



Chemistry

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IN NEW ZEALAND

PLASTICS, RESINS AND PAINTS INDUSTRY FOCUS



NZIC CONFERENCE PROGRAMME PAGE 29

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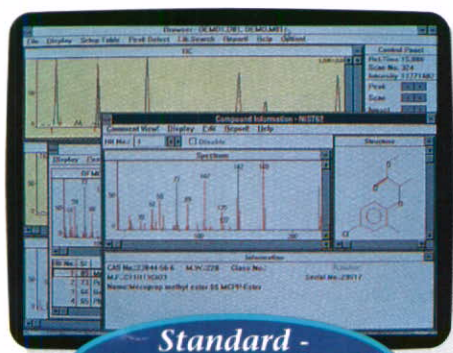
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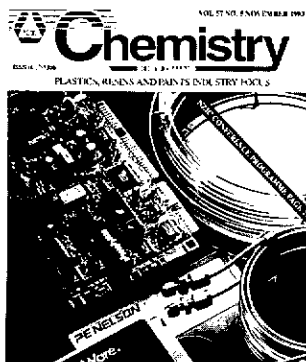
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FRONT COVER

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The Perkin-Elmer Corporation is the leading world-wide producer of analytical instrumentation systems and instruments for biotechnology. These instrument systems find application in a wide variety of fields.

For further information see the cover story on page 2



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Environmental protection is an expanding concern, as nations recognise the importance of preserving their natural resources. In order to safeguard the public and our natural resources, resource management will require careful and consistent establishment of criteria that will be supported and verified by analytical methodology. Regulations derived from legislation will specify the laboratory analyses to be implemented in order to detect and monitor pollutants. These laboratory analyses must be performed with known levels of accuracy and precision, quality control documentation, and consistency among laboratories. New environmental regulations are emerging on a global basis, fuelling the demand for more sensitive, cost-effective analytical techniques. Perkin-Elmer has entered into several collaborative programmes with government agencies, including the USEPA, permitting a complete understanding of both current and future analytical needs.

Modern agriculture depends on analytical techniques to monitor for example, the soils, fertilisers, pesticides and herbicides to optimise yields and to ensure that toxic substances do not reach the dinner table. Analytical instruments are essential to assure quality of preparation and packaging in the dairy, meat, beverage and dry food industries.

The chemical and plastic industries utilise analytical instruments for a myriad of applications in the production, processing and quality control of materials such as paints, adhesives, packaging materials, detergents, petroleum products and organic chemicals.

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HAZARDOUS SUBSTANCES AND NEW ORGANISMS: UPDATE ON PROPOSALS FOR LAW REFORM

It has been recognised for some time that there is a need for reform of the laws covering hazardous substances and new organisms. Present legislation is recognised as being outdated, complex or, in some cases, non-existent.

In October last year the Ministry for the Environment published a document which set out proposals for such reform. These included a proposed piece of new legislation and the formation of a new agency to be called the Environmental Risk Management Authority (ERMA). The stated purpose of these proposals was to both minimise the risks from hazardous substances and new organisms while retaining their benefits, and to improve the efficiency of current assessments of control measures. Some 255 submissions relating to these proposals, including a submission from the NZIC, were received by the Ministry. Most welcomed movement towards law reform. Many expressed impatience to see the new law in place although a small number of submissions expressed the view that reform was not required.

On June 3 this year the Government announced that the Bill to reform the management of hazardous substances and new organisms would be introduced into the House before the end of the year. As part of the process of ensuring that all those interested are kept informed on the progress of the reforms the Ministry has provided a series of updates.

In April of this year a summary of the submissions relating to the proposals was prepared. This illustrated the coverage of the submissions but did not attempt any analysis of the issues raised or any response to the comments made. Subsequently three progress reports have been released.

Progress Report No. 1 in June 1993 covered matters such as:

- Principles
- The proposed Environmental Risk Management Authority (ERMA)
- Assessment 1: Revised criteria and delegations (covering hazardous substances or new organisms, time of hearings)
- Assessment: Public participation, intellectual property rights, and reassessment (covering information and confidentiality)
- Controls

Progress Report No. 3 in September 1993 covered:

- Control structures proposed such as regulatory framework, exemptions, general standards and the implementation of international agreements.
- Compliance structures proposed including monitoring, compliance testing, and an integrated and efficient compliance system avoiding duplication and overlaps and utilising existing central government agencies and local authorities using standards established under the new legislation or developed in consultation with ERMA.

Readers wishing to obtain further information or copies of these reports should contact the Ministry for the Environment, P O Box 10 362, Wellington.

Norman Thom, Covenor, NZIC Environmental Committee
(C/- Environmental Science Unit, University of Auckland)

Sustainable Energy for New Zealand

Comment on seminar held at CIT, Upper Hutt, 20-21 August 1993

The seminar consisted of eight plenary sessions which addressed general questions, nine parallel workshops, each of which was allocated a specific aspect of energy utilisation and five hours of formal meeting time.

The topics of these workshops were:

- a) Fossil fuel resources and technology
- b) Renewable energy sources and technologies
- c) Energy efficiency and demand side options
- d) Transport resources and technologies
- e) Treaty issues
- f) Trade and development
- g) Pricing and economics
- h) Planning and legislation
- i) Institutional, community and politics

The purpose of the seminar was to examine what was meant by sustainable energy and how to achieve it.

The very ambitious two day programme achieved much more than I would have thought possible. To begin with it brought together in a single forum such diverse viewpoints as those of Wayne Mackeig, Chairman of the NZ Energy Foundation and Bill Falconer (Fletcher Challenge) and of Molly Melhursh (Power for our Future) and Kirsty Hamilton (Greenpeace) and of John Luxton (Minister of Energy) and Jeanette Fitzsimons (Alliance).

Surprisingly, the seminar actually reached something of a consensus with respect to what was meant by sustainability (catering for the needs of the present without compromising the ability of future generations to cater for theirs) - with more or less detailed qualifications - seemed to be an acceptable definition. It was agreed - even by the representatives of the fossil fuel industries, that fossil fuels could only be an interim source of energy, though views varied on how long we could or should go on depending on them. It was recognised that New Zealand had available to it a range of renewable energy resources and that no single resource could be the sole answer to the sustainability question. Hydro power, geothermal energy, wind energy, direct solar energy and biomass derived fuels and energy management have all got their part to play.

Many of the impediments to the implementation of a sustainable energy future were examined, including official inertia, the failure of the market to recognise the full cost of fossil fuel use, including environmental costs, and the different ways in which the market operates for large scale publicly funded systems, through to the individually financed household level options.

My own appreciation of the seminar was perhaps clouded a

little by the realisation of just how far we have fallen back since the energy conferences and the energy studies promoted in the 1970's and early 1980's by the ERDC, the LFTB and the Ministry of Energy, none of which, sadly exist today. We are not completely back to square one but not far from it. It is to be hoped that the lost ground can be quickly made up through the activities of organisations such as EECA and that this time more of the work done in the energy field bears fruit in the form of implementation, than was the case ten to fifteen years ago.

Arthur Williamson
President

Statement by the Foundation for Research, Science and Technology

Closer links between industries and research agencies are the key to success for five-year research strategies released last month by the Foundation for Research, Science and Technology.

The strategies set priorities for the Foundation's allocation of New Zealand's \$275 million Public Good Science Fund until 1998, with the emphasis on research which contributes to growth in export earnings and job opportunities.

"The strategies contain a wide range of very specific guidelines for enhancing cooperation between research and industry," Chief Executive, Dr Laurie Hammond said.

"Industries which develop research and development strategies and contribute their own finance will improve their chances of receiving public research funding. For example, equine research will be publicly funded for the first time at a level dependent on what the industry itself is also prepared to contribute".

All research in industrial technology and manufacturing will have to be conducted with active industry involvement unless it can be clearly justified otherwise.

"We have seen the benefits of researcher-industry cooperation in the \$11 million Technology for Business Growth Scheme run by the Foundation, which has resulted in participating companies increasing revenue and staff numbers," Dr Hammond said.

"There are a wide range of mechanisms by which industries can work with research agencies, such as through club groupings of several companies. The Foundation is also prepared to fund research carried out with just a single company if there are wider benefits to New Zealand and the results are publicly available"

Dr Hammond said the strategies complete the reform of Government-funded research activity. The priorities aim to give science agencies and industry clear messages about what the Government wants to fund over the next five years, although only high quality science will be funded.

12 ENERGY

Foundation Output No. 21
1997/98 funding: \$5.8 million

Energy research will have an increase in its funding from \$4.7 million in 1992/93 to \$5.8 million in 1997/98. There is a shift in funding emphasis away from non-renewable energy resources and towards non-traditional renewable resources, and energy utilisation and management.

This strategy seeks to identify areas where partnerships and the coordination of Foundation funded research, along with the activities of regional and local bodies, government departments, industry and individuals, can maximise the impact of the research effort and can improve research performance and productivity.

This strategy attempts to suggest a balanced energy research portfolio which will underpin future energy options. The strategy allows for the funding of research on all forms of energy of strategic importance, regardless of whether they are renewable or not. The portfolio may include research on resource delineation, assessment and extraction. It includes social, environmental and economic research.

The four topic areas for research are:

- Non-renewable energy resources' including energy related research on fossil fuels such as oil, natural gas, coal, peat and oil shale. Because of New Zealand's large coal resources, coal may become increasingly important as the supply of oil and gas diminishes, but this will probably depend on the ready availability of economic and efficient clean-burning technologies. This may see an expanded need for coal research in this country at some time in the future. On balance, there is probably a greater justification for public good research on coal than there is on oil and gas.
- Traditional renewable resources, including geothermal research, which is at present well supported. Currently, there is little public-good research directed at hydro resources. A greater emphasis in future on small-scale hydro may see the need for the Foundation to fund research on this topic, as may increased public resistance to further utilisation of our natural waterways for electricity generation.
- Non-traditional renewable resources, which are often actually very traditional in nature, but may play an enhanced role in the generation of electricity or provision of energy on a relatively large scale.
- Energy utilisation and management, which is envisaged to be a broad area, containing energy efficiency research, energy conservation research, energy utilisation research and research which does not fit readily within the other categories. This will include technological, social, economic and environmental research relevant to all forms of energy.

21 CLIMATE AND ATMOSPHERE

Foundation Output No. 33
1997/98 funding: \$7.7 million

Research on climate and atmosphere will receive \$7.7 million in 1997/98, slightly down on the current level. This strategy leads to the following areas of emphasis for research:

- Stratospheric ozone depletion and surface UV radiation levels
- Greenhouse gases and aerosols, their exchange at the earth's surface and ocean, and their likely effect on climate.
- Climate and weather processes and modelling for the New Zealand-Southwest Pacific region
- Monitoring, archiving and documenting New Zealand and South Pacific climate.

Increased funding for climate and weather processes and modelling research is indicated because of the sensitivity of New Zealand's economy to climate and weather fluctuations. The increase will come from a funding decrease within the climate monitoring, archiving and documenting area. Much of this can be obtained by redirecting resources and personnel between the two areas.

Climate and atmosphere research leads to useful outcomes and added value in many sectors of the economy and provides knowledge on which to base important government planning and policy decisions. The Foundation will encourage high quality strategic climate and atmosphere research which underpins such applications.

Appropriate international collaboration is regarded as particularly important for addressing global and regional climate science issues.

For further information on the Research Strategies **Contact:** Dr Laurie Hammond, Chief Executive, Foundation for Research, Science and Technology, P O Box 12 240, Wellington, Ph. (04) 499 2559 (w) (04) 384 4116 (h)



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Research on further processing of sheep meat, beef, seafood and horticultural products will be a priority, together with wood processing research. Research on treating waste from primary production and processing will aim to lessen environmental hazards and manufacture marketable products from waste.

The strategies emphasise research on energy-efficiency, renewable energy resources, transport efficiency, and environmental protection and rehabilitation.

The five-year strategies will help promote stability in science organisations which have undergone continuing change and restructuring throughout the past few years, Dr Hammond said.

The Foundation's funds go mainly to the Crown Research Institutes established last year by the restructuring of DSIR, MAF Technology and other Government research departments. Other recipients are research associations such as the Dairy Research Institute, private companies and individuals.

The universities do not yet have access to the Foundation's main fund, but bid for a separate \$10.7 million fund which is not currently covered by the new strategies but will be in future.

The strategy exercise began after the Government's Science Priorities Statement in October 1992 set the amounts of public money to be allocated to broad areas of research over the next five years. The new strategies set priorities for funding within those 24 research areas.

The strategies have been finalised after several rounds of consultation with more than 5000 interested parties, including research agencies, research users, sector groups and industries.

PUBLIC GOOD SCIENCE FUND RESEARCH STRATEGIES TO 1997/98

The Foundation for Research, Science and Technology has prepared one-page summaries of the five year research strategies for allocating the Government's \$275 million Public Good Science Fund. These strategies will guide the Foundation for Research, Science and Technology in allocating the funds until the 1997/98 financial year.

There are 24 separate strategies, covering the different research areas into which the Foundation's funding is divided.

The one-page summaries are listed below. Chemistry in New Zealand has published below strategies 9, 12 and 21 as these areas have received the largest funding related to chemistry and related research. If you wish to receive some or all of the other strategies, please contact Wendy Rhodes at the Foundation: ph (04) 499 2559, fax (04) 499 2568

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STRATEGY NUMBER	NAME	FUNDING 1997/98
1	Sheep, Beef, Meat, Wool	\$21.0M
2.	Dairy Research	\$9.2M
3.	Alternative Animal Species	\$4.0M
4.	Generic Animal Research	\$11.0M
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21.	Climate and Atmosphere	\$7.7M
22.	Antarctica	\$1.8M
23.	Space and Fundamental Knowledge	\$3.8M
24.	Science and Technology Services	\$4.3M

9 INDUSTRIAL TECHNOLOGY & MANUFACTURING

Foundation Output Nos. 16, 17 & 18
1997/98 Funding: \$22.5 million

Research into materials, industrial technology, manufacturing, electronics and instruments will receive \$22.5 million in 1997/98, up from \$21.2 million in 1992/93.

The main aims of this strategy are to develop strong bonds between researchers and industry, and to enhance the quality of research programmes and their contribution to technological performance in industry. Research teams are to form close relationships with New Zealand industry. People are important to the innovation process. Proposals involving transfer of people between research and industry and between institutions are encouraged.

Priority research areas are:

- New biomaterials, bioprocess technologies and products
- Industrial processing technologies for the non-biological industries
- Properties and performance of materials important to New Zealand industries
- Design methods and production technologies
- Automation systems for primary and processing industries
- Information and communication technologies, in areas where New Zealand has, or can develop, a competitive advantage.
- Management systems and management support tools relating to New Zealand's manufacturing industries.

NEW ZEALAND PAINT APPROVALS SCHEME (NZ Pass)

By Bob Bettison
Telarc New Zealand, Private Bag 28901, Remuera, Auckland

For engineers, architects, specifiers and all property owners the implementation of the restructured New Zealand Paints Approvals Scheme gives an assurance that paint products approved by Telarc conform to a recognised product specification and will live up to the claims of the manufacturer.

The restructured New Zealand Paint Approvals Scheme (NZ Pass) came into force on April 1, 1993. It was developed out of the Public Sector Paint Committee which was established in 1983 for public sector paint purchasers.

When government restructuring fragmented the committee's members, it was renamed the New Zealand Paint Approvals Scheme and its operation passed to Telarc, an independent body established in 1972 to identify and recognise quality in the supply of services, products and materials.

In 1992 NZ Pass was restructured as a true third party product certification programme to the requirements of:

ISO/IEC Guide 28:1982 "General rules for a model third party certification system for products"

EN45011:1989 "General criteria for certification bodies operating product certification"

NZ Pass also requires that manufacturers have certification to ISO 9002:1987 "Quality systems for production and installation".

Product certification is based on type testing by the manufacturer through a registered laboratory, and assessment and approval of the manufacturer's quality control and production facilities. A surveillance programme covers inspection of the manufacturers production facility, quality control and certified products.

NZ Pass provides an independent assurance that products are fit for use and conform to a product specification and that quality policies and procedures in management and manufacture are such that if followed, product quality will be attained.

NZ Pass maintains a close relationship with Australia's Government Paint Committee (gpc). It also provides technical advice about standards for paints, related materials and processes, and advises on the specification, standardisation, coordination, quality assurance, testing and use of paints and related materials.

The outlines of NZ Pass are published in a document titled "New Zealand Paint Approvals Scheme Criteria for Quality Paints", available from Telarc's Auckland office.

For paint specifiers Telarc publishes a product Specification Handbook which contains product specifications, NZ Pass recognised manufacturers and a listing of approved products.

Manufacturing units which already have Telarc recognition are:-

Altex Coatings Limited

Courtaulds Coatings NZ Limited

Croda Lusteroid Paints Limited

ICI Paints NZ Limited

Levene Paint Manufacturing Limited

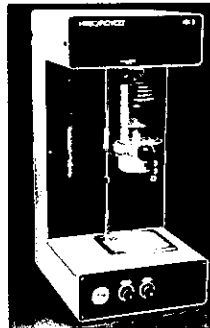
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Many products made by the above are approved under the NZ Pass programme.

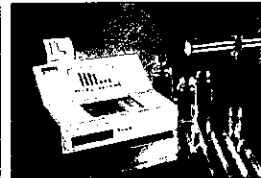
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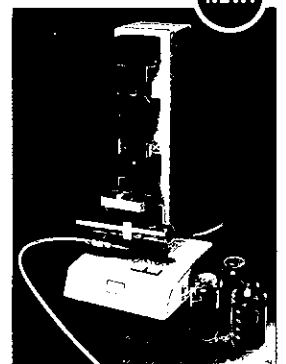
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SUNSCREENS AND THE HUMAN PHOTOMETER

By Brian Wilkins MSc(NZ), PhD(London), FNZIC

Using human skin as a photometer for ultraviolet radiation would seem like a rough and risky procedure. Yet it is the most highly regarded method for testing sunscreens. The reading depends on the presence or absence of a mild burn (erythema). To measure this minimal erythema dose (MED) of UV, adjacent areas of skin are exposed to successively longer periods of irradiation from a xenon lamp, each period usually being 1.26 times the previous period. The ratio of the irradiation time required to produce this erythema on skin covered with a 2 mgcm⁻² film of sunscreen, to the time for an equivalent reddening of untreated skin, is defined as the sun protection factor (SPF), or more correctly as the initial SPF.

Even less precise is the human photometer output in the form of accelerated skin ageing, troublesome or fatal cancer, and suppression of the immune system. Decades may elapse before some of the readings are displayed.

But the chemistry has a vital role to play in all this and chemists have produced many excellent UV absorbers and spectrophotometry, after a shaky start through misuse of data, is now coming more into prominence.

UV ABSORBERS EMPLOYED IN SUNSCREENS

Irradiation of human skin with narrow bands of UV shows that their ability to produce erythema rises sharply as the range from 320 nm to 290 nm is traversed (1). This, the main sunburn region, and the region of most damage, is called the UVB region.

Shorter wavelengths are present outside the atmosphere but are screened out mainly by ozone and oxygen. Combining the erythema sensitivity of skin and the intensity of this radiation at the surface of the earth, we can attribute most erythema to a fairly narrow band between 295 nm and 320 nm, peaking at about 307 nm.

