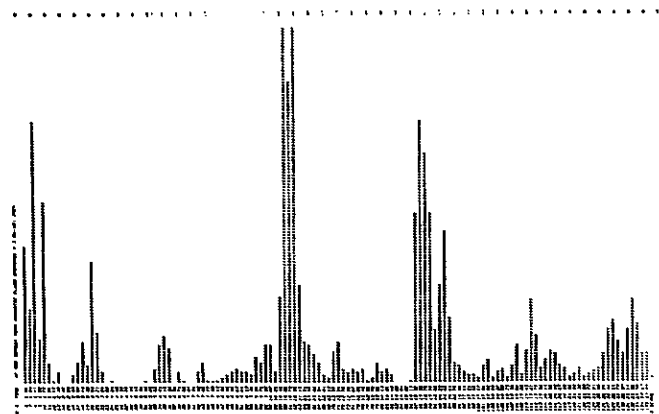


Fig. 3. Reconstructed GC of urinary steroid run

The data acquisition subroutine puts A/D samples into two 2048 word blocks in memory. While the interface is filling one block the program is rejecting samples in the other block that are below threshold and determining the area and time for each detected peak. Time is the number of samples to the peak centre from the spectrometer scan start. The output of this subroutine is thus a spectrum in memory with each peak represented by an intensity/time pair of words. The times are converted to masses by a mass conversion subroutine using a time vs mass calibration built up from the spectrum of a perfluoroalkane standard. Where masses are only required to unit mass accuracy (low resolution) this calibration is run prior to taking sample spectra. The spectrometer scan stability is such that the calibration will hold to ± 0.2 amu for several hours. Masses sufficiently accurate for elemental composition assignment (high resolution) are obtained using perfluoroalkane run with the sample and internal calibration of each scan. A minimum spectrometer resolution of about 3000 is required to separate sample peaks from those of the standard.

Spectra can be stored and retrieved from diskette in time/intensity or mass/intensity format. The mass spectra can be output in a variety of formats for use by the

operator or chemist. Subroutines implemented at present include spectrum typeout on the terminal, an 8 largest peaks spectrum summary on the terminal, bar graph plot of the spectrum on a fast recorder and a display of the spectrum on storage oscilloscope. The latter two subroutines use the digital-to-analog converter (D/A) in the interface (Figs. 1 and 2) to drive the oscillographic recorder galvanometer and the oscilloscope vertical deflection. The further functions of background subtraction, total ionisation plot and elemental composition assignment (high resolution spectra) are also available as subroutines to be called when required. The following examples illustrate the programmable nature of the system and some of the outputs provided.

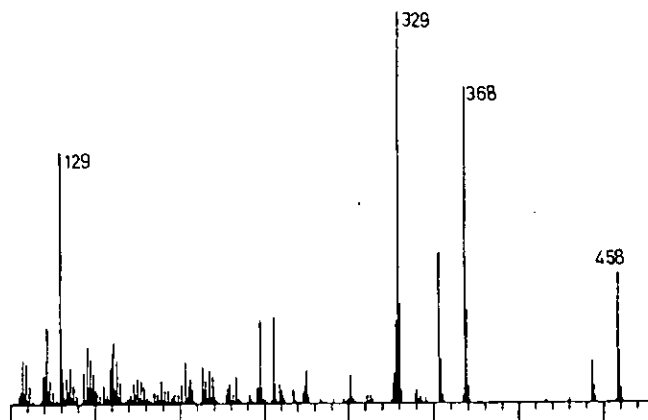


Fig. 4. Mass spectrum of cholesterol-TME ether (scan 88, Fig. 3)

To invoke the system to acquire 140 scans from the spectrometer, for example during a GC/MS run the following sequence of 2 letter cues would be entered at the terminal (* is the system prompt); *CG *MA *ST *SC *140. This causes the subroutines of data acquisition, mass conversion and spectrum storage to be carried out sequentially 140 times leaving the mass-spectra on diskette. Fig. 3 is reconstruction of the gas chromatogram for a GC/MS run of urinary steroids generated on the terminal by the command sequence RS * TI * SC * 140. This reads each scan from diskette and plots the sum of all peak intensities (total ionisation) as a histogram. From this plot the regions where components are eluting can be identified, for example scans 87-91. The command sequence RS * BK * PL * SL * 85 * 88 * 0 retrieves spectrum number 88 and subtracts spectrum number 85 from it (essentially spectrometer background and column bleed) and plots the "cleaned-up" spectrum on the recorder. Fig. 4. reproduces that spectrum and shows the component to be the TMS ether of cholesterol (mw 458, base peak 329).

High resolution spectra are generally obtained from direct probe introduction of relatively pure samples. A typical for spectra acquisition in such a mode is; CG * ST * SC * 6. If spectrum number 3 of the 6 scans taken was judged satisfactory then the command list RS * CA * MA * DE * CO * SL * 3 * 0 would read the stored spectrum, calibrate the mass scale, convert to masses, delete peaks from the perfluoroalkane standard and calculate elemental compositions to fit the measured-masses. Fig. 5 gives the output from subroutine CO for the high mass region of the high resolution spectrum of a toxic compound isolated from cultures of a fungal pathogen. The tolerance for fitting the observed masses was ± 4 millimass units. The molecular formula is apparently $C_{31}H_{40}O_8$ (m/e 508) and fragmentations leading

EPM004 FUNTRENORGEN A OR B 38/11/77									
SCAN#	S	TOL.	4MMU	LIMITS:	32/42/	1/	6		
MASS	INT	REL. INT	ERR	C/C13	H	N	O		
430.2566	316	63.07	-3.2	32/0	32	1	0		
			1.5	31/1	31	1	0		
			-0.5	29/0	34	0	3		
431.2560	189	21.76	-1.0	31/1	32	1	0		
			-3.0	29/0	35	0	3		
			1.7	28/1	34	0	3		
439.2155	501	100.00	0.5	29/0	29	1	3		
			3.2	26/0	31	0	6	m - C ₅ H ₉	
440.2201	151	30.14	-2.7	29/0	30	1	3		
			1.7	28/1	29	1	3		
			-0.0	26/0	32	0	6		
448.2689	122	24.35	-3.5	32/1	35	0	1		
			-1.3	25/0	38	1	6		
			3.4	24/1	37	1	6		
475.2457	63	12.57	-1.2	32/1	32	1	2		
			-3.0	30/0	35	0	5		
			1.7	28/1	34	0	5		
498.2738	129	25.75	1.4	29/1	34	0	5	m - H ₂ O	
499.2501	72	14.37	1.4	32/0	35	0	5		
588.2799	281	56.09	-2.8	31/0	40	0	6	molecular ion	
			1.6	30/1	39	0	6		
589.2802	92	18.36	2.1	30/0	39	1	6		

INPUT PROGRAM LIST

Fig. 5. Elemental composition printout for high resolution spectrum of a fungal metabolite

to loss of H₂O and C₄H₉ are observed. These high resolution spectra are invaluable for the identification of complete unknowns as the molecular formula can be determined on microgram quantities of material. Interpretation of the spectrum is greatly facilitated by also having the formulae for fragment ions.

Results using this system have shown that the single focussing mass-spectrometer operated at 5000 resolution, 30 sec/decade scan rate can produce masses accurate to better than 5ppm. Elemental composition assignments have proved extremely useful in the structural elucidation of some metabolites of the Facial Eczema toxin Sporidesmin (5). The ability to store and retrieve spectra in a standard format has greatly facilitated comparison of spectra to check whether a metabolite is the same as one previously isolated. The system has also proved invaluable in identification of steroid hormone metabolites in urine and the cuticular lipids and resin acids of *Pinus Radiata* needles (6). In these applications the extremely complex patterns of compounds present were separated and characterised by GC/MS with the data system acquiring and storing all data for later review.

The programmable nature and selective parameter setting of this system allows fast, flexible processing of high and low resolution data. The implementation of the interface and program package took 6 months and was greatly assisted by the diskette based operating system supporting programming tools of a high standard of reliability and sophistication. Future developments will include selected ion monitoring GC/MS where computer switching of the spectrometer accelerating voltage (7) allow several specific mass peaks to be monitored for determination of residues such as dioxins at picogram

Patrick Holland graduated B Sc (Hons) in Chemistry from Canterbury University in 1967 and gained his Ph D in Radiation Chemistry from Queens University, Kingston, Ontario, in 1970. He gained an interest in mass spectrometry from using a simple gas analysis device during his doctorate research. He furthered this by 2 years with Dr A. Burlingame, University of California, Berkeley, studying fundamentals of high resolution mass spectrometry and applications to lunar sample analysis. He returned to NZ in 1972 and set up the Ruakura GC/MS facility with analytical applications to pesticides, mycotoxins and general organic microanalysis.

levels (8). Another possible enhancement is library searching where computer matching of spectra with files of standard spectra leads to rapid and objective identification of unknowns without the need for detailed spectrum interpretation (9). The relative slowness and limited capacity of diskettes makes large libraries impractical and precludes long, fast scan GC/MS runs using capillary GC. The problems could be overcome with a larger but considerably more expensive disc drive.

Acknowledgements

The purchase of the minicomputer was made possible by a grant from the Golden Kiwi Lottery Scientific Grants Committee.

R. Rieg carried out much of the interface design and implementation. Mrs. A. France and Dr. E. P. White provided samples for the examples given.

