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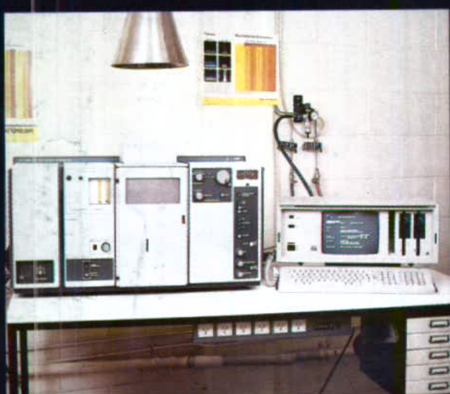
chemistry in new zealand



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Editor: Dr Bruce Graham, c/- Dept of Health, 2 Edenvale Rd, Mt Eden, Auckland

Branch Editors:

Auckland: Dr Roger Whiting, Auckland Technical Institute, Private Bag, Auckland.

Waikato: Dr Max Sutton, Ruakura Soil and Plant Research Station, Private Bag, Hamilton.

Manawatu: Dr Cecil Johnson, DSIR Applied Biochemistry Division, Private Bag, Palmerston North.

Wellington: Dr Peter Cropp, Chem. Div. DSIR, Private Bag, Petone.

Canterbury: Jeff Plowman, Chem Div. DSIR, P.O. Box 29-181, Christchurch.

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

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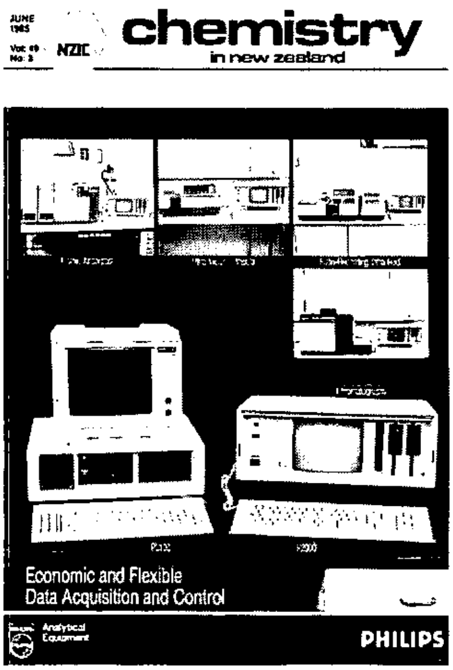
FRONT COVER STORY: PAGE 83



Chemistry in new zealand

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Outline of the Institute

The New Zealand Institute of Chemistry is the primary professional and learned society for chemists, biochemists, chemical engineers, and chemistry technicians in New Zealand. Membership is open to all with appropriate tertiary qualifications in chemistry, biochemistry, or chemical engineering. There is also a student grade of membership, while those persons with a general interest in chemistry, but without the necessary qualifications, may be local members.

Institute activities are many and varied. At the local level, regular Branch meetings, lectures, and social functions provide opportunities for members to meet informally with their colleagues, as well as to keep abreast of developments within the professsion. Branches are also active in promoting chemistry in schools with various competitions and participation in science fairs. The Annual Conference of the Institute is held at a different venue each year. The programme includes invited plenary lectures, specialist lecture sessions and workshops for the presentation of current research findings, trade displays, and social activities. In the public arena the Institute has a number of committees to present members' views on chemical hazards, the environment, chemical education, and public affairs generally. The Institute also has representatives on bodies such as SANZ, AAVA, and the Royal Society of New Zealand.

To assist its members in their profession, the Institute surveys salaries periodically and publishes a Code of Ethics, and Guidelines to Professional Employment. The professional achievements of individual members are recognised each year by the awarding of a number of Institute prizes.

The NZIC has links with the Royal Society of Chemistry, the American Chemical Society, the Royal Australian Chemical Institute, the Federation of Asian Chemical Societies, and the International Union of Pure and Applied Chemistry. Members may therefore have the opportunity of participating in their activities and meeting chemists who visit this country under the auspices of the Institute. In particular, a visiting speaker scheme is currently operated with the RACI.

Application for membership of the Institute is made on a form available from the Registrar (PO Box 29-183, Christchurch). Current (1985) subscriptions for the main membership grades, including the cost of this Journal, are:

Fellows and Members (less $5 if paid before 31 Aug.)	$60
Associates (less $5 if paid before 31 Aug.)	$50
Graduates and Technicians (less $5 if paid before 1 Aug.)	$35
Students	$10

EDITORIAL

This and That

This issue marks the start of my second year as Editor. No special celebrations are planned!

Producing an editorial for each issue is probably one of the chores of this position. It's nice to be able to pass the task on to somebody else from time to time, but for this issue I'm afraid that no-one has taken up the challenge. Nonetheless the remaining space must be filled, so I offer you the following — a few snippets from the recent experience of an editorial chemist.

Two of Council's committees have been active recently. The Environmental Committee has prepared comments on the NZ Ecologic-document on nuclear warfare (Chem. in NZ, **49**, 44, (1985)), and the Hazardous Chemicals Committee has prepared a submission on the ICI fire, for the investigation by the Commission for the Environment. Space does not allow details of these to be presented here, but I hope to incorporate them into future articles that will look at the two issues in more detail.

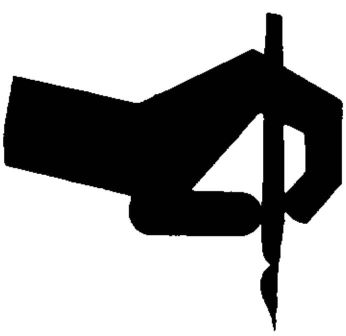
On the subject of the ICI fire, that company has recently published a report by Gordon Maxwell, a consultant ecologist on the environmental effects of the fire. The report concentrates on the Tamaki estuary, and perhaps the most significant finding is that the fire has not been alone in producing observable damage to the area. The effects of the fire will be short-term and highly localised. Much more widespread are the effects of irresponsible dumping of domestic and industrial rubbish. Boaties also come in for some flak, in contributing to a marked decline in numbers in a resident shag colony.

On a completely different tack. . . I was recently talking to a colleague who was surprised to learn that it is not necessary to wait to be asked to submit articles for publication in Chemistry in NZ. True, many of the articles we publish are by invitation, but the major reason for that is that insufficient material comes otherwise to fill these pages.. So, to all of you who have been too modest to offer until now — my address is on the first page of each issue.

Finally, an item for all chromatographers. The NZ Medical Journal, recently published a letter entitled "Leafy-green coloured infant stools". It seems that a number of mothers in the Manawatu area, who have been feeding their children a product known as Yokit, have been alarmed to observe the above result. Intrepid researchers at Massey have traced the problem to the chocolate-flavoured variety of Yokit. Apparently this contains three dyes, two of which (red and yellow) are absorbed or neutralised, but a third (blue), is not. This combines with "other yellow compounds" to give the final effect. Fascinating! My question is, how to classify this phenomenon? GC — surely not; HPLC — where's the high pressure (or performance); reaction chromatography — perhaps; but more likely an example of traditional open column low pressure chromatography, with irreversible adsorption of some of the components — I think!

Bruce Graham.

LETTERS TO THE EDITOR



PAC-CHEM 84

Sir,

Although it is not unusual to read reviews or reports of concerts or rugby matches that one has attended which raise doubts that the events reviewed were indeed those which had been witnessed, we would have thought it unlikely that we should read a report by the President of the Institute in your issue of February 1985 which raised doubts in our minds that we had attended the 1984 International Chemical Congress of Pacific Basin Societies.

We went knowing that this was the twice yearly jumbo get-together of the American Chemical Society held in conjunction with the Chemical Society of Japan and incorporating kindred smaller societies from Pacific Basin countries of which NZIC was one. We were quite expecting 4,000 registrants and innumerable symposia and papers, and we knew the topics covered would range over applied, economic and administrative aspects of chemical science and scientific co-operation of special significance to the countries taking part, but we also knew that the chance to attend would afford us the opportunity to hear a plethora of excellent new science much of it from some of the biggest names in modern chemistry. In short, this was a chemistry Conference and, to put matters in perspective, the "Economics and Management" symposium to which the President alluded exclusively attracted 23 contributions (including his own) of the 3,000 or so that were given during the week.

Our major reason for writing is to express disappointment that the part played at the Conference by other New Zealand chemists was entirely disregarded by the President. Some New Zealanders were invited members of the organising committees of specific symposia, and we feel that the 15 papers given by chemists and the 3 by administrators from this country was no mean contribution, and we wish to point out that these ranged from good, contributed papers on a range of topics — some New Zealand inclined, some not so — to specifically invited full lectures selected for specific symposia of the highest quality. To say the least, we believe these additively deserved more than complete disregard.

We and our colleagues in the Universities in this country are finding chemical life hard these days, and we would appreciate any encouragement — not least from industry, which is not unknown for its view that academic chemists can be aloof. Our President has unfortunately just illustrated the magnitude of the gulf between the two aspects of our subject in New Zealand, and we regret that he did not reveal a broader understanding of, and sympathy with, all of those he represented.

Professor R.C. Cambie
Professor R.J. Ferrier
Dr. M.H.G. Munro
Professor B.H. Robinson

Departments of Chemistry,
Universities of Auckland, Wellington, Christchurch and Otago

THE PRESIDENTIAL RESPONSE

Sir,

My comment on Pac Chem 84 gives my personal impressions of the Congress. I was not asked to review contributions from any one sector, or, more specifically, from the New Zealand sector. Had I been asked to make such a review I would have declined since I am not competent to do so.

It is unfortunate that an inference should be drawn that my report illustrates that a gulf exists between industry and academia. In my view such a gulf exists only in the minds of the academics, but surely if there is such a feeling some positive approach to industry by those suffering the "hard chemical life" would be logical.

It is perhaps worth noting that this was not "the twice yearly jumbo get-together of the American Chemical Society held in conjunction with the Chemical Society of Japan". Pac Chem 84 grew out of a conference in 1979 involving the American Chemical Society, Chemical Society of Japan, Royal Australian Chemical Institute, the Chemical Institute of Canada and the New Zealand Institute of Chemistry. At that time it was resolved to broaden the scope of a follow-up congress by inviting chemical societies in all countries bordering the Pacific Ocean to participate formally. The result was Pac Chem 84 bringing together 22 chemical societies and the Asian and Latin American federations of chemical societies.

A major objective of Pac Chem 84 was to foster co-operation among chemists from developed and developing countries. This dimension was regarded as especially important since disparities in conditions between developed and developing countries represent one of the most important threats to peace facing the world today.

The above paragraph is taken from the message by Dr. Glenn Seaborg (General Chairman of Pac Chem 84) which is recorded in the front of the programme. I suggest that our friends should read this so that they will clearly understand the nature and objectives of the Congress which, presumably, they attended and to which they undoubtedly made an important academic contribution. I, personally, am in some doubt that the broad objectives, as outlined, were achieved.

Yours sincerely

A.W. Mackney
PRESIDENT

1985 NZIC/NZBS/NZACB CONFERENCE

Joint Conference of the New Zealand Institute of Chemistry, the New Zealand Biochemical Society and the New Zealand Association of Clinical Biochemists

University of Canterbury, Christchurch
26-30 August

The registration form and general information have been distributed with the annual subscription mailings and an early return would be appreciated. The programme outline and the Computer Workshop programme are shown below. The Biochemistry and Clinical Biochemistry sessions will begin on Tuesday morning at 11.00 a.m. and run in parallel with other sessions through until 5.15 p.m. on Thursday. The organisation of the other Specialist Sessions will only be possible after the receipt of all abstracts. Each contributor will be notified of their time slot with the registration receipt. It may be advisable to make provisional transport reservations in advance as the school holiday period is always a popular travel time. The 10% Air N.Z. travel discount vouchers which will be included with the receipt are required when payment is made; one month prior to departure.

Biographical details of two of the plenary speakers, Professor Smith and Associate Professor Napper, were published in the April issue of the Journal and details for the three remaining plenary speakers, Professor Schreiber, Dr Robinson and Dr Gainsford are presented here.

Enquiries to: Dr Peter W. Harland, 1985 Conference Secretary, Chemistry Department, University of Canterbury, Private Bag, Christchurch.

Gerhard Schreiber
The Russell Grimwade School of Biochemistry, University of Melbourne, Australia

Gerhard Schreiber is Professor of Biochemistry (Medical) at the University of Melbourne, Australia. He studied experimental physics and medicine at the University of Mainz and Freiburg, i.Br., West Germany, from 1951-1959. After two years internship he received an M.D. for a thesis on the metabolism of acetoin in pig heart muscle carried out at the Department of Biochemistry at the University of Freiburg. After Postdoctoral Fellowships in the Department of Biochemistry at the University of Freiburg, and the McCardle Laboratory for Cancer Research at the University of Madison, Wisconsin, he was Assistant Professor of Medicine at Columbia University, New York. In 1967 he returned to Freiburg in Germany and became a Dozent for Biochemistry in 1970. In 1973 he went to Australia to take up the Chair of Biochemistry (Medical) in the Russell Grimwade School of Biochemistry at the University of Melbourne. Since 1965 he has been studying the mechanism and the regulation of the synthesis and secretion of plasma proteins. The title of Professor Schreiber's lecture will be Synthesis and Processing of Plasma Proteins.

Graeme J. Gainsford
Chemistry Division DSIR
Petone, New Zealand

Graeme Gainsford is Leader of the Computing and Statistics Section at Chemistry Division and a graduate of the University of Canterbury, B.Sc. (Hons) and Ph.D. Since graduating Ph.D. in 1969 Graeme has held a Postdoctoral Fellowship at Ohio State University, a Science Research Council Fellowship at the University of Sussex and Research Fellowship at the Australian National University in Canberra during 1972 and 1978 and study leave at the National Research Council of Canada in Ottawa in 1981-82. Research interests cover all aspects of computing and single crystal X-ray crystallography. His lecture will be entitled Computing Applications in Chemistry Division, DSIR.

Ward T. Robinson
Department of Chemistry, University of Canterbury, Christchurch, New Zealand

Ward Robinson is a Reader in Chemistry at the University of Canterbury from which he graduated Ph.D. in 1964. Since then he has worked in the United States at Brown University, Northwestern University and Stanford University and, most recently, spent some study leave at Bristol University in England. He is interested in all aspects of crystal structure analysis and is now concentrating on developing and using state-of-the-art X-ray equipment to provide structure solving services to New Zealand chemists who do not have these facilities. Dr Robinson will present a lecture on Computers in Crystal and Molecular Structure Research.

Dr Jurgen Moller, Tecator Laboratories, Sweden

Another overseas visitor to the conference will be Dr Jurgen Moller, Head of Applications, R & D and Product Quality Control for Tecator Laboratories, Sweden. Dr Moller will deliver a major lecturer on Flow Injection Analysis to the Analytical Specialist Group on the Tuesday morning.

Dr Moller is travelling from Sweden to an international conference on F.I.A. in Birmingham U.K., but has agreed to detour via Christchurch thanks to the efforts of the staff of Wilton Instruments.

COMPUTER WORKSHOP PROGRAMME OUTLINE

Computers in Chemistry Workshop
Friday, 30 August 1985
University of Canterbury, Science Lecture Theatre Block

9.00 a.m.	Preview of displays and demonstrations
9.30 a.m.	Dr. B. Peake, University of Otago, "Overview of Interfacing Microcomputers to Chemical Instruments"
10.15 a.m.	Morning Tea
10.45 a.m.	Demonstrations and Discussions
1.00 p.m.	Lunch
2.00 p.m.	Professor S. Smith, University of Illinois, 'Computers in Chemical Education"
2.45 p.m.	Demonstrations and discussions
3.15 p.m.	Afternoon Tea
5.00 p.m.	Conclusion

PROGRAMME OUTLINE FOR 1985 CONFERENCE: NZIC, NZBS, NZACB

26 — 30 AUGUST

UNIVERSITY OF CANTERBURY

TIME	Monday 26	Tuesday 27	Wednesday 28	Thursday 29	Friday 30
a.m. 9.00	Registration	Plenary Napper; Plenary Schrieber	Vaughan Sympos.; Pharmacia; Specialist	Plenary Smith; Plenary Gainsford	Computer Workshops
10.30	Tea/Coffee	Tea/Coffee	Tea/Coffee	Tea/Coffee	Tea/Coffee
11.00 – 11.40	Opening Ceremony Presidential Address	Specialist Sessions	Vaughan Sympos.; Specialist	Educ; Specialist	Computer Workshops
p.m. 12.30	Lunch	Trades Lunch	Lunch	Lunch	Lunch
1.45	Plenary Robinson	Posters Session #1	Visits	Posters Session #2	Computer
2.45	Specialists AGMs etc				
3.15	Tea/Coffee	Tea/Coffee		Tea/Coffee	Tea/Coffee
3.45	Easterfield followed by AGM	Specialist Session		Educ; Specialist	Computer Workshops
5.15	Dinner	Dinner	Dinner	free	
	Mixer	free	free	Conference Dinner	

CATALYSIS AND ENERGY

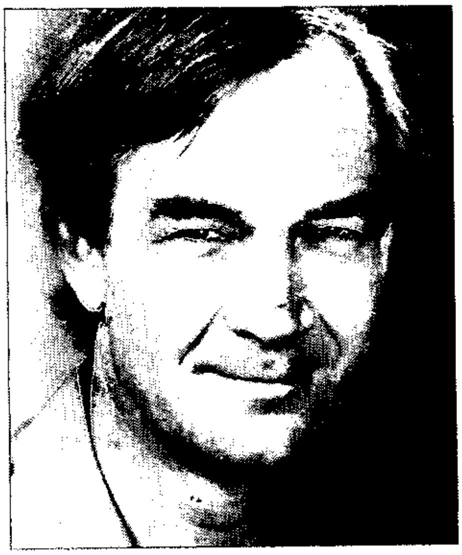
D.L. Trimm
School of Chemical Engineering and Industrial Chemistry, University of New South Wales, Australia.