The erythema sensitivity of human skin at longer wavelengths 320 nm to 400 nm peaks at about 380 nm but is less than that in the UVB region by a factor of one thousand to several thousand (1).

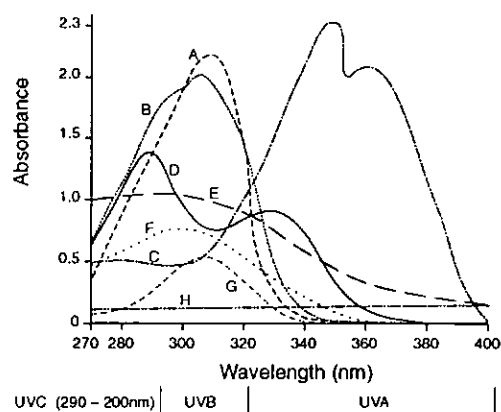
A natural constituent of human cells with a UV absorption peak coinciding with the erythema sensitivity peak, and possessing a high standard absorbance value, would seem to be the ideal suncreening agent. Therefore when it was realised that para-aminobenzoic acid (PABA) met these requirements the place of PABA was assured in sunscreens for many years. Chemical sunscreens have been in use for 60 years and PABA has been popular for about 40 years, but it has now disappeared almost entirely from use. It is useful to look at the reasons for this because they tell us that UV absorption is not the only requirement for acceptability.

PABA was oxidisable under the conditions of use. It was also relatively insoluble in the lipophilic components of emulsions

and cosmetics, and when administered in the rather inconvenient vehicle of an ethanolic solution was likely to crystallise on the skin (2).

When the related dimethylaminobenzoate ester (A) was employed these problems were overcome and it is now in widespread use. However A is not accepted by all manufacturers because it has been implicated as a cause of contact dermatitis in a small proportion of users. The literature is confusing on this and the whole matter of sensitivity is complicated by the possibility of sensitisation induced by some other previously used agent, including drugs (3, 4).

Figure 1.
Ultraviolet Absorbance of Some Commonly Used Sunscreening Agents



Key:

- A 2-Ethylhexyl paradimethylaminobenzoate
- B 2-Ethylhexyl paramethoxycinnamate
- C 1-(4-tert-Butylphenyl)-3-(4-methoxyphenyl) propane-1,3-dione
- D 2-Hydroxy-4-methoxybenzophenone
- - E Titanium dioxide (Tioveil Brand, ICI, Ultrafine, Particle size approx. 0.02 microns.)
- F 2-Ethylhexyl 2-cyano-3,3-diphenylacrylate
- G 2-Ethylhexyl salicylate
- H Titanium dioxide (R-HD2 Tiioxide ICI, Particle size approx. 0.25 microns.)

All were measured at the same concentration (2mg/100ml of Universal Sunscreen Solvent which is a mixture of 2-propanol, cyclohexane, and dichloromethane in the volume ratio of 11/7/2). The two titanium dioxide samples were suspended in the same solvent mixture.

Thousands of conjugated structures exist allowing suitable transitions and possessing absorption maxima in the UVB. Chemists have not been slow in drawing on existing compounds and making new ones. Fifty nine compounds were listed in 1978 and screened for toxicity (5). Nearly all of the compounds in use today have been employed in sunscreens for 25 years or more.

The most common types are based on structures shown in Figure 2. Other structures are used including derivatives of camphor and 1,3,5-triazine. One of the latter is 2,4,6-trianilino- p- (carbo-2'-ethylhexyl-1'-oxi)-1,3,5-triazine which

was recently approved for use in EC countries (6). In the USA the FDA in 1978 approved 25 active ingredients for use. Australian health authorities approve 40 compounds in a list compiled a few years ago and this is the present guideline for New Zealand manufacturers.

Most compounds are more or less lipophilic, but a few, e.g. those with sulphonic acid groups are designed for solubility in the aqueous phase of emulsions.

The UVB is well catered for, but because of the relatively late attention being given to the possible dangers from UVA radiation, and the continuing lack of agreement concerning the extent of that danger, the number of agents is very limited. The dibenzoyl methane derivatives e.g. C are the most effective on a weight for weight basis, but C (trade name Parsol 1789) is likely to face competition from the less costly microfine TiO_2 . C has not been approved for general use in the USA.

The benzophenones such as D (generic name oxybenzone) were the original "broad spectrum" UVA absorbers, but their standard absorption in the region is only moderate (Figure 2) and they no longer dominate the field.

The question has been raised recently as to whether sunscreens can act as photosensitisers and cause harm. UV damage to DNA via thymine dimerization is well documented as a potential precursor to skin cancer. It is known that thymine triplets react with ground state thymine to yield thymine dimers. It is suggested that sunscreens whose lowest triplet is higher than or similar to that of thymine could be a danger. However recent measurements have shown that the triplet energy levels of the two commonly used sunscreen agents studied (B and C) lie below that of thymine.

THE PARTICULATE UV BLOCKERS

Sunscreens based on titanium dioxide and zinc oxide have retained, until recent years, an aura of total impenetrability; the proverbial brick wall. If users were prepared to look like white painted circus clowns they could achieve total protection, but the reality was not as clear cut. If used in the same concentration and film thickness as the visibly transparent sunscreens these so-called opaque agents were not nearly as effective as organic-based products. Even when plastered thick on the skin they frequently melted away rapidly in the heat.

The pigment grade TiO_2 and ZnO used in these products normally had a particle size of at least 0.25 microns. Theory predicts a different cause of scattering for particles of this size compared to finer particles. Particles in the 0.02 - 0.05 micron range display a critical difference in behaviour in that they act by UV absorption as well as UV scattering and are relatively transparent in the visible range. Absorption curves of the fine TiO_2 (E) compared to the coarser TiO_2 (H) in Figure 1 show the advantage of smaller size. TiO_2 is a semi conductor and UV radiation excites an electron from the valence band to the conduction band.

Several brands of microfine TiO_2 and ZnO are now on the market. The near transparency in the visible region eliminates the undesirable whiteness on the skin except when high percentages are used. The UV absorbance of microfine TiO_2

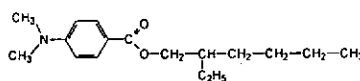
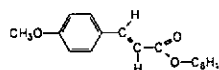
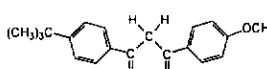
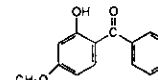
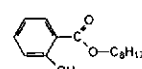
is better in the UVB region than in the UVA but not as effective on a weight for weight basis as is the organic UVA blocker C. Microfine TiO_2 on its own can provide very adequate UVA protection. A useful brief review of TiO_2 as a UV absorber recently appeared in Chemistry in Britain (8). However the relative absorbance values published in that paper should be treated with some reservation.

Formulators must always be conscious that there is no gain to be had from microfine ingredients if at any stage in the process the fine particles flocculate. Nephelometry, where suspended particles are shown to exhibit Beers Law-type behaviour in the spectrophotometer, has a useful part to play in sunscreen development but some form of *in vivo* testing, indoors or outdoors, would seem to be a necessary confirmation of success in maintaining the fine particles as separate entities right up to the time of use.

CHROMATOGRAPHIC ANALYSIS

References are given to thin layer analysis of some 200 sunscreens (5), GLC of 16 commonly used absorbers (9) and reverse phase HPLC of common UV absorbers and some of their degradation products (10).

FIGURE 2
Structures and standard absorbance values (A_1^1)^{*}
of suncreening agents named in Figure 1

		A_1^1	
		307nm	360nm
A		1040	—
B		800	—
C		260	1100
D		400	110
E		180	—

*measured in universal sunscreen solvent (Figure 1).

Spectrophotometric Analysis

Routine spectrophotometry in the range 295-400 nm is the principal method of quality control. Of great interest is the question of whether those results enable us to predict the performance of a sunscreen in use. But first we need to consider the behaviour of sunscreens on the skin.

Sunscreens vary in their ability to maintain an intact protective layer on, or partly in, the skin. This property is called substantivity and it depends on a totality of properties related to all the constituents of the formulation. Substantivity is not related to UV absorption except insofar as some of the UV actives may influence substantivity through other properties, e.g. hydrophobicity, that they may possess.

Substantivity and SPF measurement are inevitably linked to some extent because, other factors being equal, the longer the irradiation time, whether it be seconds under a lamp or hours in field testing, the lower will be the recorded SPF because of the progressive deterioration of the film. Any information we obtain from spectrophotometry can therefore relate only to the initial SPF that has been determined under artificial lamps requiring short exposure times. Since this latter description applies to nearly all published SPF's, it is worth pursuing.

Since the output from most spectrophotometers is either in the form of per cent transmittance (%T) or absorbance (A) we must choose which of these is more useful in relation to the photobiology of human skin. If SPF was directly proportional to %T then a sunscreen with a transmittance of 1 per cent should also have an SPF of 99. However the true SPF of a 20 micron film, which is the standard thickness for most *in vivo* testing, is nearer 5 or 6 for a product with 1 per cent transmittance.

Mistaken attachment to %T led the Australian authorities during the 1970's, and subsequently, to classify as "maximum protection products" and "high protection products" sunscreens with up to 3 per cent T in the UVB at 305 nm for an eight micron layer. As a result this list placed users in danger by including many mediocre products. New Zealand authorities appear always to follow Australia.

Absorbance expressed as the absorbance of a film of sunscreen 10 microns in thickness is a more appropriate parameter to relate to SPF. Correlations, useful in sunscreen design up to about SPF 12, were published by Nearn and Bell (31) and by Wilkins (32).

Successful prediction of SPF from spectrophotometry has been achieved by Diffey and Robson (18) who dispensed with the normal design of spectrophotometer and expressed the result neither as %T nor A but simply as the ratio of transmitted to incidental UV. The transmitted radiation was then expressed in terms of the energy that would be passed by the sunscreen in each 5 nm band of radiation between 290 and 400 nm. Finally this energy was combined with data on the relative effectiveness of each of the 5 nm bands in producing erythema. A novel feature of this method is the use of dimpled polymeric tape to support the sunscreen film. In view of the weak erythemic effect of radiation in the 330-400 nm region the approach appears to be unnecessarily elaborate.

In pursuit of absorbance values we should note the practical issues in arriving at a suitable method for collecting this *in vitro* data and expressing it in a useful form. The literature contains mistakes to be avoided. Sandwich techniques, where a very thin film of sunscreen is held between two quartz plates, involve such a small amount of material being held in the beam that the sampling is inadequate and the results on emulsions which by their nature are not homogeneous, are inconsistent. Furthermore in the case of an emulsion the unbroken emulsion is not the form in which the sunscreen resides after being spread out on the skin.

Then there is the impractical procedure set out in the Australian Standard for sunscreen products AS-2604 which

requires the preparation of a test solution containing an exact weight.

The following method is an adaptation of that of Schulze (11) and from normal solution spectrophotometry allows the calculation of the absorbance of a neat film of the sunscreen. Ten microns is the chosen thickness. Twenty microns is the thickness applied to skin for *in vivo* testing but experience indicates that users generally apply less than that. Skin, being a highly uneven surface, has a proportion of area covered by a thickness of even less than 10 microns.

Method: About 50 mg of sunscreen is weighed into a 50ml volumetric flask and dissolved in solvent (USS Fig. 1). Ultrasonification is essential where particulate suncreening agents are present. 3ml is transferred to a 25ml volumetric flask and diluted to volume with USS. The absorbance (A) is measured in a 1 cm cell.

$$A \text{ (calculated for 10 micron film)} = \frac{A \text{ (Found)}}{\text{Final Concentration in mg/ml}}$$

The most useful wavelength at which to apply this method is 307 nm because it lies at the centre of the erythema-producing UVB region. The peak height of most UV-actives in the UVB is roughly proportional to peak area, but not so for the flattish curves of the particulates.

The A(10 micron film) is also convenient for those interested in determining whether their product meets the suggested figure for classification as a broad spectrum product in the Australian Standard AS-2604.

The AS-2604 suggestion is that broad spectrum classification requires that "an 8 micron layer of the product does not transmit more than 10% of UV radiation at any wavelength from 320-360 nm". Converting this to absorbance units and a 10 micron film, the minimum suggested absorbance in the range is 1.25 units. Since absorbance is directly proportional to concentration, the absorbance method allows the formulator/manufacturer to adjust the level of UVA absorber accordingly.

A serious weakness of the AS-2604 method is that the 360 nm result tells us little about the total integrated area in the 320-360 nm range. A flattish curve from a particulate signifies much less protection although it may pass the test.

THE LIMITATIONS OF SPF TESTING

The spectrophotometer reacts to the same radiation that burns the skin. We would expect the results to relate to each other and they do. Where substantivity is good, spectrophotometry also relates well to field tests where users display themselves to the sun with weighed amounts of sunscreen carefully applied to measured areas of skin.

Although the xenon lamps employed in *in vivo* indoor testing imitate the spectral range and energy of the sun the following results of Pathak (12) ring the alarm bells.

COMPARISON OF SUN PROTECTION FACTORS FOR THE SAME GROUP OF PRODUCTS MEASURED IN DIFFERENT WAYS.

	SPF claimed on packaging	SPF from artificial lamp method	SPF in field tests in the sun	
			Passive sunbathing for 1 hour	Active swimming & sweating for 1 hour
Mean	9.00	10.84	5.93	3.51
Standard Deviation	5.04	5.56	2.73	1.44

We can understand this rapid fall off in protection to half or less during use only by analysing the time factor as it applies to artificial as compared to natural methods of testing.

Contrary to much of the advertising copy we read, the Sun Protection Factors (SPF) do not tell us how long we can stay out in the sun without burning. This is because the tests to measure SPF are carried out with UV lamps about a hundred times the intensity of sunlight and are completed in such a short time that the all-important time factor in the protection afforded by the sunscreen is ignored.

I can illustrate this point with typical data from a recent test with which I was associated. One of the subjects in the testing panel required 10 seconds exposure to the xenon lamp, to receive a just detectable burn. The same subject, with the standard amount (2mgcm⁻²) of sunscreen on the skin, required 240 seconds of exposure to produce the same redness. The SPF is the ratio of these two times, 240:10=24.

Since the exposure time is a mere four minutes this type of test could tell us only about the protection we get beyond that time if the protective film remains fully intact throughout the longer period. In fact it does not, and it has been known for twenty years that the protection afforded by sunscreens falls off with time.

The SPF therefore tells us only what we start with. A more useful application of the xenon lamp burn technique is to find the SPF at the end of a specified period rather than at the beginning. In this way we can check on the all-important lasting qualities which vary tremendously among the different products on the market. Very few commercial sunscreens carry information on this final SPF.

Another question concerns the reliability of the human photometer with respect to registering damage other than the inflammation related to redness. Kligman (15) has demonstrated that precancerous cell damage occurs as a result of exposure to UV radiation of only one quarter that required to produce erythema. This calls into question the whole ethos of testing employing the erythema end-point. Therefore we are now forced to redefine just what constitutes a good sunscreen. The human photometer is no longer totally adequate and we must rely to a greater extent on the laboratory spectrophotometer.

The latest blow to the once sacred dictum that SPF 15 represents maximum protection and suberythema doses of UV are safe, comes from research on immunosuppression. A

rapidly growing body of work now attests to the ability of UVB radiation to suppress vital immune reactions in animals and in man (20-24).

van Praag et al. (21) state that their "results suggested that the minimal erythema dose is not an accurate method to determine protection against UV-induced immunologic alteration". The mediocre performance of certain commercial sunscreens as reported in work in this area is also a cause for concern.

DESIGNING A SUNSCREEN

Good sunscreen design requires that we put enough UV absorber on the skin and ensure that it stays there during the period of use. The focus on initial SPF and the relative lack of attention to substantivity has resulted in many inadequate products.

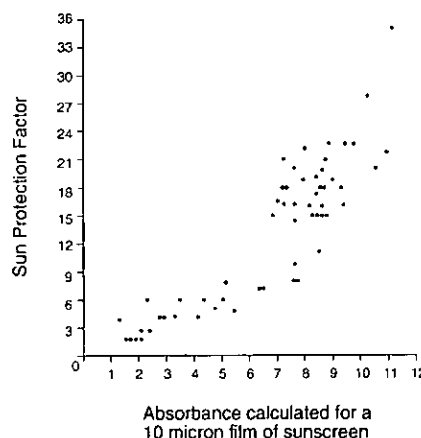
Thirty years ago it was thought that because a day's solar radiation equated to about 15 MED's then an SPF of 15 provided maximum protection. Since SPF's drop in value during use, then if we continue to use formulations of doubtful substantivity, it would be prudent to begin with SPF's greater than 15. Better substantivity also ensures a more efficient use of the UV-actives.

Which UV absorber or combination of absorbers to use depends both on the degree of protection and the desired spread of protection across the UVA and UVB range. The choice also depends on which UV actives are approved for use in a particular country, and on the maximum allowed concentration. These maxima appear to bear little relation to the standard absorbance values of the various compounds. A certain active may also be chosen for its good solubilising effect on other components of the mixture, or for its effect on the physical properties of a gel formulation.

Since most sunscreens are emulsions, formulators are faced with the limitation that the emulsifying surfactants ending up on the skin will act against good substantivity in the presence of water, including sweat.

Figure 3.

Relationship Between Sunscreen Absorbance and Initial Protection Factors



Using spectrophotometry in aid of design for a certain initial SPF is simple and effective within its limitations. We must accept that UV damage is possible at suberythemal levels and that the initial SPF tells us nothing about substantivity. Nevertheless, absorbance, unlike per cent transmittance, relates to SPF in a useful manner. The points plotted in Figure 3 derive mainly from published SPF data and also from some personally-owned results. The absorbance values for the published data have been calculated from the published percentages of absorbers present in each product. Whilst the accuracy and precision of spectrophotometry is not in question the same cannot be said about all SPF data. This unreliability and the complication of the influence of different substantivities as longer exposure times are required blur the picture at SPF's of 15 and above.

Since the A (10 micron) value is ten per cent of the standard absorbance value for a component or for a whole product, we can calculate the required amounts approximately from data in Figure 2 and combine in simple additive fashion the absorbance contributions from more than one active ingredient.

Although numerous formulas and their accompanying initial SPF values are available from suppliers of raw ingredients the calculation method is helpful when juggling the consequences of using various mixtures, the constraints of SPF and possible broad spectrum requirements, cost and regulatory and solubility limitations.

Designing for good substantivity has involved formulating emulsions containing water repellent polymers including silicones or avoiding emulsions altogether. Published formulas are available in which the oil phase of emulsions consists entirely of silicones (16). Not unexpectedly, water-in-oil emulsions provide better substantivity than oil-in-water emulsions (19).

Dr F Greiter, a pioneer of outdoor sunscreen testing, and one who was very aware of the time factor in SPF's developed a non-emulsion formula which has been popular for many years. A few other products of that type are now on the market and there appears to be a good future for well designed, longer lasting nonaqueous formulations.

STABILITY OF SUNSCREENS

Long term stability for aqueous emulsions requires that the active ingredients, many of which are esters, survive hydrolysis. Even if the loss of the lipophilic side chains has little effect on the absorbance, the formulation of the free acid may lead to precipitation or at least to a more polar entity with reduced substantivity. Non-aqueous formulations are inherently more stable chemically and microbiologically.