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STANLEY NELSON SLATER, 1915-1979

Emeritus Prof Stanley Slater was born in Ngaruawahia and received his secondary education at Wanganui Technical College. After completing his M Sc degree at the University of Otago he went to Oxford on a postgraduate scholarship in science. He completed his D.Phil. working with one of the great figures in English organic chemistry, the late Sir Robert Robinson, before returning to Dunedin to take up an appointment as assistant lecturer in the Chemistry Department. He moved to Victoria University College in 1950 to take up the Chair of Chemistry, which became vacant on the retirement of

the late Prof P. W. Robertson, and spent the rest of his working life at Victoria University, becoming over the years more deeply involved with top administration until at the time of his retirement in 1975 he occupied the office of Assistant Vice-Chancellor.

Slater's own research interest lay principally in the field of natural products chemistry (perhaps a reflection of his days at Oxford) and in particular much of his published work was concerned with structural studies on amaroids, the non-nitrogenous "bitter principles" typified by the well known (and commercially available) picrotoxin.

Stanley Slater had many fine personal qualities. He was an outstan-

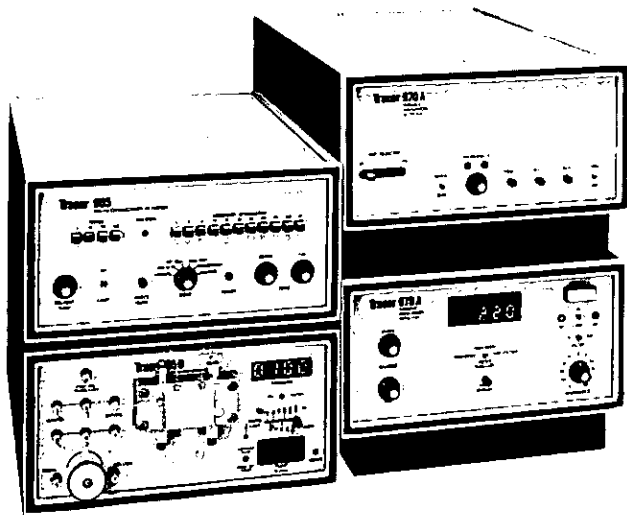
ding lecturer and his meticulous approach to all matters whether theoretical or practical was never better exemplified than in the care which he devoted to practical work in the laboratory, to the construction of hi-fi equipment and, in latter years, to the building of catamarans of successively increasing dimensions.

He was a vigorous supporter of the Institute concerned both with its "learned society" and "professional body" activities at both local and national level and was made an Honorary Fellow in 1975. In 1945 he married Jenny (nee Miller) who survives him as do their three daughters: their only son was killed in an accident late in 1978.

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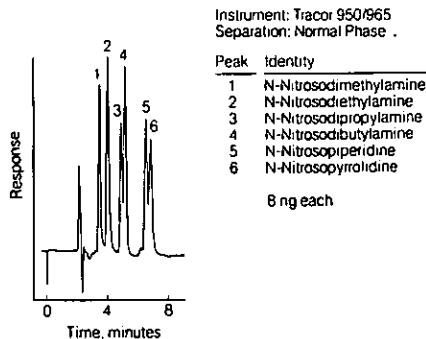


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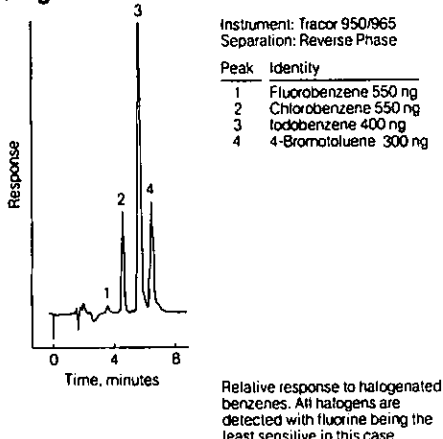


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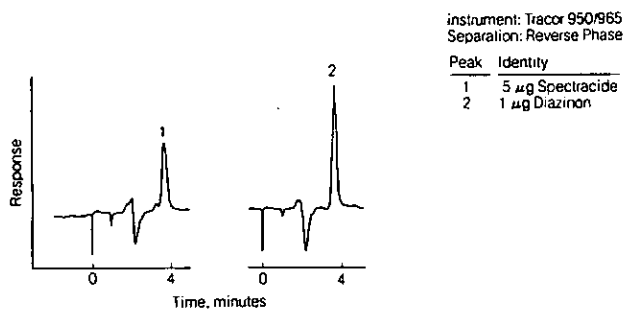
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DSIR's Chemistry Division complex, Gracefield, Lower Hutt

CHEMISTRY IN WELLINGTON

Stan Brooker reviews the current scene

"100 Years of Chemical Research" was published by the DSIR as Information Series No 46, copies of which are available on request. There are branch laboratories at Auckland and Christchurch, which have their own fields of work, complementing the activities at Gracefield.

While in the past the work of the Chemistry Division and its predecessor, the Dominion Laboratory, was mainly regulatory, there is now a much greater amount of true research undertaken. Staff members presented 5 papers at ANZAAS in Auckland on subjects ranging from a new polymorph of silica to organic sulphur compounds from the anal gland of the stoat. Cadmium stannates developed as part of a programme on new oxide materials from petrochemical conversion of solar energy were the subject of another paper. A typical example of the current emphasis on research is shown in the food section, where work done at one time was almost wholly regulatory at the behest of the Health Department; this part of the work is now handled by 2 technicians, while 4 of the staff are engaged in research on pesticides in foods and new crops and 4 more on nutritive values in food, this work at present being concentrated on fish and on wheat and its products. One result has been to show that "high fibre" bread has no advantage nutritionally over wholemeal. Work on pesticides is aimed at ensuring protection of the environment and the quality of food, while still meeting the needs of increasing agricultural production. The food section is also looking at Chemistry in New Zealand

Any review of chemistry in Wellington must start with Chemistry Division, which employs more chemists than any other establishment in NZ and has also a great investment in apparatus and ancillary services. Despite the transfer of staff of the Industrial Processing Division, there are about 120 qualified chemists, some 55 technical and 50 supporting staff. Besides the IPD, the Institute of Nuclear Sciences, and the Physics and Engineering Divisions of DSIR are close by, while the Coal Research Association and the Pottery and Ceramics Research Association also employ a number of chemists who benefit from their proximity to Chemistry Division.

The visitor to the Gracefield campus is first impressed by the fact that the Division is in a number of smallish single storey buildings which, while they take up a large surface area, have several advantages. The risk of fire spreading from one section to another is greatly reduced; evacuation in an emergency presents no problems; structural changes are easily made and hazardous materials such as gases under pressure can be placed outside and serviced easily through the walls. For these reasons, a major building reconstruction programme involving a multi-storey edifice is not universally welcomed by the staff.

The Chemistry Division is proud to trace its ancestry back to the Colonial Museum and Laboratory established in 1865 with **Dr (later Sir) James Hector** as Director and **William Skey** as Analytical Chemist. The Division thus celebrated its centenary in 1965, when the booklet,

fatty acid composition, minerals and vitamins in processed baby foods.

Another area of work is the development of methods of analysis especially suited to the research programmes; particularly their automation. A good example of this is in the blood alcohol set-up in the toxicology section. Forensic work involving drugs is important and this section was involved in nearly 1000 cases in 1978; while most cases required investigation for cannabis, there has been a significant growth in the work on heroin and LSD. Samples of heroin can be characterised by the degree of acetylation of the morphine used as a base and by the amount and type of the diluent used. From the analyses for these factors it can be found whether batches of undiluted heroin are from the same source and whether dilution has been carried out by one or more operators in NZ. For this purpose Chemistry Division is using its latest acquisition, automated HPLC, which can handle 100 analyses in a 24-hr period.

In analytical work there has been a great advance with a wide variety of spectral techniques. Atomic absorption spectroscopy enables a large number of samples to be handled, e.g. for testing mercury levels in fish. Because of the laboratory's access to viscera from unexplained deaths, accidents and suicides examined for the Coroner, the levels for trace metals in normal individuals can be established and here the Division is in a rather unique position. Development of the newer automated techniques has enabled a diet survey to be undertaken in conjunction with the Health Department and the Nutrition section of Otago University. In fact spectroscopic techniques cover such a wide range, such as optical emission, nuclear magnetic resonance and Mossbauer spectroscopy, that a whole section with