David Trimm is Professor and Head of the School of Chemical Engineering and Industrial Chemistry, University of New South Wales.

His research interests lie in the field of catalysis with an emphasis on the applications of catalysts to applied problems such as synthetic fuel production, coal conversion as well as catalyst and reactor design. He has also served as consultant for a number of industrial firms.

He has published a wide range of papers in the catalytic field, is the author of "Design of Industrial Catalysts" and an Editor of the journal "Applied Catalysis".

This paper is based on a plenary lecture given by Professor Trimm at the 1984 NZIC Conference. We are indebted to Dr David Bibby, Chemistry Division, DSIR, Wellington, who prepared this version for publication in the Journal.



1. INTRODUCTION

The energy industry as we know it today is almost entirely based on fuels derived from coal, oil, shale oil, natural gas, wood or biomass; the major energy-producing process is combustion. Catalysts are extensively used to convert starting materials to more desirable forms, to improve the efficiency of combustion and to clean up combustion effluents. It is convenient to consider each of these roles in turn. We also consider some possible developments of catalysis in energy production in the future.

2. CATALYSIS AND THE INTERCONVERSION OF FUELS

Nearly every carbon- and hydrogen-containing material is a potential fuel. However, combustion devices, designed for fuels with specific compositions, have accumulated to the point where in many cases it is cheaper to convert the fuel to suit the appliance rather than to introduce major changes in the devices to suit a given fuel. Such fuel conversion relies on adjustment of the C:H ratio and alteration of the molecular structure of a fuel to obtain better combustion characteristics while avoiding pollutant emissions.

Perhaps surprisingly, the most widely used method of altering the C:H ratio is gasification, which involves the conversion of raw materials to carbon oxides and hydrogen, followed by reassembly of these molecules to produce desired materials. Reasons for this include the relative ease of production of carbon oxides and hydrogen, the well established routes from these chemicals to desired products and the ease of removal of potential pollutants during processing. Another method of producing fuel is hydrogenation which involves the addition of hydrogen to high carbon content materials. A third route, the removal of carbon from high carbon content materials by pyrolysis, is not discussed here.

a) Gasification

Transportation fuels are seen, from figure 1, to lie in the middle of the range of C:H ratios and, as a result, may be produced either from methane or from heavy oils or carbonaceous solids. Carbon oxides and hydrogen can be produced from these starting materials by reaction with steam or with oxygen, and the processes may or may not be catalytic. These gaseous products can be used as fuels in their own right or can be used as feedstocks for other processes. In the latter case the mixture of $CO + H_2$ is commonly referred to as synthesis gas.

Perhaps the best known reaction is the production of hydrogen by the steam reforming of light hydrocarbons. This process has been operated industrially for many years as part of the production of ammonia or of methanol[1,2] and the overall reactions may be represented as

$$CH_4 + H_2O \longleftrightarrow CO + 3H_2 \quad (1)$$
$$CO + H_2O \longleftrightarrow CO_2 + H_2 \quad (2)$$

In the context of fuel production, methane is the most economic starting material, although heavy oils have been steam reformed using a cyclic process.[3] The thermodynamics of the system are such that hydrogen production is favoured at high temperatures (ca.800°C) and the most cost-effective catalyst involves supported nickel. Supported nickel is not the most effective catalyst, catalytic activity decreasing in the order

Rh, Ru > Ni, Pd, Pt > Re > (Ni_2Cu alloy) > Co

but, for industrial operation, Ni is used universally as a result of the lower costs involved.

Supports are not just a cheap way of making a catalyst go that much further. They play an important role in the catalytic process and some of the most exciting recent developments in catalysis have been in the area of catalyst/support interactions. Steam reforming is complicated by coke formation[4,5,6] and the choice of a support is often made on the basis of temperature- and steam-stability coupled to some activity for coke removal. Magnesia, which promotes the reaction between steam and coke (or coke percursors), is often used, while other catalysts incorporate complex supports which slowly release KOH, a catalyst for coke gasification.[2] Simple but robust supports are favoured for the steam reforming of methane, and the rate of coke formation is low. However, coke formation does occur and

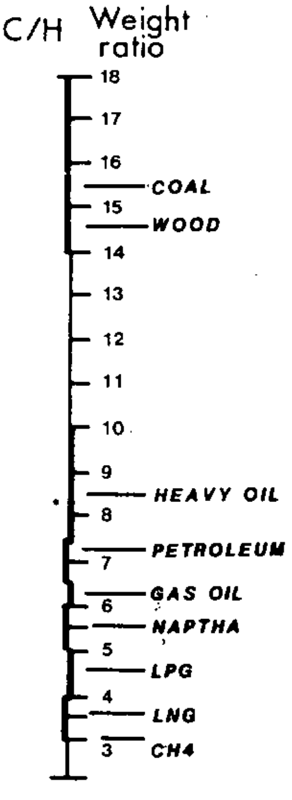


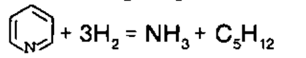
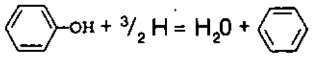
Figure 1
Carbon/hydrogen ratios in different fuels.

deactivation of the catalyst is observed over long periods. In this connection, interesting work has recently appeared in which the ensemble size has been used to control coking.[8] Although sulphur is a poison for nickel, if added in very small amounts it will absorb on the surface in a regular array[9] leaving 'islands' of free nickel atoms on the surface delineated by nickel-sulphur species. Careful control of the amount of sulphur allows ensembles of nickel atoms of such a size that steam reforming can proceed and coking cannot.[8,10] As a result, industrial operations are possible for many months without interference by coke formation.

The reaction between steam and solid raw materials is well known but has not been used industrially to the same extent.[3] Gasification of coal, for example, is promoted by transition metals and by alkali carbonates[11,12] and work continues in the search for even more efficient catalysts.[13] At least part of the problem lies with the chemical and physical structure of the solid, particularly as gasification proceeds. Too often, a matrix of inorganic material is left behind by gasification and forms an efficient trap for the catalyst. As a result, catalyst-coal contact is lost and gasification slows down. At the same time, recovery of the catalyst from the inorganic residue becomes more difficult and the overall cost of the process increases. This is a theme that recurs frequently — the cost efficiency of the interconversion of fuels is always the most important factor of any process. A major advantage of the gasification of solids and heavy oils lies in the cleaner fuels produced: inorganic material is removed during processing since the inorganic components are left behind in the ash; in addition contaminants in the gas mixture, such as SO_2, H_2S, NH_3, etc. can be readily removed. The liquid fuel synthesised from such mixtures is therefore of high purity.

b) Hydrotreating

Rather than producing carbon oxides and hydrogen, it is also possible to upgrade heavy raw materials and remove undesired impurities by the addition of hydrogen. Catalytic processes have been developed for the hydrotreating of coal,[14] wood[15] and heavy oils,[16] the overall processes being typified by the sequence of reactions

Hydrogenation	$RHC{=}CHR^1 + H_2 = RCH_2 - CH_2R^1$	(3)
Hydrocracking	$RHC{=}CHR^1 + 2H_2 = RCH_3 + R^1CH_3$	(4)
Hydrodesulphurisation	$RSR^1 + 2H_2 = H_2S + RH + R^1H$	(5)
Hydrodenitrogenation		(6)
Hydrodeoxidation		(7)
Hydrodemetallation	$RM + \frac{1}{2}H_2 = RH + M$	(8)

The last reaction is much more complicated than shown, primarily because it appears to involve hydrocracking of an organic group attached to a metal.

In general, the reactions involve three stages, all of which may be, but usually are not, carried out in the same reactor. Taking coal as an example, the first stage involves liquefaction after which residual solid matter may be filtered off. The second stage involves removal of most of the hetero atom compounds, while the final stage is concerned with upgrading the products to meet specifications for the desired final products. These processes were used during the Second World War, but have not been developed to the extent of the gasification alternative.

The difficulty of separating catalysts from the inorganic material in coal usually leads to the use of a 'throwaway' catalyst for the first stage. There is debate whether such catalysts are more active than inorganic material present in the coal, but investigation of cheap iron-based catalysts (e.g. 'red mud' from alumina processing) has been widespread.[14] Liquefaction makes it possible to remove most of the inorganic mineral material mixed with the coal, but does little to remove chemically bound oxygen, sulphur and nitrogen. The liquid therefore requires considerable upgrading.

3. CATALYSIS AND THE UPGRADING OF FUELS

There is no question that crude oil remains and will remain the major source of fuels and organic chemicals for many years to come, and that conventional refinery operations will be of paramount importance. It is also obvious that supplies of crude oil will eventually become depleted and that, when this happens, natural gas, coal, oil shale and to a lesser extent, biomass will take over as major raw materials. In this context it is necessary to examine catalysis in the refinery and catalytic processes which will be needed in the future.

Most refinery processes are well established, and it is necessary only to summarise their characteristics and to indicate areas where improvements can be expected. We can also compare a conventional refinery to a refinery geared up to include the wider range of raw materials that will result from the conversion of natural gas or solid fuels.

a) Catalysis and the conventional refinery

A conventional refinery processes crude oil to produce fuels and chemicals in the amounts required by the local market. A refinery must always be in balance. However, the relative amounts of products must vary with the market demand which can change, for example, with the season. As a result, a degree of flexibility in refinery operations is essential.

It is impossible to deal with all the refinery processes in detail given the space available here. Because of the importance and scale of refinery operations, small improvements are cost effective and considerable efforts are made to obtain them. Recent advances have been made in the areas of cracking, reforming, steam reforming and isomerisation but more work is needed in hydrogenation, alkylation, hydrotreating and hydrocracking. The importance of these operations is emphasised by the 1982 US demand for catalysts which exceeded 1.3 billion dollars.

b) Catalysis in a future refinery incorporating upgrading of liquefaction products

In considering future developments, the refinery can be viewed as a basic unit to which can be added the various processes needed to handle alternative raw materials.

The most important of these alternatives are likely to be the heavy oils from liquefaction processes. For these enhanced hydrotreating operations are required in order to produce a material that can be processed in a conventional refinery. These operations differ from petroleum oil hydrotreating largely as a result of the need for more severe hydrogenation and hydrocracking and the need to remove larger amounts of nitrogen and oxygen from the oil (reactions 3-8 above). Further problems arise in that the heavy oils produce more coke and, usually, more inorganic deposits on the catalyst, resulting in catalyst deactivation — or the need to design non-deactivating catalysts.

Although such catalytic deactivation remains a problem which requires attention, the efficiency of hydrotreating can be reasonably high. Heterocyclic oxygen and nitrogen have proved the most difficult to remove, but studies of coal liquids and shale oil hydrotreating show that good quality transport fuels can be produced despite the severe requirements.

In terms of the overall process, introduction of coal- or shale-derived materials depends on cost, and hydrogen consumption in the hydrotreating processes is a major part of that cost. As a result, it would be very beneficial to find a catalyst suitable for the direct removal of O- and N- atoms from organic molecules, but this has yet to be achieved.

c) Catalysis in future refineries incorporating synthesis gas conversion

Carbon monoxide/hydrogen mixtures (synthesis gas) may be used to prepare both chemicals and fuels. In the context of catalysis and energy, the Fischer-Tropsch reaction, the production of methanol and the production of gasoline from methanol are currently important. The production of higher alcohols could be significant in the near future. Of these, probably only the products of the Fischer-Tropsch reaction would be suitable for conventional refinery processing.

The most direct route from synthesis gas to potentially useful fuels lies in the production of methanol, which can be used as a blend with gasoline as a fuel or as a feedstock for further conversion. The history of catalyst development for methanol production is a classic case study in which the activity and selectivity of $Cu/ZnO/Al_2O_3$ catalysts has been improved over many years.[17]

Although the direct combination of carbon monoxide and hydrogen is widely used throughout industry, attention has recently been refocused on other routes to methanol. The reasons for this lie in the reaction conditions needed for direct combination: even current improved catalysts are operated at 250-300°C and 5,000-10,000 kPa.[17] As a result, studies have been initiated, of a two stage synthesis first reported by Christiansen in 1919.[18]

$$CH_3OH + CO \rightleftharpoons HCOOCH_3 \qquad (9)$$

$$HCOOCH_3 + 2H_2 = 2CH_3OH \qquad (10)$$

The carbonylation reaction is catalysed by alkali metals and proceeds at 4000 kPa and 70°C,[19] while hydrogenolysis, catalysed by copper chromite, gives high yields of methanol at 160°C and 101 kPa.[20] Using this route the energy saving can be very significant.

Methanol is a valuable product — both as a fuel and a chemical — but interest is also growing in the production of higher alcohols. Mixtures of C_1 to C_6 alcohols avoid many of the miscibility problems of methanol and gasoline in the presence of trace amounts of water, and one process designed to produce such mixtures has been tested at a pilot plant level.

The most interesting use of methanol is, however, as a feed for the Mobil ZSM-5 zeolite catalyst based process for gasoline synthesis. The fact that methanol can be converted to hydrocarbons over acidic catalysts has been known for many years,[21] but the process was inefficient and non-selective. By contrast the acidity and pore structure of ZSM-5 make it a particularly suitable catalyst for the selective production of gasoline.

ZSM-5 catalysts are most effective with alcohol feedstocks, but it is possible to use the zeolite as one component of a dual function catalyst. Combination of catalysts for methanol production with ZSM-5 leads to the production of gasoline directly from carbon monoxide and hydrogen[22] but there are disadvantages. One of these is that olefinic intermediates produced during methanol conversion may be hydrogenated over the methanol-synthesis catalysts, thus reducing the yield of desired aromatics. The second is that the optimal conditions for methanol and gasoline formation are significantly different. It appears therefore that the balance of economics favours a two step reaction for gasoline production.

However, this conclusion may be too premature, in view of studies now in progress. Careful control of $CO:H_2$ ratios fed to a dual function system has led to a situation where coke formation can be almost eliminated. As a result, the overall economics may swing in favour of the dual function system.

Turning to the Fischer-Tropsch reaction, it is clear that major advances in the understanding of the mechanism of reaction have been developed in the last few years.[24] Fischer-Tropsch processes have been established since the 1920's and current industrial operations are practised on a very large scale in South Africa. What has become clear only recently is the role of carbonaceous intermediates in the reaction and the role of the catalyst in forming and promoting the chain growth of these intermediates. The present understanding of the reaction rests on four reasonably well established observations:

i) Fischer Tropsch reactions (and methanation) involve, as a first step, the dissociative adsorption of carbon monoxide on the catalyst to form a surface carbidic carbon and CO_2 or H_2O depending on the $CO:H_2$ ratio and the catalyst used.[24,25,26]
ii) The activity of catalysts is closely related to the metal-carbon and metal-oxygen bond strengths, with an optimal value existing.[24,27]
iii) Oxygen free species are the most probable intermediates in chain growth.[24,28]
iv) The most essential step involves CO dissociation. This is a multisite reaction and requires large ensembles on the catalyst surface.[24,29] Surface defects affect ensemble size and CO adsorption.