Stability to UV is also required but it is unlikely to be a problem in the few hours of possible exposure, and at the relatively high concentrations employed in sunscreens. Little work has been published on sunscreen stability in formulations and there would seem to be a need to look more closely at the stability of C in some emulsions. A case came to the authors notice recently which pointed to a substantial loss of C during two years storage.

UVA CONTROVERSIAL WAVELENGTHS

The total solar energy (irradiance) in the UVA region reaching the surface of the earth is about three times that in the UVB (18).

SURPLUS ANALYTICAL EQUIPMENT

- * CSI Supergrator 2 Integrator
- * Unicam SP-3 IR spectrophotometers with 050 interface
- * Wilks 20 metre variable path length gas cell (2) for IR analysis of gases
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Why then is there a lack of agreement on how much protection we need against it, or in fact whether we need to be protected from it at all?

For the chemist, the Grotthus-Draper Law is a good place to start. This tells us that only radiation absorbed by a system is effective in producing photochemical change. We also know that absorption of radiation depends on molecular structure. The total quantity of radiation present per se is therefore irrelevant.

Ill-informed sales literature promoting the UVA blocking products depicts UVA penetrating the skin to a much greater depth than does UVB. We know that the biological effects of UVA are relatively mild compared to those from UVB. Rather than demonstrating the danger from UVA this deeper penetration in fact shows the opposite. UVA penetrates because of its lesser absorption by the molecules in the tissue. If it is not absorbed, Grotthus and Draper tell us that it is having no effect; no more effect than when we shine a torch light through our hand. UVB and UVC radiation penetrates less because it is absorbed by some of the cell constituents to produce many harmful biochemical effects.

Nevertheless, UVA is absorbed to some extent and does have a number of effects (26) including erythema production, pigmentation, dermal connective tissue alterations, and tumour production in animals. Phototoxic and photoallergic reactions have also been reported (26). But the weakness of these effects compared to those associated with UVB has prevented agreement on the amount of protection, if any, we need against UVA.

An extreme view is that taken by the Garland brothers (27) who claim that by using UVB-blocking sunscreens with poor UVA-blocking ability we are encouraged to stay longer in the sun and therefore suffer harm from UVA. In support of this argument they quote the rising rates of melanoma in countries where sunscreens have been in use for many years. A more mundane explanation does not seem to have occurred to them. This is simply that the figures may merely be demonstrating the inadequacy of most commercial sunscreens.

Attempts have been made to arrive at protection factors for UVA using the erythema or tanning response (28, 29, 30). The amount of protection found in these studies is roughly what one would expect from an inspection of the absorbance curves in Figure 1.

As indicated earlier, some Australians have made a guess at what might be a desirable degree of UVA protection, but there is as yet insufficient evidence on the matter, and as a result the FDA authorities in the USA have refused to back a UVA standard.

Dose and spectral response studies of skin tumour production in irradiated hairless mice have shown that the action spectrum for photocarcinogenesis coincides approximately with the action spectrum to produce erythema (17). This and other studies showed that wavelengths above 330 nm have virtually no carcinogenic effect in animals. There does not appear to be any strong reason as yet for serious concern about UVA.

ACKNOWLEDGMENT

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SYNTHESIS OF DIAMOND FILMS FROM ACETYLENE FLAMES

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INTRODUCTION

The mechanical, electrical, thermal and optical properties of diamond make it attractive for use in a variety of applications, ranging from wear resistant coatings on tools and engineered components, to advanced semiconductor structures for integrated circuit devices. Diamond has a large band gap (5.5 eV), a low dielectric constant, high carrier mobility, high breakdown voltage, and is resistant to high temperatures and radiation. This resistance to radiation induced degradation is coupled with optical transparency in the visible and infra-red regions. These characteristics make diamond a material of major technological importance and potential, if suitable methods of fabrication, particularly of semiconductor quality thin films, can be developed.

The synthesis of diamond from graphite within its field of thermodynamic stability (ultrahigh pressures 60,000 atm. and temperatures >1500°C) was developed by General Electric in the 1950's and has been widely used for diamond production, particularly of abrasives, at the rate of about 100 tons per year. Although it was not widely reported until much later, shortly after the GE development, Spitsyn et al. [1] developed a method of synthesis in the "thermodynamically hindered" low pressure region [2] i.e. well outside the stability field. Many workers have attempted to synthesize diamond in the hindered region [1-3] and attempts have increased many fold since the Spitsyn publication in 1981 [3]. A typical method of synthesis has been Chemical Vapour Deposition (CVD), using a tungsten filament to generate reactive species from methane hydrogen mixtures at pressures of around 1 Torr. [4]. Plasma assisted CVD using microwave or radio frequency (RF) devices [5,6] and ion beam sputtering methods have been reported as alternatives for the activation of the gaseous hydrocarbon [7,8]. Variants on these methods are steadily being reported, most driven by the need to achieve higher growth rates and better mechanical properties. A number of relatively high pressure (100-760 Torr) techniques such as dc plasma jet CVD [9], thermal RF plasma deposition [10] and arc discharge plasma CVD [11] have emerged for successful diamond deposition.

Thin diamond films with a variety of morphologies and physical properties are now being produced and their properties investigated at a number of research laboratories. Despite the relative immaturity of the technology, in certain applications, the technological feasibility of producing diamond coated components has been established. Companies such as Asahi Industrial Diamond, and Shinetsu Chemical Co. are already coating small areas of drills, dies, cutting knives and some bearing surfaces with CVD diamond films. Sony, Onkyo and Sumitomo Electric are using diamond films on loudspeaker tweeters. Sumitomo also report making preproduction diamond thin film base semiconductors, and Crystallume in Menlo Park,

California, appear to be the first company devoted entirely to diamond film manufacture.

The techniques that are mentioned above have succeeded in achieving deposition rates as high as 180 µm/hr [12] but are still quite expensive, as they require high vacuum chambers and sophisticated plasma or sputtering sources. Also vacuum deposition techniques do place some restrictions on the type and size of substrates for film deposition.

In 1988, Hirose and Kondo [13] reported the synthesis of diamond in an oxygen-acetylene flame, in the ambient atmosphere, and with growth rates averaging ~100-200 µm/hr. Reports confirming the combustion synthesis process followed soon afterwards [14]. It is essentially another variant on the CVD route, but in this case, combustion generates the activation of the hydrocarbon in a remarkably simple experimental configuration. This method appears to offer a number of advantages in reaction control and cost over conventional CVD and has become another growing area of diamond film research.

Because of existing interests in plasma, combustion and surface chemistry, we have initiated a research programme in this area. Although in its infancy, we have been successful in making diamonds and diamond films, and readily achieving deposition rates greater than 100 µm/hr. Our aim is to elucidate the nucleation and growth mechanism of diamond on hetero-epitaxial substrates and thus improve diamond film quality and commercial viability in selected applications. We report here on the early progress in diamond film synthesis at the University of Auckland, highlighting some of the results, and the techniques used for characterising the material produced.

EXPERIMENTAL

Diamond films have been prepared using oxy-acetylene flames of different O₂/C₂H₂ ratios, varying between neutral (molar ratio 1:1) and acetylene rich (0.85:1), at various substrate surface temperatures in a 650-900°C growth window. The experimental set-up used for this is shown in Figure 1. Mechanically polished silicon wafers were used as the substrates. The deposition temperature was measured with an Infra-red, two-colour optical Pyrometer and controlled by changing the cooling rate of the substrate holder. The heat transfer and distribution in the reaction zone above the surface is critical in the selective growth of diamond, as it is a major factor in determining the speciation of the reactants. Temperatures involved have to be high enough to provide sufficient energy for the initial activation of the hydrocarbon and maintain sufficient concentrations of, for example, atomic hydrogen, to allow diamond growth after dissociation of the hydrocarbon starting gas.

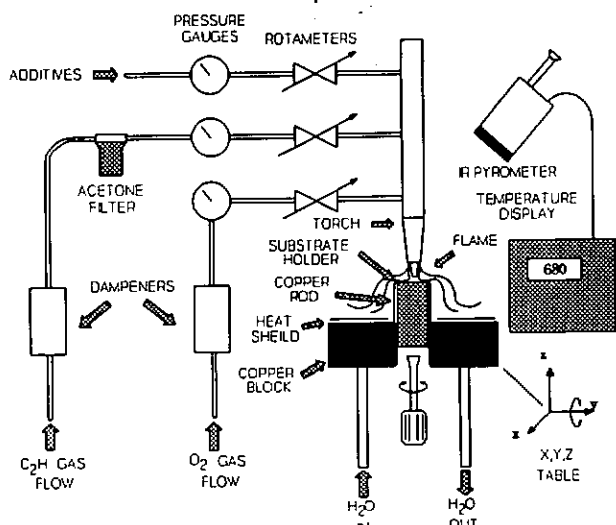


Fig.1 A schematic diagram of the deposition system used for growth of diamond films using acetylene flames.

SEM (scanning electron microscopy) and XRD (x-ray diffraction) were used to establish presence of crystalline diamond and Raman and electron energy loss (EELS) spectroscopy were used to distinguish between the various forms of carbon present. SEM was also used to study the physical morphology of the products. The morphology of diamond can vary from cubic to octahedral, with a variety of cubo-octahedral intermediates as shown in Figure 2, and most of these have been observed in our experiments.

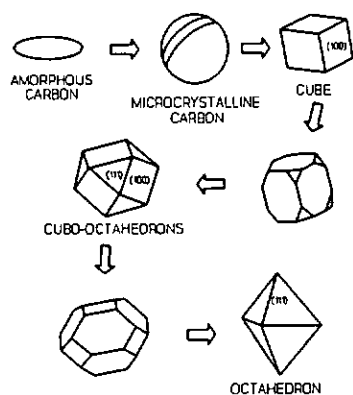


Fig.2 Representative morphologies and structural transformations of diamond.

RESULTS

Figures 3a & 3b show SEM micrographs of two early oxy-acetylene grown diamond samples. As can be seen from the larger density of the crystals growing near defect sites/scratches on the substrate, surface preparation is critical in assisting nucleation. Figure 4 shows SEM micrographs of typical large crystals in which the crystal faces can be well resolved. For the growth of such discrete diamonds, the observed crystals are of the order of $\sim 100 \mu\text{m}$ after 1 hour of deposition. This is comparable to the best reported values for crystal sizes in diamond films grown by any technique in comparable time. Surface preparation by silicon carbide polishing results in relatively low nucleation densities and large discrete diamonds. Polishing with finer abrasive increases the nucleation densities,

but by far the highest nucleation densities, resulting in continuous films, result from polishing with diamond paste. In all cases, samples were carefully ultrasonically cleaned after the abrasive treatment, so direct seeding is not the dominant nucleation mechanism. (There are some diamond film techniques which do mechanically imbed fine diamond crystals into the surface to act as seed nuclei).

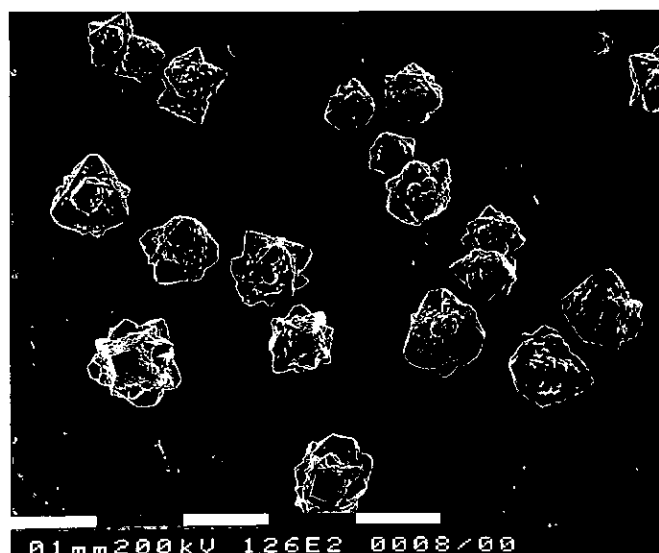
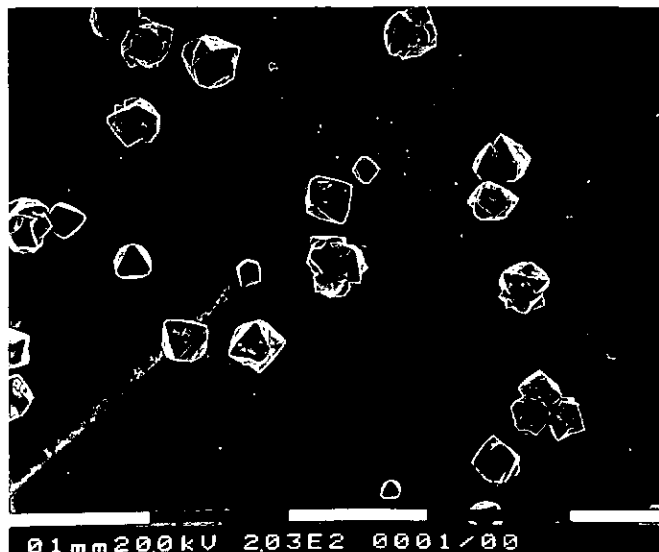


Fig.3a,b Scanning electron micrographs of diamond particles on a silicon carbide polished silicon substrate deposited by the oxy-acetylene flame method, and observed at the edges of the deposition region.

Fig.5a shows the Raman spectrum of a highly transparent film, which shows the F_{2g} triply degenerate diamond mode at 1332 cm^{-1} and the sharp peak at 518.5 cm^{-1} corresponding to the silicon substrate. The broad peak at $\sim 1482 \text{ cm}^{-1}$ is due to non-diamond carbon, referred to in the literature as NDC [15,16]. Fig.5b shows the Raman spectra of a more typical film, with the diamond mode at 1332 cm^{-1} and the first order doubly degenerate E_{2g} mode of graphite at approximately 1524 cm^{-1} . Raman efficiency of the detection of the graphite phonon is 50 times higher than that of diamond [17,18], so that even a very small amount of sp^2 carbon present in the film gives a large signal. Though Raman spectroscopy is very sensitive to carbon hybridisation, it has limited surface sensitivity and some limitations in spatial resolution.

A novel application of electron energy loss spectroscopy (EELS) was used in an attempt to identify areas giving signals attributed to graphitic or amorphous carbon. EELS spectra of the films were taken using a Kratos XSAM 800 spectrometer normally used for XPS/AES analysis and located in the Research Centre for Surface and Materials Science. Spectra were taken in the reflection mode with incident electron beam energies $\sim 500\text{eV}$, and the energy losses from the elastic peak were examined. The most useful loss structure is the $\pi \rightarrow \pi^*$ resonance observed $\sim 5\text{ eV}$ below the elastic peak. This is characteristic of graphite as shown in figure 6a. The use of the reflection mode renders these spectra extremely surface sensitive, so EELS spectra taken in this mode can be used as a sensitive tool to detect any graphitic deposition in the films. Before taking the EELS spectra, films were checked for other chemical impurities using Auger electron spectroscopy and were found to contain no impurities other than adsorbed oxygen. The films were SEM imaged to observe the microstructure and different spots were chosen for EELS spectra, with a spatial resolution of 10-100 μm . Fig.6b shows the EELS spectrum of a diamond grain, while Fig. 6c is the EELS spectrum of the film at the edge of the deposition zone, indicating that carbon is present in both sp^2 and sp^3 forms in this region. The presence of sp^2 carbon at the edges is attributed to poorer control on the deposition parameters, particularly uniformity of temperature and gas mixing, at the edges of the area on which the flame impinges.

One of the current areas of interest in all the deposition techniques in the thermodynamically hindered region is the uniformity of deposition. Most of these methods are as yet far from being fully optimized and attempts are directed not only toward making larger area uniform films, but also to reducing the substrate temperature without significant sacrifices in growth rate. A further issue is deposition on non-planar or convoluted surfaces. Answers to many of these questions will depend largely on progress on some of the underlying scientific problems regarding the growth mechanism.

One of the many issues that has yet to be resolved unambiguously is how diamond is nucleated on the surface of non-diamond substrates [19].

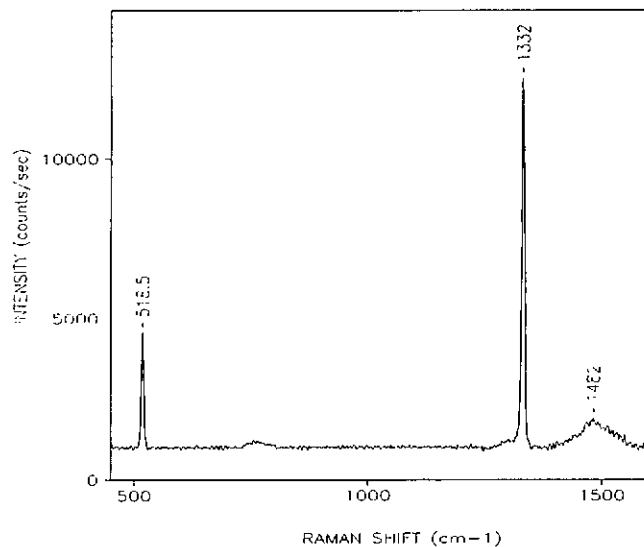
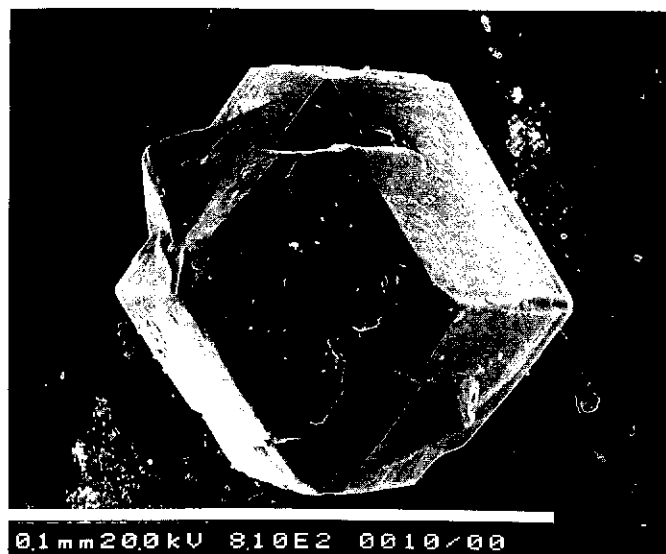


Fig.5a Raman spectrum of a highly transparent polycrystalline diamond film on a silicon substrate.

The deposition of diamond can be separated into two critical steps, nucleation and growth. It is likely that on silicon wafers, the intermediate formation of silicon carbide provides the high energy surface sites and the "pseudo epitaxial" surface on which diamond nucleates [20,21].

The exact mechanism of subsequent diamond growth in the combustion method is also not resolved, however the reactions which select the kinetically unfavoured "diamond like" carbon are probably shared with CVD. The critical species is a surface carbon radical generated by the abstraction of a hydrogen from a terminal CH by a gas phase radical. In the case of hot filament CVD, and probably in combustion synthesis, this is atomic hydrogen from the gas phase. The tetrahedral geometry is then defined and maintained by the geometry of this surface radical. Jackman and Chua [22] have identified adsorbed acetylene on the surface of Si(100) after hot filament activated dissociated methane/hydrogen mixtures and observe reaction with adjacent methyl species to form C_3 species. Subsequent H abstraction leads to regeneration of the acetylenic intermediate and carbon chain propagation.