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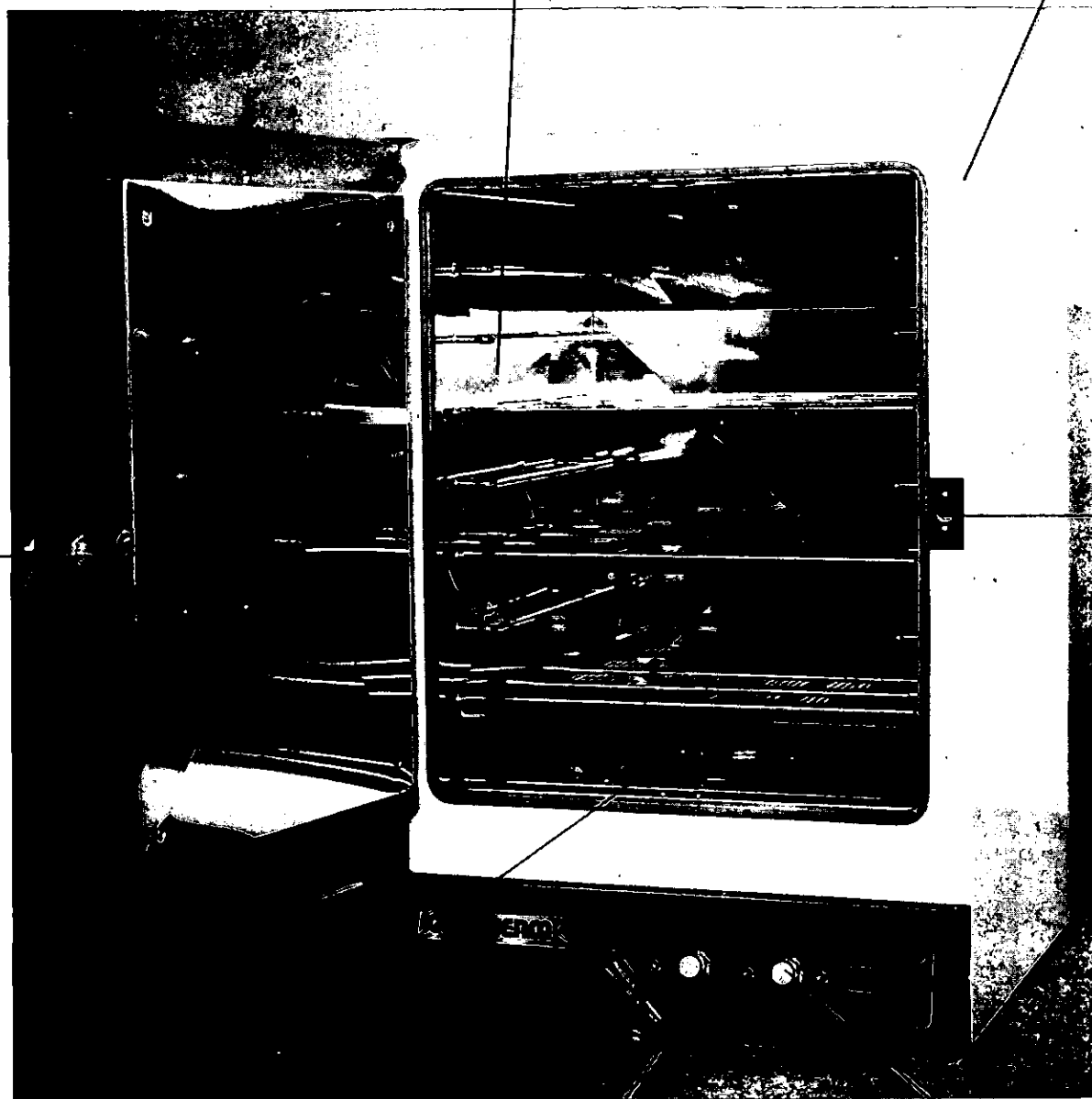
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Chemistry in Wellington (Cont)

a staff of 11 has been set up to deal with them. The methods have been applied to such areas of applied chemistry as the determination of detergents and wool grease in scour liquors; characterisation of coloured effluents from paper mill bleach plants, and the physical and chemical properties of NZ coals.

Some examples taken at random from the Division's 1979 Handbook, now in the press, indicate the diversity of the work. The applied chemistry section tests a variety of materials for the Government Stores Board and other departments, with a recent emphasis on detergents and their biodegradability. This section is also looking at graffiti-resistant coatings, and at coconut oil soap produced in Tonga under a foreign aid project. The geochemistry section handles a wide range of inorganic analyses, as well as dealing with environmental pollution, both from industrial and natural geothermal discharges. Arsenic, sulphur, lead, cadmium, beryllium, thallium and uranium pollution have all been studied. The head of the geothermal section, **Mr W. A. J. Mahon**, and the Director, **Dr A. J. Ellis** have written a book, "Chemistry and Geothermal Systems" (400 pages, Academic Press, 1977) showing the special place of NZ in this work; personnel from the section have also been seconded to UN and other projects in Argentina, Chile, Djibouti, El Salvador, Ethiopia, Fiji, India, Indonesia, Kenya, Mexico, Nicaragua, Panama, Peru, Philippines, Solomon Islands, Taiwan, Thailand and Turkey. It is divided into two groups, one in Wellington, and one at Wairakei, where a new building is being constructed.

The information section is the first point of contact for general enquiries and collects material from the literature on subjects not covered by other sections. It works closely with the library on information retrieval systems. Recently it has prepared in-depth reports on the history of motor vehicle gas producers and products from the *Rhodophyceae* seaweeds. It has a general interest in the utilization of waste materials, and has developed a system for recycling thermoplastics.

The natural products section has been studying plant flavonoid glycosides as part of plant tax-

onomic studies in conjunction with Botany Division, Crop Research and Massey University. It has been looking at the separation of lignin from carbohydrate in wood to produce materials suitable for ruminant digestion and for liquid fuel production. In conjunction with the Entomology Division, a number of naturally occurring moth attractants, such as *cis* and *trans* isomers of a variety of C_{12} alkenes have been used in a project to control kiwifruit leaf roller moths. Another activity has been the development of HPLC techniques for the analyses of sugars and mycotoxins in foodstuffs.

The organic chemistry section aims to provide a pool of information and instrumental techniques in this branch of chemistry. Particular studies are directed to polyphenolic polymers in outer pine bark and other polymers in seed coats which potentially have commercial value. Pathways in the breakdown of pesticides and other organic chemicals in the environment are being studied, as also is the chemistry of NZ lichens on which little work has been done. The section has also developed a head space gas chromatography method for estimating alcohol in beer, which is of particular significance now that beer is taxed directly on its alcohol content.

The toxicology section has been particularly concerned with blood alcohol determinations for which is handled 16,000 samples last year. An investigation of methods for testing blood alcohol for Transport Department officers has resulted in the selection of a pocket-sized fuel cell which was introduced at the end of 1978. Driving skills may also be impaired by drugs, and gas chromatographic techniques have been adapted so that common drugs can be measured in 1ml of blood.

The water section monitors potable waters and is involved in a collaborative programme with other laboratories examining the quality of water analyses in NZ. It has also taken a considerable part in organising studies of land disposal of sewage effluents in several parts of the country.

Ancillary services and administration involve about 50 people. The library with 16,000 books, 35,000 bound volumes of periodicals and 250,000 other items is an important resource. It subscribes to 650 scientific journals.

At Victoria University there are impressive facilities shared jointly

between the physics, geology and chemistry departments for investigating reactions at high temperatures and pressures which has now been installed in the new Cotton building on the campus.

Equipment includes nickel alloy pressure vessels capable of being used at pressures up to 5000 bars and temperatures up to 800°C, a 500-ton hydraulic press with tungsten carbide pressure vessel assemblies for synthesis and phase equilibrium studies at pressure up to 25,000 bars and temperatures up to 1600°C and a high pressure spectrometer cell for visible and infra-red spectroscopy up to 6000 bars. Some of the work with this equipment is generated by the University's close association with research in Antarctica and interest in vulcanology. Among other chemistry staff involved, **Dr Alan Freeman** has been particularly interested in Antarctic geochemistry including a study of volcanic activity of Mt Erebus.

Another field of interest at VUW's Chemistry Dept. is the use of spectroscopic methods. **Dr. Garry Burns** uses resonance Raman spectroscopy to investigate structures of natural and synthetic photochromic dyes. **Prof. James Duncan**, HOD, is interested in the application of X ray and Mossbauer methods to problems in inorganic chemistry. The electron microscope and X ray diffraction have been used to investigate the mechanism of dental decay in association with **Dr John Featherstone**, now with the Wellington Dental Research Unit. In collaboration with Pilkington Bros. Ltd., **Prof. Duncan** is also interested in the use of electric fields to confer anisotropic properties on lead oxide and silicate glasses.

Drs John Craig and Brian Halton are interested in organic compounds containing strained ring systems, while **Prof. Neil Curtis** is working on coordination chemistry. **Prof. Ferrier** of the organic chemistry section is particularly interested in carbohydrate chemistry.

Lester Stonyer showed us around the ICI Tasman Vaccine complex at Upper Hutt. Activities on the biological side are impressive, but chemical activities rather static and confined to a few, but widely used, antiseptics in various forms based on quaternaries. ICI are winding down activities at Seaview in favour of Christchurch and Mt Maunganui; some plant was recently given to DSIR for work on Montan wax.

At Unilever's Petone plant, guide **Ted Jakobsson** told us of new developments in detergents and deodorant sprays.



Parliamentary Point Of View By Ian Shearer, MP



Antarctica

Ever since I returned from a brief 6-day visit to Antarctica, I have managed to keep in contact, in a "distant" sort of way with the activities of McMurdo Base and Scott Base through copies of unclassified reports received by the American Embassy in Wellington.

In 1976 I was invited to accompany a group of scientists from the American National Science Foundation, the National Academy of Science and the US Antarctic Research Programme to Antarctica. It was a trip I will never forget and the frequent messages I receive from the Embassy serve as a constant reminder of the time I spent on the ice.

Recently the message read as follows:- "Independence Day. Detachment McMurdo and civilians from the US and NZ Antarctic Research programs assembled in the Station Gym for official observance of Independence Day. During the formal ceremony detachment McMurdo personnel were awarded the Antarctica service medal with "wintered over" clasp. Dr Lysakov our Soviet exchange scientist and veteran of 4 Antarctic winters addressed the detachment and assembled guests presenting a gift to each individual."