The realisation of the importance of the dissociative adsorption of CO has led to re-examination of Fischer-Tropsch catalysts and to the use of alloys or metal-support combinations that can be expected to favour the desired products.[24] Although this has not, as yet, led to new catalysts of commercial interest, there is little doubt that improvements in yield and selectivity will result from a better understanding of the reaction mechanism. For the first time in many years, there appears to be hope of a quantum leap in the design and use of novel catalysts for the Fischer Tropsch reaction.

4. CATALYSTS AND THE PRODUCTION OF ENERGY

Energy production depends primarily on combustion, but combustion has many drawbacks. Gas phase oxidation can be inefficient and unwanted pollutants can be produced. The reaction occurs only within the flammability limits of a fuel and, within those limits, is difficult to control. As a result it is not surprising to find that combustion over a catalyst (catalytic combustion) has been the focus of much attention.

Perhaps the best known use of catalytic combustion is in car exhaust systems, where unburnt hydrocarbons and carbon monoxide can be completely oxidised to water and carbon dioxide.[31] These systems are used not for energy production but for pollution control and can be disregarded in the present context. However, similar systems are used in circumstances where energy is a desired product, for example, catalytic combustion devices used in industrial deodorising,[30,31] wood stoves[32,33] and waste gas treatment.

Applications of catalytic combustors in engines are aimed at achieving efficient and complete oxidation and thus avoiding pollution by controlling it at source. During conventional combustion nitrogen oxides are produced mainly by the direct combination of nitrogen and oxygen, a reaction which is favoured at temperatures greater than ca. 1650°C. However, the use of a catalyst allows operation at far lower temperatures. The control of nitrogen oxide emission has become important recently with the realisation that it plays a significant role in the production of acid rain in certain areas of the world.

There is little doubt that catalytic combustors will become more important in energy production in the future, particularly as a result of their ability to handle a wide variety of fuels over a wide variety of concentrations.[30] New developments can be expected, ranging from catalytic cylinder heads to catalytically powered hot air balloons.

5. CATALYSTS AND ENERGY: PAST, PRESENT AND FUTURE

The application of catalysts to the production and use of energy covers a multitude of areas and yet only a fraction of the potential applications have been considered. Complex catalysts used for biomass processing or for photochemical applications have not been touched on here, despite the fact that intensive efforts are in progress to develop commercially useful materials. The advantages of selectivity and controllability introduced by the application of catalysis make the whole field a vibrant and exciting venture for the future.

Where can the major breakthroughs be expected? There is no doubt that further applications of acidic and, probably, zeolitic catalysts will be developed in the very near future, and that a range of new industrial reactions will emerge. It also seems certain that greater understanding of the role of ensembles of metallic catalysts will lead to enhanced selectivity and improved performance for a range of mono-, bi- and multi-functional catalysts. All of these developments will improve our conversion of various energy sources to other, more desirable, forms. At the same time, the possibility of more stable catalytic combustion units will lead to better energy recovery and to the production of fewer pollutants.

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APPLICATION OF INFRA-RED TECHNOLOGY TO BREATH ALCOHOL TESTING

by

G. L. Dick, Chemistry Division, DSIR, Gracefield.

Graeme Dick is a Scientist in the Drugs & Alcohol Section of Chemistry Division DSIR at Gracefield. His involvement in breath alcohol testing began in 1977 with evaluation of the Alco-Sensor II, now used for evidential breath testing in New Zealand, and has since progressed to evaluation of recent developments, including those described in his paper.

In this article, a brief account is given of the application of infrared measurement to breath alcohol analysis. Mention of particular products should not be taken as endorsement of them, and, conversely, failure to mention other similar products does not mean that they are regarded as inferior. The unmodified term 'alcohol' means ethanol.

'Evidential' of course means that the result of the analysis can be used in evidence. This may seem a trivial point, but there is an important implication to bear in mind, and this is that an acceptable level of accuracy must be met in the analysis. This can be compared with 'screening breath tests', commonly used on the roadside as the first step in alcohol testing, which are semi-quantitative at best.

The first attempt at infrared breath alcohol analysis appears to have been made about 1965 [D. W. Hill, cited in ref. 1]. This study used an infrared laser energy source, but its instability was too great to enable accurate quantitation at the low alcohol levels encountered. In 1971, Harte[1] reported the development of the Omicron Intoxilyzer (TM), and subsequent instruments have largely followed the same basic principles. Most instruments measure absorption at a wavelength of about 3.39 microns (2950 cm^{-1}) using, for example, a quartz iodide source (Intoxilyzer) or heated nichrome filament (Intoximeter 3000). Some specificity is obtained by use of narrow bandpass filters to isolate the wavelength of interest.

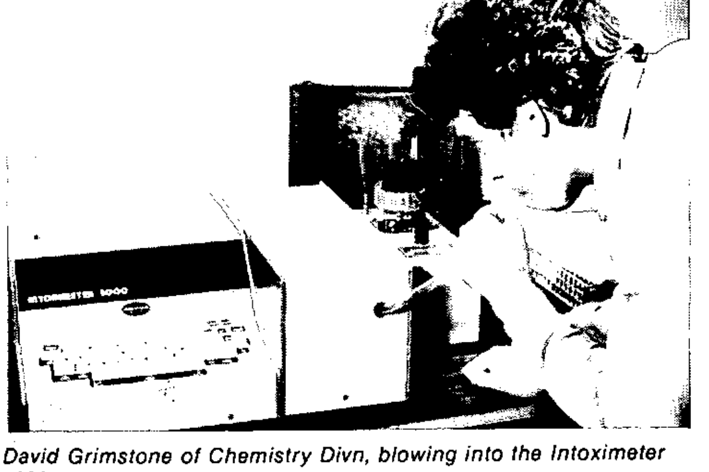
"But", I hear you saying, "2950cm^{-1} corresponds to the C-H asymmetric stretching vibration, and this will clearly be non-specific for alcohol." You'd be quite correct, and it is the way in which manufacturers have attempted to overcome this non-specificity that gives the topic an added interest.

Initially no allowance was made for interference on the grounds that to produce a reading equivalent to a blood alcohol level of only 10 mg/100mL it would be necessary for the concentration in the blood (and hence the breath) to exceed the LD50 values for the interferents[1]. This may be so in many cases, but lawyers (or consulting chemists?) were quick to realise the potential of (or for) interference by acetone, produced for example by some diabetics under some circumstances, and manufacturers have since in practice been forced to improve the discrimination of their instruments, to eliminate acetone as a possible interferent.

One approach, used in the Intoxilyzer and the BAC Verifier, is to measure absorption at two wavelengths, one more sensitive to alcohol and the other more sensitive to acetone. The ratio is compared with that obtained from a known alcohol standard, and deviation from the ratio is taken to indicate interference. A correction can then be applied to the result to deduct the contribution of the interferent. This method of discrimination copes well when something is known about the interferent, i.e. when the presence of a particular interferent is assumed — and it is usually assumed to be acetone. Acetone is the only endogenous volatile compound that could be present in a sufficiently high concentration to interfere with alcohol analysis, so this assumption will usually be correct.

The Intoximeter 3000 instrument uses an entirely different approach. Instead of a second wavelength, a semi-conductor is used to detect interference. This is the Taguchi Cell, widely used in gas detection equipment and which is well known for its non-specificity. The Taguchi Cell catalyses oxidation of absorbed molecules and changes conductivity. The ratio of infrared/semi-conductor response is then compared with that for a known alcohol standard. This is essentially the format in the Intoximeter 3000 instruments used for evidential breath testing in the UK. A recent rather ingenious development has been to make use of the dependence of the alcohol oxidation on the temperature of the semi-conductor surface[2]. The heater voltage applied to the detector is programmed to decrease in a series of discreet steps. Oxidation of different compounds will have different temperature dependences, and thus a characteristic voltage step can be determined at which maximal oxidation of a compound occurs. This detector consequently has the potential to discriminate against a wide range of interferents[2].

The problem with any method requiring interference detection is that it is necessary to show that the interference detector was working properly when a test was conducted. Put another way, if interference was not indicated was there none present or had the detector failed? Most, if not all, infrared breath alcohol instruments now available are microprocessor-controlled, and it should therefore be a relatively simple matter to incorporate



David Grimstone of Chemistry Divn, blowing into the Intoximeter 3000.

the necessary checks into an automatic routine. This difficulty may have been circumvented with a recent development by Drager in their model 7110 instrument, which apparently measures absorption of the C-O stretching vibration at 9.5 microns (1050 cm^{-1}). Interference by acetone would then no longer pose a problem.

Infrared breath alcohol testing offers the advantage of a non-invasive method of analysis which therefore minimises inconvenience to the subject; it can be performed rapidly, has long term calibration stability, and lends itself to microprocessor control and consequent simplification of operation. Although other methods are available, infrared analysis increasingly appears to be the method of choice worldwide.

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INFRA-RED ANALYSIS OF FREON IN AIR — TESTING A FIRE PROTECTION SYSTEM

by

J. W. Mitchell, Chemistry Division, DSIR, Auckland.

Jim Mitchell is a scientist, in charge of the Applied Chemistry Section of Chemistry Division, DSIR, in Auckland. He is involved in a wide range of chemical work, mostly for other government departments, but has a particular developing interest in polymer chemistry. He was previously in the Food Section of the laboratory where his interests involved trace metals analysis and wine chemistry.

Our laboratory was recently involved in an extensive test of a gas flooding fire protection system at a computer installation. The system used BTM (bromotrifluoromethane), but for economic reasons the gas used in the actual test was Freon 12 (dichlorodifluoromethane).

The objectives of the test were to establish:—

1. Whether the freon, after its very rapid initial release, was adequately mixed (freon being much heavier than air, layering is possible).
2. Whether a freon concentration sufficient for fire protection was attained quickly and then maintained for a specified time.
3. The effectiveness of the smoke clearance system (an air-conditioning system which operates when the fire hazard has been eliminated).

The ideal method for monitoring concentrations of freon in the air of the test area would have been capable of continuous measurement at each of several sites. No such system (eg several mobile IR spectrophotometers) was available to us, so grab samples were taken by feeding plastic tubing from each sampling point to electric pumps and Tedlar (polyvinyl fluoride) gas sampling bags outside the test area.

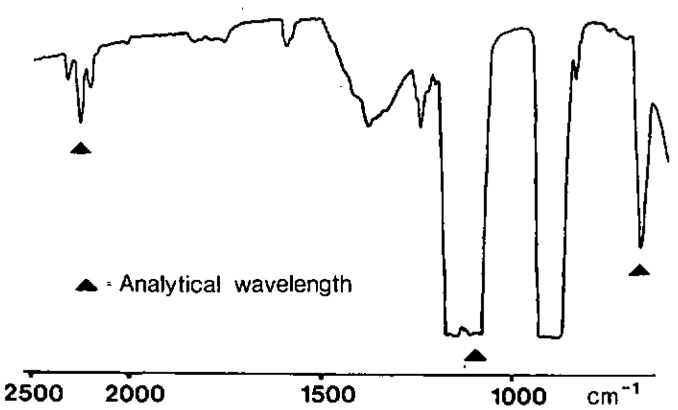

Figure 1

IR spectrum of 10% Freon 12 in air.

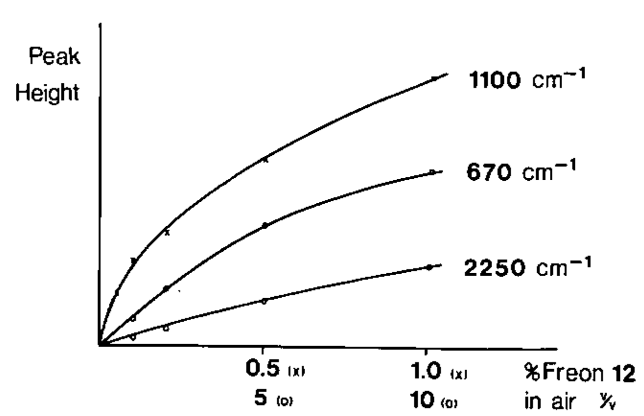

Figure 2

Calibration curves (1100 cm^{-1}, 0-1% freon; otherwise 0-10%).

A series of standard mixtures of Freon 12 in air was prepared using gas-tight syringes and gas sampling bags, and infra-red spectra were recorded using a 10 cm pathlength Pyrex gas cell with NaCl windows. A spectrum is shown as an example in Fig. 1. Study of these spectra showed that analysis could be performed over the range of concentrations required (0.02 to 15% by volume) by constructing calibration curves at each of 3 different wavelengths (see Fig.2).

The results of our tests showed that freon concentrations of 7-9% by volume in air were rapidly established throughout the room where the test took place. The freon levels remained above the required level of 5% for 10 minutes, except at the ceiling, where new air entered as the heavy freon-air mixture slowly sank away through cracks in the floor and around doors. The freon level was reduced to 0.02% after the smoke clearance system had operated for 10 minutes.

This work shows that a 10 cm cell, a relatively inexpensive accessory, can substantially extend the scope of an IR spectrophotometer. The obvious alternative analysis method (gas chromatography with thermal conductivity detection) was not available to us at the time, and would have offered no advantages for this application.

MONITORING OF FUMIGANT VAPOURS

(The Foxboro Miran 801 Infrared Analyser at the MAF Fumigation Plant at Auckland Airport)

by

C. Van Pelt, W. Arthur Fisher Ltd, Auckland

Chris Van Pelt is National Service Manager for W. Arthur Fisher Limited, and has been with the company for six years since emigrating from Holland. He is particularly involved with the servicing of process instrumentation and control systems supplied by the company throughout New Zealand.

INTRODUCTION

In a fumigation plant exposure to residual fumigant vapours is of major concern because of the possible ill effects on human health. Staff may be exposed to toxic vapours such as ethylene dibromide, methyl bromide or formaldehyde. The concentration of fumigant vapours therefore needs to be monitored to guard against this.

All of the vapours have one or more absorption bands in the infrared spectral region of 2.5 through 14.5μm. By passing an infrared light beam of the proper wavelength through a cell containing the sample to be analysed, the concentration of the vapour present can be determined by measuring the amount of infrared energy absorbed. Excellent sensitivity is achieved by using a multi-pass, long-pathlength cell.

THE MIRAN-801 MULTIPOINT CONTINUOUS ANALYSER

At the fumigation plant operated by MAF at Auckland International Airport, a Miran-801 infrared analyser is used for monitoring fumigant vapours. This is a central air monitoring system consisting of a microcomputer built around the Intel 8080A microprocessor and integrated with an infrared spectrometer and a multipoint sampling manifold (Figure 1). The system is designed to measure and record the concentration of air contaminants at up to 24 sampling locations. The microprocessor control can be programmed to simultaneously monitor any desired selection of up to 10 individual gases.

The microcomputer controls the spectrometer, signal averages the infrared transmission measurements at each programmed wavelength, calculates absorbance and uses a stored coefficient matrix to calculate the concentration of components in the air sample. Solenoid valves of the alarm system are also controlled by the microcomputer.

Incorporated into the system is a program to generate a printed record showing the time-weighted average concentration of each gas, summarized for each shift and on a monthly basis. An alarm system warns personnel when gas concentration exceeds a preset level. The typical analysis time for a six component sample is about two minutes.

OPTICAL SYSTEM (Figure 2)

The infrared head provides a beam of chopped monochromatic infrared radiation. Wavelength variation is achieved by means of a circular variable filter (CVF) which is mounted on the shaft of a high resolution potentiometer and coupled to a D.C: servo motor. The position of the CVF is controlled by a digital wavelength number which is output from the microcomputer. This system has excellent wavelength stability and it can be set to any wavelength in less than one second.

The 20 metre gas cell has entrance and exit windows, a field mirror and two objective mirrors with a pathlength control to vary the number of times that the infrared beam passes through the sample. (The cell itself is less than 0.4m long).

After passing through the gas cell, the attenuated infrared beam is focused onto a pyroelectric-type detector. This is composed of a lithium tantalate semiconductor, chosen for its infrared bandwidth, speed of response, long-term stability and durability. The detector response is not temperature dependent, however, its inherent sensitivity to thermal radiation requires that it be shielded from drafts and sudden temperature changes. The detector also exhibits a microphonic effect which requires isolation from acoustic noise.