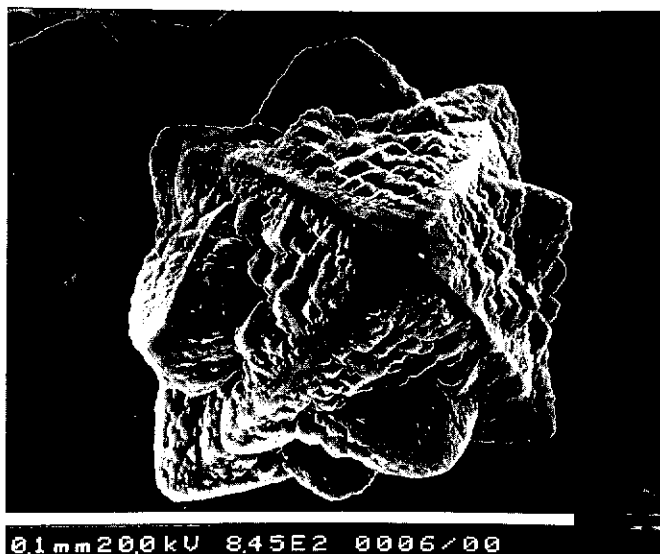


Fig.4a,b Scanning electron micrographs of diamond growth on a silicon wafer after 1 hour of deposition in the oxy-acetylene flame.

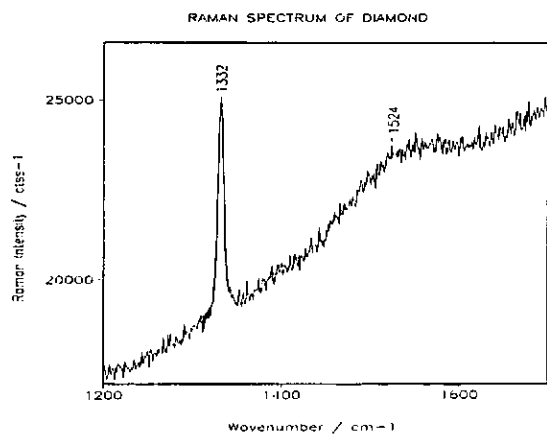


Fig.5b Raman spectrum of a typical coarse polycrystalline diamond film.

Our present efforts are directed towards understanding the growth mechanism of diamond crystallites. We are using X-ray photoelectron spectroscopy (XPS) to chemically identify the nucleating species. Efforts are also directed towards correlating microstructures of diamond and diamond-like films with the gas compositions and temperatures at which the films are formed. If such diamond films are to be used in the micro-electronic industry, a high degree of structural control is necessary. For most applications, production, at an acceptable growth rate, of films with very little graphitic or amorphous carbon component is required.

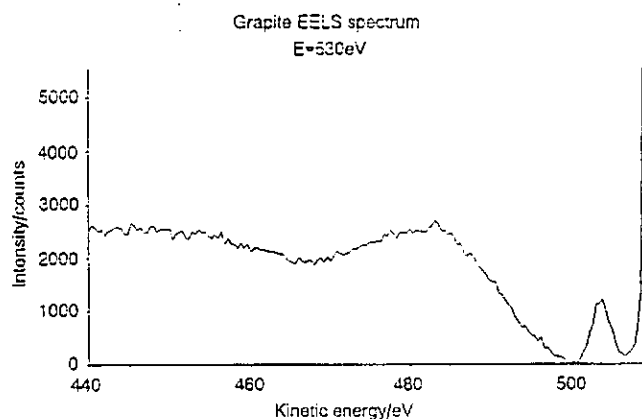


Fig 6a Electron Energy Loss spectra of a graphite film. The structure $\sim 5\text{eV}$ below the elastic peak is due to π resonance. This is characteristic of sp^2 type carbon as observed in graphite.

CONCLUSION

Production of quality diamond films using a relatively simple technology, appears to be quite viable and has been demonstrated in our laboratory. The characterisation methods we are using allow us to address the important questions regarding the structure and growth mechanism of these diamond films. Moreover, even at these early stages of our work, diamond films with, in general, lower 'non-diamond' carbon level, as compared to CVD films, have been grown by this route and there is still substantial room for further development. The critical factor is clearly controlling the earliest stages of deposition, so that acceptable nucleation densities are achieved.

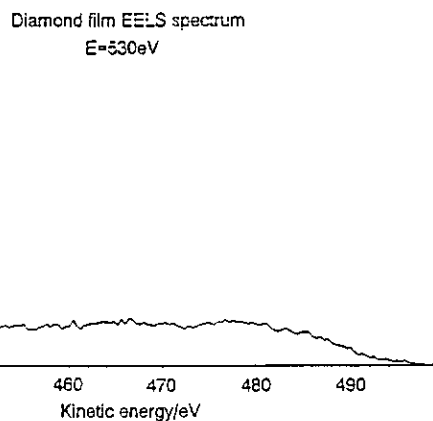


Fig 6b Electron Energy Loss spectrum of a typical good quality diamond film grown by the combustion method. Note the absence of any resonance structure below the elastic peak. This indicates the virtual absence of sp^2 bonding and is typical of diamond.

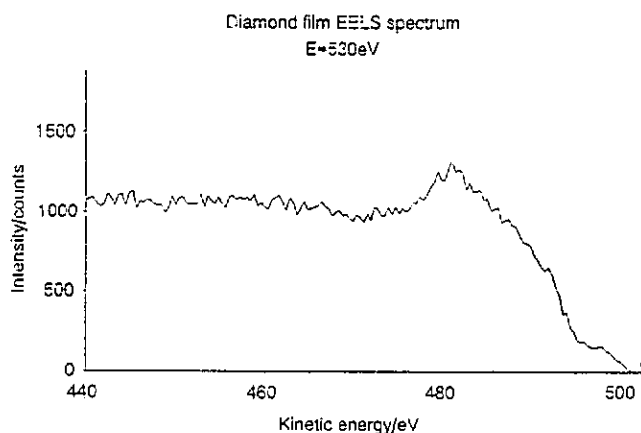


Fig 6c Electron Energy Loss spectra of a diamond film taken near the edge of the deposition zone. This indicates the presence of carbon in both graphitic and diamond form.

At the moment, the major international research effort in such technology is centred in Japan, U.S.A and Russia. Although industrial application of diamond films and diamond-like films is just beginning, predictions put the value of overall global shipments of commercial diamond film products over US\$1 billion by 1997 (International Resource Development Inc., IRD) and the market for diamond-like films at over US\$100 million by 1995 (Technical Insight Inc.).

Acknowledgements

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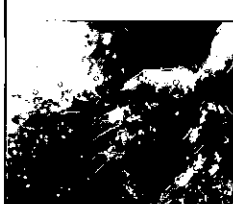
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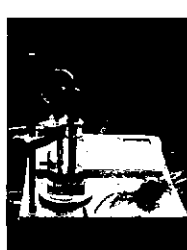
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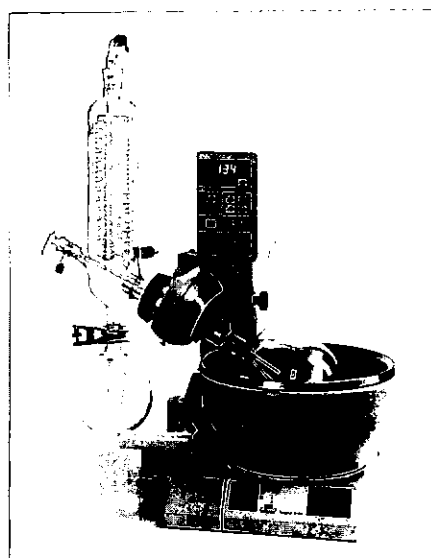
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HP developed HP DrugQuant drug-analysis software to meet the specialised needs of drug analysis laboratories using HP MS systems to confirm and quantitate drugs or their metabolites in specimens. HP DrugQuant drug-analysis software strengthens HP's MS system solutions for laboratories performing drugs-of-abuse and sports doping testing, as well as therapeutic-drug monitoring and clinical testing.

Intelligent batch sequencing of HP DrugQuant makes real-time decisions, without the intervention of an operator, to correct the problems laboratories typically encounter when analysing a batch of drug-analysis samples. For example, intelligent batch sequencing can automatically reinject specimens and controls if ion ratios, retention times or internal standard criteria fall outside of a laboratory's limits. Intelligent batch sequencing improves laboratory productivity because operators do not have to remain close to the HP MS system in order to monitor problems. This allows operators to complete other tasks. It also enables laboratories to analyse more samples because operators do not have to re-extract, reinject and rerun samples or entire batches when drug analysis problems occur. Intelligent batch sequencing ensures consistent analyses because it makes consistent decisions based on analytical results. Chain-of-custody is ensured because samples are reinjected by the system - not by an operator.

Automated reports and statistical charts allow drug-analysis laboratories to integrate quality assurance into their analytical methods and to eliminate transcription errors. One of these

automated reports, the batch summary report, gives the operator reviewing the batch a quick look at the status of the run and flags samples where ion ratios or retention times fall outside the laboratory limits. HP DrugQuant drug-analysis software can automatically track up to three levels of control values with Levey Jennings and percentage-control charts. Using Westgard Rules, HP DrugQuant drug-analysis software flags controls that are outside limits. Control charts increase detection of both random and systematic analytical errors and help the laboratory comply with certification requirements.

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The new models also feature an innovative high performance 60° Michelson mechanical interferometer incorporating dynamic alignment during every scan. The spectrometers offer resolution to 0.25 cm^{-1} and a maximum scanning rate in excess of 20 scans/second.

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The new spectrometers are controlled by HP Vectra Workstations running "WIN-IR", a powerful Windows-based programme that links seamlessly with popular word processors and spreadsheets. The software enables the user to operate the spectrometer at a number of levels depending on the experience of the user, and the application required.

For the routine user, the display screen can consist of a series of "buttons" that implement specific commands using the point and click mouse technique. These commands typically include "SCAN" and "PLOT" and may also implement arithmetic routines, library search or quantitative programmes.

For the first time, users are not limited to an interface designed by the spectrometer manufacturer, each screen and command set can be custom designed for the user who owns the unique application.

The FTS-175 and FTS-185 FT-IR Spectrometers are designed for operation in the mid-IR region with the flexibility of operating in other spectral ranges. The high energy optics employed in these new spectrometers are ideal for use with hyphenated techniques such as GC/FT-IR, IR microscopy and TGA.

Contact: Bio-Rad Laboratories, P O Box 100 051, NSMC, Auckland, Ph. (09) 443 3099, Fax (09) 443 3097 **or circle no. 48 on the reader reply card**

PERKIN-ELMER'S NEW UV/VIS SPECTROMETERS

Based on the successful model Lambda 2 spectrometer are two new UV/Visible spectrometer systems from Perkin-Elmer.

The Lambda 11 is a single beam instrument designed for laboratories in the educational, industrial and pharmaceutical market. Special attention was given in the design to simplicity of operation. Five preprogrammed standard methods on the keyboard can be executed simply by pressing the START button. These methods include quantitative analysis with factor concentration or simple calibration methods, absorbance versus time (time drive analysis), wavelength program method and spectra monitoring. Additional methods can be derived easily from the basic method, then stored and reused at any time.

The Lambda 2S double beam spectrometer is the basis for a variety of applications systems including:

- dissolution testing in the pharmaceutical industry
- flow injection analysis for environmental and food industry applications where on-line sample preparation and derivatisation is performed
- kinetic analysis for enzyme and substrate determinations on multiple samples simultaneously with several options for sample temperature control
- automated analysis with sample transfer systems and autosamplers
- remote sampling with the fiber optic system and dedicated optodes

The quality of these two new instruments is proven in an instrument certificate, the starting point for Good Laboratory Practice following the ISO 9000 regulations.

Contact: Perkin-Elmer New Zealand, P O Box 22 159, Otahuhu, Auckland, Ph (09) 276 2230, Fax. (09) 276 5602 **or circle no. 49 on the reader reply card**

ANALYSIS OF PCB'S IN INDOOR AIR

A new application note is now available from Perkin-Elmer detailing a thermal desorption/capillary GC/MS analytical procedure for monitoring vapour phase polychlorinated biphenyls in indoor air.

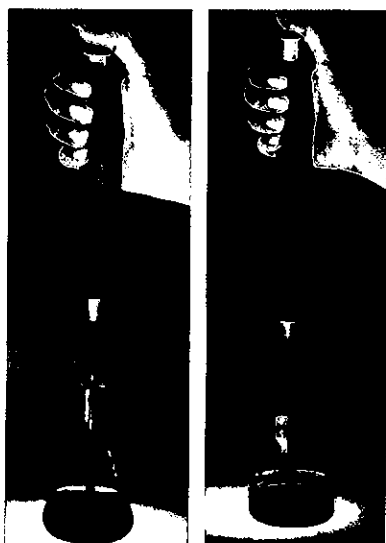
Method development and evaluation work was conducted by the Federal Office for the Environmental Protection and Trade Inspection (LFUG) in Germany. The method specifies pumped sampling onto tubes packed with Tenax™ GR followed by thermal desorption with a Perkin-Elmer Model ATD 400. Analysis is by capillary GC/MS and detection limits are in the order of 1.0 ng/m^3

Contact: Perkin-Elmer New Zealand, P O Box 22 159, Otahuhu, Auckland, Ph (09) 276 2230, Fax. (09) 276 5602 **or circle no. 50 on the reader reply card**

MACRO PIPETTING

Labsystems designers have drawn on all the expertise gained developing the renowned Finnpiquette range to produce the macro range of Digital Finnpiquettes, (1-5mL and 2-10mL). The designers have succeeded in building all the features of the Digital range into a 2-10mL pipette which is of a manageable weight and size, resulting in an easy to use and convenient unit.

A feature of both pipettes is the uniquely designed piston assembly which eliminates vortex contamination, a common problem when pipetting large volumes. Additionally the 2-10mL pipette has a dampened piston action which prevents foaming normally associated with dispensing large volumes of liquid.



These surprisingly light macro pipettes are comfortable to use and easy to hold on to. The handles have been designed to prevent overall hand strain when pipetting for long periods. A streamlined separate tip ejector prevents accidental detipping and the digital volume control enables rapid single-handed adjustment over the volume range.

Calibration certificates are supplied with each pipette as a guarantee of its accuracy and precision. Pipettes can be easily recalibrated in the laboratory to meet GLP and routine maintenance can also be performed easily by the user.

Contact: Douglas Scientific, P O Box 45 027, Auckland 8, Ph: (09) 837 5447, Freephone (outside Auckland) 0800 735 725, Fax (09) 836 0668 **or circle no. 45 on the reader reply card**

ELGA ENHANCE THEIR OPTIONS

Elga, the Pure Water people, have re-launched their well-proven Elgastat Option range of laboratory water purifiers with new styling and improved technical features. Comprising four compact models the Option range has been used worldwide either to enhance the performance and operation of distillation units or replace them with self-contained, cost-effective systems. Option 1 provides primary-grade feedwater for a still - minimising downtime and operating costs, and improving distillate quality - whereas Option 2 enhances the purity of water pre-treated by distillation or reverse osmosis. Both Options 3 and 4 are independent multiple-technology

systems providing low cost high purity water by utilising a combination of pretreatment, reverse osmosis, ionic/organic removal and photo-oxidation.

The new 1993 Options are a darker shade of grey and have been restyled to complement the modern laboratory. The purification media have been upgraded to provide more efficient organic removal, and the photo-oxidation chamber has been enlarged, extending the contact time between the water and the ultraviolet radiation. As a result, bacteria are destroyed more effectively, and organic molecules are split more readily, facilitating their removal by the purification media.

The Elga range of water purification systems has been further enhanced by the newly released Optima range which produces general laboratory grade water with a flow rate of 30 or 60 litres per hour.

Contact: Douglas Scientific, P O Box 45 027, Auckland 8, Ph: (09) 837 5447, Freephone (outside Auckland) 0800 735 725, Fax (09) 836 0668 **or circle no. 46 on the reader reply card**

ENHANCED PERKIN-ELMER SYSTEM 2000 FT-IR PERFORMANCE AND APPLICATIONS

A new colour brochure available from Perkin-Elmer outlines the enhanced capabilities of the System 2000 FT-IR. The resolution specification has been increased to better than 0.3 cm^{-1} (upgradeable to 0.15 cm^{-1} in the field) and the signal to noise has been increased to typically better than 30,000/1 RMS; 6000/1 peak to peak for 5s measurement, 4 cm^{-1} resolution (DTGS detector, KBr beamsplitter). A cutaway view of the System 2000 illustrates its unprecedented optical and sampling flexibility, with a detailed key showing the range of options which allow the user to select a configuration to match particular applications precisely.

A new Applications Brochure is also available which discusses many example applications and includes well established performance tests. While by no means exhaustive, these demonstrate the versatility and capabilities of the System 200 FT-IR.

Contact: Perkin-Elmer New Zealand, P O Box 22 159, Otahuhu, Auckland, Ph (09) 276 2230, Fax. (09) 276 5602 **or circle no. 47 on the reader reply card**

CHROMATOGRAPHY NEWSLETTER FROM PHENOMENEX

The "Resolution Times" is a 12 page chromatography newsletter published quarterly by Phenomenex. Focusing on the separation sciences, the newsletter is designed primarily for the technical education of its readers. Advances in science and separation technology are covered along with new chromatography products from Phenomenex. Column Applications, Chromatography Calculations, Troubleshooting, Science News, Chiral Corner, and "Did You Know?", are just a few of the columns included in each issue.

Contact: Chromspec Distributors Limited, P O Box 367, Warkworth Ph. (09) 425 9032, Fax (09) 425 9032 **or circle no. 57 on the reader reply card**

THERMAL ANALYSIS WITH THE FLEXIBILITY OF WINDOWS

Shimadzu have complemented their range of modular thermal analysis instrumentation with flexible, easy to use, Windows based software, TA-50WS for Windows.

TA-50WS gives you more. More channels. More features. More control. It is the only thermal analysis software that gives you simultaneous control of up to four thermal analysis modules using Microsoft Windows v3.1.

The easy to learn software gives complete control over the Series 50 range of modular thermal analyzers from Shimadzu (DSC, TGA, DTA & TMA).

TA50WS software enables you to check on your sample without having to wait for it to finish its run. With SnapShot, you can perform real time analysis for quick Pass/Fail determination. This exclusive feature of Shimadzu's software lets you take an advanced look at your thermogram while still in the measuring mode. Three clicks of the mouse captures a snapshot of the still acquiring thermogram, analyses and reports your findings and then returns you to the measuring display.

Not only does the TA50WS software enable you to control four instruments, but the quad screen display lets you view those analyses simultaneously on your screen. When you are ready for closer examination of one analysis in progress, point and click on the desired channel and a larger screen appears with on-screen cross-hair cursor display.

Compare multiple thermograms in the same display. Multiview lets you overlay up to twelve thermograms by clicking on the desired files. Perform unlimited additions or replacements of existing files easily for continuous comparison.