The message ended with a few words about a birthday party and associated festivities while, outside, I noted the temperature had risen for the minimum of -30.9°C . 4 days earlier to a maximum of -13.1°C !

Budget

What did this year's Budget have in it specifically for the scientist? Well, as far as the actual Budget document is concerned, little if anything. However, the accompanying Estimates of Expenditure, which outline departmental spending for the year ending March 31, 1980, was a little more hopeful. The DSIR, for instance, go a lift of just under \$4½ million which is about 10% and just keeping up with inflation. Beleaguered scientists, short on technician support, would also note

that a slight increase in the staff ceiling occurred over the last 12 months (an extra 10 scientists but only 1 technician), but that a further increase of 13 positions is planned for the next year.

In the Agriculture and Fisheries vote, Science — Fisheries Research — received an extra \$500,000 over last year while Science — Agriculture Research — received an extra \$1 million more than last year.

Scientists not connected with these two major areas of scientific endeavour might find some consolation in the \$700,000 increase in the financial allocation to the National Research Advisory Council which has the task of advising the Minister of Science and Technology on the promotion, development, and planning and co-ordination of scientific research and services in NZ.

Lead In Petrol

Recently, Friends of the Earth (FOE) launched an all-out attack on the use of lead in petrol. It is a topic of conversation which usually centres on the detrimental effects of lead on human health but seldom have I seen a discussion on why it is used as an additive and what alternatives there are by way of substitution.

The Minister of Energy revealed that, by adding 0.84 gm Pb/litre the octane number of gasoline is increased from 82 to 96. If the much lower level suggested by FOE of 0.06 gm Pb/l is used the octane number would be no more than 84.5. Other organometallic compounds of manganese, iron, nickel, tellurium, chromium, selenium and cobalt have been studied in detail but most of these compounds are nothing like as cost effective or as technically effective in increasing the octane number as the lead tetra-ethyl and lead tetra-methyl at present used.

Substances such as methanol and methyl tertiary butyl ether (MTBE) while not strictly additives in that they form part of the base gasoline could be used for octane improvement when added in considerable

quantities (5-15%) but their addition can displace other high octane components such as butane.

Brief Note (DSIR Annual Report 1979) Phosphorite for Chatham Rise

Late last year 2 major areas on the central Chatham Rise were assessed to contain, in total, 15 million tonnes of phosphorite. NZ's imports of rock phosphate currently average about 1 million tonnes/year.

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Chemistry in the Market Place (2nd Edition)

Ben Selinger, Australian National University Press, P.O. Box 4, Canberra, A.C.T. 2600 Australia, 1978, 454 + xxxiii pp., Recommended Aust. Retail Price \$8.50 plus postage.

This book, an expanded version of the first edition, fits comfortably between being a reference text on the chemistry of consumer products and entertaining general interest reading. After a short chapter on introductory chemistry, the wide range of topics include products used in the laundry (soaps and detergents), kitchen (fats, oils and waxes), boudoir (sic) (cosmetics, sunscreens and baby care preparations), garden (pesticides) and the medicine cabinet (drugs). The chemistry, properties and applications of plastics, synthetic fibres and paints are discussed in three chapters called The Chemistry of Hard-and Soft-ware I, II, and III. Energy is considered in a very non-mathematical chapter mainly devoted to the car and mentioning lead batteries as an alternative power source but not alternative fuels such as ethanol. A chapter on heavy metals is followed by suggestions for fourteen experiments in consumer chemistry (eg food colours in jelly beans by paper chromatography, measurement of water in detergents) most of which require only simple apparatus and will be of interest to teachers looking for experiments with "relevance".

As the author admits in the preface, a book of this nature and size must have limitations and the choice of topics and their coverage reflect Ben Selinger's interests and concerns. The author has attempted to cater for an audience with widely varying chemical knowledge and a good bibliography, often to Aust. and N.Z. sources, is given at the end of each chapter.



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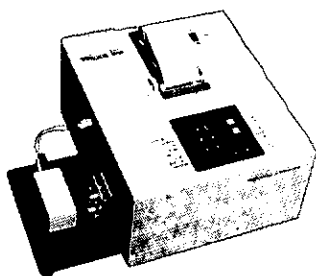
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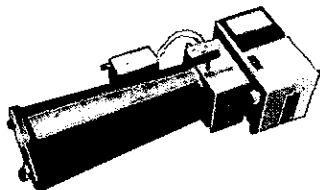
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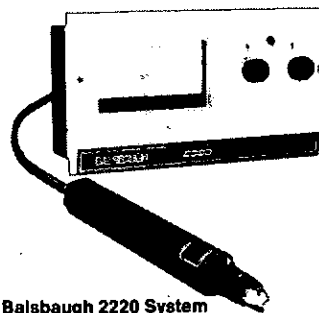


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SHOULD CHEMISTS TENDER FOR WORK?

The Editor,
Sir,

At the risk of being ostracized, I wish to express my strong disagreement with Dr Sprott's remarks (see April issue, P.79) that analytical chemists should decline to tender for Government or any other analytical contracts.

Furthermore, I feel that our members should oppose strongly his suggestion that our Institute should legislate against this practise and stop any member from tendering his services. That would constitute yet another infringement of the dwindling rights of the individual in our already over-legislated country.

My main contention is that no individual or profession must command respect — they must earn it. If we call ourselves professionals, let's not emulate the labour unions — or any other monopolistic organisations — in that respect.

I agree with Dr Sprott that we as chemists are a professional group. But I would not like to think that he made his suggestions in order to ward off competition to his well established and respected analytical enterprise from the newer analytical chemists who could

possibly provide the same services more cheaply.

As I see it providing a professional chemical service to industry, Government or the public comes in three forms — chemical analyses, professional advice on and solution of chemical problems and the development of chemical products and processes.

Of these, only the simple routine chemical analyses could ever be considered for Government or any other contract tender, because only these can be undertaken by the so-called "non-professionals" and then only if they have the equipment, the methods and the experience in the operations involved.

Let's not delude ourselves; we are but one of many industrial services and that narrow function of the "simple" analysis may well be left to the contract tenderers, the price cutters and those less qualified entrepreneurs. In the chemical marketplace, the simple routine analyses are the commodity merchandise and I feel that Government departments and industry have a right to save on costs.

Professional chemists have a much wider role to play in our society, for example, in providing expertise in the analysis and solution of chemical problems, work that could never be open to tender.

There is no doubt that industry will continue to need professional chemical analysts so long as complex and instrumented analyses are required — and so long as they can continue to provide goodwill and reliable service.

But it would be wrong for Dr Sprott and any other established analysts to impose their wills through legislation in order to stop competition, albeit in contract tenders. The outcome could well be bad publicity for them and the Institute — and they would still have competition from the non-professionals and the non-members.

In any event, TELARC registration should be adequate protection for the professional analysts and their clients.
KEES MOOYMAN
Christchurch.

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Fig. 1.

Gas-Liquid Chromatography is a very powerful and simple analytical technique, yet the necessary interpretation and calculations based on peaks on a strip chart recorder can be very tedious and time consuming. The modern trend is to use a dedicated electronic integrator or a minicomputer to acquire and process the data.

At the UEB Technical Centre, the decision had been taken to purchase a NOVA 3 minicomputer to carry out many other duties. A comparison of an analogue data subsystem for the NOVA and dedicated integrators was carried out and the decision was in favour of using the NOVA for the following reasons.

- a) Initial capital cost of an analogue subsystem for the NOVA (including 4 channels A/D and two channels D/A) was lower.
- b) It is necessary to monitor 2 detectors simultaneously.
- c) Greater flexibility in calculation and reporting would be possible.
- d) Data from a large number of runs could be stored for future reference and/or comparison.

The NOVA 3 (Fig. 1) was purchased with 32k bytes of memory, Real Time Clock, Analogue Data Subsystem and dual floppy disks. This system was interfaced to a Pye GC 204 gas chromatograph (Fig. 2) and a Varian 9176 strip chart recorder using twisted pair cabling.

Unfortunately no suitable software was available for the NOVA, making it necessary to write a program in FORTRAN IV, with assembly language subroutines to handle the A/D and D/A conversion. **Chemistry in New Zealand**

Acquisition, Processing Of GLC Data Using A Minicomputer

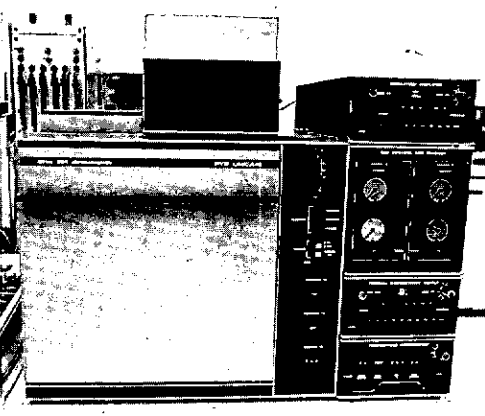


Fig. 2.

The initial program was written in a single task mode due to DOS system limitations. This had the disadvantage of tying up the system completely during a series of GLC runs. Following the addition of a 10m byte disk and RDOS the program was modified into a multitasking laboratory application package.