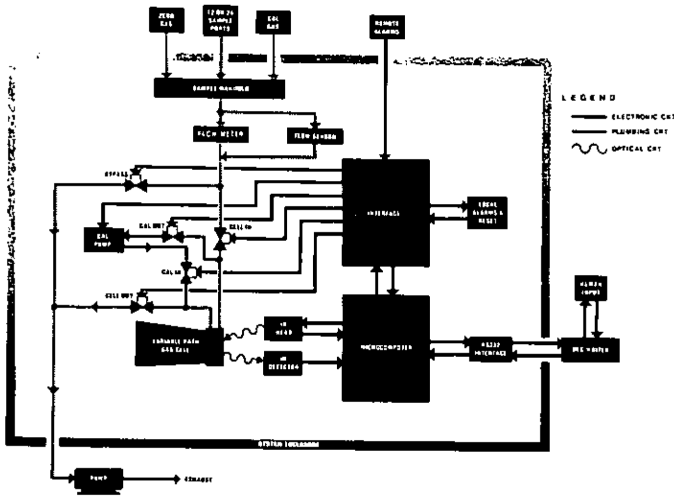

Figure 1 MIRAN-801 FUNCTIONAL BLOCK DIAGRAM

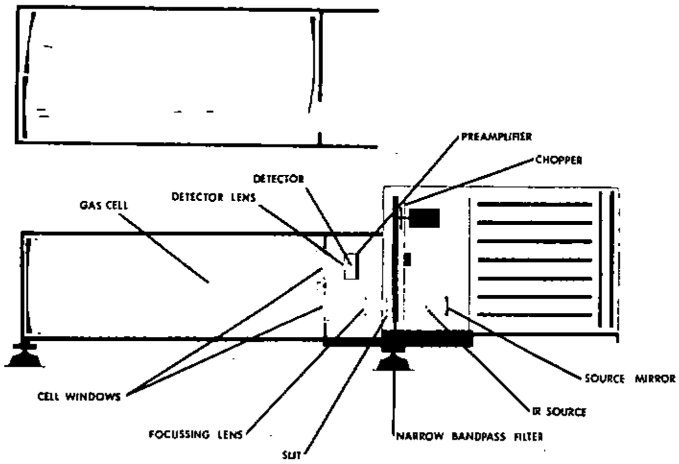

Figure 2 MIRAN-801 OPTICAL DIAGRAM

SENSITIVITY OF INFRARED SYSTEMS

The amount of infrared absorption is proportional to the pathlength of the infrared beam through the sample. For low-concentration ambient measurements, a cell is used through which the infrared beam traverses many times. With a pathlength of 20.25m, the minimum detectable level of most fumigants is 0.5ppm or less, as shown in Table 1.

Table 1. Analysing Fumigants With The Miran 801 Ambient Air Monitoring System

Fumigant	Analytical Wavelength in µm	Min. Detectable Concentration at 20.25m* (ppm)	Max. Detectable Concentration at 20.25m* (ppm) approx.
Carbon disulfide	4.55	0.5	1450
Carbon tetrachloride	12.6	0.06	32
Acrylonitrile	10.5	0.4	330
Chloropicrin	11.5	0.05	50
Ethylene dibromide	8.4	0.1	300
Ethylene dichloride	8.2	0.3	550
Methylbromide	7.6	0.4	945
Sulfuryl fluoride	11.5	0.1	57
Formaldehyde	11.9	0.2	50

*Pathlength of Gas Cell

CALIBRATION OF INFRARED SYSTEMS

The calibration of an infrared analyser system is simple and does not require standard gas samples. A "closed-loop" method is used, in which the cell is filled with clean air, and a bellows pump is connected in such a way that it circulates the air from the outlet of the cell, past a tee connection containing a septum, and back into the cell at the inlet. Known amounts of the (liquid) fumigant are injected by means of a syringe and the absorbance is recorded. Since the volume of the system is known, the vapour concentration resulting from each injection can be calculated.

COUNCIL NEWS

During March and April Mr Alan Mackney spoke to members in Invercargill, Dunedin, Christchurch, Nelson, Wellington, Palmerston North, Hastings, New Plymouth, Hamilton and

At these meetings the President expressed Council's concern at our Institute's poor record, for many years, in recruiting newly qualified chemists. Research and Development Management in New Zealand, The Forest Industries and A Growth Strategy for New Zealand were the subjects of his addresses.

AAVA Chemistry V Prize. Mr Martin B. Hunt of Palmerston North has been awarded the Institute's prize of $50 for the student obtaining the highest marks in the Chemistry V examination for NZCS conducted by the Authority for Advanced Vocational Awards at the end of 1984.

Chemistry Syllabus Committee. It is proposed that the Chemistry Syllabus Committee widen its scope to cover Chemical Education in general. The Committee has made a submission to the Department of Education's Committee of Enquiry into Forms 5 and 7.

Mr G. Valpy is convenor and Messrs Best and Freitag, Drs Sharman and Tennant are members of this Committee.

Environmental and Hazardous Chemicals Committees. Council has forwarded to the Commission for the Environment five comments on the ICI fire prepared jointly by the Environmental and Hazardous Chemicals Committees (see April issue p.41 and p.44). This material dealt with the Availability of Hazardous Chemical Data in Chemical Emergencies, Fire Service Management Procedures, Environmental Considerations (fire runoff and environmental research), Public Education on Hazardous Substances and Storage of Hazardous Materials.

In submitting the comments Council noted that members of the Institute in Auckland, through their employers, for example DSIR, the Department of Health and the ARA, also had contributed to the Commission's investigation.

In April the Council sent the Hon. C. R. Marshall, Minister for the Environment, our Environmental Committee's comment on the statement of concern by the New Zealand Ecological Society about "The Environmental Consequences to New Zealand of Nuclear Warfare in the Northern Hemisphere". This report was summarised in the April issue, p.44.

Copies of our submission were also sent to the Ecological Society and the Ministers for Agriculture and Fisheries and Science and Technology.

Although the Environmental Committee was unaware of any expertise within the Institute that could add to or comment on the Ecological Society statement with any authority or to any significant degree, it urges all members be aware of the statement and its implications. It suggested that a Conference committee arrange a session on this topic.

"Considerations of survival must not however be allowed to overshadow the main argument, that nuclear war of any kind would be catastrophic, is not inevitable and must not be allowed to happen".

The President and Dr D. E. Wright of the Public Affairs and Science Policy Committee attended the launching in Wellington on 29 April by the Prime Minister of the Royal Society of New Zealand's publication: The Threat of Nuclear War: A New Zealand Perspective". A review is planned for the Journal later in the year.

Thomson Medal and Fund. The Royal Society of New Zealand has introduced a new award to commemorate the contributions made to science by G. M. Thomson and his son, J. A. Thomson. The medal is to be awarded in recognition of outstanding contributions in the fields of the organisation, administration or application of science, or without restriction to the above, to the furtherance of science generally.

This years recipient is A.W. Mackney, President, NZIC.

DSIR — Ross Dependency Research Committee. An information package on research directions, available facilities and how to prepare a proposal is available along with support information for members wishing to put forward proposals for research projects for the 1986/87 NZ Antarctic Research Programme from the Secretary, RDRC, c/o DSIR, Head Office, Private Bag, Wellington.

TV — New Zealand. Larry Podmore, producer of "Fast Forward", screened at 7 p.m. on Saturday evenings, invites members to contact him about any new discoveries or breakthroughs that have an impact on the community. It is suggested this be done through the General Secretary.

General Secretary. Denis Hogan will act as General Secretary from 25 May until 5th August during the absence of John Rogers in the UK and Europe.

DSIR BIOTECHNOLOGY DELEGATION TO JAPAN

DSIR wish to learn of organisations interested in joining 10-12 senior scientists, three of whom will be from DSIR, to make contact with Japanese company and government workers in developmental biotechnology.

Genetic manipulation of organisms of industrial importance, enzyme and protein technology, microbial fermentation systems, plant and animal tissue and suspension culture systems, and the use of computers in these biotechnological processes, are proposed as specific topics for attention.

The 10-14 day visit in April-May 1986 will cost about $5,500 per person. NZIC members interested in joining this delegation should write to Dr J. G. Robertson, Applied Biochemistry Division, DSIR, Private Bag, Palmerston North offering contacts and noting places in Japan they prefer to visit. Formal invitations will be issued later to joint the delegation.

DEADLINE FOR SHELL AND ESSAY PRIZES

Council has postponed the deadline for entries for the Shell and Essay Prizes to 31 July. Entries should be sent to the Registrar, Box 29-183, Christchurch.

INTERNATIONAL CHEMISTRY

FACS. Dr H. J. K. Powell of the Chemistry Department, University of Canterbury, represented Council at the 3rd Biennial Assembly of the Federation of Asian Chemical Societies. This was presided over by Dr M. H. Hnoosh of Iraq in Singapore during the Asian Chemical Congress 8-11 April.

Professor H. H. Huang of Singapore was elected President of the Executive Committee of FACS and Professor Sang Up Choi of Korea as President-Elect. The 4th Biennial Assembly will be held in Seoul, Korea, late June 1987.

The Papua New Guinea Institute of Chemistry and the Brunei Chemical Society were admitted to FACS which now has 20 members. All were represented at Singapore.

The Asian Network on Analytical and Inorganic Chemistry (ANAIC), sponsored by FACS and supported by UNESCO, held its first regional seminar and the Inaugural Board Meeting in Singapore on 10 April. Dr Powell represented NZIC.

Professor Arthur Campbell has accepted nomination as the analytical chemist to act as one of NZIC's two contact persons on the Board of ANAIC. An inorganic chemist is also to be nominated.

RACI — Eighth Analytical Division Conference. Kip Powell represented NZIC at the Eighth Australian Symposium on Analytical Chemistry held in Melbourne 15-19 April.

RACI-NZIC Joint Conference. At its meeting in February Council considered a suggestion from the RACI that a joint Conference be held in 1988 to mark Australia's Bicentenary. Council expressed a preference for Hobart as a venue early in 1988 and suggested a number of topics for the programme.

A firm proposal was received in May from RACI for a RACI-NZIC Bicentenary Conference in Hobart during the week 19-25 January 1988. Council has been asked to appoint a liaison secretary to work with the President of the Tasmanian Branch of the RACI regarding organisation and development.

Members are asked to comment on the proposed date of the Conference. Members who propose to attend — families are welcome — are asked to advise the General Secretary by 1 August and to indicate their preference for University/Wrest Point/Motel accommodation.

INTERNATIONAL CHEMISTRY:

NZIC-RACI Visiting Speaker Award. The holder of the 1985 Award, Dr Charles Barnes, will be visiting Auckland, Hamilton, Palmerston North, Wellington, Christchurch, Dunedin and Invercargill 15-27 June.

His address "Chemical Adventure in Biotechnology" will describe work by Biotechnology Australia Pty Ltd. Topics included are genetic engineering a vaccine for neonatal diarrhoea, bacterial leaching of sulphide minerals, structure of an antibiotic and gene/peptide synthesis.

The RACI and NZIC Councils have agreed that selection for this award will be made in August. This will allow NZIC Branches to include the 1987 Visiting Speaker from Australia, who will be chosen in August 1986, in their programmes for 1987.

The Councils have also agreed to accept nominations for these awards from members of both RACI and NZIC each year through their Branches. Details of these proposals which are designed to make the awards more useful to members of both Institutes have been sent to Branch Secretaries.

IUPAC Affiliate Membership Scheme. At the request of the Royal Society of New Zealand and Professor Campbell, chairman of its National Committee for Chemistry, it will be recommended to Council that this Institute administer the IUPAC Affiliate Membership Scheme for our members.

This provides for NZIC members who so wish to "belong" to IUPAC as Affiliate Members on payment of approximately $20 NZ to cover NZIC administration and postage costs and the $7.50 US charge for six copies per year of Chemistry International.

Members interested in becoming Affiliate members of IUPAC are asked to advise the General Secretary before 1 August 1985.

J. Rogers Honorary General Secretary
12 May 1985

MEMBERSHIP:
At a meeting of Standing Committee on 16 May, the following applications and changes in status were approved:

Fellowship:
BOYD, Peter David William, BSc(Hons) (Tas) PhD(Monash). Chemistry Dept. University of Auckland. (Senior Lecturer).
BROOKER, Edgar George, MSc PhD(NZ). Ivon Watkins-Dow Ltd. New Plymouth. (Chief Research Chemist).
NELSON, Peter Edward, BSc(Hons) PhD (Otago). Chemistry Divn. DSIR, Auckland. (Government Analyst).

Membership:
GUMLEY, Stewart John, BSc(Hons) (Massey) D.Phil(Waikato). ICI (NZ) Ltd. Mt Maunganui. (Research Chemist).
KODY, Paulus Cornelius Maria, Analystor School, Amsterdam. Petralgas Chemicals, NZ Ltd. (Laboratory Supervisor).
McGAVESTON, Dean Arthur, NZCS BSc. Ruakura Agric Res Centre, Hamilton. (Supervisor, Plant Analysis Lab.).
PRITCHARD, Nathaniel Eames, LRIC. NZED, Huntly. (Station Chemist).
ROWLAND, Ian Arthur, BSc(Hons) (Wales) MSc(Aberdeen). Chemistry Divn. DSIR, Christchurch. (Scientist).
TENNENT, David James, BSc(Hons) (Cantuar). Linwood High School, Christchurch. (Teacher).
WATSON, Douglas James, BSc(Hons) PhD (Otago). NZ Synthetic Fuels Corpn. New Plymouth. (Chief Chemist).
WONG, Ooi, M Pharm PhD(Otago) Malaysia. (Post-Doc Res Fellow, Kansas Un.)
McKITRICK, Karen Sue (Mrs), MAOAC. AHI Technical Centre, Auckland (Analyst).

Graduate to Membership:
BENNETT, Adrian Francis MSc(Massey). Building Research Assn. of NZ, Porirua (Scientist).
BOWMAN, Nigel John, MSc(Cantuar.). DYC Foods Ltd., Christchurch. (Plant Chemist).
CARDILE, Clay Mitchell, NZCS BSc(Hons. Well), Chemistry Dept. Victoria University of Wellington (Junior Lecturer).
DENT, Barry Roy BSc(Hons. Well), Chemistry Dept. Victoria University of Wellington (PhD Student).
PURCHASE, Nigel Garth, BSc(Hons) PhD. (Cantuar.) Coal Research Assn. of NZ, Lower Hutt (Research Chemist).
WESTON, Grant Campbell, BSc Dip.Tchg. Stevens, Fitzmaurice & Partners, Auckland. (Laboratory Manager).
WONG, Lisa BSc, Dip.Sci(Otago) Dental Research Unit, MRC, Wellington (Research Asst. and MSc. Student).
LYNDON, Rex Murray, BSc., Gamlen Chemical Co (NZ) Ltd, Auckland (Chief Chemist).
YANG, David Chin Ming, MSc.(Cantuar). Wilfrid Owen (NZ) Ltd, Christchurch (Senior Chemist).

Graduate Membership:
COLLINGWOOD, Trevor Neale BSc. Chemistry Dept. University of Waikato. (MSc. Student).
DE RAADT, Anna BSc(Hons) (Well). Chemistry Dept. Victoria University of Wellington. (Ph.D. Student).
HAMILTON, Pamela Margaret, NZCS, BSc. Chemistry Dept. University of Auckland. (MSc. Student).
HERRINGTON, Philip Raymond, BSc(Hons) (Well). Chemistry Dept. Victoria University of Wellington. (Ph.D Student)
SIRIWARDENA, Asokamali (Mrs) BSc(Hons) (Massey). Chemistry Dept. Victoria University of Wellington. (PhD. Student).
YOUNG, Leslie, MSc.(Auck). Chemistry Dept. University of Auckland. (Teaching Fellow)
WELSH, Ian Kenneth, BSc. Dip.Sci.(Otago). Alliance Freezing co. Invercargill. (Bio chemist).

Technician to Associate:
BRIGGS, Paul Murray, NZCS. Aerosol Products Ltd, Auckland (Production Coordinator).

Deaths:
O H Keys Hon.FNZIC (Auck); W A Joiner Hon.FNZIC (Wgtn); G C Martin (Canty); H W Crozier, Hon.,FNZIC (Canterbury).

Resignation:
R A Hall, Waikato; A Haines (ex-O/S); R J Madden, Auck; J Samundsen, Otago.

PEOPLE

Lester Stonyer, long-time stalwart of the Institute, is to receive a prize for the best paper given at the Cosmetic Chemists' Conference in Rotorua earlier this year. Lester's paper was on the "Preservation of Shampoos". He says that he gave the topic a humorous presentation and was heartened by the number of people who said they had enjoyed it ("although few indicated that they gained much technical information").

Mr Alan Sheath has been appointed chief chemist of Lusteroid Paints Limited, the largest New Zealand-owned manufacturer of industrial coatings. Mr Sheath, 36, joined Lusteroid from the United Kingdom in April 1981 as an industrial chemist. In 1982 he was appointed deputy chief chemist, and in 1983, works chemist with responsibility for quality control.