Contact: Douglas Scientific, P O Box 45 027, Auckland 8, Ph: (09) 837 5447, Freephone (outside Auckland) 0800 735 725, Fax (09) 836 0668 **or circle no. 51 on the reader reply card**

MELT FLOW - DENSITY - FRICTION - IMPACT

Lloyd Instruments have incorporated Davenport Instruments into their range of materials testing instrumentation.

Now along with tensile testers, low force gauges, torque gauges and chart recorders,

Lloyd Instruments offer:

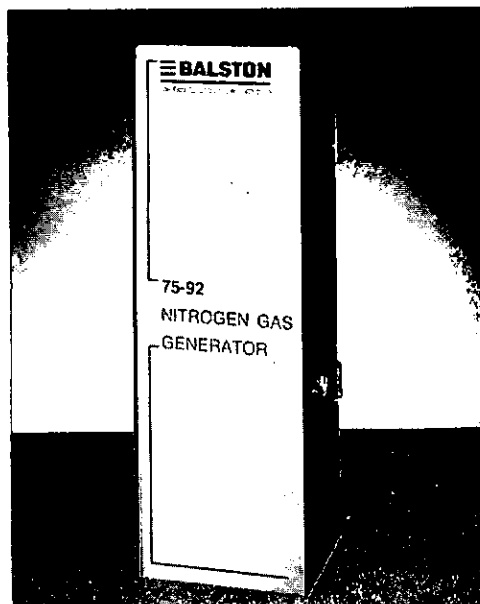
- Melt Flow Indexers
- Density Gradient Columns
- Melt Viscometers
- Falling Dart Impact Testers
- Pneumatic Impact Testers

Contact: GBC Scientific, P O Box 68 330, Newton, Auckland, Ph: (09) 373 5765, Fax (09) 360 0683 **or circle no. 52 on the reader reply card**

BALSTON GAS GENERATORS AN ALTERNATIVE TO DANGEROUS AND INCONVENIENT CYLINDERS

Now available in New Zealand are the Balston range of laboratory gas generators to produce high purity gases for analytical instrumentation. Balston provides the safest and purest source of >99.9998+% purity hydrogen, 99.9995% purity nitrogen and purified air for GC, FT-IR, TOC, AAS, NMR and other techniques.

Balston Gas Generators eliminate the need for dangerous and inconvenient cylinders and free up valuable laboratory floor space. All the systems are easy to install, operate and maintain, even by personnel not trained in instrumentation.



Also available are explosion-proof models suitable for instruments located in potentially explosive environments.

Balston quality products are manufactured by Balston Inc., one of the Whatman Group of Companies in the USA. Each model incorporates the best quality components available to ensure long term reliability and trouble-free operation.

See the Balston and Whatman product ranges on display at the Labsupply Pierce (NZ) Ltd stand at the NZIC Conference or:

Contact: Labsupply Pierce (NZ) Ltd, P.O. Box 34-234, Birkenhead, Auckland. Ph. (09) 443 5867 Fax (09) 444 7314 **or circle no. 53 on the reader reply card**

NEW DIGESTION SYSTEMS

Tecator is launching a new generation of its well known digestors. The basic concept, of doing multi-sample digestions like Kjeldahl and other wet digestions on limited bench space with the assistance of a broad range of accessories, is still the same. The new generation of digestors has improved performance and even more accessories to give better working conditions as well as savings in the use of water and energy.

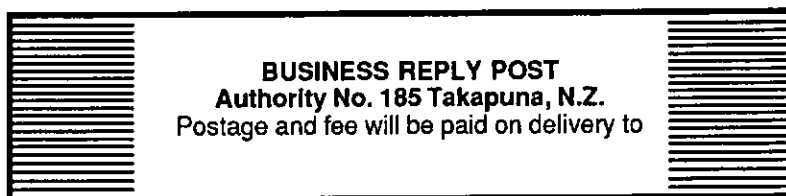
Contact: Sci Tech, P O Box 663, Dunedin, Ph. (03) 477 7860, Fax. (03) 477 7870 **or circle no. 54 on the reader reply card**

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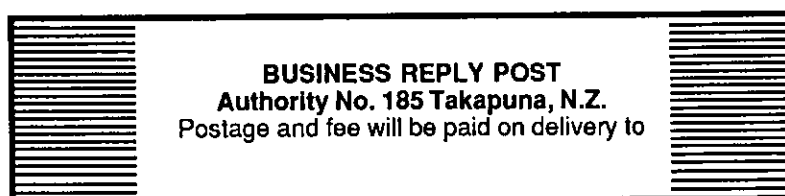
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THE NEW OPTIFIX® RANGE OF BOTTLE TOP DISPENSERS

For many years OPTIFIX® dispensers have been renowned for their functionality, safety, precision and reliability.

OPTIFIX® now introduce a new generation range of dispensers with models to suit all laboratory applications.

OPTIFIX® *BASIC* - with PTFE coated glass pistons for dispensing aqueous solutions and weak acids.

OPTIFIX® *SOLVENT* - for dispensing organic solvents and other solutions that cause PTFE to swell.

OPTIFIX® *SAFETY* - with PTFE coated glass pistons possessing an extra lip seal on the piston end, and a PTFE valve ball for ventilation. These dispensers are ideal for strong, fuming acids and other media with strong pungent odours.

OPTIFIX® *HF* - both cylinder and piston are made of PTFE for dispensing hydrofluoric acid.

All the new OPTIFIX® dispensers feature a modern ergonomic design and a new volume setting system including an additional fine adjustment control for rapid and accurate volume setting. The corrosion resistant scale rod is made of polypropylene and has graduations on both sides to suit both left-handed and right-handed operators.



Contact: Labsupply Pierce (NZ) Limited, P O Box 34 234, Birkenhead, Auckland, Ph. (09) 444 5867, Fax. (09) 444 7314 **or circle no. 37 on the reader reply card**

NEW FROM METTLER: THE FP900 THERMOSYSTEM

The research and development of new materials often calls for exact knowledge of the thermal behaviour. In quality assurance or production monitoring experimental results are compared with a standard.

The new FP900 Thermosystem from Mettler with five measuring cells for various analytical procedures is an efficient and appropriate tool for the numerous analyses in this field. In comparison with the earlier Thermosystem, the temperature range of several cells has been extended by 50°C to 375°C thereby expanding the range of possible applications.

The FP90 Processor is the central unit of the FP900 Thermosystem; it functions as the control and communication device of the system. Any one of five measuring cells can be attached to it: the FP181HT Measuring Cell for melting, boiling and cloud points, the FP83HT Measuring Cell for dropping and softening points, the FP82HT/FP84HT Thermal Microscopy Hot Stages or the FP85 Measuring Cell for DSC (differential scanning calorimetry).



The operation of the system is simple, yet flexible. The analysis is started at a keystroke after entry of the required parameters. The FP90 then controls the attached measuring cell according to the set method. The measurement is performed fully automatically, rapidly and objectively due to electronic detection of the final signal.

Calculation of the results from the experimental data is automatic. An attached printer generates a record, an analog recorder can be used to plot the measured signal during the analysis. An interface built in as standard also allows bidirectional data interchange with a computer or an LIMS.

Contact: Watson Victor Ltd, P.O. Box 1180, Wellington, Ph. (04) 385 7699, Fax (04) 384 465 **or circle no. 38 on the reader reply card**

HEIDOLPH SHAKING AND MIXING MACHINES

The four large shaking and mixing machines from Heidolph give impressive performance.

The electronic speed control gives constant speed regardless of load and the LCD speed display allows reproducible speed setting. All systems have an in-built timer and a capacity of up to 10kg allowing the machines to handle up to 108 conical flasks.

A full range of easily fitted or removed accessories is available and the machines suit a wide range of applications.

Contact: John Morris Scientific Limited, P O Box 6348, Wellesley Street, Auckland, Ph (09) 444 5836, Fax (09) 444 0974, Freephone 0800 651 700 **or circle no. 39 on the reader reply card**

LOW PRICED LABORATORY BALANCES AND ACCURATE ELECTRONIC SCALES

EMC Industrial Weighing announce the arrival of a new range of UWE electronic laboratory balances and industrial scales ranging in capacity from 300g x 0.01g up to 20kg x 0.02kg and wholesaling from \$185.00 plus GST up to \$825.00 plus GST.

All models operate off batteries or standard 3 pin power using a 230/240 VAC to 9 VDC adaptor which is included in the price. Each scale has a rigid foam container for protection when not in use.

Many useful features are included with various models, including auto-shut off, zero/tare function, percentage mode, hold key, counting mode, etc. Descriptive leaflets are available on request and most models are ex-stock.

Contact: EMC Industrial Weighing, P O Box 31 145, Milford, Auckland, Ph. (09) 444 9229, Fax (09) 444 1145 **or circle no. 40 on the reader reply card**

PATCH TESTING MEMBRANE

Sartorius offer 5mm or 8mm membrane filters made of cellulose nitrate in either 25mm or 47mm diameter, for patch testing of oils and other hydrocarbons. A standard volume of oil sample is filtered through the specified pore size membrane at a set pressure. After filtration the membrane filter is removed and compared with a standard to determine the level of particulates in the oil. The test is also commonly referred to as the filth test.

Contact: Medic Corporation Ltd, Private Bag, Lower Hutt Ph. (04) 569 3539 Fax (04) 569 7984 **or circle no. 41 on the reader reply card**

ALL GLASS HPLC VACUUM FILTER UNIT

The Sartorius all glass HPLC vacuum filter unit offers the following features:

- * All surfaces in contact with the medium are glass.
- * The 6mm wide glass rim above the ground glass neck prevents filtrate from contacting the ground glass and thus becoming contaminated when decanting from the side arm flask.
- * The safety connector for the vacuum hose is made of polypropylene. No more cut hands if there is a "slip-up"!
- * A centering rim on the filter support simplifies mounting the funnel and prevents the membrane filter creeping.

Contact: Medic Corporation Ltd, Private Bag, Lower Hutt Ph. (04) 569 3539 Fax (04) 569 7984 **or circle no. 42 on the reader reply card**

PERSEPTIVE BIOSYSTEMS FOR PERFUSION CHROMATOGRAPHY

PerSeptive Biosystems designs, manufactures and markets advanced proprietary products and systems for the purification and analysis of biomolecules. These bioseparation products are designed to reduce significantly the time and cost required for the development and manufacture of biopharmaceuticals. Three core technologies make these productivity gains possible. Perfusion Chromatography, a system of specially engineered chromatographic particles: Immuno Detection:, a continuous flow immunoassay technology for the real-time assay of biomolecules: and, Rational Surface Design, a proprietary technique used to create highly specific synthetic surfaces that mimic the binding characteristics of antibodies.

The need for rapid separations systems to purify and analyse biomolecules has become increasingly important since the biotechnology revolution began in the early 1980's. Major advances in biopharmaceutical drug discovery, however, have not been matched by advances in the technology necessary for the purification and analysis of biomolecules. PerSeptive Biosystem's technologies represent the first separations that are 10 to 1,000 times faster than conventional technology for applications from discovery through manufacturing and quality control.

Contact: Sci Tech, P O Box 663, Dunedin, Ph. (03) 477 7860, Fax. (03) 477 7870 **or circle no. 43 on the reader reply card**

RELIABLE MEASUREMENT OF PARTICLE SIZE WITH SALD-2001

The SALD-2001 Laser Diffraction Particle Size Analyser by Shimadzu provides fast reliable measurement of particle sizes ranging from 0.03 to 700 μm using a single optical system.

The laser diffraction method for particle size measurement is fast (short measurement times), provides high reproducibility, and gives you the capability to measure particles in a liquid stream. The Shimadzu SALD-2001 is designed to ensure higher accuracy than conventional instruments. Its noteworthy features include adoption of a semiconductor laser system, a diffracted/scattered 76 element light sensor (of Shimadzu's original design), and highly flexible software compatible with IBM PCs.

The SALD-2001 uses a personal computer for data processing (a set of software programs are supplied as standard) to handle and display particle size distribution data as well as compare them and treat them statistically. A program is available to recalculate previously processed particle size distribution data with, for example, a different refractive index.

A wide variety of data presentation formats are also available using various information besides ordinary particle size distribution data. The SALD-2001 Particle Size Analyser is a quick, easy to use and flexible instrument for a wide variety of applications.

Contact: Douglas Scientific, P O Box 45 027, Auckland 8, Ph: (09) 837 5447, Freephone (outside Auckland) 0800 735 725, Fax (09) 836 0668 **or circle no. 44 on the reader reply card**

DIONEX ION CHROMATOGRAPHY

Dionex revolutionized detection technologies that have become established techniques for analysis of inorganic and organic ions. DX 500 conductivity, electrochemical and UV/Vis absorbance detectors mark another advance in IC detection technology, offering the ultimate in performance and ease of use.

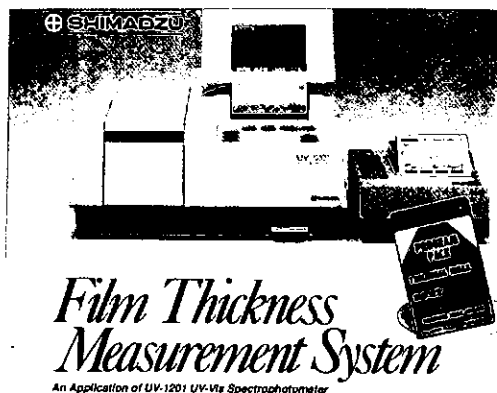
New signal processing electronics improve signal-to-noise ratios and reproducibility. Programmability and methods storage increase user convenience. And features such as data buffering, diagnostics and leak detection ensure trouble-free operation. DX 500 conductivity and electrochemical detectors fully support AutoSuppression using the SRS (Self-Regenerating Suppressor); AutoSuppression dramatically improves conductivity detection limits without effort or maintenance.

For expanded capability, the DX 500 is compatible with a wide range of detector technologies, including fluorescence, photodiode, multiwavelength, radiochemical, chemiluminescence, retractive index (RI), and IC/ICP.

Contact: Sci Tech, P O Box 663, Dunedin, Ph. (03) 477 7860, Fax. (03) 477 7870 or circle no. 55 on the reader reply card

FILM THICKNESS MEASUREMENT SYSTEM

Shimadzu have recently designed and released a further application system for the UV-1201 ultraviolet/visible spectrophotometer. Using special accessories film thickness measurement can be made through a simple operation. The UV-1201 spectrophotometer system with its plug in programme pack leads the user through the process with step by step instructions on its large display.



Film Thickness Measurement System
An Application of UV-1201 UV-Vis Spectrophotometer

Film thickness is calculated from the interference pattern obtained from reflectance or transmittance measurement. Reflection spectra are obtained with the 5° relative specular reflectance accessory. The user then inputs the refractive index of the material being analysed and the thickness of the material is calculated.

Spectra can be stored on a data pack for later use and results can be recalculated using a different area of the interference spectra. The results display the calculated thickness data together with the spectrum. Hard copies may be obtained using a Epson printer or compatible.

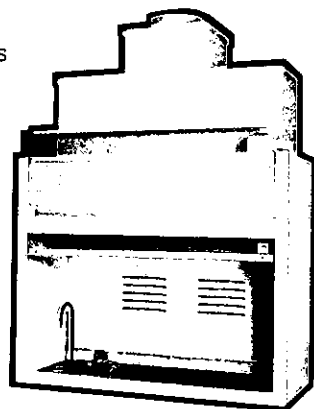
Contact: Douglas Scientific, P O Box 45 027, Auckland 8, Ph: (09) 837 5447, Freephone (outside Auckland) 0800 735 725, Fax (09) 836 0668 or circle no. 56 on the reader reply card

Smoothflow Fume Cabinets

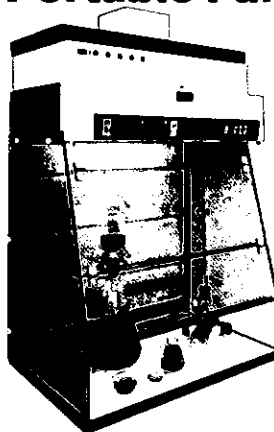
New Zealand made **Smoothflow** Fume Cabinets comply with NZS 7203 (1992) and NZS 6101 Part 3, and are Classified Non-Hazardous.

The **Sensor-Flow** controls fan purge cycles, and constantly monitors airflow and temperature, for complete electrical safety.

Available with **Fumeflush** scrubber mounted above the fume chamber.



Captair Ductless Portable Fume Hoods



Toxic gases eliminated by 99.99% efficiency filtration.

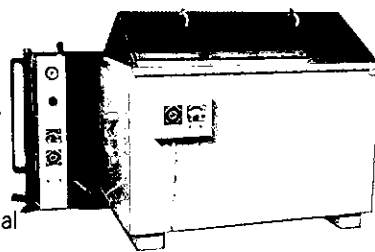
Captair hoods meet AS 2243.9.

Captair recirculating fume hoods can be set up on any convenient bench in less than 30 minutes for immediate protection.

There are over 30,000 Captair hoods in service world-wide.

Saltron Salt Spray Cabinet

New Zealand made **Saltron** cabinets have given rigorous service in industrial laboratories for over 7 years, providing a facility for neutral and acetic salt spray tests to more than 30 international standards.



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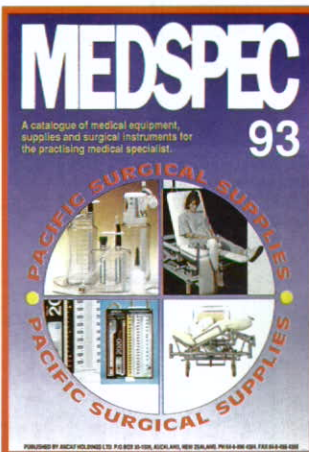
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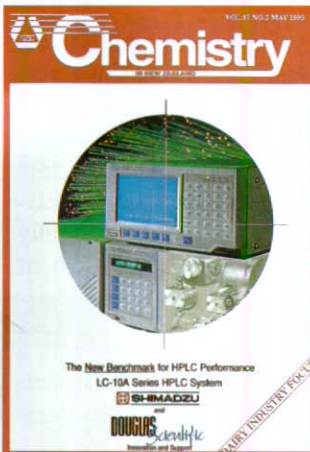
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EXTRACARE is without question the fumecupboard most in demand today. Developed in advance of the legal requirements of the new Occupational Safety and Health Act and in anticipation of the 1992 revision of NZ Standard 7203, it has literally taken the market by storm.

No wonder because no other fumecupboard is superior in overall safety and few, if any excepting our Labrocure IV and Econocare II come close to it. All three fumecupboards also comply with NZ Standard 6101 Part 3.

And now that the Occupational Safety and Health Act is LAW, it is more important than ever that your fumecupboard can stand up to any test.

What other fumecupboard offers...

- Microprocessor control of start-up and shut-down cycles, automatic isolation of power and gas in the event of electrical power failure, automatic shutdown should airflow become inadequate and an audible and visual warning system.
- Automatic temperature control.
- Heat resistant recessed Friduric ceramic floor (alternatives on request).
- Superior fume containment with easily removed baffles.
- Full width exhaust outlets providing more even air extraction.
- Condensate trap - ergonomic base beam - turbulence reducing columns - armour toughened 2-part glass doors.

...THE LIST GOES ON AND ON!