A. F. Peacock
Section Head: Building Products
Technology
UEB Technical Centre, Auckland.

Automation In The Laboratory

This package runs 5 tasks simultaneously; each have a priority level. The high priority (low number) tasks interrupt tasks of lower priority when necessary to carry out their function then allow the lower priority tasks to continue. The five tasks and their functions are:

TASK NAME	FUNCTION	PRIORITY NUMBER
LABPACK	Initialises variable and starts other tasks.	0
ADCON	Obtains Real Time sampled data using A/D converter.	2
GC PROCESS	Detects peaks and records times and areas.	5
GC OUT	Outputs data to the console and/or a disk file	10
CONTROL	Allows execution of a library of programs.	15

Task ADCON runs at 10HZ using the Real Time Clock, a message is then passed to GC PROCESS to process this data, any peak information then being passed to GC OUT to out-

put to the console and/or a disk file. Once the data has been processed and output, any cpu time left is used by CONTROL to execute other programs as selected. These programs include GC PARAM for setting parameters using stored data. Programs called by CONTROL are overlaid onto disk to keep the size of the program to a minimum.

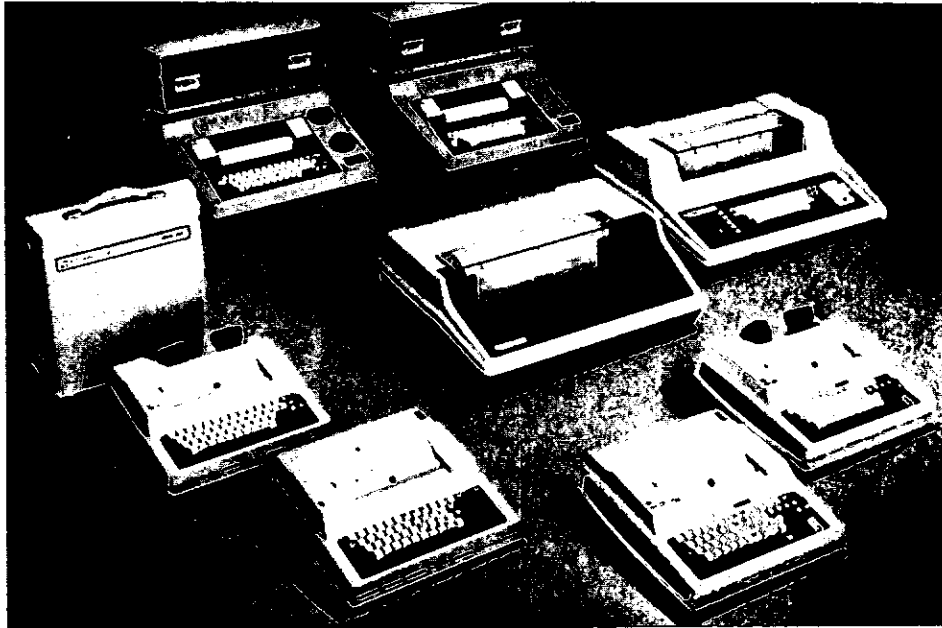
The detailed operation of the GC PROGRAM task, which carries out peak detection, is beyond the scope of this article. However a brief description will be given. Initial setting up of parameters allows sizing of a moving statistical window, setting of initial and timed sampling rates, setting an integration delay etc. Peaks are detected using first derivatives and threshold techniques; this may be extended later to using second derivatives to improve performance. Peak start, maximum and finish times are recorded, with a signal optionally being sent to the event marker(s) on the strip chart recorder. The latter facility enables easy recognition of any errors in parameters set, and permits greater confidence in results. As the responses of the 2 detectors (TC and FID) differ, the signal from each is processed completely independently and reported separately. This prevents a poor response from one detector affecting the results from the other.

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2. "Computer-Controlled Chromatographs". P. P. BRIGGS. CONTROL ENGINEERING VOL 14 — 1967.
3. "Microprocessors in Instruments and Control". R. J. BIBBERO. WILEY INTERSCIENCE PUBLICATION.

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Uses of Desktop Graphics Computer In Automated Geochemical Analysis

Bernard M. Gunn
W. & K. McLean Ltd

The production of large amounts of accurate geochemical element concentration data became possible in the early 1960's with the advent of X-ray fluorescence spectrometers with stable electronic circuitry and digital output. The method depends on comparing the secondary, emitted X-ray intensity of an excited element with that of a known standard. Unfortunately the X-ray intensity/concentration relationship is not linear due to differential absorption of the emitted characteristic radiation and a complex, iterative "matrix correction" involving about 2500 arithmetic operations is necessary. In 1960-65 sample changing, spectrometer goniometer settings and excitation power setting was still largely done by hand, the resultant X-ray intensity-time data entered on cards by hand and to compute the results for a group of 20 analyses for 10 elements each meant an afternoon's work on an IBM 1620. At the University of Montreal, by 1967, spectrometers in use, e.g. the Philips PW1220, were semi-automatic, the machine operating conditions being preset mechanically and the data being output on-line to an IBM card-punch, with matrix computation made off-line by a CDC 6600, along with line printer, drum plotter and electrostatic "Versatek" graphics.

In 1970 a PDP-11 8K word minicomputer was interfaced to control the goniometer and sample-changing stepping motors, and to print out approximate element percentages together with replicate comparison errors as analysed at 10 sec. - 1 min. intervals.

Though a matrix of results for up to 20 elements for 50 samples could be stored in memory, these were "saved" on paper tape daily in case of power failure. The final matrix correction calculation took 22 sec/sample.

As up to 30,000 element determinations were being made per year, the final results were downloaded to the CDC 6600 to be added to a data file which came to include over 30,000 world-wide rock and mineral analyses for 10-50 elements each.

Preparation for publication demanded previews of several hundred data-plots and statistical treatments of which perhaps 6-30 plots would be selected for publication. Thus, though perhaps only 50 publishable plots were required per year their production became the most time-consuming aspect of any one project. In the Deep Sea Drilling Program of 1974, three long drill cores were obtained of sea-floor basalts from the Mid Atlantic Ridge. Our contribution was to analyse 400 samples for 20 chemical elements in 3 months. The afternoon the project was completed about 200 preview line-printer plots were run off at a cost of about \$10.00, from these a dozen were selected for accurate plotting on a flat-bed plotter, and the results were presented at the American Geophysical Union Meeting in Washington 2 days later.

The recent development of the desktop graphics computer of the Tektronix 4050 series type has enabled this process to be greatly simplified, the central mainframe, now a Cyber 74, being no longer required except for major data file

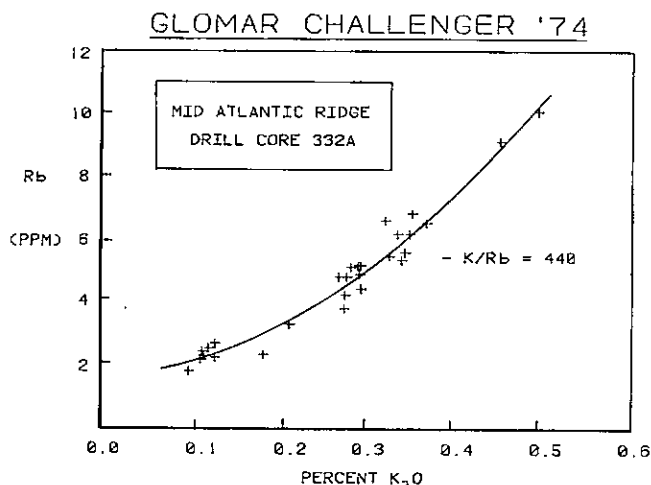


Fig. 1 A very common type of representation of geochemical data with second order curve printed. Plotted on Tektronix 4662 plotter in a time of about 25 sec.

Automation In The Laboratory

searches.

The graphics microcomputer offers several advantages over the minicomputer as an on-line data processor. A necessary preliminary test before beginning a new analytical project is to run a series of known standards (supplied by the US Geological Survey) as unknowns. Correct for matrix effects each element concentration must vary linearly with concentration within the statistical counting uncertainty. If any one does not, or a curve results, then any one of a series of faults may be present ranging from a dirty analytical surface, to power instability, counter gas leakage etc and obviously the project cannot proceed. A plot of standard concentration (%) against X-ray intensity (counts/sec) for, e.g. the element Ca, may be displayed on screen for visual checking, in less than 1 sec after pressing a User Defined Key. The BASIC interpreter resides in ROM firmware, a distinct advantage over bootstrap loading from papertape, and programs are loaded from built-in magnetic tape. Due to the new bit-slice bipolar microprocessor in the Tektronix 4052, each 10-element iterative matrix correction takes only 3 sec., a speed beginning to approach that of the batch-process Cyber.

With final data stored on magnetic tape, to display a preview plot of 400 data points of, say, Rb against K₂O concentration, takes less than 5 sec; to add a second order polynomial best fit curve, about 5 sec; to plot out a publishable quality copy on a flat-bed plotter about 1 min.

If a spectrometer is required to be run on a 16hr/day basis, obviously the computer is off-line when being used as for plot preview and statistical computation. Fully automatic, hardwired spectrometers are more expensive by \$30,000 and it is probably more efficient to control the machine settings and sample-changing by a cheap dedicated microcomputer board such as an Intel SBC-80/10 or SDK-85, store sample number, time and intensity in RAM and download at intervals. The program may be "burned" into ROM but as different operating conditions may be needed, several binary programs may be stored on tape in the graphics computer and loaded into the microcomputer as required via the RS232 port.