Greg Stratton has shifted from NZ Farmers Fertiliser to Johnsons Wax.

Mr Roger Harvey, has been appointed General Manager of the Printing and Packaging Division of Whitcoulls Limited. Mr Harvey was formerly the marketing controller for New Zealand Industrial Gases, and holds a degree in food technology from Massey University.

New Managing Director for Du Pont (New Zealand) Ltd

Mr Maxwell (Max) C. Lloyd-Jones has been appointed managing director of Du Pont (New Zealand) Ltd, a subsidiary of E.I. Du Pont de Nemours and Co Inc. He transferred from Du Pont (Australia) Ltd to take up the new appointment which became effective on February 1. **Mr Lloyd-Jones** succeeds **Mr Peter A. Scott** who has retired from the company.

Senior Appointments at BJN Industrial

Two senior staff appointments have been made at the industrial division of paint and surface coatings manufacturer BJN. The appointments are part of a shift in orientation for the industrial division towards more complex technology and a heightened awareness of professional industrial marketing.

Mike Lennane, who has 27 years' experience in the industrial paint market, has been appointed Sales Manager, Industrial Coatings and Automotive.

John Hutchinson is Sales Manager, Protective Coatings and Heavy Duty Maintenance Coatings. He is responsible for the sales of industrial coatings under the 'Protection' brand name, and 'Torpedo' brand marine coatings.

BRANCH NEWS

Auckland

The President addressed a meeting of the branch in April, on the subject "The Forestry Industries". He pesented a review of the history of forestry in New Zealand, followed by an outline of the development of industries based on the exotic forests. The economic problems facing the industries in utilising the forests which will mature by the end of the century were also discussed. Mr Mackney also raised the question of recruitment of new members to the Institute, a subject which engendered much discussion.

Waikato

Alan Mackney gave his Presidential Address at a very well attended meeting of the branch in March. (See above). Also at the meeting, **Dr Don Llewellyn** was presented with an Honorary Fellowship of the Institute, and J.E. Allan Memorial Prizes were presented to the joint winners **Mark Plant** and **Leslie Arnold,** the best 2nd year chemistry students at the University of Waikato in 1984.

Dr Terry Fullerton, Forest Research Institute, Rotorua, described "The Development of Catalysts for Alkaline Pulping Processes" at the April branch meeting. Reactions of organometallic complexes with lignin model compounds were investigated and the discovery was made that simple reducing sugars are capable of promoting the lignin cleavage reaction which is believed to be primarily responsible for the dissolution of lignin during pulping. Dr Fullerton discussed the mechanism by which this is believed to occur and the implications which these results may have on the development of new pulping catalysts.

Manawatu

The Branch's prizes for the best students of 300 level chemistry and of biochemistry at Massey University were presented to **Caroline Colville** and **Fraser Fleming** respectively, by **Mr Alan Mackney** when he visited the Branch on 14 March.

The Institute's Shell Industrial Chemistry Prize for 1984 was presented to **Dr John Ayres** (Department of Chemistry and Biochemistry, Massey University) by **Mr Graham Wilson,** Technical Service Manager of Shell (NZ) Holding Co. Ltd., at a Branch meeting on 1 April. Dr Ayres then addressed the meeting on the subject: "Troubleshooting in Protein Purification by Ion Exchange", in which he described the development of ion exchange chromatography from applications of the softening of water to protein purification. Particular emphasis was placed on the development and use of the Grant Resin for the clean-up of meat works' waste, and the recent development of high capacity cellulose resins by Dr Ayres.

"The Use of Drugs to Treat Cancer: Where Are We After Fifty Years?" was the subject of an address given by **Dr Bill Denny** of the Cancer Research Laboratory, University of Auckland School of Medicine, to a Branch meeting on 30 April. Dr Denny discussed the use of drugs in cancer therapy under three headings: 1. Why use drugs to treat cancer? 2. Why aren't they very effective? and 3. What's being done to improve them? He described the development of various drugs, problems of their application to the different forms of cancer, in particular solid tumours, and current work, both in New Zealand and overseas, aimed at producing more selective and less toxic drugs.

Wellington

The Presidential address was delivered to a meeting of the branch in March. Mr Mackney spoke on "A Growth Strategy for New Zealand; The Need for Innovation." In this address Mr Mackney discussed recent proposals concerning growth opportunities in New Zealand, and drew attention to the need for consistent and far-sighted general economic policies to permit planning for the future. The support provided by both Government and private sector agencies towards R&D was examined and compared with that in other countries.

The April branch meeting was addressed by **Dr Ken Mackenzie** of the Chemistry Division, DSIR. Dr Mackenzie described the labour intensive research done in China, e.g. in one thermocalorific experiment there were 40 reaction vessels during the test, 40 technicians would be positioned at each bath each reading and recording results of one thermometer. Although the research buildings were dilapidated Dr Mackenzie was impressed with the practical and advanced research done in ceramics and how quickly the research was applied. He contrasted the research done in Japan where vast amounts of money and latest equipment means the Japanese are doing fundamental research. At one of the larger research institutes each research group was required to finish the research topic they had chosen at the end of five years, then they would move onto another one. Mackenzie finished the evening on a light note describing the eating of the famous Peking Duck where all the parts of the duck are served up in different dishes.

The following students have been awarded the Wellington Branch prizes for study at Victoria University of Wellington: **S.I.D. Barrett** (Chem 100), **K.A. Larking** (Chem 200), **R.J. Collier** (Chem 300), **S.L. Davies** (Biochem 201), and **F.M. Foster** (Biochem 300).

Canterbury

In April, **Dr Wayne Temple** talked to the Branch and the N.Z. Association of Clinical Biochemists about the types of information available at the N.Z. Poisons Information Centre in Dunedin and their efforts to computerise it.

Otago

Assoc. Prof. Jim Simpson from the University Chemistry Department lectured to a meeting of the Branch in April. His topic was, "X-ray Crystal Structure Determination — a "Routine" Analytical Procedure?".

On the schools scene, a Science Quiz was held at Moreau College, Dunedin on Friday, 26th April. Fifteen teams from high schools in Dunedin and Central Otago took part. The finalists were teams from Kings, Queens and Logan Park High Schools and The Taieri High School, the winners ultimately being the team from Logan Park High School. They received cash prizes from the Bank of New Zealand who sponsored the quiz.

GENERAL NEWS

A.C. KENNETT MEMORIAL AWARD

Nominations are now open for this year's A.C. Kennett Memorial Award, which will apply for work presented or published during the 12 months ending July 31. Full details of the conditions for the Award were published in Chemistry in NZ, **48,** 64, (1984).

IUPAC DOCUMENTS

Table of Atomic Weights to Four Significant Figures

This table has been specially prepared by IUPAC for use in secondary schools. Copies are available from Professor D.J. Waddington, Department of Chemistry, University of New York, Heslington, York, YO1 5DD, UK.

Provisional Recommendations

IUPAC is seeking comments on the following documents: Reporting Data on absorption from solution at the solid/solution interface; Specifications for Infrared Reference Spectra of Molecules in the Vapor Phase; A Descriptive Classification of the Electron Spectroscopies.

The Editor has copies of the summaries of these documents, which are also printed from time to time in Chemistry International. Full copies of the recommendations are available from: Prof. Huang Hsing Hua, The Singapore National Institute of Chemistry, c/o Chemistry Department, National University of Singapore, Lower Kent Ridge Road, Singapore 0511.

Wanted

Dr Ruth Ferguson, of the School of Pharmacy, CIT, Heretaunga (Private Bag, Trentham) is scouring the country for a Zeta meter, used for measuring the zeta potential on suspended particles. This is needed for use in student teaching laboratories, and age and condition (possibly) not important. So, any of you readers who just happen to have one of these cluttering up your benches, and just begging to be let loose on a few suspended particles, telephone Ruth on Wellington 288-169, ext 846.

CONFERENCES

1986 NZIC/NZBS Annual Conference
1986 10th Conference of the A & NZ Society for Mass Spectrometry

The NZIC/NZBS Annual Conference will be held in Dunedin, Monday, August 25 — Thursday, August 28, 1986. The Conference theme will be Applications of Modern Instrumentation. There will be a one day Symposium on Applications of Nuclear Magnetic Resonance Spectroscopy on Monday, August 25.

The Australian and New Zealand Society for Mass Spectrometry will also hold its meetings in Dunedin starting with an evening meeting on Tuesday, August 26 and closing with the afternoon session on Friday, August 29. A joint ANZMS/NZIC/NZBS Symposium on Applications of Mass Spectrometry will be held on Wednesday, August 27.

Those interested in both the NZIC/NZBS and the ANZSMS meetings will be able to apply for a joint registration.

Secretary for both conferences is: Dr J.F. Cutfield, Department of Biochemistry, University of Otago, Dunedin, New Zealand.

Australasian Corrosion Association — one-day symposium on **Process Industry Corrosion,** 18 July, 1985, Auckland.

This Symposium is being held to outline some of the corrosion problems faced by process industry staff, and to discuss the strategies available to help avoid the recurrence of these problems.

Symposium Convenor: L. H. Boulton, P.O. Box 5961, Auckland. Tel: (9) 34-116.

UNIVERSITY NEWS

Overseas Visitors

A number of distinguished chemists have visited chemistry departments throughout the country over the past four months, presenting lectures both within the universities and to meetings of some of the Branches of NZIC as well. Amongst these visitors were:

Professor J.P. Collman from Stanford University in the U.S.A. Prof. Collman researches in the field of organometallic chemistry and has a particular interest in the chemistry of oxygen transport by myoglobin-like Fe(II) porphyrins, and of oxygen utilisation by the oxygenase enzyme — cytochrome P-450. He lectured on "Fundamental Analogues of Cytochrome P-450", and "The Structural Chemistry of Multiple Metal-Metal Bonded Porphyrin Dimers."

Professor Max Herberhold, from the University of Bayreuth in Bavaria, who gave seminars entitled, "Stabilisation of Small Sulphur-containing Molecules in Transition Metal Complexes". He is the author of a two-volume monograph on mono-olefin pi complexes of transition metals, and has wide research interests which also embrace the chemistry of sulphur-nitrogen compounds and the synthesis of ferrocenyl compounds.

Professor Ron E. Hester from the University of York recognised principally for his contributions to Raman and infrared spectroscopy of short-lived reaction intermediates by using high powered pulses of radiation of very short duration from excimer U.V. lasers. The title of his lecture was "Spectroscopic Studies of Photochemical and Electrochemical Reaction Intermediates".

Cancer Research, Auckland

Dr Bill Denny is to be a plenary lecturer at the 4th RACI National Conference on Medicinal and Agricultural Chemistry in Melbourne during May.

Waikato

Dr Malcolm Carr and **Ms Valda Kirkwood** (Teaching Fellow) have prepared a position paper on internal assessment of laboratory work in 7th Form chemistry for distribution to all schools by the Universities Entrance Board, (the revised prescription proposes 20% internally assessed laboratory work). Dr Carr is joint Director (with Dr R.J. Osborne — Physics) of a three-year research project, funded by the Department of Education, to investigate learning about and teaching about energy in primary and secondary schools — the Learning in Science; Energy Project.

Canterbury

The University of Canterbury Chemistry Department and Chemistry Division, DSIR, are jointly funding the purchase of a Kratos MS80 gas chromatograph — mass spectrometer system. The instrument, which will have facilities for capillary GCMS, chemical ionisation, and fast-atom bombardment, will be installed later this year, and a data system will be added during 1986.

Professor Leon Phillips has been awarded a contract by DSIR for research on the analysis and monitoring of anaesthetic gas mixtures.

Otago

Four members of the Chemistry Department recently talked about their research activities on radio. **Assoc. Prof. David Fenby** introduced the programme in which **Prof. P.K. Grant** spoke on the chemistry of perfume compounds, **Prof. B.H. Robinson** discussed organometallic catalysts for the oil industry, **Assoc. Prof. D.J. Brasch** talked about his studies of polysaccharides extracted from seaweeds, and **Dr K.A. Hunter** talked aout the estimation of trace metal contents of natural waters.

In May, a one-day symposium on the Chemical Analysis of Water will be held in the Chemistry Department in association with TELARC. Speakers will include **Dr J.M. Robertson** (Government Analyst with the DSIR in Christchurch), **Dr E.T.J. Bathurst** (Head of the Water Section at the DSIR in Christchurch), **Dr J.B. Macaskill** from the Hamilton Science Centre, **Mr L.R. McKenzie** from the Southland Catchment Board, and **Dr J.H. Garside** (Director of TELARC in Auckland).

Dr Richard Beyer, formerly a student in the Nutrition Department, has returned from a post with the Australian Armed Forces Food Research Institute in Tasmania to a lecturing position in the School of Home Science's Foods Department. Richard plans to continue his research on polysaccharide gums.

Dr Don Ferry, of the M.R.C. Toxicology Unit, returned early this year after 15 months on study leave in the Division of Clinical Pharmacology at the University of North Carolina. He collaborated in studies on in vivo and in vitro pharmacokinetics of several drugs.

The Department of Biochemistry welcomes two visitors who have arrived this Autumn. **Dr Brian Catley** is from the Department of Brewing and Biological Sciences, Heriot-Watt University in Edinburgh. He is interested in the synthesis of the cell wall glucans of Candida albicans and will be joining Dr Sullivan's group during his six-month stay. **Dr Berthold Kastner,** from the Max Planck Institute for Molecular Genetics in Berlin, is a recipient of a Feodor Lynen Fellowship from the Alexander von Humboldt Foundation and a University of Otago Postdoctoral Fellowship. Dr Kastner is an immuno-electron microscopist who has developed novel techniques to determine the orientation of subunits in macromolecular complexes. He has worked specifically with the ribosome, and will spend a year in the research group of **Dr Warren Tate.** They will be attempting to map where the polypeptide chain release factor binds to the ribosome during protein synthesis.

From the Pharmacy Department, Head of Department, **Prof. D.G. Perrier** will be leaving in December to become Dean of Pharmacy at the University of Toronto in Canada. He will have been at Otago for a little over three years. **Richard J. Prankerd** has now completed his Ph.D. while working under **Dr R.H. McKeown.** He will now proceed to postdoctoral studies in pharmaceutical chemistry with **Prof. V. Stella** at the University of Kansas in the U.S.A. Dr McKeown will present papers at the R.A.C.I.'s Division of Medicinal and Agricultural Chemistry 4th National Conference to be held at Lorne, Victoria, in May.

GOVERNMENT DEPARTMENTS & RESEARCH INSTITUTES

FOREST RESEARCH INSTITUTE

Dr Terry Fullerton has been awarded a Gendron Fellowship by the Pulp andInstitute of Canada in Montreal to enable him to spend six months at the Institute later this year. While there he will study the interactions that occur between carbohydrates and lignin during pulping with the objective of using this information to improve existing pulping processes and develop new ones.

Wheat Research Institute

Dr Howard Dengate left in May to take up the position of Director of the NSW Department of Agriculture's Agricultural Research Institute at Wagga Wagga.

MAF, Ruakura Agricultural Research Centre

Dr Denis Lauren will be on leave in Canada for 12 months from the end of May. He will spend this time at the Chemistry and Biology Research Institute of Agriculture Canada in Ottawa. Dr Lauren will be part of a combined research team from Agriculture Canada and Carleton University involved in the isolation and structural characterisation of mycotoxins and secondary metabolites from *Fusarium* fungal species. He will also attend a Gordon Research Conference on Trichothecenes and present data on techniques for carotinoid analysis by HPLC at the annual conference of the Association of Official Analytical Chemists. Major travel funding for Dr Lauren's trip has come from the Stapledon Memorial Trust in England, the Trimble Agricultural Research Fund, and also the Corday-Morgan Memorial Fund to cover additional travel to visit ICI research facilities in England.

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Building Research Assn

P.K. Foster is attending a meeting of the board of the Council for International Building Research and Documentation (CIB) in Moscow on 16 and 17 May. He is returning to New Zealand the following week through Beijing to make contact with the China Academy of Building Research.

Health Department, NECAL

The National Environmental Chemistry and Acoustics Laboratory was officially opened by the Minister of Health, **Dr Bassett** in March of this year. Although occupation of the building was completed during 1984, the opening was delayed by the snap election. (Fortunately, the official plaque was not prepared until the election result was known).

The building finally brings together all of the various sections of NECAL on the one site — chemistry, electro-acoustics, engineering, library, and administration. The Northern Region Air Pollution Control Group, and the Regional Noise Engineer are also housed on the site.