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UNIVERSITY OF AUCKLAND

CONFERENCE PROGRAMME

From the Conference Chairman

It is a great pleasure to welcome delegates to Auckland for this conference, jointly sponsored by the New Zealand Institute of Chemistry and the Medicinal and Agricultural Division of the Royal Australian Chemical Institute. Particularly pleasing is the large number of delegates from overseas, particularly from Australia. We hope that your stay in Auckland will be professionally valuable and that you will make some time to see our city and its environs and perhaps to travel further afield.

The NZIC has, for many years, held its conference in August. We hope that this early December conference proves popular with delegates - registrations as of mid-November indicate no lessening of interest. Your comments to any member of the Organising Committee will help shape future planning. Moves for cooperation between the Australian and New Zealand Institute have been growing in recent years and we hope that this conference containing, as it does, very substantial trans-Tasman input will be the fore-runner of other joint ventures. Increasing numbers of New Zealanders have been attending RACI Divisional conferences and National Conventions. We hope that this conference will provide the opportunity for delegates to discuss the possibilities of RACI meetings in New Zealand, perhaps following the pattern of the very successful Inorganic Chemistry meetings held in 1981 and 1991.

Writing immediately after New Zealand's General Election we see much uncertainty over many aspects of our country's future. It is not known yet whether the visitor for Thursday 9 December, the Hon Simon Upton, will be Minister for Science, Research and Technology - or even whether he will be a member of the government. However, we assure him of a very warm welcome as he has shown himself to be a strong supporter of scientific research, both pure and applied. It is pleasing to note that in many aspects the political parties have adopted a common approach on science policy. After the extensive restructuring, particularly of government funded science, in recent years many feel that a period of stability is necessary in order to allow us to focus on our real concerns in scientific research.

And that brings me back to the primary reason for this conference - the opportunity for you to share your latest results, to meet colleagues and discuss future plans and to learn something of recent advances outside your own research speciality. The four Plenary Lecturers are all leaders in their fields and bring a high international profile to this conference. The invited keynote speakers represent active researchers in their various fields both within Australia and New Zealand and from further afield. The level of international participation is a noteworthy and pleasing feature of this conference and we hope it will be a continuing feature of this country's conferences...

Likewise, we are pleased with the blend of pure and applied chemistry. We as scientists are fully aware not only of the challenge and excitement of "blue-sky" research but also of the very substantial long term benefits that it conveys. In a period of funding uncertainties and an emphasis on research perceived to be immediately applicable it is satisfying to note the very substantial body of fundamental research being reported at this conference. At the same time, much important and novel research is coming from industrial labs and research institutes and we look forward to some very significant contributions from this area. Tomorrow's scientists must not be forgotten and we see a big Chemical Education programme scheduled for Thursday.

To you all - and particularly our visitors - we extend a very warm welcome. We hope that your week in Auckland will be intellectually stimulating and socially enjoyable and that you will carry away happy memories of this year's conference.

Brian Davis



NZIC CONFERENCE PROGRAMME TIMETABLE

TIME	MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY
8:30 - 9:00		OPENING			
9:00 - 10:00		PLENARY LECTURE PLE1 Raymond Baker	PLENARY LECTURE PLE3 Bob Bergman	PLENARY LECTURE PLE4 Ronald G Prinn	PLENARY LECTURE PLE5 John Albery
10:00 - 10:30		TEA	TEA	TEA	TEA
10:30 - 10:50		Medicinal Chemistry MED Organic Synthesis OSY Reaction Mechanisms REM Physical Chemistry PHY Forensic Chemistry FOR	Marine Natural Products NAP Medicinal Chemistry MED Marine Chemistry EAC Organic Synthesis OSY Inorganic Chemistry INO Physical Chemistry PHY	Marine Natural Products NAP Medicinal Chemistry MED Education EDU Polymer Chemistry POL Atmospheric Chemistry EAC Inorganic Chemistry INO Organic Synthesis OSY Physical Chemistry PHY	Marine Natural Products NAP Medicinal Chemistry MED Analytical Chemistry ANA Reaction Mechanisms REM Physical Chemistry PHY
10:50 - 11:10					
11:10 - 11:30					
11:30 - 11:50					
11:50 - 12:10					
12:10 - 12:30				Address by Simon Upton MP	
12:30 - 13:30		LUNCH	LUNCH / WOMENS LUNCH	LUNCH	LUNCH
13:30 - 13:50		PLENARY LECTURE PLE2 Ian Paterson	EASTERFIELD LECTURE Margaret Brimble	Lipid Natural Products NAP Medicinal Chemistry MED Education EDU Inorganic Chemistry OSY Atmospheric Chemistry EAC Polymer Chemistry POL Physical Chemistry PHY	Marine Natural Products NAP Physical Chemistry PHY Reaction Mechanisms REM
13:50 - 14:10					
14:10 - 14:30					
14:30 - 14:50		TEA	TEA		
14:50 - 15:10			TOUR 15:00 - 17:30	TEA	TEA
15:10 - 15:30		Terrestrial Natural Products NAP Organic Synthesis OSY Reaction Mechanisms REM Physical Chemistry PHY Forensic Science FOR Inorganic Chemistry INO	BARBECUE 17:30 - 19:45	Terrestrial Natural Products NAP Medicinal Chemistry MED Education EDU Inorganic Chemistry INO Riverine Chemistry EAC Polymer Chemistry POL Lipid Natural Products NAP Organic Synthesis OSY	Marine Natural Products NAP
15:30 - 15:50					
15:50 - 16:10					
16:10 - 16:30					
16:30 - 16:50					
	AGM 17:00 -	POSTER SESSION 17:00 - BUFFET 18:30 - 20:00		CONFERENCE DINNER (Barbecue) 19:00 -	

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PLENARY LECTURERS

Professor Ray Baker is Executive Director of Medicinal Chemistry at the Neuroscience Research Centre of Merck Sharp & Dohme, situated just north of London. He was born in Derbyshire and graduated from Leicester University before going on to do postdoctoral studies at the University of California.



Professor Baker

He was previously Professor of Organic Chemistry at the University of Southampton, where his work ranged from studies of organometallic chemistry to insect chemistry and organic synthesis. The first eight years of independent research was involved with physical organic chemistry. The culmination of this period was the publication of a standard text on the mechanisms of organic chemistry. A major change of emphasis was made into a study of insect pheromones. This involved the determination of the structure and synthesis of a range of insect pheromones and the demonstration of their role in insect behaviour.

The synthetic chemistry involved with the preparation of insect pheromones led, in due course, to the synthesis of more complex natural products. New synthetic procedures were developed for the construction of spiroacetals, a group commonly found in a range of natural products.

Professor Baker joined Merck Sharp & Dohme in 1984 as Director of Medicinal Chemistry at the beginning of the new research centre. The major emphasis of the work is the search for new drugs for the treatment of diseases such as Alzheimer's, schizophrenia, depression, neurodegeneration of the brain and the treatment of pain particularly that associated with migraine and inflammation.

He is the author of over 250 scientific publications and has filed over 30 patents since 1985. He was recently awarded the 1991 Royal Society of Chemistry Prize for Medicinal Chemistry and the 1992 Hugo Müller Medal for Chemistry associated with Biology.

Dr Ian Patterson, from the Cambridge University's Chemical Laboratory, is a Cambridge graduate with interests in the synthesis of natural products, particularly the polyether and macrolide antibiotics. After a Ph.D with Dr Ian Fleming he spent a post-doctoral period with Professor Gilbert Stork at Columbia University before taking a post at University

College, London. From there he moved to Cambridge where he has now established a strong research record. He has focused his synthetic researches both on methodology - such as bisepoxide cyclisation and the directed aldol reaction - and on synthetic targets, such as the erythronolides and rifamycin. He has been an invited speaker at a number of international conferences and - linking him with this conference - at least three of his recent postdoctoral workers have been Auckland graduates.

Professor Bob Bergman is Professor of Chemistry at the University of California, Berkeley. Born in Chicago in 1942, he received his PhD at the University of Wisconsin with Professor J.A. Berson. After post-doctoral work with Ronald Breslow at Columbia his teaching career began at Caltech, moving to Berkeley ten years later, in 1977.

Professor Bergman was trained as an organic chemist and spent the first part of his independent career at Caltech investigating the mechanisms of organic reactions. He also developed methods for the generation and study of unusually reactive molecules, such as 1,3-diradicals and vinyl cations. In 1972 he discovered the thermal cyclization of *cis*-1,5-hexadiyne-3-enes to 1,4-dehydrobenzene diradicals, a transformation that has recently been identified as a crucial DNA-cleaving reaction in several antibiotics that bind to nucleic acids. In the mid-1970's his research broadened to include organometallic chemistry. Since that time he has made contributions to the synthesis and chemistry of several types of organotransition metal complexes and to improving our understanding of the mechanisms of their reactions. In this area he has focused on migratory insertion and oxidative addition reactions, the chemistry of new dinuclear complexes, the investigation of organometallic compounds having metal-oxygen and metal-nitrogen bonds, and the reactions of organotransition metal enolates. He is probably best known for his discovery of the first soluble organometallic complexes that undergo intermolecular insertion of transition metals into the carbon-hydrogen bonds of alkanes, and the use of liquefied noble gas solvents in the study of these reactions.



Professor Bergman

He is the author of over 200 scientific publications and has received a number of awards and honours. He was elected a member of the National Academy of Sciences and the American Academy of Arts and Sciences in 1984. He has held a large number of visiting lectureships and has given extensive service to the profession of chemistry.

Dr Margaret Brimble joined the staff of the Department of Chemistry at the University of Auckland at the beginning of 1993, after seven years with Massey University.



Dr Margaret Brimble

Margaret Brimble was born in Auckland in 1961 and topped the Science Faculty at the BSc and MSc level. Her MSc research was undertaken with Professor Brian Davis (Conference Chairman), and her PhD research at Southampton University with Professor Ray Baker (Plenary Lecturer). Her doctoral studies involved work on the polyether antibiotic salinomycin; she has maintained and developed her interest in that area of spiroacetal synthesis. She was then appointed to a lectureship at Massey University and in her research in conjunction with a growing group of research students undertook the total synthesis of a number of natural products. The Easterfield Medal is not the only recognition of her work; she has recently received the Hamilton Award of the Royal Society of New Zealand and spent the 1992 Fall Semester at the University of California, Berkeley with Professor Clayton Heathcock. She is the author of 30 scientific papers.

Professor Ron Prinn is TEPCO Professor of Atmospheric Chemistry in the Department of Earth, Atmospheric, and Planetary Sciences at MIT; Director of the MIT Center for Global Change Sciences and Co-Director of the MIT Joint Program on Science and Policy of Global Change. He was born in Hamilton, New Zealand in 1945 and graduated MSc with first class honours in chemistry, from the University of Auckland in 1968, and ScD from MIT.



Professor Ron Prinn

Professor Prinn's principal research interests are broad, incorporating the chemistry, dynamics, and physics of the atmospheres of the Earth and other planets and the chemical evolution of atmospheres. He leads the Global Atmospheric Gases Experiment (GAGE) in which the rates of increase of the concentration of the trace gases involved in the greenhouse effect and ozone depletion have been measured continuously over the globe since 1978. In the 1970s he and his colleagues

developed the first comprehensive global three-dimensional dynamical-chemical-radiative model of the ozone layer and applied it specifically to elucidating the effects of supersonic aircraft on ozone. He is a Fellow of the American Geophysical Union (AGU), a 1981 recipient of the AGU's Macelwane Medal, and the 1984 V.I. Vernadsky Memorial Lecturer of the USSR Academy of Sciences. He is currently the Chairman of the Steering Committee for the International Global Atmospheric Chemistry Project and he has served as the chairman of the National Research Council Committee on Earth Sciences. Professor Prinn is also very active in planetary science including participation in the Pioneer Venus mission and co-authorship of the Academic Press book, *Planets and their Atmospheres: Origin and Evolution*.

Professor John Albery is Master of University College, Oxford and Professor of Physical Chemistry at that University. He was born in 1936, educated at Winchester College and Balliol College, Oxford, gaining his DPhil with Professor RP Bell. He was then elected to a Fellowship at University College, Oxford, and during his time there also held visiting research positions in Britain and the United States. In 1978 he was appointed Professor of Physical Chemistry at Imperial College, London, where he later held the post of Dean of the Royal College of Science and Head of the Chemistry Department. He was elected to Fellow of the Royal Society in 1985.

John Albery has made major contributions to the fields of electrochemistry, the kinetics of proton and electron transfer, and the development of polymer modified electrodes as sensors. In his early work on ring-disk electrodes he showed how convection-diffusion processes were coupled with electron transfer at electrode surfaces, and in some cases fast homogeneous reactions. These techniques were extended to time resolved electron spin spectroscopy and photochemistry. He is widely known for his pioneering investigations into photo-galvanic cells, which convert solar energy into electricity and stored chemical energy. This research led to the discovery of modified electrodes, which carry films of conducting polymers, and which can be adapted as sensitive sensors for biomedical applications.



Professor John Albery

Dr. Albery has published several major reviews and monographs, and a large number of seminal papers. His textbook on "Electrode Kinetics" (1975) is a model of an original and lucid introduction to the field. In addition to his scientific contributions, John Albery has a reputation for his humorous and satirical writing of scripts for television and the theatre. In 1989, he was elected Master of University College, Oxford and in 1992 was President of the Chemistry Section of the British Association. He is the author of 2 monographs and over 200 research papers.

PLENARY LECTURES

Venue: Large Chemistry Lecture Theatre

PLE1 Tues 9:00 - 10:00

Receptor Sub-Types - Innovations in Drug Discovery

Raymond Baker

Merck Sharp & Dohme Research Laboratories, Neuroscience Research Centre, Terlings Park, Eastwick Road, Harlow, Essex CM20 2QR, England

PLE2 Tues 13:30 - 13:50

Progress and Problems in the Synthesis of Marine Macrolides

Ian Paterson

University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, UK

PLE3 Wed 9:00 - 10:00

A new Intermolecular C-H Activation Reaction of Methane and Other Hydrocarbons with Ir (III) Complexes

Peter Burger, Bruce A Arndtsen, Yinong Ma and Robert G Bergman

Division of Chemical Sciences, Lawrence Berkeley Laboratory and Department of Chemistry, University of California, Berkeley, California, USA 94720

PLE3 Thurs 9:00 - 10:00

Global Atmospheric-biospheric Chemistry

Ronald G Prinn

Massachusetts Institute of Technology

PLE4 Fri 9:00 - 10:00

New Electrochemical Sensors for Medicine and Biology

Professor John Albery FRS

EASTERFIELD LECTURE

Tues 13:30 - 14:30

Target Synthesis: From Insect Antifeedants to Ionophores

Margaret Brimble

Department of Chemistry, University of Auckland, Private

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SYMPOSIA

MEDICINAL CHEMISTRY SYMPOSIUM

Venue: Small Lecture Theatre

In conjunction with the Medicinal and Agricultural Chemistry Division of the Royal Australian and Chemical Institute)

SESSION 1. Tues 10:30 - 12:30: ANTICANCER DRUGS

Chair: Hollis Showalter

MED - OR1

10:30 - 10:50 INVITED LECTURE: *The synthesis and characterisation of boron-containing bibenzimidazoles related to the DNA minor groove binder, Hoescht 33258.*

David P Kelly, Stuart A Bateman, Roger F Martin, Monica E Reum, Michael Rose and Antony R D Whittaker.

School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia

MED - OR2

10:50 - 11:10 *Screening for natural anti-mitotic agents: development of a microtitre-based tubulin binding assay.*

Stephen J Kellam, John W Blunt and Murray H G Munro

Department of Chemistry, University of Canterbury, Christchurch and Nigel B Perry, Plants Extracts Research Unit, Crop and Food Research, Department of Chemistry, University of Otago, Dunedin, New Zealand.

MED - OR3

11:10 - 11:30 *Antitumour lignans and cytotoxic .asin acids from kawaka; Libocedrus plumosa*

Nigel B Perry and Lysa M Foster

Plant Extracts Research Unit, Crop and Food Research, Department of Chemistry, University of Otago, Dunedin, New Zealand

MED - OR4

11:30 - 11:50 *Analogues of CC-1065; cytotoxicity and mechanism*

Peter J Parson, Rodney H White and David J Young

School of Science, Griffith University, Brisbane, Australia

MED - OR5

11:50 - 12:10 *Synthesis of 2,3-dihydro-2-thioxo-1H-indole-3-alkanoic acids, 2,2'-dithiobis (1H-indole-3-alkanoic acids) and some related ester and amide derivatives as inhibitors of the epidermal growth factor receptor tyrosine kinase.*

Andrew M Thompson, David W Fry, Alan J Kraker and William A Denny

Cancer Research Laboratory, University of Auckland School of Medicine, and Parke-Davis Pharmaceutical Research Division, Warner-Lambert Company, Ann Arbor, USA

MED - OR6

12:10 - 12:30 *Lithiation routes to oxindole and 2-indolinethione precursors to 2,2'-dithiobisindoles: novel compounds with potent tyrosine kinase inhibitory properties.*

Gordon W Rewcastle, William A Denny, Brian D Palmer, Ellen M Dobrusin, H D Hollis Showalter and Alan J Kraker

Cancer Research Laboratory, University of Auckland School of Medicine, and Parke-Davis Pharmaceutical Research Division, Warner-Lambert Company, Ann Arbor, USA

SESSION 2 Wed 10:30 - 12:20 HYPOXIA-SELECTIVE DRUGS

Chair: Bill Denny

MED - OR7

10:30 - 11:10 **INVITED LECTURE:** *The preclinical development of PD 144872, the R-enantiomer of the novel dual function 2-nitroimidazole radiation sensitizer, RB 6145*

H. D Hollis Showalter

Parke-Davis Pharmaceutical Research, Division of Warner-Lambert Co., Ann Arbor, USA

MED - OR8

11:10 - 11:30 *Hypoxia-selective cytotoxins: synthesis of novel alkylamino bisnitroimidazoles*

Michael P Hay and William A Denny

Cancer Research Laboratory, School of Medicine, University of Auckland, Auckland, New Zealand

MED - OR9

11:30 - 11:50 *Hypoxia-selective cytotoxic agents based on nitrogen mustard derivatives of isomeric dinitrobenzamides*

Brian D Palmer, Stephen Cliffe, William A Denny, Philip Kestell and William R Wilson

Cancer Research Laboratory, School of Medicine, University of Auckland, Auckland, New Zealand

MED - OR10

11:50 - 12:10 *Nitrobenzyl mustard quaternary salts as hypoxia-selective cytotoxins*

Moana Tercel, William R Wilson, William A Denny, Pierre Van Zijl and Susan M Pullen

Cancer Research Laboratory and Department of Oncology, School of Medicine, University of Auckland, Auckland, New Zealand

MED - OR11

12:10 - 12:30 *Synthetic approaches to mitomycins*

Hazel J Dyke and H W Moore

Centre for Drug Design and Development, University of Queensland, Brisbane and Department of Chemistry, University of California, Irvine, California, USA

SESSION 3 Thur 10:30 - 12:10 MODELLING AND STRUCTURE

Chair: David Boykin

MED - OR12

10:30 - 11:10 **INVITED LECTURE:** *Structural approaches to the rational design of DNA-recognition drugs*