A complete graphics and data processing unit for one to several automated X-ray fluorescence, electron microprobe, NMR and or gamma spectrometers together with printer and plotter now costs about \$20,000, only 10-20% of the cost of a single spectrometer, thanks to microprocessor LSI technology.

Automation Of Blood Alcohol Analyses

N. M. Stone & P. P. Williams

In 1969, legislation came into effect to enable blood samples to be taken from vehicle drivers suspected of being under the influence of alcohol. The responsibility for analysing these samples was given to Chemistry Division, DSIR.

Initially, samples were analysed at laboratories in the four main centres using manual injection gas chromatographs. By 1974, about 10,000 samples per year were being analysed, and such large numbers were placing a heavy, and increasing, load on equipment and staff. The importance of the results required a significant number of high-calibre staff to be employed on a relatively simple, highly repetitive and very dull task.

The Solution

The critical factor leading to the development of the present analytical system was the emergence of the automatic sampling, head-space analysing gas chromatograph. The Perkin-Elmer F40 and F42 instruments in use hold 30 samples, and since only the vapour phase over a diluted blood specimen is sampled, the working life of the columns is very long.

The potential for a high throughput with these instruments led logically to a decision to centralise all the blood alcohol work in one laboratory, in order that this potential might be fully exploited and that efficient methods of handling large numbers of samples could be introduced.

The decision to centralise called for the provision of at least three GCs to handle the volume of work. It was therefore decided to install a mini-computer to collect and process the fairly large amounts of data which the instruments would produce and to calculate alcohol levels in samples.

An analysis of the time taken and the operations required for the complete processing of a specimen of

blood revealed that the clerical work involved in receiving, recording and certifying samples required at least as much effort as the analytical procedures and contributed more to the time taken. A specification for the computer configuration was therefore developed which would also allow the input, storage and collation of clerical data and the printing of the final certificate of analysis.

The Present System

The main equipment now in the blood alcohol unit comprises five F40 or F42 gas chromatographs equipped with an integrated gas system, a Data General Nova 840 computer with disk storage, visual display unit (VDU) terminal, teletype, lineprinter and Olivetti printing terminal. The GCs are all interfaced to the computer through an analogue to digital converter and an external interrupt device.

Samples of blood arrive at the laboratory in two sealed specimen bottles, one of which is held for independent analysis if required, the other being used for analysis. Each sample is accompanied by a form detailing the source of the sample: the name of the donor, date and time of sampling, the names of the enforcing officer, the doctor and the ultimate recipient of the analytical certificate. A laboratory sample number is assigned to the blood sample, and this, with all the descriptive information, is entered into the computer through the VDU.

For analysis, samples are grouped into batches containing 13 samples in duplicate together with 4 standard alcohol solutions. Aliquots of the samples are accurately machine diluted with a diluent containing isopropanol as an internal standard, sealed in vials, and loaded with the rest of the batch into the water bath of a gas chromatograph. The analyst instructs the computer to accept data arising from this batch, identifies himself to the computer as the analyst in charge, and lists the samples which constitute the batch. The GC is then set in operation and the samples in the batch are analysed in the following 90 min. The current from the flame ionisation detector in the GC is monitored by the computer so that peaks may be detected and measured.

A record of the chromatogram of each sample is stored in the com-

puter as a list of the integrated areas and retention times of the peaks. At the conclusion of the batch, the mean of the results held for the standard alcohol solutions is used to calibrate the FID response and hence calculate the alcohol contents of each of the blood samples. These values are then stored with the other information already held about the sample. In addition, the computer receives the result of a check analysis, performed by a different analyst using a different method. Finally, the computer types a certificate of analysis for each sample, ready for signature and posting.

A number of facilities are available for the detection and correction of errors. For example, during the analysis of a batch, the computer checks that chromatograms from duplicate samples are similar and prints warning messages on finding discrepancies. Opportunities are offered at several points for checking and editing the information held on a sample, and for repeating faulty or inconsistent analyses.

Benefits

Prior to the introduction of the computer based system, the turnaround time for a sample was on average about 11 days. Now it is about 4 working days. In high demand periods, e.g. during a Ministry of Transport "blitz" the throughput of the system can be very high — up to 600 samples per week.

Since all the information and results for all samples are held on computer disks, it is possible to retrieve the data for an old sample very quickly and easily. This is particularly useful when the laboratory is requested to release the reserve sample for independent analysis, sometimes months after the original analysis was performed.

The large amount of information now held on the transactions of the unit has made it possible to assess in some detail the consistency and reliability of the analytical procedures. The stored information has also been processed by the computer to provide important statistical data which can be used to assess the effectiveness of the drinking-driver legislation and evaluate new legislative proposals.

But the most striking benefit to the laboratory is that the number of staff allocated to this work has been halved and that in the year following its commissioning, the system was able to cope with a 60% increase in the number of samples without difficulty.

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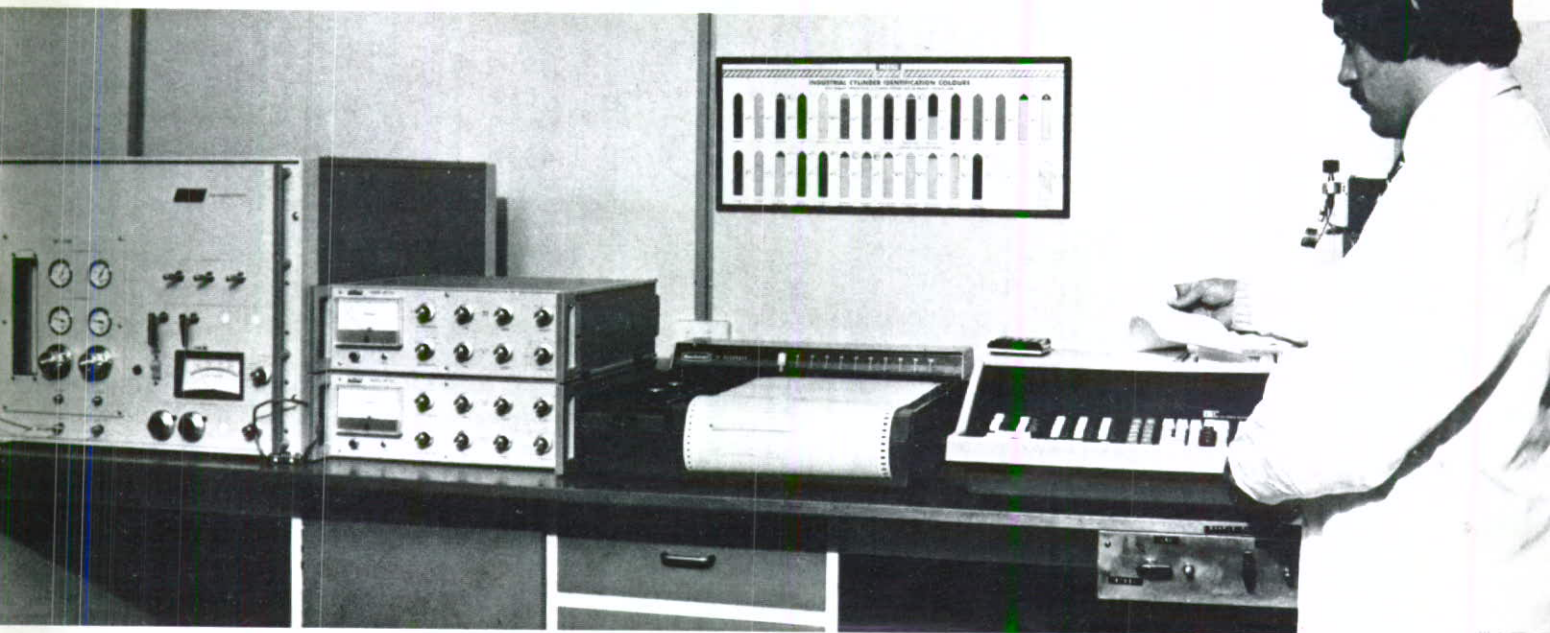
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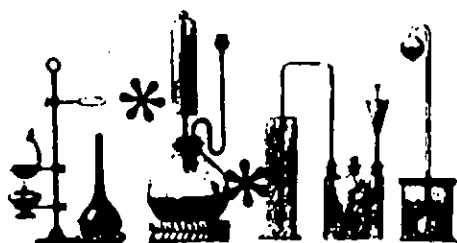


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Contamination control systems are required throughout the pharmaceutical industry and also, of course, in hospitals and medical research laboratories. At Guys Hospital, London, for example, four screens protect the main operating theatre suite and the renal diaysis unit. Early tests proved so successful that the operating theatres of all four hospitals in the Guys group are now equipped with them.

Several ways of controlling floor-contamination have been tried with partial success. The use of overshoes or mechanical shoe-brushing (with or without dust-removal by suction) can deal with part of the problem but cannot, of course, be applied to trolley wheels. Rugs impregnated with chemicals are suitable for gross contamination, but soon disintegrate; and the contamination they collect may be ground to dust, then become airborne or adhere to shoe-soles and wheels. Disposable sticky mats in metal or plastic frames have also been used; but the frames tend to harbour contamination and are difficult to clean, while the adhesive itself may sometimes be carried over into the clean area.

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Tests have shown that removal of all harmful contamination from shoes and trolley wheels requires that each foot should land at least three times and each wheel rotate three times over the surface of a Dycem screen. Therefore standard screens are 3 or 4m long x 1.2m wide and usually 7mm thick, though screens 14mm thick can be provided to deal with unusually heavy vehicles, and they can be made to any length for particular applications.