The chemical activities of NECAL are in the areas of air pollution monitoring, industrial hygiene, hazardous waste disposal, and general areas of environmental chemistry as they relate to public health.

D.S.I.R. Applied Biochemistry Division:

Mr Martin Hunt was awarded the Institute's prize for the student obtaining top marks in the AAVA Chemistry V NZCS examinations for 1984. Since joining the Division in 1981 Mr Hunt has been involved in a wide variety of projects, as well as working in the Division's Analytical Laboratory for a year.

Dr Warren Holloway has taken up a postdoctoral fellowship at the Chemistry Department, Faculty of Science at the Australian National University, Canberra. The position is supported by the Australian Centre for International Agricultural Research and is concerned with the improvement of the staple food crops and the nutritional status of the peoples of the South Pacific.

DSIR, Chemistry Division, Gracefield

Dr A.R. Gainsford visited Melbourne during April to attend the Eighth R.A.C.I. Analytical Chemistry Conference. While he was in Australia Dr Gainsford also visited a number of organisations where A.R.L. Optical Emission Spectrometers are used as primary analytical equipment.

Dr G.J. Gainsford attended a computing school and the Crystal XV Conference in Adelaide, organised by the Society for Crystallographers in Australia. He also visited other organisations in Sydney, Canberra and Melbourne to look at computer systems; particularly those with interactive graphics.

Dr N.B. Milestone is spending the next year at the Brookhaven National Laboratory in New York where he will be studying the durability of geothermal well grouting systems. Neil will be investigating systems which will withstand high temperature and acidic conditions, some of the factors contributing to the problems encountered in the new geothermal development at Ohaaki.

Dr N.K. McCallum has transferred from the Natural Products section to the Drugs and Alcohol section at Gracefield.

The Food section at Chemistry Division has recently installed a Hewlett-Packard 5970B Mass Selective Detector. This instrument will be used to detect trace contaminants, particularly TCD Dioxin in the environment and in food samples.

Dr G.J. Sutherland has returned to the Drugs and Alcohol section after working for seven months in the Laboratory of the Government Chemist in London. At the LGC Graham examined methods for the examination of illicit heroin as an aid to the identification of batches or country of origin.

Dr L.P. Aldridge has recently returned to Chemistry Division after a year visiting the Institut fur Physik, Medizinische, Hochschule, in Lubeck, West Germany. In Germany Laurie calculated spectral parameters for ferrous and ferric ions in minerals using extended Huckel and Multiple Scattering X-L molecular orbital methods. He recently attended the International Workshop on 'The Theoretical Approaches to the Description of the Electronic Structures of Transition Metal Compounds' at San Miniato near Florence in Italy.

Chemistry Division Seminar on Cementitious Materials

Thirty-nine participants from industry, MOWD, Research Associations and Chemistry Division attended an all day seminar on the 23rd April to discuss current work in the field of cementitious materials.

Talks were given on current work at the Building Research Association of N.Z. by Dr Sharman, at the N.Z. Concrete Research Association by Mr Gaerty and the Central Laboratories of the MOWD by Mr Smith. The seminar was opened by Dr Leary, Director of Chemistry Division, and a general overview of past and present research activities in the Division was given by Dr Bibby. The two technical speakers from Chemistry Division, DSIR were Mr St John who spoke on Petrography and the Durability of Concrete and Dr Milestone who reviewed the Division's work in Cement Chemistry.

Chemistry Division, Christchurch

Dr Mike Taylor is leaving on 13 June to spend 15 months in the Forensic Science Laboratory in London working on computer based methods for analysing physical evidence from crime scenes.

Dr John Bathurst attended the RACI Analytical Conference in Melbourne in April and visited other water laboratories in Melbourne and Adelaide.

SAFETY Guidelines to Chemical Safety

There are three routes by which chemicals may enter the body: skin contact and absorption, ingestion, and inhalation. In the workplace the first two of these are relatively easy to control, the third presents more difficulties. Inhalation of airborne vapours can be controlled by means such as ventilation, the use of some form of respirator or breathing apparatus, or substitution of a less hazardous material. But before such steps are taken, how can we tell whether they are really necessary?

Threshold Limit Values (TLVs)

TLVs are the criteria used in this country as guidelines for exposure to airborne contaminants in the workplace. Published annually by the Department of Health, these are based on, with minor modifications, exposure limits established by the American Conference of Governmental and Industrial Hygienists in the USA. Copies of tables of the TLVs are readily available from District Offices of the Department, and their interpretation and use are fully explained in the TLV booklet.

Knowledge of the TLV for a particular chemical does not tell us whether that limit will be exceeded in a particular situation. There is only one way that can be determined — by measurement of the airborne concentration. This will be the subject of a future article in this series. There are however two other indices that one can use to at least get a "feel" for the likely probability that a hazard will exist or not.

Odour

In some cases odour can provide a reliable indication of the concentration of a vapour in air, although it should be recognised that sensitivity to odours can vary between individuals. There are a number of tabulations of odour data in the literature — two of the most extensive being Vershueren, Handbook of Environmental Data on Organic Chemicals — 2nd edn, New York: Van Nostrand Reinhold, 1977, and Amoore and Hautala, J. App. Toxicol, **3**, 272, (1983).

The most reliable use of odour data will apply when the threshold of perception is less than the TLV. If one cannot smell the chemical, the concentration in air is probably quite safe. Conversely, if the TLV is less than the odour threshold, detection of an odour indicates an unsafe concentration.

Two additional points should be recognised. One cannot readily judge concentrations above the odour threshold, and, with a number of chemicals the sense of smell may be anaesthetised by exposure (H_2S being the prime example). Mixtures of chemicals may also present special problems.

Vapour Hazard Index

A number of authors have attempted to relate the degree of vapour hazard from a chemical to a combination of the TLV and the liquid vapour pressure. The rationale is that the vapour pressure is indicative of the rate at which the material evaporates, and therefore the relative ease with which it will attain any concentration in the air. This concept was raised as far back as 1959 in an approach to recommending face velocities for laboratory fume hoods (J.E. Peterson, Ind. Hygiene J., 259, (1959)), and again in 1963 in a paper on ventilation requirements for the oven-curing of surface coating materials (J.F. Boyle, N.P. Novak, Ind. Hygiene J., 606, (1963)). More recent publications have included those by Reed and Scala (Paint, Oil and Colour J., 778, (1971)), Meadows (Processing, 13, (1976)), Pitt (Chem. and Ind., 804, (1982)), and Popendorf (Am. Ind. Hygiene Assn. J., **45**, 719 (1984)).

In principle the concept seems quite reasonable, and allows a useful ranking of the relative degree of hazard from a range of materials. However, as pointed out by Coker (Chem. and Ind., 91, (1983)) there are some pitfalls: "TLVs are not intended as a relative index of hazard or toxicity. (They) are set for a variety of different toxic effects, some for acute reactions such as irritation, some for chronic effects such as damage to body organs and cancers, and some to prevent allergic sensitisation." In addition, evaporation of a material may well be influenced by the way in which it is used (e.g. high temperatures, increased air movement, thin films, aerosol generation) and may not follow the simple behaviour predicted by vapour pressure data. The presence of a mixture of chemicals will also produce complications.

The use of a vapour hazard index is probably quite acceptable if one confines the application to groups of related chemicals with similar toxic affects. It can serve as a pointer to the substitution of a "safer" material, and would allow one to predict changes in ventilation requirements in a "known" system.

(Note: copies of most of the papers referred to above are available on request.)

Bruce Graham

INFRA-RED

INFRARED SPECTROSCOPY — WHAT'S AVAILABLE?

A.C. Herd, Auckland Technical Institute

Once again it is necessary to commence an intrumental overview with the statement that there is insufficient space to do justice to the wide range of instruments, applications, data handling methods, and acccessories available on the New Zealand infrared scene. Interested readers wishing further information are invited to use the reader reply card or to contact the listed agents directly (but please give Chemistry in New Zealand a mention). For those who have ignored the IR scene for a year or so, be prepared for a shock, Fourier Transform IR is just one of a number of advances that have come to fruition in the last few years. Until recently, seen as a technique that had passed its best years, in 1983 infrared spectroscopy was referred to as "the most nearly universally useful of all instrumental techniques."

Dispersive Systems

Conventional grating or filter spectrometers are facing a considerable challenge from FTIR but partly because of this competition are markedly improving in quality and are competing effectively on a cost basis and in most analytical applications.

Jasco — NZ agents Watson Victor Ltd, circle on the reader reply card. Looking very unlike the first Jasco spectrophotometer I ever used, a battleship grey monstrosity in the bowels of Tokyo University, Jasco offer a number of models, the IR-810 which is a ratio-recording instrument measuring over 4000-400cm^{-1} (Figure 1). Model A-702 is a high performance model with a resolution of better than 0.25 cm^{-1} at 1000cm^{-1}. The model A-100 is an economical instrument for quality control, student use etc. A Jasco data system is also available for automatic baseline correction, differential spectra etc.

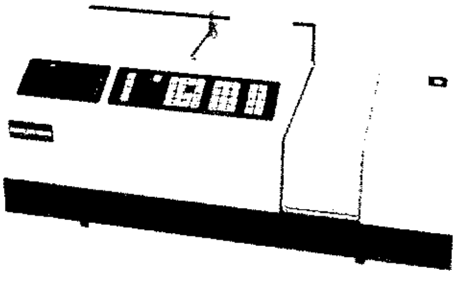


Figure 1. The Jasco IR-810.

Philips — Sold and serviced by Philips NZ Ltd, circle **17** on the reader reply card. The SP3 series of ratio-recording instruments has fast pyro-electric detectors and high emissivity sources. Data processors and data control consoles (Fig 2) are also available. The PU9510 and PU9520 series offer high resolution ratio recording down to 200cm^{-1}.

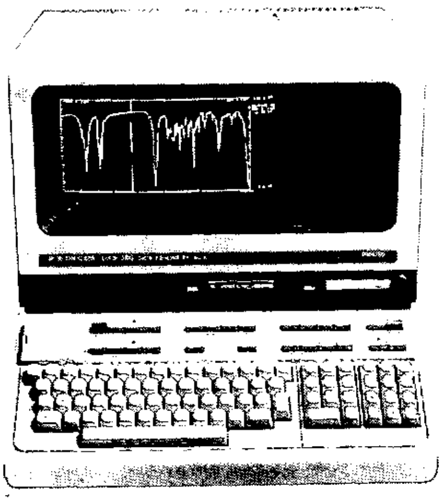


Figure 2. The Philips SP3-080 Data Control Console.

Perkin Elmer — New Zealand agents John Morris Scientific Ltd, circle **18** on the reader reply card. Perkin Elmer have a large number of models, the 983 G has a wavelength range 5000-180cm^{-1}, stores two complete spectra and has built in data handling. The 780 series has background correction, four slit programs, allows the storage of up to ten analytical parameters, and features pre-sample chopping on the 783. Samples, particularly polymer films can experience sufficient heating for the resulting emission to cause significant errors at longer wavelengths with strongly absorbing samples. Pre-sample chopping eliminates this problem (Fig 3). The 1400 series is again ratio recording with ordinate scale expansion and automatic gain set. They are based on the 1300 series, double beam optical null units with microprocessor control. Perkin Elmer also offer the 710B, a low cost instrument for routine use.

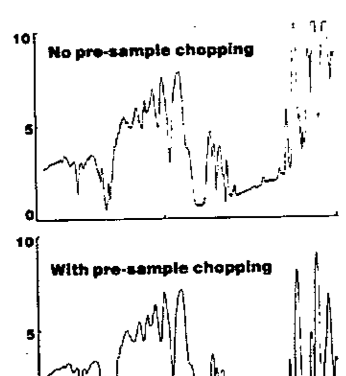


Figure 3. The effect of pre-sample chopping on the Perkin Elmer 783.

Shimadzu — NZ agents Sci-Med NZ Ltd, circle **19** on the reader reply card. The Shimadzu IR-435 has a parallel head printer which give simultaneous spectrum and frame printout. A built-in data processor accommodates seven files, each of which holds 1000 point data. Output signals can also be processed directly and instrumental parameters are stored in backup memory.

Fourier Transform Systems

Although not fully supporting a 1983 prediction that grating instruments will be entirely superceded by FTIR systems, the Analytical Chemistry's 1984 Fundamental Reviews notes that all U.S. manufacturers of dispersive instruments now have an FTIR product line, and one of them has stopped manufacturing dispersive instruments entirely. A number of commercial FTIR spectrometers can produce a complete IR spectrum on a video screen at 2-4cm^{-1} resolution and with a S/N ratio of 500-1000:1 less than half a minute from the time of introduction of the sample.

Bruker — NZ agents Sci-Med NZ Ltd, circle **20** on the reader reply card. This West German company manufactures a range of FTIR spectrometers. The IFS-45 is a bench-top model for routine application, a single beam instrument, it ratios the measured sample spectrum against a stored background. Model IFS-85 (see Fig 4) is an applications orientated instrument designed with automation in mind. It is also suitable for GC-IR and HPLC-IR work. The IFS-100 series is the research FTIR spectrometer line, fully automated so that changeover of beamsplitters, sources, apertures etc can be controlled by computer command.

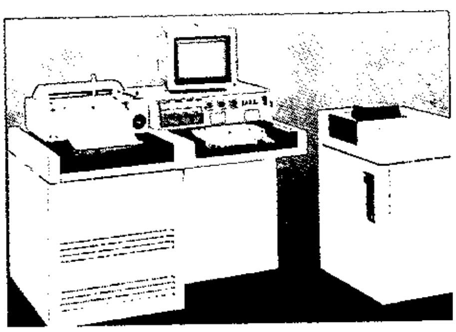


Figure 4. The Bruker IFS 85 FTIR.

Mattson Instruments — NZ agents Advanced Electronics Ltd, (supported by Mattson Instruments in Australia), circle **21** on the reader reply card. The Sirius 100 FTIR claims a resolution of 0.125 cm^{-1} and a variety of beam splitter and detector combinations enable operation over the range 25000 to 10 wave numbers. The Cygnus 25, like its sophisticated stablemate has been designed with a large sample space so that with the addition of removable pre-aligned optics, techniques such as ATR are not forced into unfavourable configurations.

INFRA-RED

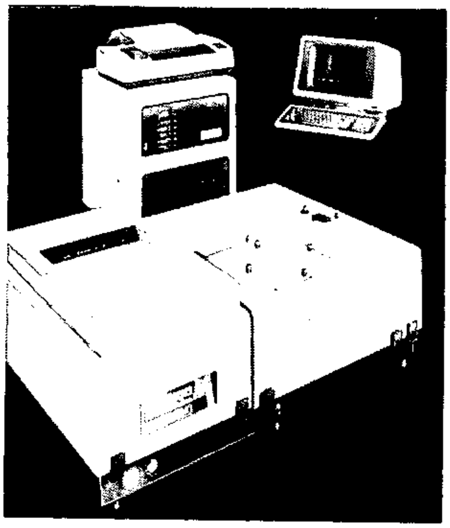


Figure 5. Mattson Instruments' Sirius 100.

Nicolet — NZ agents, Watson Victor Ltd, circle **9** on the reader reply card. A Nicolet FTIR spectrophotometer featured on the front cover of Chemistry in New Zealand in October 1982 (Fig 6) and Nicolet claims to have installed more FTIR instruments in more laboratories world-wide than any other manufacturer. The wide range of models extends from the compact, economical 5MX to the high performance 170SX with spectral resolution to $0.06cm^{-1}$.

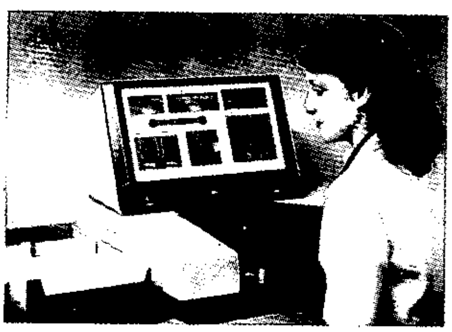


Figure 6. The Nicolet 5MX.

Perkin-Elmer — John Morris Scientific Ltd, circle **10** on the reader reply card. There are two series of FTIR spectrophotometers from Perkin Elmer, the 1800 series, and the 1700 series (See Fig 7).