Stephen Neidle

Cancer Research Campaign Biomolecular Structure Unit, Institute of Cancer Research, Sutton, UK

MED - OR13

11:10 - 11:30 **INVITED LECTURE:** *The interaction of ruthenium (III) antitumour complexes with human lactoferrin: a model for site-specific drug delivery.*

Edward N Baker

Department of Chemistry & Biochemistry, Faculty of Science, Massey University, Private Bag 11222, Palmerston North, New Zealand

MED - OR14

11:30 - 11:50 **INVITED LECTURE:** *Conformational studies of the blood group determinant D- α -fucopyranosyl-(1,2)-O-B-D-galactopyranosyl- β -OMe*

Edward M Coxon, D Ross Boswell and James M Coxon
Department of Chemistry, University of Canterbury, New Zealand

MED - OR15

11:50 - 12:10 *The structure of ferredoxin from Clostridium pasteurium; NMR and model building*

S. D. B. Scrofani, Robert T C Brownlee, N S A Hoogenraad, G A Vincent, P S Brereton, A M Hamer, M J Lavery, S G McDowall, A G Wedd
Department of Chemistry, La Trobe University, Bundoora, Australia

SESSION 4 Thur 1:30 - 2:50 DRUG DEVELOPMENT TECHNOLOGIES

Chair: Michael West

MED - OR16

13:30 - 13:50 **INVITED LECTURE:** *^{13}C NMR Spectroscopy - applications to organic and medicinal chemistry*

David W Boykin

Department of Chemistry, Georgia State University, Atlanta, Georgia 30303, USA

MED - OR17

13:50 - 14:10 *Structural diversification of bioactive lead compounds*

Paul F Alewood and Wim Meutermans

Centre for Drug Design and Development, University of Queensland, Queensland 4072, Australia

MED - OR18

14:10 - 14:30 *Synthesis of some analogues of chlorhexidine*

G T Wernert, David A Winkler, Brian C Elmes and G Holan
CSIRO Division of Chemicals and Polymers, Private Bag 10, Rosebank MDC, Clayton, Victoria 3169, Australia

MED - OR19

14:30 - 14:50 *The feasibility of licit production of morphine, some of its derivatives and certain other opium alkaloids in New Zealand; Codeine and Pholcodine in particular*

Rob H McKeown, H C Atkinson, I G Buchanan, Y C Gopal, M D Mochan and J T Price

Pharm Chem Research Laboratories Limited, P O Box 5313, Dunedin, New Zealand

SESSION 5 Thur 15:10 - 16:50 p.m. ADRIEN ALBERT MEMORIAL LECTURE AND RACI BUSINESS MEETING

Chair: Bob Brownlee

15:10 - 15:20 *Introduction*

MED - OR20

15:20 - 16:20 **ADRIEN ALBERT MEMORIAL LECTURE:** *Applications of NMR in drug design*

David J Craik

Victorian College of Pharmacy, Parkville, Australia

16:20 - 16:50 RACI Business Meeting

SESSION 6 Fri 10:30 - 12:30: ANTI-PARASITIC, ANTI-VIRAL AND ANTI-BACTERIAL AGENTS

Chair: Bill Denny

MED - OR21

10:30 - 10:50 *INVITED LECTURE: New targets for new drugs*

Prapon Wilairat

Department of Biochemistry, Faculty of Science, Mahidol University, Bangkok, Thailand

MED - OR22

10:50 - 11:10 *3,6 Diamino-9-anilinoacridines as potential antimalarials*

Swarna A Gammage, Prapon Wilairat, David P Figgitt, Raymond K Ralph and William A Denny

Cancer Research Laboratory and Department of Developmental Biology, School of Biological Sciences, University of Auckland, Private Bag, Auckland, New Zealand

MED - OR23

11:10 - 11:30 *INVITED LECTURE: Total Synthesis of (±)-calanolide A, a non-nucleoside inhibitor of HIV-1 reverse transcriptase*

Balan Chenera, Michael L West, Joseph P Finkelstein and Geoffrey B Dreyer

Department of Medicinal Chemistry, Smith Kline Beecham Pharmaceuticals, 709 Swedeland Road, King of Prussia, Pennsylvania 19406, USA

MED - OR24

11:30 - 11:50 *Modifications at C-6 of castanospermine*

Richard H Furneaux, Jennifer M Mason, Peter C Tyler, Oliver Hartley and Brian Winchester

Industrial Research Ltd, P O Box 31 310, Lower Hutt, New Zealand, and Institute of Child Health, University of London, London, UK

MED - OR25

11:50 - 12:10 *Chemical modification of the glycosidase inhibitor castanospermine*

Richard H Furneaux, Jennifer M Mason and Peter C Tyler

Industrial Research Ltd, P O Box 31 310, Lower Hutt, New Zealand

MED - OR26

12:10 - 12:30 *Design and synthesis of antiviral agents*

L Bui, M N Iskander and Sebastian Marcuccio

Department of Pharmaceutical Chemistry, Victorian College of Pharmacy, Monash University, Parkville, Australia

ORGANIC SYNTHESIS SYMPOSIUM

Venue: Physics Lecture Theatre II

SESSION 1 Tuesday 10:30 - 12:30

Chair: David Larsen

OSY - OR1

10:30 - 11:10 *INVITED LECTURE: Synthetic and structural studies on diterpenoid plant growth regulators and pheromones*

Lewis N Mander

Research School of Chemistry, Australian National University, Canberra, ACT 0200 Australia

OSY - OR2

11:10 - 11:30 *One-step synthesis of glycosidic spiroketals from 2,3-epoxybutyl glucosides*

Robert J Ferrier and David W Hall

Department of Chemistry, Victoria University of Wellington, Wellington NZ

OSY - OR3

11:30 - 11:50 *Asymmetric hydrogenation of prochiral C=N bonds*

Cornelius Lensink

Industrial Research Limited, Lower Hutt, New Zealand

OSY - OR4

11:50 - 12:10 *Fluorine chemistry: A fascinating tool in organic synthesis*

L. Streckowski, A.S. Kiselyov, M. Hojjat, J. Nguyen, S.E. Patterson, K. and J. Cramer

Department of Chemistry, Georgia State University, Atlanta, Georgia 30303, USA

OSY - OR5

12:10 - 12:30 *An evaluation of Hofmann and Cope elimination routes to (±)-2-n-propylthietane*

A.D. Woolhouse^a, G.J. Gainsford^a, D.R. Crump^a, J M Coxon^b, and K Lundie^b

^a Industrial Research Limited, Lower Hutt, New Zealand

^b Department of Chemistry, University of Canterbury, Christchurch, New Zealand

SESSION 2: Tuesday 14:50 - 16:50

Chair: L N Mander

OSY - OR6

14:50 - 15:30 *INVITED LECTURE: A stereoselective approach to the angucycline antibiotics*

David S Larsen

Department of Chemistry, University of Otago, Dunedin, New Zealand

OSY - OR7

15:30 - 16:10 *INVITED LECTURE: Macroring contraction methodology in natural products synthesis*

Takashi Takahashi

Tokyo Institute of Technology, Meguro, Tokyo 152, Japan

OSY - OR8

16:10 - 16:50 *INVITED LECTURE: Diels-Alder reactions: from chemistry to chemotherapy*

Andy Pratt, Carolyn Coulter, Jolon Dyer and Sian Fayle

Department of Chemistry, University of Canterbury, Christchurch, New Zealand

SESSION 3 Wednesday 10:30 - 12:30

Chair: R J Ferrier

OSY - OR9

10:30 - 10:50 *Synthesis and characterisation of boric acid derivatives of biguanide*

Robert A Franich^a, Hank W Kroese^a, Kathryn B Anderson^a, Roger Meder^a, Richard Meinhold^b, and Cliff Rickard^c.

^a NZ Forest Research Limited, Rotorua, New Zealand

^b Industrial Research Limited, Lower Hutt, New Zealand

^c Department of Chemistry, University of Auckland, New Zealand

OSY - OR10

10:50 - 11:10 *Michael-Wittig condensations of arsonium - and phosphonium ylides*

Cornelius M Moorhoff

Department of Chemistry, University of Tasmania, Australia

OSY - OR11

11:10 - 11:50 **INVITED LECTURE:** *Mechanism of Mukaiyama-Michael reaction of ketene silyl acetal: electron transfer or nucleophilic process?*

Junzo Otera

Department of Applied Chemistry, Okayama University of Science, Ridai-cho, Okayama 700, Japan

OSY - OR12

11:50 - 12:30 **INVITED LECTURE:** *Total synthesis of allosamidin*

R H Furneaux^a, R Blatner^a, T Kemmit^a, P C Tyler^a, R J Ferrier^b and A-K Tiden^b

^a Industrial Research Limited, Lower Hutt, New Zealand

^b Department of Chemistry, Victoria University of Wellington, Wellington, New Zealand

SESSION 4 Thursday 10:30 - 12:10

Chair: A Pratt

OSY - OR13

10:30 - 10:50 *Design and synthesis of rigid internally functionalised cavitands*

M J Stoermer and D P Fairlie

Centre for Drug Design and Development, University of Queensland, Qld 4072, Australia

OSY - OR14

10:50 - 11:10 *A new and efficient cycloaddition strategy for the synthesis of [n] ladderanes*

Giovanni Abbenante and Ronald N Warrener

Centre for Molecular Architecture, University of Central Queensland, Rockhampton, Australia

OSY - OR15

11:10 - 11:30 *Applications of microwave technology to organic synthesis*

C R Strauss^a, K D Raner^a, R W Trainor^a, and J Thorn^b

^a CSIRO Division of Chemicals and Polymers, Clayton, Victoria 3169, Australia

^b CSIRO Division of Applied Physics, Lindfield NSW 2070, Australia

OSY - OR16

11:30 - 11:50 *A possible synthetic route to C60?*

Robert J Ferrier

Department of Chemistry, Victoria University of Wellington, New Zealand

OSY - OR17

11:50 - 12:10 *Synthesis and characterisation of double-chain second generation cleavable surfactants*

Sarah G G Russell and David A Jaeger

Department of Chemistry, University of Wyoming, Laramie WY82071, USA

SESSION 5 Thursday 13:30 - 14:30

Chair: R F Furneaux

OSY - OR18

13:30 - 13:50 *The retro-ene desulfination reaction of allylsulfinate esters*

Malcolm D King and David J Young

Faculty of Science and Technology, Griffith University, Nathan 4111, Brisbane, Queensland, Australia

OSY - OR19

13:50 - 14:10 *Annulations of podocarpic acid via aryne intermediates*

Paul I Higgs and Paul D Woodgate

Department of Chemistry, University of Auckland, Auckland, New Zealand

OSY - OR20

14:10 - 14:30 *Asymmetric synthesis of, pharmacological evaluation of, 2-phenyl-3-benzazepine alkaloids, and structural analogues via novel chiral sulfoxides*

A R Hajipour and S G Pyne

Chemistry Department, University of Wollongong, Australia 2522

OSY - OR21

14:30 - 14:50 *Preparation of neem tree diterpenoids; a structural constation, confirmation, refutation and alteration*

Justin G Bendall and R C Cambie, Department of Chemistry, University of Auckland, New Zealand

SESSION 6 Thursday 15:10 - 16:50

Chair: M A Brimble

OSY - OR22

15:10 - 15:30 *Gibberellin chemistry: A lesson in serendipity*

Michael S Sherburn and L N Mander

Research School of Chemistry, Australian National University, Canberra, ACT 0200, Australia

OSY - OR23

15:30 - 15:50 *Annulations of diterpenoids via (n6 - arene) tricarbonyl complexes*

Ralph J Stevenson and Paul D Woodgate

Department of Chemistry, University of Auckland, New Zealand

OSY - O24

15:50 - 16:10 *Asymmetric intramolecular cyclizations using chiral acetal auxiliaries*

K C Higgs, Rachel M Lorimer, J J Rustenhoven and P S Rutledge

Department of Chemistry, University of Auckland, New Zealand

OSY - OR25

16:10 - 16:30 *Asymmetric synthesis of amino acids via exo-diastereoselective Diels-Alder reactions*

Javad Safaei-Ghomi and Stephen G Pyne

Department of Chemistry, University of Wollongong, NSW 2522, Australia

REACTION MECHANISMS SYMPOSIUM

Venue: Medium Lecture Theatre 2

SESSION 1 Tues 10:30 - 12:30 SOLUTION CHEMISTRY OF METAL COMPLEXES

Chair: James Wright

REM - OR1

10:30 - 11:10 *Model compounds for the Raman spectroscopic study of metal ions - DNA interactions*

Rodrigue Savoie and Junusz Stangret

Département de Chimie, Université Laval, Quebec, Canada G1K 7P4

REM - OR2

11:10 - 11:30 *The solution chemistry of cisplatin and related complexes*

D A House

Chemistry Department, University of Canterbury, Christchurch

REM - OR3

11:30 - 11:50 *Competition between metal ion and neighbouring group catalysis in the hydrolysis of diamino acid methyl esters*

Geoffrey D Beresford, Gary J Depree and Peter J Morris

Chemistry Department, University of Waikato, Hamilton

REM - OR4

11:50 - 12:30 **KEYNOTE SPEAKER:** *The solution chemistry of Mo₃S₄ and related mixed metal cuboidal complexes*

A G Sykes

Department of Chemistry, The University, Newcastle upon Tyne, NE1 7RU, UK

SESSION 2 Tues 14:50 - 16:30 SPECTROSCOPY AND DYNAMICS

Chair: Rodrigue Savoie

REM - OR6

14:50 - 15:30 **KEYNOTE SPEAKER:** *Spectroscopy, dynamics and function of heme-copper oxidases*

William H Woodruff

Los Alamos National Laboratory, Los Alamos, NM 87545, USA

REM - OR7

15:30 - 15:50 *Effect of tetraiodofluorescein on lactate dehydrogenase*

Rachel Vallanie and Robin Ledger

School of Pharmacy, University of Otago, P O Box 913, Dunedin

REM - OR8

15:50 - 16:10 **INVITED SPEAKER:** *Thermal-induced structural change of AOT reversed micelles and H-D exchange reaction between AOT-proton and solubilized-D₂O deuterium*

Akihiro Yoshino, Toshibisa Uchida, Takayoshi Yoshida and Hirofumi Okabayashi

Department of Applied Chemistry, Nagoya Institute of Technology, Gokisocho, Showa-ku, Nagoya, Japan

REM - OR9

16:10 - 16:30 **INVITED SPEAKER:** *Direct conversion of microscopic chemical energy into macroscopic vectorial motion utilising nonlinear dynamics*

Kenichi Yoshikawa

Graduate School of Human Informatics, Nagoya University, Nagoya 464-01, Japan

SESSION 3 Fri 10:30 - 12:50 PHYSICAL-ORGANIC REACTION MECHANISMS

Chair: Duncan McLennan

REM - OR10

10:30 - 10:50 **INVITED SPEAKER:** *Mechanisms of organometallic reactions with application to synthetic organic chemistry. A rational approach to asymmetric synthesis?*

Robin A J Smith, A Samuel Vellekoop and Celia L Kingsbury
Chemistry Department, University of Otago, P O Box 56, Dunedin

REM - OR11

11:10 - 11:30 **INVITED SPEAKER:** *Addition of aluminium hydride to carbonyls*

James M Coxon and Richard T Luibrand

University of Canterbury, Christchurch

REM - OR12

11:30 - 11:50 **INVITED SPEAKER:** *Ground state stereoelectronic effects involving silicon*

Jonathan M White and Yew Leong Kuan

School of Chemistry, University of Melbourne, Parkville Victoria 3052, Australia

REM - OR13

11:50 - 12:10 *The use of membrane mimetic media for elucidation of reaction mechanisms of enzymes*

Charmian J O'Connor and Douglas R Cleverly

Department of Chemistry, The University of Auckland, Private Bag 92019, Auckland

SESSION 4 Fri 13:30 - 14:50 BIO-ORGANIC REACTION MECHANISMS

Chair: Charmian O'Connor

REM - OR14

13:30 - 14:10 **KEYNOTE SPEAKER:** *Biological activity of poly (MA-CDA): a synthetic polycarboxylate*

Raphael Ottenbrite

Department of Chemistry, Virginia Commonwealth University, Richmond, VA 23284-2006, USA

REM - OR15

14:10 - 14:50 **KEYNOTE SPEAKER:** *Synthesis of artificial antigenic lipids and their immunogenicity*

Ei-ichi Kato, Shin-ichi Sakashita, Kazunari Akiyoshi and Junzo Sunamoto

Division of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University, Sakyo-ku, Yoshida Hommachi, Kyoto 606-01, Japan

FORENSIC SCIENCE SYMPOSIUM

Venue: Chemistry Seminar Room

SESSION 1 Tues 10:30 - 2:30

FOR - OR1

10:30 - 11:30 *Forensic Dentistry - From Bites to Bytes!*

M C Churton

FOR - OR2

11:30 - 11:50 *Fingerprint Developments*

Dr A Lavis

Institute of Environmental Health and Forensic Sciences,
Private Bag 92-021, Auckland

FOR - OR3

11:50 - 12:10 *Chemical Aspects of Blood Detection Reactions*

Robert Winchester

ESR Forensic, Mt Albert Science Centre, Private Bag 92021,
Auckland

FOR - OR4

12:10 - 12:30 *Use of Polymerase Chain Reaction (PCR) in Forensic Science*

Marion Savill

ESR:Forensic, Christchurch Science Centre, P O Box 29181,
Christchurch

SESSION 2 Tues 15:00 - 16:40

FOR - OR5

15:00 - 15:20 *Drug Screening by Capillary Electrophoresis*

Eric R Cairns

ESR, Wellington Science Centre, P O Box 30547, Lower Hutt

FOR - OR6

15:20 - 15:40 *The use of Deuterated Drug Internal Standards in Forensic Toxicology*

Donna Smith

ESR, Wellington Science Centre, P O Box 30547, Lower Hutt

FOR - OR7

15:40 - 16:00 *Homebaking, The first decade*

Rodney Norris

Institute of Environmental Health and Forensic Sciences,
Private Bag 92 021, Auckland

FOR - OR8

16:00 - 16:20 *Forensic Chemistry - An Investigation of the Impurities found in Methamphetamine produced by various synthetic routes*

K L Harrison¹, M McTigue¹, J R Pearson², E M Sear¹ and
J E Rowe¹

¹ Department of Chemistry, La Trobe University, Bundoora,
Victoria 3083, Australia

² Victorian State Forensic Science Laboratory, Macleod,
Victoria 3083, Australia

FOR - OR9

16:40 - 16:40 *Substance abuse in the racing industry*

G D Beresford

Official Racing Analyst, Institute of Environmental Health
and Forensic Sciences

PHYSICAL CHEMISTRY SYMPOSIUM

Venue: Medium Lecture Theatre

SESSION 1 Tues 10:30 - 12:30

Chair: Peter Schwerdtfeger

PHY - OR1

10:30 - 11:10 *Recent Advances in the Quantum Chemical Coulomb Problem*

Peter M W Gill

PHY - OR2

11:10 - 11:30 *Dependence of Diatomic Properties on Vibrational - Rotational States*

Michael Seth and Peter Schwerdtfeger

PHY - OR3

11:30 - 11:50 *A New Look at Organic Thermochemistry: C-C Bond Energy Variations explained by Electronegativity Equilibration*