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BUBBLE MEMORY

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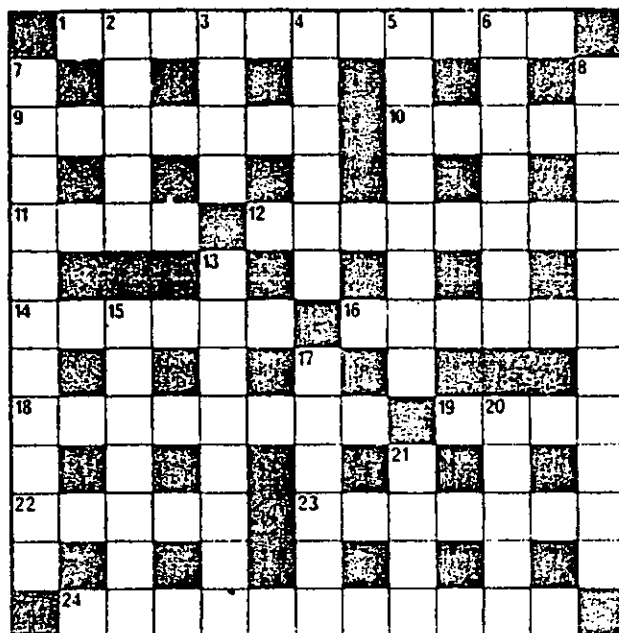
The bubbles are actually cylindrical magnetic islands polarised in a direction opposite from that of the film in which they function. Bubble memory has no moving parts and, because it works magnetically, it retains information even when the power is turned off, important for portable equipment.

Bubble memory terminals can access anyindexed record in memory in less than 15 millisecond. Further information is available from the NZ distributors, Data Communications & Management Ltd., Auckland. (See also advertisement on Page 170).

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Chemical Crossword

By Mike
(with help
from
Laurie)



Across

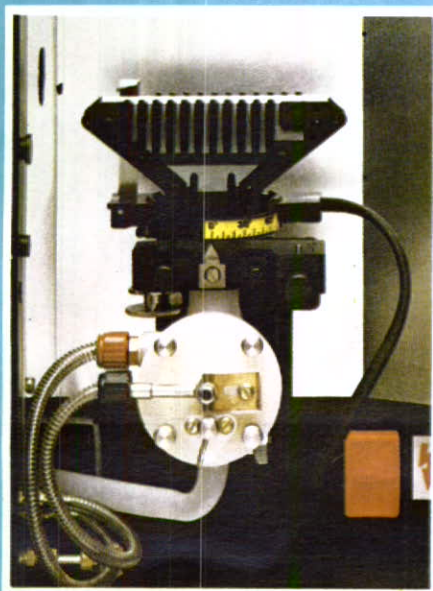
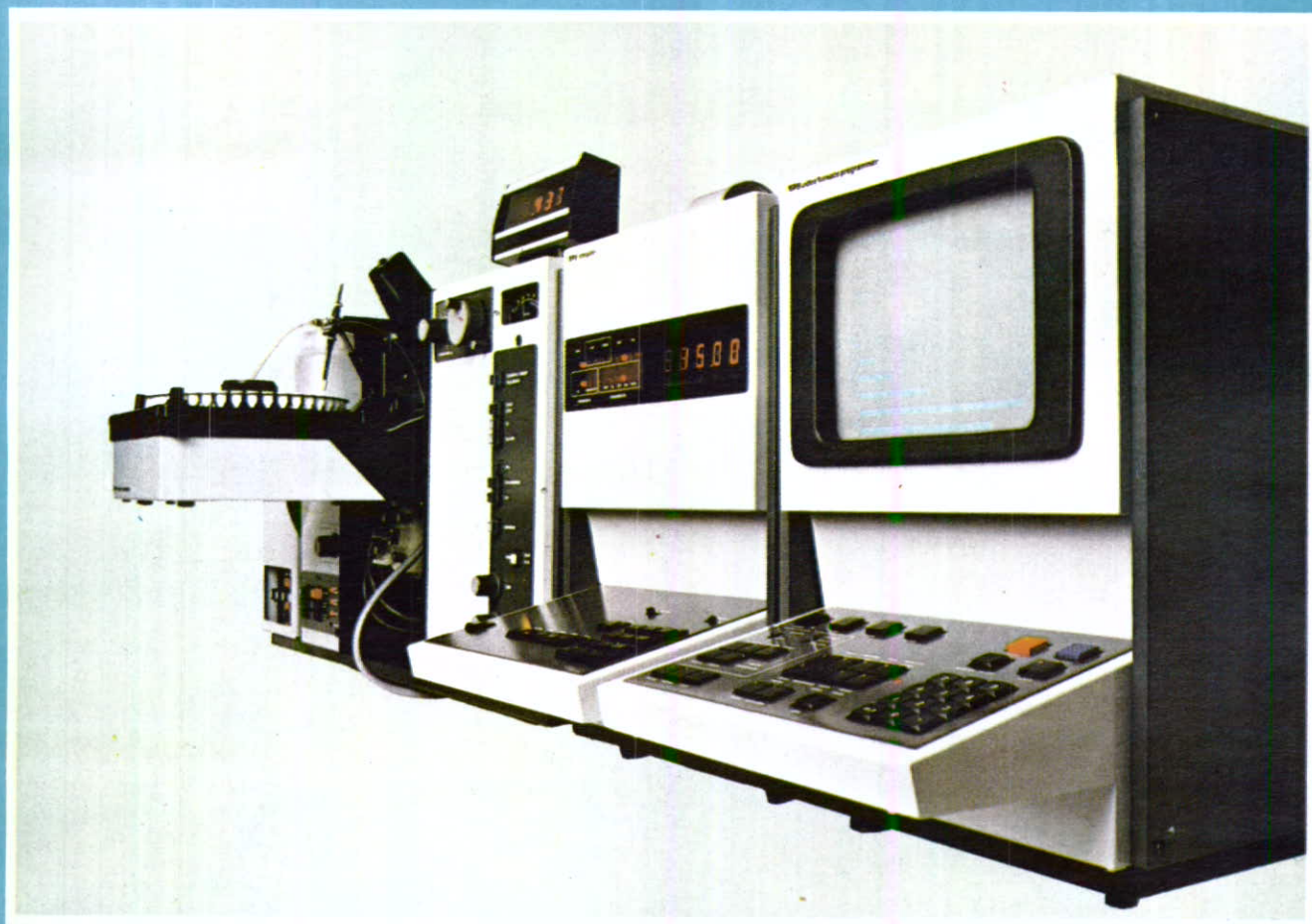
- 1 See 9
9,1,15 A ship cruise goin' o' the puddle (or pool) of a biosynthetic intermediate (7, 11, 7)
10 False silks from trees (5)
11 Fats in court by the sound of it (4)
12 Results of 23 breakdown (8)
14 Scientific prediction of the month (6)
16 Those in vessel — or driving it (6)
18 Cut-rate to a point - or just cut (8)
19 Bimetallic island (4)
22 Lifeless nitrogen coloured chip (5)
23 6's mate for life (7)
24 Family of Mann? (11)

Down

- 2 Ten American cents forms acids derivative (5)
3 Keratinaceous extrusion (4)
4 Rocky view, past and present (6)
5 Tough going for 16's insides (4,4)
6 9 and me, without rib, basically (7)
7 Salts in a tub become solid (11)
8 Cities' rents cause empty spaces (11)
13 Augmented velocipede from e.g. Twistane? (8)
15 See 9
17 Hallowed tree forms layers (6)
20 Start of 22 and end of 2 is an anion (5)
21 Half a chemist? (4)

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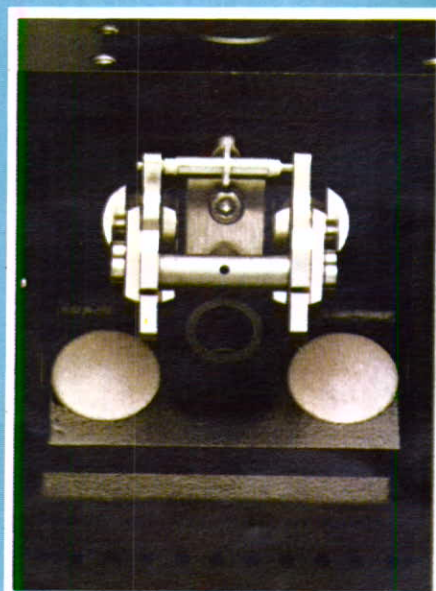
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Waters Associates Pty. Ltd., a wholly owned subsidiary of Waters Associates, Inc., Massachusetts, U.S.A., was established on 1 January, 1977, to better serve the interests of the Australasian Liquid Chromatographers.

With over 15 years experience in manufacture and application of Liquid Chromatographs Waters expertise is available to you through:

- **Technical assistance**
- **Frequent seminars and workshops**
- **Regular L.C. Schools**
- **Continuing publication of literature**
detailing L.C. separations in practically all industries and fields of research.

Waters factory trained staff assemble instruments locally from imported components, subsequently extensive spare parts and supplies are immediately available.

Laboratories in Sydney, Melbourne, Brisbane and Auckland, New Zealand, staffed by qualified chemists provide "on-going" service to clients.