Special IR Applications

i) Milk Analysers — Foss Electric, NZ agents Watson Victor Ltd, circle **11** on the reader reply card. Foss market a range of Milko-Scan automated instruments that utilise infrared to analyse milk products for fat, protein, lactose and water and for calculating total solids and non solids fat (Fig 8). The systems are single beam, using filters to choose suitable sample and background wavelengths.

ii) Ambient Air Analysers — Miran, W. Arthur Fisher Ltd are agents for the Foxboro Miran infrared ambient air analysers. Mention of the Miran range was made in the feature on Portable Gas Detection Methods in the August 1984 issue of Chemistry in New Zealand. The range includes the 101 Specific Vapour Analyser, factory calibrated for the measurement of a single vapour, the portable Miran IB with liquid crystal display, the computing Miran 80 and the microcomputer controlled Miran 980A (Fig 9).

Figure 7. The 1700 Series from Perkin Elmer.

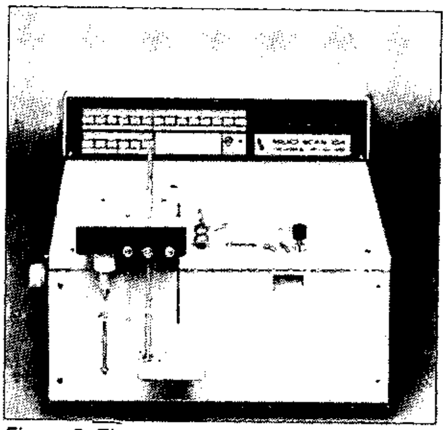


Figure 8. The new Milko-Scan 104 from Foss.

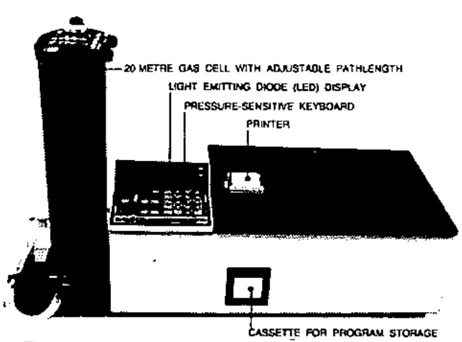


Figure 9. The Miran 980A Ambient Air Analyser.

iii) Near Infrared — Dickey-john, marketed by Watson Victor Ltd, circle **12** on the reader reply card. Two instruments, the Instalab 800 and 600, utilise reflectance measurements in the near infrared (750 to 2500 nm). Solid or semisolid samples can be measured and the instruments are calibrated against a range of representative samples of the material to be tested. Initially used by the food industry, it is increasingly finding applications in areas such as pharmaceutical, petroleum and cosmetic manufacturing.

Accessories

i) IR Chromatography Detectors Several FTIR spectrometers allow for connection to a GC or LC system. Nicolet's GC-IR package for example, shows a series of IR spectra in real-time as the GC run proceeds (Figure 10). Mattson's Cryolect approaches the problem in a different way by freezing the GC eluent at 12K on a gold collector. This method has no time constraints on IR parameters and claims 100 times the sensitivity of GC-IR methods.

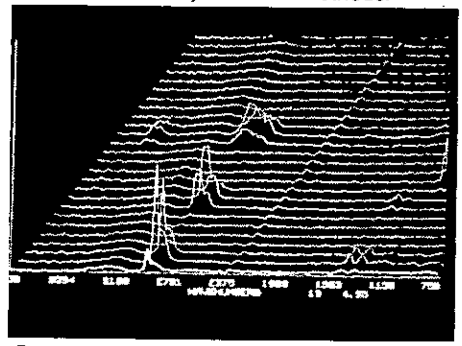


Figure 10. The colour raster display of a series of real time IR scans as a GC run proceeds.

ii) Accessory Catalogs A number of manufacturers produce accessory catalogs, for example the Philips catalog lists various sample holders and windows, presses for KBr disks, and ATR units. The Perkin Elmer accessory catalog, as well as the more conventional accessories mentions a diamond anvil cell which allows IR spectra to be recorded while the sample is under high pressure, an example of a single textile fibre pressed into a film is given. Foxboro Wilks have a catalog which, as might be expected, contains a large selection of gas cells, but also windows and reflectance attachments for a variety of spectrophotometer brands.

iii) Data Processing Too much to mention. Readily available computing power, search facilities etc have contributed to the upswing in IR's popularity. All manufacturers previously mentioned will supply information on request.

iv) Applications Brochures Again the wide variety makes a comprehensive survey impractical. Instead, one example which helps to show how far IR has come since most of us puzzled over the spectrum of an unknown organic solvent. Figure 11 says it all, 1% w/v asprin in water, the strong water absorbances subtracted out, 3000 to 900 cm^{-1} in 30 seconds on the Perkin Elmer 1700 series.

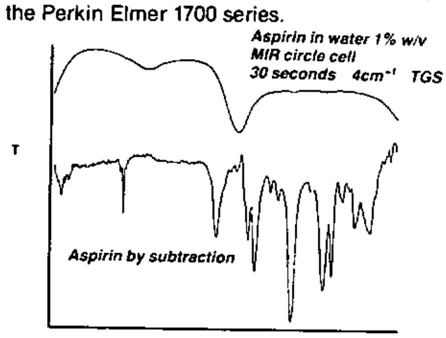


Figure 11. Asprin in water in 30 seconds.

Conclusion This brief look at the IR power available to chemists today does not claim to be comprehensive, just because a particular feature is not accredited to a particular manufacturer does not necessarily mean it's unavailable. Contact your local branch and ask.

INFRA-RED

CC/IR ON THE PERKIN/ELMER 1700 series

Perkin-Elmer Limited announce the availability of a major new accessory for the 1700 Series FTIR spectrometers; the 1700 SERIES GC/FTIR INTERFACE.

The GC/FTIR Accessory consists of:
Temperature Controlled Heated Light Pipe
Temperature Controlled Transfer Line
Accessory Controller Unit
GC/FTIR Software

The accessory will run on a basic Model 1710 FTIR Spectrometer!

The ability to combine Gas Chromatography and FTIR spectroscopy offers the chemist a unique and powerful system for the analysis of both simple and complex chemical mixtures. The strengths of both analytical techniques are brought together in an integrated system. For mixture analysis the gas chromatograph is used to separate a sample into its individual components and the FTIR spectrometer used to detect each component, obtain its spectrum and identify it.

Accessory Hardware

The accessory works by splitting the GC gas stream after the column. Part of the flow is passed to the standard GC detector and the bulk is passed through a heated transfer line to the heated light pipe in the Model 1700 sample compartment. When a peak enters the light pipe it is detected by a unique IR peak detection system, its spectrum is obtained and stored in the 1710 memory. Spectra from up to 63 peaks can be stored.

Temperature controlled Heated Transfer Line

A critical part of the GCIR accessory is in the transfer of the GC column eluant from the gas chromatograph to the IR light pipe in the interferometer. It is important that the transfer line is long enough and flexible enough to connect to a variety of gas chromatographs and be suitably designed to minimise any adverse effects on the chromatographic resolution. We have adapted technology developed by the ATD 50 to make a 1.3m long transfer line from the GC to the heated light pipe. The line is constructed from a 0.3mm internal diameter de-activated quartz capillary tube running down a nickel sleeve. This is wrapped with a heating element and then surrounded with 50mm of silicone rubber insulation. The nickel sleeve offers mechanical protection to the quarts capillary and ensures an even temperature along the transfer line length. The operating temperature of the line is controlled from a separate Accessory Control unit and sensed by two thermocouples in contact with the nickel sleeve. Heating of the line is boosted at its ends to ensure any heatsink effects from couplings are minimised, and the temperature is controlled to within 1°C.

Temperature Controlled Light Pipe

After the transfer line the GC eluant passes into the temperature controlled IR light pipe. This is a miniature heated gas cell constructed from a gold coated glass tube, 19cm x 0.2cm, held in a thermostatted oven. The light pipe and oven are fitted in the sample compartment of the spectrometer. Suitable transfer optics are used to ensure a high optical throughput and allow the instrument to scan routine samples while the accessory is fitted. simply removing a mirror mount and replacing it with a kinematically mounted sample slide. The whole accessory can be removed very readily and replaced without the need for realignment.

Temperature Control Module

The accessory includes a temperature control module for independently regulating the transfer line and light pipe temperature. The temperature can be set in 25°C increments up to 275°C. The control module is also used to set a data acquisition trigger level derived from the F.I.D. output on the chromatograph.

GC/IR SOFTWARE

The GC/IR software is on a printed circuit board which fits into the processor unit of the 1710 and adds a further five pages to the VDU controller screen. The software is used to set up the data acquisition, collect the data, display the IR generated chromatogram and finally to review the IR spectra after the run has finished.

IR peak detection

The presence of a peak in the light pipe can be detected from its effect on the interferogram. This provides a unique method of detection and allows an "IR" generated chromatogram to be displayed in real time on the 1710 VDU screen.

GC peak detection

The presence of peaks in the light pipe can be detected from the GC detector signal and a suitable delay incorporated in the system prior to data acquisition.

IR chromatogram

The signal from the IR peak detector is displayed on the VDU controller screen during the experiment and generates an IR chromatogram.

The GC/IR accessory has been designed to work with most modern gas chromatographs and fitting kits are available for all current Perkin-Elmer instruments as well as a universal fitting kit. The accessory has been optimised to work with a Perkin-Elmer 8300 Series gas Chromatograph using the latest technology in capillary columns.

The use of wide bore capillary columns allows a combination of good chromatographic resolution and higher column loadings to be achieved allowing detection limits of around 100 ppm with the FR-DTGS detector.

MCT Sensitivity

Although we believe that many real analytical problems can be solved with the FR-TGS detectors, for maximum sensitivity a narrow band MCT detector should be used. The first results on our own MCT detector show sensitivity equal to that specified by Nicolet for the 20 SXB — not bad for the lowest cost system available!

Miran IA for ethylene oxide monitoring

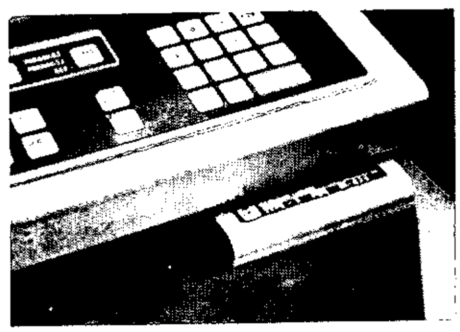
The January/February 1985 issue of the Journal of Hospital Supply, Processing and Distribution featured an article on the use of the Foxboro Miran IA general-purpose gas analyser in an American Hospital's risk management program. For further information contact W. Arthur Fisher or circle on the reader reply card.

SHIMADZU IR—435 INFRARED SPECTROPHOTOMETER

Plug-in optional program units further enhance the versatility of the Shimadzu IR-435 microprocessor-controlled IR spectrophotometer.

The program cassette CIR-1 features:
Spectrum smoothing on either stored or real-time spectra
First and second order derivative spectra (stored or real-time)
Peak detection mode: Wavenumbers and photometric values are printed out by the peaks as they are recorded by the printer.
Accumulation mode: Allows recording of multiple scans and by attenuating the noise from run to run, obtaining spectra with a very high signal to noise (S/N) ratio.

The program cassette CIR-2 features:
Quantitative analysis programs — effect quantitative analysis of the concentration of a compound and prints out the result. Also draws a working curve of standards with axes. — can calculate and print out the ratio of concentrations of a sample made up of two components. — inclined baseline correction program. — area integration program.



These program cassettes simply plug into the front of the IR controller unit and may easily be exchanged with each other depending on your application requirements.

These additional features neatly complement the impressive array of functions already built into the standard IR-435 spectrophotometer, which include: spectral storage; arithmetic manipulation of stored or real-time spectral data; framing of spectra; print-out of spectra, analysis results, and operating parameters on the same sheet.

For further information contact Sci Med or circle on the reader reply card.

NEW "SHORT-BEAM" INFRA-RED TECHNOLOGY FROM FOSS ELECTRIC

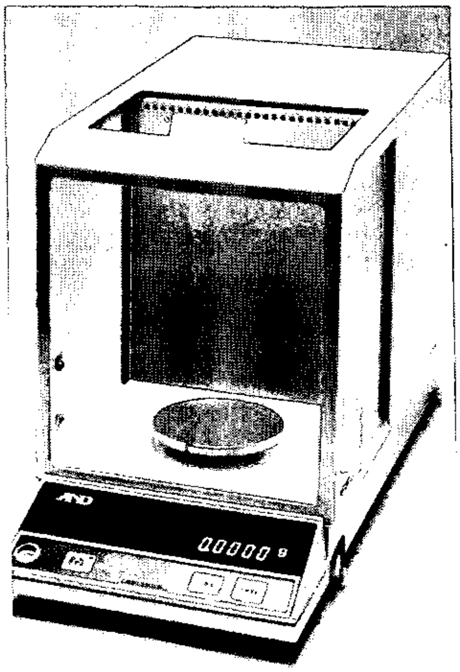
In order to meet the high quality requirements of the modern dairy industry, an entirely new "short beam" infra-red technology has been developed. The "short beam" optics of the latest Foss Milkoscan's make it possible to fit the entire optical system into a small, but highly stable and sturdy box which forms the "HEART" of the instrument. This design yields unprecedented reproducibility and stability of calibration.

The compact "short beam" system contained in the "HEART" of the instrument has reached the ultimate in simplicity. Using no mirrors except the two conical reflectors, and having an optical way length of only 27 cm, it represents a dramatic departure from traditional systems using as many as ten mirrors. In spite of its simple design, the "short beam" system uses the proven single cell, single beam, dual wave length Milko-Scan principle.

PRODUCT NEWS

NEW ALSEP ANALYTICAL BALANCES

E. C. Gough Ltd are pleased to announce the release of two new analytical balances from A. & D. Alsep Ltd. The ER-120A (120 grams x 0.1mg) and the ER-60A (60 grams x 0.1mg) offer the same accuracy, versatility and convenience of their forerunner, the ER-180A, but allow the end-user to more clearly define the weighing capacity required and, in the case of the ER-60A, save up to 100% on the possible initial investment. The ER series offers 0.1 mg resolution over the entire range, a linearity of ± 0.2 mg over the entire range and a sensitivity drift of ± ppm/degree C. Other features include one touch tare up to balance capacity, pressure sensitive liquid and dust proof controls, large 7 digit cobalt blue display, internal automatic calibration, large glass walled weighing chamber, weighing under the balance capabilities, external taring block, and a whole host of adaptor and peripheral options.



For further information please contact E. C. Gough Ltd or circle on the reader reply card.

New Portable Low-Voltage air samplers for indoor, outdoor or underground sampling

Northrop Instruments has introduced a new range of portable low and high volume air-samplers which will find application in many fields including industrial hygiene and air pollution studies. Several different sampling techniques can be employed:

Filter sampling for dust, particulates, chemicals and aerosols,
Impinger sampling with liquid media,
Sorbent tubes — for collection of chemical vapours,
Colour tubes.

The pumps can be battery or mains operated with some models being intrinsically safe and therefore suitable for use in hazardous locations.

A wide range of filters, and sorbent tubes are available and Northrop can also supply a catalog which details recommended procedures for the collection and analysis of some 500 different compounds.

For further information contact, Northrop Instruments & Systems Ltd, or circle **1** on the reader reply card.

A NEW MODULAR SAMPLING SYSTEM FOR LIQUID CHROMATOGRAPHY

Spectra-Physics announces the introduction of its liquid chromatography sampling system, the SP8780XR Automatic Sampler. This stand-alone module automates any modular LC system, while also providing fully integrated operation with other Spectra-Physics LC modules, including the SP8700XR Extended Range Pump. Control and communication are provided via the company's local area network, LABNET™, RS-232-C, and contact closure circuits.

Unique to the SP8780XR is the ability to use bar code labels on each individual sample vial. The bar codes provide each vial with a unique identification to aid in sample tracking and eliminate errors in tray loading. The bar code also carries analysis file information for each vial, thereby automating instrument setup in LABNET systems.

Capabilities of the Automatic Sampler include:

Setup either by the function keypad on the sampler, or via dialog by remote computer.

Capacity for 80 samples in four removable trays for continuous, non-stop operation.

Coded individual sampling and analysis conditions for each vial.

Injection volumes with fixed loop from 10 to 500 microliters, and in variable volume mode from 1 to 250 microliters.

Variable draw and dwell rates for the analysis of samples of high viscosity.

For further information or a demonstration please contact: Watson Victor Ltd, Wellington or circle **2** on the reader reply card.