**WATERS
ASSOCIATES**
PTY. LTD.



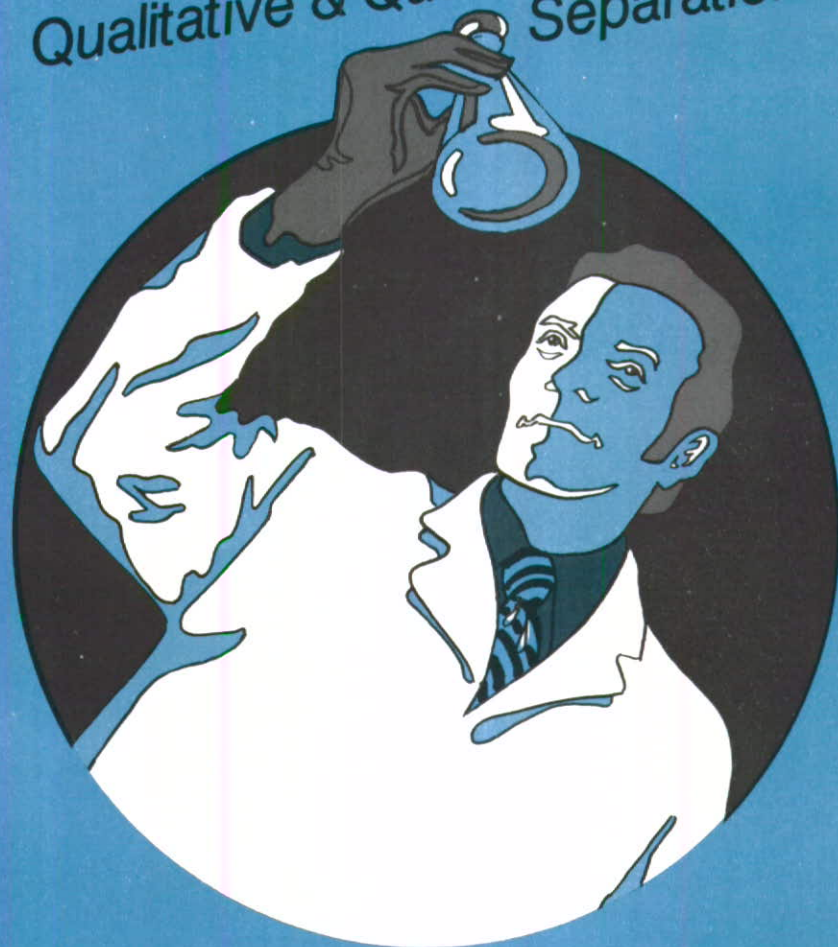
82-96 Myrtle Street, Chippendale,
Telephone: (02) 699 1377
P.O. Box 145, Chippendale,
Australia, 2008
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64 Elgin Street, Carlton,
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901 Kingsford Smith Drive, Eagle Farm,
Telephone: (07) 268 6488
P.O. Box 71, Hamilton Central,
Australia, 4007
Telex: AA42788

83 Wakefield Street, Auckland,
Telephone: 77 0392
P.O. Box 5565, Auckland, 1,
New Zealand
Telex: NZ21433

Sample Preparation
Solvent Purity
Qualitative & Quantitative
Separations



**3 Brochures
from Waters
will solve your
Problems**

The Liquid Chromatography People

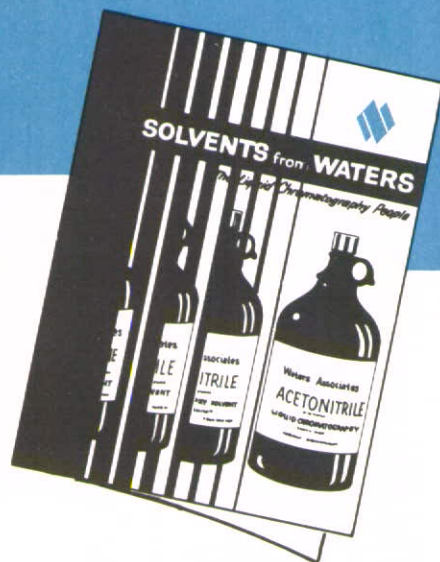
Solvents from Waters

Waters Solvents are quality controlled by Liquid Chromatography to meet or exceed all conventional standards of High Quality Solvents.

These standards include:

- **Minimum residue**
- **Controlled moisture content**
- **Particulate free**
- **Minimum lot to lot variation**
- **Low background absorbance**

Waters Solvents have been produced specifically to meet the stringent requirements of Liquid Chromatography but may be used in a wide range of laboratory procedures that require quality and reliability.



Request Brochure No. A100 detailing Waters L.C. Grade Solvents, Paired Ion Reagents and useful chemical data.

All Waters Solvents and Reagents are available EX-STOCK at your nearest Waters Office.

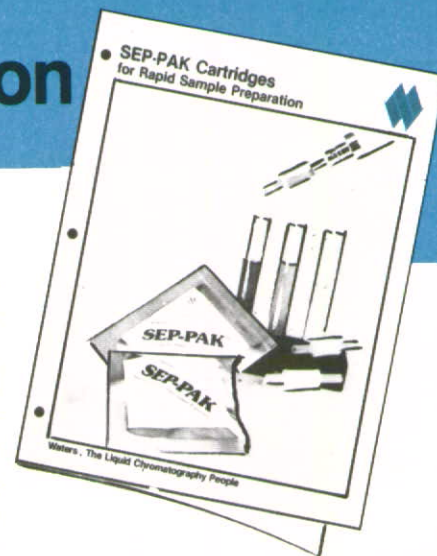
SEP-PAK Cartridges for Rapid Sample Preparation

SEP-PAK™ Cartridges permit rapid sample preparation and save valuable time. These small self-contained cartridges can reduce complex sample preparation schemes to a few simple steps requiring only minutes to complete.

SEP-PAK Cartridges are ready-to-use, prepacked with chromatographic materials, optimized for sample preparation. A 10 ml syringe with luer end fitting and collection vessels are all the equipment you will need to prepare samples for analysis.

SEP-PAK Cartridges:

- **reduce consumption of costly Solvents and Reagents**
- **facilitate on-site sampling**



- **minimise handling of toxic compounds**
- **eliminate the chance of cross-contamination**
- **permit detection of trace compounds**
- **eliminate interferences**
- **make sample preparation fast, easy, efficient and convenient**

If you would like to receive free samples of SEP-PAK Cartridges for your own evaluation please request together with Brochure No. F82.

WATERS total Software Support

You would expect "the Liquid Chromatography People" to consider the complete L.C. system — that's the intelligent approach.

The optimum high performance Liquid Chromatography system certainly starts with quality instrumentation. Applications support, customer training and responsive service are also essential for success.

A dependable source of high quality columns, solvents and supplies is also required to complete the system.

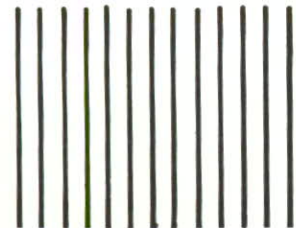
Waters can offer you:

- **Solvents**
- **Packed Columns**
- **Solvent and Sample Clarification Kits**
- **L.C. Packings**
- **Syringes**
- **Recorder accessories**
- **Stainless steel tubing**
- **PTFE tubing**
- etc, etc.**

Waters Associates Pty. Ltd. is your single source for all L.C. needs.

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What Liquid Chromatography can do for YOU

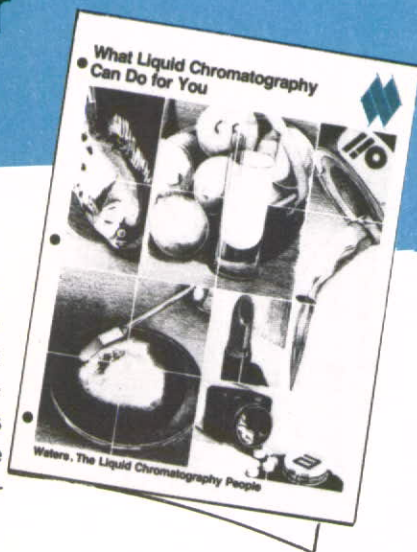
Liquid Chromatography is an instrumental technique which separates complex mixtures into their component parts and provides qualitative and quantitative information on each component.

Because L.C. separates very similar compounds from each other, it provides interference-free analytical information on quantities of pure material from complex matrices.

Once an L.C. technique has been developed, typical methods take from three to twenty minutes. Sample preparation is minimal, usually solution and filtration are all that is required.

And we can get you started quickly. Waters Associates' files contain details of thousands of developed L.C. methods and our four applications laboratories in Australia and New Zealand are here to support you.

Ask for the 16-page Brochure "What Liquid Chromatography Can Do For You", No. N65.



WATERS ASSOCIATES PTY. LTD.



I would like to receive the following brochure(s):

- Waters "High Purity Solvents".
- "SEP-PAK Cartridges" together with free samples of the C18 and Silica Sep-Paks for my evaluation.
- "What Liquid Chromatography Can Do For You".

Please have a Waters' Chemist phone me; my application is

I currently have access to an L.C. Model

My instrument needs are:

- Purchase in six months. Budget/Grant Planning.
- Purchase in twelve months. Literature Files only.

NAME

ADDRESS

STATE..... POSTCODE.....

TELEPHONE.....

Colleagues who would like information:

.....
.....

The Liquid Chromatography People