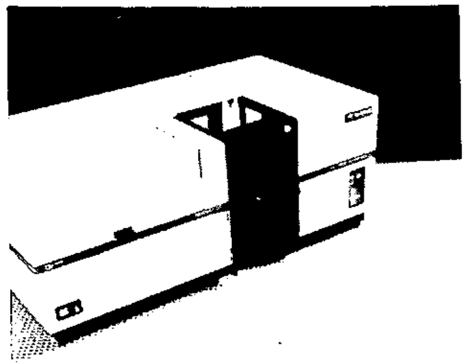
NEW SALES REP. FOR JOHN MORRIS

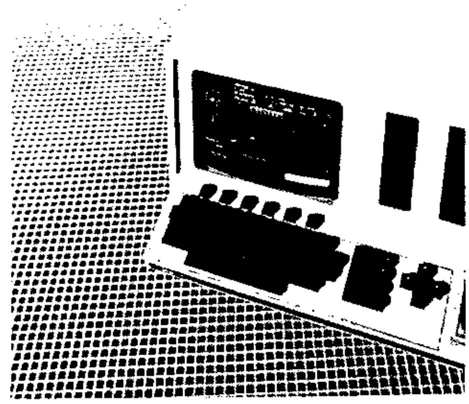
Derek Squires, well known in the Auckland region has recently joined John Morris Scientific Ltd as Sales Representative. John Morris Scientific hold a number of equipment agencies, including Perkin Elmer, Parr, Ingold, and Endecotts. Derek can be contacted at (09) 444-5836.

AUSTRALIAN SPECTROPHOTOMETER SYSTEM RELEASED AT THE PITTSBURGH CONFERENCE

A new concept in atomic absorption analytical systems was launched world-wide by Melbourne-based Varian Techtron at the Pittsburgh (USA) Conference on Analytical Chemistry in February.

Totally designed and manufactured in Australia the system, known as SpectrAA, features 'central control'. A single computer terminal is the sole point of interface between the operator and all components of the system. This concept provides a high level of automation, data handling and flexibility, while at the same time simplifying operation. The system includes a user oriented protocol — requiring the operator to simply 'fill-in-the-form' to set up even the most complex analysis.





The SpectrAA-40 model provides for fully automated analysis of up to 12 elements using flame, furnace and hydride atomization. The extensive software available provides such capabilities as graphics, error detection, data storage, editing and archiving to floppy disk. Of particular value is the ability to generate complete reports of an analysis — reports configured by the operator to include as much or as little information as may be considered appropriate for the expected audience.

For further information contact Wiltons or circle **3** on the reader reply card.

AUSTRALIAN MADE HPLC EQUIPMENT

ETP Kortec Pty Ltd, have appointed Advanced Electronics Limited as New Zealand distributors for their range of High Performance Liquid Chromatography equipment.

The product range includes:

Single and Dual Piston Pumps, Binary Gradient controller, Variable UV and Fluorescence detectors, and a 45 Tube Automatic sampler.

For further information circle **4** on the reader reply card.

PRODUCT NEWS

NEW FLASK HEATERS

Isopad have introduced their exciting new range of Labsafe flask heaters and controls. Labsafe instruments are designed for safety and have no difficulty living up to their name. Their advanced ceramic construction offers excellent insulation properties, — both electric and thermal — ensuring a cool outer surface.

The modular control system is designed to save both time and money. A selection of Labsafe controls can be easily interchanged with a flask heater, making it fully adaptable to different types of equipment.

Further advantageous features of the Labsafe include a broad base and rubber feet for maximum stability, a power-on red neon indicator and a watertight cable gland, which ensures maximum security of electrical connections.

The range of Labsafe heaters comprises three different models with flask sizes of 250,500 and 1000ml.

For further details please contact: Watson Victor Limited or circle **6** on the reader reply card.

SEALED ROTORS

Heraeus Christ, offer for their range of Centrifuges a unique sealed Rotor to guard against the possibilities of infection during Centrifugation.

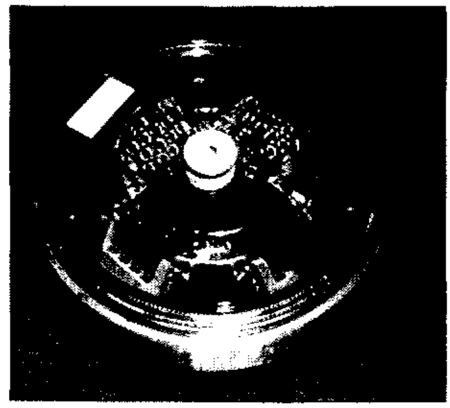
The stainless steel shield, enclosing head and carriers, plus the tightly closing polycarbonate lid, safely prevents any hazardous aerosols or sample material from broken containers from getting into the Rotor chamber or out into the Laboratory.

The clear polycarbonate lid enables the operator to identify broken specimen tubes. If necessary the entire sealed Rotor can be transferred to the autoclave for decontamination.

In contrast to the traditional windshielded Centrifuge heads the sealed Rotor can be removed from the Centrifuge without having to open its lid first. Loading and emptying of the carriers, can if necessary, be carried out in a safety cabinet such as an Email airpure cabinet. It is then sealed and carried back to the Centrifuge for Centrifugation.

The sealed Rotor is recommended for many applications and includes Blood tube spins in immunology and Biochemistry, microbiology applications, Tissue culture and Radio immuno assay work.

For further information, contact Smith-Biolab Ltd, or circle **7** on the reader reply card.



Ultracentrifuge on your bench

Beckman have again reinforced their claim to leadership in development of Ultracentrifuge technology by introducing the Model TL-100 tabletop instrument for cost saving small samples at high G forces and K. factors.

The TL-100 goes anywhere — needing only 24 inches of bench space and 230V mains outlet to perform DNA banding, rate-zonal separations or pelleting and lipoprotein isolation. It will operate in a glove box or fume cupboard for bio-safety.

The TL-100 follows the trend of modern liquid scintillation counters and clinical analyzers to perform reliable assays on reduced sample volumes.

For further information contact: Alphatech Systems or circle **8** on the reader reply card.

FRONT COVER STORY — ECONOMICAL DATA ACQUISITION & CONTROL CENTRE FOR ANALYTICAL EQUIPMENT

by Ron Smith Production Manager, Analytical Instrumentation, Philips New Zealand Ltd.

Some laboratory analysts have recently been appreciating the ability of computers to greatly speed their work with data acquisition, analysis, control and interpretation.

But there is often a considerable gap between defining the advantages offered by computing in the laboratory and justifying it as an economic proposition.

Current analytical computing equipment has traditionally been extremely expensive, providing total dedication to a particular discipline — such as infra-red spectrophotometry or atomic absorption etc.

A computer used for data control and analysis in one field, could not be used in the other, and the purchase of inflexible equipment was often ruled out on the grounds of cost.

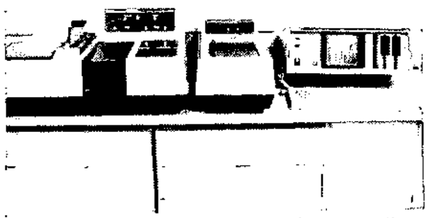
However, this situation has now changed. It stemmed from a realisation by our Philips Analytical team in New Zealand that a rethink was needed if the majority of laboratory analysts were ever to fully experience the tremendous advantages which computerisation has provided for so many other high technology fields.

In August of last year our Scientific and Industrial software specialists began work on producing a low-cost, versatile, data acquisition and control centre. The major building block already existed — the highly acclaimed P2000C portable professional computer. But the vital software which would make the whole project viable for New Zealand conditions had to be built from scratch.

Less than a year later, several analytical packages have been completed and are in use in many laboratories throughout the country. These laboratories have been able to acquire a multi-discipline, computerised, data acquisition and control centre, and in the process have saved themselves many thousands of dollars.

So what is this special equipment, and what can it do? As we have said, its primary component is the P2000C, a fully professional portable computer with a huge range of options. It can run eight and sixteen-bit applications. With up to 1.6 megabytes of storage on floppy disk alone, and thirty megabytes on hard disk, its storage capacity is virtually unlimited. It runs the CP/M operating system and can use the optional MS-DOS, plus all languages. In addition to the hardware — already used in thousands of professional applications world-wide, are a suite of programmes designed specifically for the use of New Zealand laboratory analysts. But more detail about that later.

In the sense that the P2000C data centre runs a number of analytical software packages — changed simply by inserting a floppy disk — it is unique. There is no other computer dealing with all the techniques which we cater for. Normally you would have to buy a completely different computer for each discipline, so we are talking about a highly versatile system. Of course it is also very inexpensive. A typical system would cost $6,000 or less, including word processing and spreadsheet software.



Philips Pye Unicam SP3 ratio recording infra-red spectrophotometry series : with P2000 data acquisition and control centre (U.E.B. Technical Centre)

As any analyst who has fought for budgetary approval of a data centre in the past would know, the normal price for a dedicated machine is usually in excess of twenty thousand dollars. If another instrument was needed, so then was another costly data centre — and most New Zealand companies could not afford such expenditure.

The software does away with the need for that duplication. One computer is all that is needed, even for a laboratory using a number of Philips instruments over a range of disciplines. It can be easily connected to all Pye Unicam analytical equipment in the laboratory and be used for data acquisition, post-run calculations, and control functions. The P2000C is portable and moved easily within the laboratory.

An extra incentive is the data control centre's ability to run the huge range of CP/M and MS-DOS software available on the market, including spreadsheet packages, data base managers, word processors and so on. Such programmes can be integrated with the specialist software supplied with the machine, allowing for example stored data from sample analysis to be pulled through into a word processing programme, to make up fully formatted laboratory reports. In almost all cases, the P2000C can be linked to a mainframe computer to give it even greater flexibility and performance.

But to return to the all-important software . . . included in the packages is one for infra-red spectrophotometry, which includes facilities for spectral acquisition and display, together with expansion facilities, spectral addition and subtraction. Spectra may also be compared by recalling a previously run spectra from memory and overlaying it on the screen with that of another sample or standard. A cursor can be run along spectra to determine peak positions and intensities. Finally, a library search function can be carried out, providing an invaluable interpretation aid for unknown samples.

There is atomic absorption software, allowing signal integration and statistics, and the calculation and display of calibration graphs. Up to three mathematical models can be used post-run to achieve the best fit with available standards and results can be achieved in the units required. Naturally the storage/retrieve facility is available within this discipline, as in all others.

A "Cookbook" facility has also been provided which is accessed by simply typing in the atomic symbol, and the computer will display three pages of information on the relevant elements. That information is stored in the software itself and so doesn't take up computer or data disk memory.

There is also a chromatography programme suitable for use with both GLC and HPLC, allowing data acquisition and graphical display at a sampling rate of fifty times per second. The programme provides integration consisting of peak area, height, and retention time, along with additional peak information — for instance, fully unresolved or fused etc. Soon, we will add to that software the ability to calculate concentrations using external or internal standardisation, along with other post-run calculations such as column efficiency etc.

Finally, we also have a UV software package which provides a scanning capability while using only a single beam instrument. Simply by the use of software commands, the P2000C can be used to control the new Philips PU 8600 single beam spectrophotometer for the generation of spectra, a function which represents a considerable hardware cost saving to the user who only performs the occasional scan.

The software is powerful and sophisticated, despite its ease of use and this is one of the prime reasons for the success of the data control centre in the market place.

As the software systems have been designed by a team of people who know both fields — Chemistry and Computers — we believe analysts have at last a computerised system which is suited to our New Zealand requirements.

SITUATIONS VACANT

Chemical Manufacturing Manager

Salary NZ$50,000 Housing/Car

We have been requested by a well established, respected and profitable, privately owned company established in 1970 to assist in the appointment of a Chemical Manufacturing Manager.

The permanent position is situated in the company's Head Office in LAE, Papua New Guinea. The senior management is comprised of both New Zealanders and Australians.

The position would suit a career-minded manufacturing Chemist who would be responsible for the management of a modern plant manufacturing a range of industrial, janitorial and general chemicals. The company is also in the process of installing a new sodium hypo plant.

This appontment is regarded as a permanent position with the initial term of engagement being 3 years with right of renewal. Accommodation conditions, security and total remuneration package are excellent.

Please reply in writing, giving full work history and personal details, quoting Assignment No. 4487, to:

W. R. A. Thornton,
Peat Marwick Consultants Limited,
1st Floor, Grand Building, 9 Princes St.,
P.O. Box 1220, Auckland.

PEAT MARWICK

Management Consultants
Ph. 774-690

Research Chemist

Ivon Watkins-Dow Ltd, a leading international agricultural chemicals company with substantial manufacturing facilities at New Plymouth wishes to appoint a graduate research chemist in the research division.

The successful applicant will be responsible for the design and execution of chemical research projects related to process improvements and new products from laboratory via pilot plant to full scale production.

Literature searches, the interpretation of patents and communications with other research groups world wide are important facets of this position.

Qualifications include a Ph.D or MSc in organic chemistry and several years post graduate experience, preferably in industry or some position which had a reasonable level of independence. Must have initiative and ability to work with a minimum of supervision.

We offer attractive conditions of employment and a salary commensurate with qualifications and experience.

Written applications stating age, marital status, qualifications, experience and interests should be sent to:—

The Employment Officer
Ivon Watkins Dow Ltd
Private Bag
New Plymouth

Johnson WAX

Development Chemist

Johnson Wax is a well-established and highly successful manufacturer of household and industrial products.

We seek a person to join our technical department, as chemist, to develop and implement plans that will take a project from a marketing concept to finished formula and packaging. The development chemist also provides technical support and advice to the sales force and customers.

The successful applicant will have appropriate qualifications and some previous experience in a manufacturing environment, preferably food or consumer products.

Working conditions are excellent and we offer a good salary and many benefits that will be discussed at an interview.

Please write, giving personal details and work history, to:

The Personnel Manager.
Johnson Wax New Zealand Ltd,
Private Bag,
Onehunga.

Laboratory Manager

• South Auckland • R & D Testing Laboratory

A well-known, highly respected New Zealand-based international leader in the manufacture and marketing of home heating equipment is presently strengthening their research and development team. It is well recognised that their present market position can largely be attributed to their very successful product design and development programme. To meet the demands of an international market, the research and development commitment is regularly increasing and they currently seek a Laboratory Manager.

This is an opportunity to develop and control their test programmes using equipment specifically developed for their needs. This includes managing a new TELARC registered Calorimetry room, maintaining computer and electronics-based reporting/recording equipment and performing other tasks associated with a modern test environment.

While interpersonal and organisational skills are important, experience in a laboratory environment is essential, preferably with electronic or computer-based test equipment. Applicants will possess a tertiary qualification, BE, BSc or similar and an understanding of thermodynamics will be an advantage.

Career development prospects are excellent and the salary and benefits package is most attractive.

For further information please contact John K. Williams, phone 795-550 Auckland (days), or 544-596 (evenings), or write to PO Box 579, Auckland.

LAMPEN

Lampen Associates Ltd, Management Consultants, Box 579, Auckland.
Phone 795-550.

Wellcome

Chemist Project Work

Wellcome New Zealand, a multinational pharmaceutical company, is seeking a qualified chemist to undertake a variety of project work.

The major responsibilities include validation of production processes, insecticide development, and some laboratory analytical work. The position is based in our well equipped laboratory.

This is a career opportunity which offers involvement in many operational aspects of a manufacturing company and we would welcome applications from people with relevant laboratory experience who hold a tertiary qualification and are motivated by variety and challenge.

If you believe you could fill this interesting position, please write enclosing full details to:

The Quality Assurance Manager,
Wellcome New Zealand Ltd,
P.O. Box 22-258,
Otahuhu.

Business Reply Card

Authority No. 3000
AUCKLAND, N.Z.

Postage will be paid by:

CHEMISTRY IN NZ
P.O. BOX 9072
Newmarket
AUCKLAND

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36 37 38 39 40 41 42 43 44 45 46 47 48 49 50

R = Rep To Call

L = Literature Only

Classification Data

Indicate total employed:

☐ Under 20 ☐ 20-49 ☐ 50-99
☐ 100-199 ☐ 200-499 ☐ 500 +

What is your organisation's principal activity:

....

What is your principal classification?

☐ MANUFACTURER
☐ SUPPLIER CHEMICALS
☐ SUPPLIER INSTRUMENTS
☐ SUPPLIER LAB. EQUIPMENT
☐ RESEARCH
☐ OTHER

SPECIFY

TICK BOX ☐ I WOULD LIKE TO SUBSCRIBE TO CHEMISTRY IN NEW ZEALAND
Please bill me $15 for annual subscription NZ$25 overseas.

☐ I would like to become a member of the New Zealand Institute of Chemistry
Please forward me details