Derek W Smith

PHY - OR4

11:50 - 12:10 *Inversion mechanisms for EX₃ molecules*

Patricia Hunt, P Schwerdtfeger and P Boyd

PHY OR5

12:10 - 12:30 *Electronic Structure and Properties of Complexes of the Group II Metals with CO or PH₃*

Graham Bowmaker, Peter Schwerdtfeger, M Pabst and Notker Rösch

SESSION 2 Tues 14:50 - 16:50

Chair: Robert Maclagan

PHY - OR6

14:50 - 15:30 *Reactions of Spatially Oriented Molecules in Crossed Molecular Beams*

Peter W Harland

PHY - OR7

15:30 - 16:10 *Time Resolved Vibrational Spectroscopy of Inorganic Complexes*

Keith Gordon

PHY OR8

16:10 - 16:30 *Probing the Interlayer of Synthetic Fluorohectorite and Zn-substituted Fluorohectorite Clay Catalysts using Cu(II)-ion Electron Spin Resonance*

Vittorio Luca, Richard Bramley

PHY - OR9

16:30 - 16:50 *Ion molecule reactions of Isomeric C₃H₃ Ions*

Murray J McEwan, Cara L McConnell, Colin G Freeman

SESSION 3 Wed 10:30 - 12:30

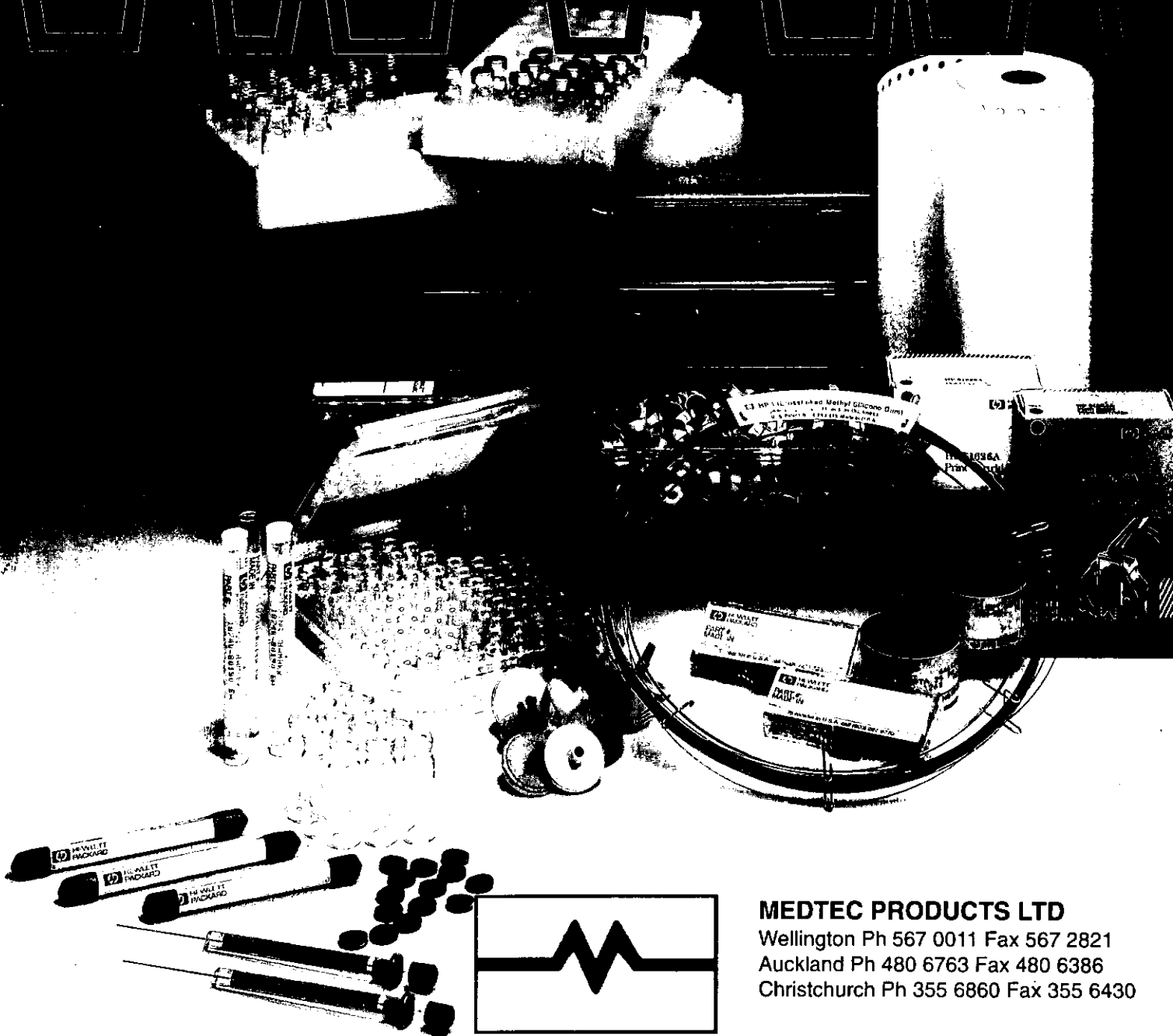
Chair: Margaret Hyland

PHY - OR10

10:30 - 10:50 *The use of SIMS Imaging in Studies of the Low Temperature Oxidation of Coals*

R R Martin

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CHEMISTRY IN NEW ZEALAND/NOVEMBER 1993

PHY - OR11

10:50 - 11:10 *Polarization Curves of Raney Nickel Electrodes for Liquid Fuels of Hydrazine or Methanol and their Surface Characteristics*

Ichiro Nakabayashi and E Nagao, K Miyata, N Minami, T Tomida, T Moriga, M Hyland and J Metson

PHY - OR12

11:10 - 11:30 *Catalysts for Low Temperature Oxidation of Ethylene*

Linda M Parker and John E Patterson

PHY - OR13

11:30 - 12:10 *Single Crystal Studies of Zeolite ZSM-5*

Kenneth T Jackson, Russell F Howe

PHY - OR14

12:10 - 12:30 *The Design and Construction of a Specimen Isolated Secondary Ion Mass Spectrometer*

James B Metson, P A W van der Heide and J Singh

SESSION 3 Thurs 10:30 - 11:50

Chair: Jim Metson

PHY - OR15

10:30 - 10:50 *Activity Coefficients of Sparingly Soluble Salts*

K H Khoo, L-H Lim, K.R.Fernando

PHY - OR16

10:50 - 11:10 *Electrochemical Kinetics of Batteries*

Graham A Wright

PHY OR17

11:10 - 11:30 *X-Ray Photoelectron Spectroscopy of Metallurgical Grade Alumina*

Allistair R Gillespie, J B Metson, R G Haverkamp, M M Hyland

PHY OR18

11:30 - 11:50 *Changes in Pinus Radiata Wood and Lignin on Acetylation and Exposure to Ultra-Violet Radiation using X-ray Photoelectron Spectroscopy*

Kirk M Torr, Bernard S W Dawson

SESSION 4 Thurs 13:10 - 14:50

Chair: Peter Gill

PHY - OR19

13:30 - 14:10 *Ab Initio Calculation of Gas Phase Ion Mobilities*

Robert G A R MacLagan

PHY - OR20

14:10 - 14:30 *Ab Initio Studies of Alkylammonium ylides and their Rearrangement Products*

George L Heard, Brian F Yates

PHY - OR21

14:30 - 14:50 *Theoretical Studies of Electron-Molecule Collision Processes*

H Struthers

SESSION 5 Fri 10:30 - 12:30

Chair: Peter Harland

PHY - OR22

10:30 - 11:10 *Kinetic Modelling of Titanium Carbide Synthesis in Thermal Plasma Reactors*

John S McFeaters

PHY - OR23

11:10 - 11:50 *Structures and Stabilities of RN=C=C=O and RN=C=C=S: Theory and Equipment*

Ming Wah Wong, R Flammang, D Landu, S Laurent, M Barbieux-Flammang, C Oliver Kappe and C Wenstrup

PHY - OR24

11:50 - 12:10 *Can AuF be Synthesised? A theoretical study using relativistic configuration interaction and plasma modelling techniques.*

Peter Schwerdtfeger, J S McFeaters, R L Stephens, MJ Liddell, M Dolg, B A Hess

PHY - OR25

12:10 - 12:30 *Classical and Non-Classical Adducts of AlX₃ with Fluorinated and Chlorinated Amines and Phosphines*

Janet E Barton and C J Marsden

SESSION 6 Fri 13:30 - 14:30

Chair: Graham Bowmaker

PHY - OR26

13:30 - 14:10 *A Computational Study of Organometallic 1,3-Dipolar Cycloaddition Reactions*

Michael Liddell

14:10 - 14:30 *General discussion on the establishment of an NZIC Physical Chemistry Specialist Group*

NATURAL PRODUCTS SYMPOSIUM

Venue: Physics Lecture Theatre I

SESSION 1 Tues 14:50 - 16:50 TERRESTRIAL NATURAL PRODUCTS

Chair: Con Cambie

NAP - OR1

14:50 - 15:30 *INVITED LECTURE: Highlights in phytochemistry in bryophytes-biologically active substances*

Yoshinori Asakawa

Faculty Pharmaceutical Sciences, Tokushima Bunri University, Tokushima 770, Japan

NAP - OR2

15:30 - 15:50 *Relative stereochemistry of the A/B rings of the tremorganic mycotoxin lolitrem B*

Richard Ede, Christopher O Miles, Lucy P Meagher, Sarah C Munday and Alister L Wilkins

Ruakura Agricultural Centre, NZ Pastoral Agriculture Research Institute Ltd, Private Bag 3123, Hamilton, New Zealand

NAP - OR3

15:50 - 16:10 *Isolation, characterisation and biological activity of some natural products from Ophiorrhiza and Hedyotis species*

Ahmad S Hamzah and Nordin Hj Lajis

Chemistry Department, Universiti Pertanian, Malaysia 43400, Serdang, Selangor, Malaysia

NAP - OR4

16:10 - 16:30 *Constituents of Trichomanes reniforme*

Nobutoshi Tanaka, Richard C Cambie and John E Braggins
Faculty of Pharmaceutical Sciences, University of Tokyo,
Inchigaya, Tokyo 162, Japan; Department of Chemistry,
University of Auckland, Private Bag 92019, Auckland, New
Zealand, Department of Botany, University of Auckland,
Private Bag 92019, Auckland, New Zealand

NAP - OR5

16:30 - 16:50 *New pigments from indigenous New Zealand
toadstools of the genus Dermocybe*

Melvyn Gill, Peter M Morgan and Jin Yu
School of Chemistry, University of Melbourne, Parkville,
Victoria 3052, Australia

SESSION 2 Wed 10:30 - 12:30 MARINE NATURAL
PRODUCTS

Chair: Murray Munro

NAP - OR6

10:30 - 11:10 *INVITED LECTURE: Biologically active
marine natural products: Structure elucidation and
biosynthesis*

Raymond J Andersen
Department of Chemistry, University of British Columbia,
Vancouver, BC, Canada

NAP - OR7

11:10 - 11:30 *The slime saga. Natural products from blue-
green algae*

Michelle R Princep, Richard E Moore and Gregory M L
Patterson
Department of Chemistry, University of Waikato, Hamilton,
New Zealand; Department of Chemistry, University of Hawaii,
Honolulu, USA

NAP - OR8

11:30 - 11:50 *Marine sesquiterpene quinones/quinols:
Mechanistic, stereochemical, and biosynthetic investigations*

Sylvia Urban and Robert J Capon

NAP - OR9

11:50 - 12:10 *Relationships between the in vitro mode of
biological activity of marine natural products and their
defensive role in situ*

Christopher N Battershill, John W Blunt, Murray H G Munro,
Mary J Garson and Peter Murphy
New Zealand Oceanographic Institute, P O Box 14 901,
Kilbirnie, Wellington, New Zealand

NAP OR10

12:10 - 12:30 *Novel brominated phenols and cyclic peptides
from ascidians of the genera Synoicum and Lissoclinum*

Anthony R Carroll, John C Coll, Bruce F Bowden
Department of Molecular Sciences, James Cook University of
North Queensland, Townsville, Qld 4811, Australia

SESSION 3 Thurs 10:30 - 12:10 MARINE NATURAL
PRODUCTS

Chair: John Coll

NAP - OR11

10:30 - 11:10 *INVITED LECTURE: Marine natural
products: a Southern Australian prospectus*

Robert J Capon
School of Chemistry, University of Melbourne, Parkville,
Victoria 3052, Australia

NAP - OR12

11:10 - 11:30 *New halichondrin compounds from the
Kaikoura sponge, Lissodendoryx sp.*

John W Blunt, Robin J Lake, Marc Litaudon, Li Shangxiao,
Murray H G Munro and Ronald J M Thow
Department of Chemistry, University of Canterbury,
Christchurch, New Zealand

NAP - OR13

11:30 - 11:50 *Structure activity studies in the halichondrin
series*

Joanne B Hart, John W Blunt and Murray H G Munro
Department of Chemistry, University of Canterbury,
Christchurch, New Zealand

SESSION 4 Thurs 13:30 - 13:50 LIPIDS

Chair: Graham Ryburn

NAP - OR14

13:30 - 14:10 *INVITED LECTURE: The development of
Linola and its potential application in New Zealand*

Allan Green
Institute of Plant Production and Processing, CSIRO Division
of Plant Industry, GPO Box 1600, Canberra, Australia

NAP - OR15

14:10 - 14:30 *Enzyme catalysed alcoholysis of tallow to
value-added products*

David E Stevenson, Roger A Stanley and Richard Furneaux
Industrial Research Ltd, P O Box 31 310, Lower Hutt, New
Zealand

NAP - OR16

14:30 - 14:50 *Unusual lipid biochemistries in some marine
microalgae*

John K Volkman, Stephanie M Barrett, Graeme A Dunstan,
Susan L Blackburn and S V Jeffrey
CSIRO Division of Oceanography and CSIRO Division of
Fisheries, GPO Box 1538, Hobart, Tasmania 7001, Australia

SESSION 5 Thurs 15:10 - 16:50 TERRESTRIAL NATURAL
PRODUCTS

Chair: Melvyn Gill

NAP - OR17

15:10 - 15:30 *Insect feeding deterrents: a New Zealand
perspective*

Graham Russell
Horticulture Research Institute, Palmerston North,
New Zealand

NAP - OR18

15:30 - 15:50 *The composition of the flavour volatiles of
Australian unifloral honeys*

Bruce D'Arcy and Gavin B Rintoul
Department of Food Science & Technology, The University
of Queensland, Gatton College, Lawes, Qld 4343, Australia

NAP - OR19

15:50 - 16:10 *From phytochemical survey to bioactive natural products at Universiti Pertanian*

Nordin Hj Lajis

Chemistry Department, Universiti Pertanian Malaysia, 43400 Serdang, Selangor, Malaysia

NAP - OR20

16:10 - 16:30 *Novel enzyme inhibitors from New Zealand plants - a review*

Stephen J Kellam and John R L Walker

Department of Plant and Microbial Sciences, University of Canterbury, Christchurch, New Zealand

NAP - OR21

16:30 - 16:50 *Biosynthesis of 2-ethyl-1-aminocyclopropane-1-carboxylic acid and coronatine by Pseudomonas syringae pr. glycinea*

Robin E Mitchell, S A Young and C L Bender

The Horticultural and Food Research Institute of NZ, Mt Albert Research Centre, Private Bag 92169, Auckland, New Zealand; Department of Plant Pathology, Kansas State University, Manhattan, Kansas 66506; Department of Plant Pathology, Oklahoma State University, Stillwater, Oklahoma, 74075, USA

SESSION 6 Thurs 15:10 - 16:10 LIPIDS

Chair: Allan Green

NAP - OR22

15:10 - 15:30 *Fatty acid selectivity of lipases*

R L Ravenhall and Peter J S Bain

Industrial Research Ltd, P O Box 31 310, Lower Hutt, New Zealand

NAP - OR23

15:30 - 15:50 *Analysis of cholesterol autoxidation products*

Cecil Johnson

Horticulture and Food Research Institute of NZ Ltd, Private Bag 11030, Palmerston North, New Zealand

NAP - OR24

15:50 - 16:10 *Protecting innovation*

M L Van Tiel

James & Wells, Patent Attorneys, P O Box 759, Hamilton, New Zealand

SESSION 7 Fri 10:30 - 12:30 MARINE NATURAL PRODUCTS

Chair: Robert Capon

NAP - OR25

10:30 - 11:10 *INVITED LECTURE: Sponge chemistry and the role of symbionts*

D. John Faulkner

Scripps Institution of Oceanography, University of California, San Diego, La Jolla, CA 92093-0212, USA

NAP - OR26

11:10 - 11:30 *Biosynthesis of chlorinated alkaloids in the tropical marine sponge Dysidea herbacea*

Eric J Dumdei, Mary J Garson and John Gerhmann

Department of Chemistry, The University of Queensland, Brisbane, Qld 4072, Australia

NAP - OR27

11:30 - 11:50 *Macrocyclic alkaloids: a three year odyssey in structural elucidation*

Leanne M Murray, T K Lim, G J Currie and R J Capon

School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia

NAP - OR28

11:50 - 12:10 *Sesterterpenes from a new Hyrtios species*

Allick Lal, Richard C Cambie and Clifford E F Rickard

Department of Chemistry, University of Auckland, Private Bag 92019, Auckland, New Zealand

NAP - OR29

12:10 - 12:30 *Investigation into the taxonomy of an alien fed alga by polysaccharide analysis*

Andy Falshaw, R Falshaw, and R H Furneaux and W A Nelson
Industrial Research Ltd, P O Box 31 310, Lower Hutt; Museum of New Zealand, P O Box 467, Wellington, New Zealand

SESSION 8 Fri 13:30 - 14:30 MARINE NATURAL PRODUCTS

Chair: John Faulkner

NAP - OR30

13:30 - 14:10 *INVITED LECTURE: Marine natural products: DNA damaging agents*

Chris Ireland

University of Utah, 308 Skaggs Hall, Salt Lake City, Utah 84112, USA

NAP - OR31

14:10 - 14:50 *INVITED LECTURE: Chemical variability in soft corals - a function of time and place*

John Coll, Mauro Maida, Pricila Leone, Anthony Carroll and Bruce F Bowden

Chancellory, University of Central Queensland, Rockhampton, Qld 4702; Department of Molecular Sciences, James Cook University of Northern Queensland, Townsville, Australia

SESSION 9 Fri 15:10 - 16:10 MARINE NATURAL PRODUCTS

Chair: Mary Garson

NAP - OR 32

15:10 - 15:50 *INVITED LECTURE: Biologically active marine alkaloids*

Nigel Perry, Brent Copp, Laurent Ettouati, Marc Litaudon, Julie Rea, John Blunt, Murray H G Munro; Golakoti Trimurtulu, John Faulkner; Hakon Hope; Geoffrey Jameson
Department of Chemistry, University of Canterbury, Christchurch, New Zealand; Scripps Institution of Oceanography, University of California; San Diego, CA, USA; Department of Chemistry, Georgetown University, Washington DC, USA

NAP - OR33

15:50 - 16:10 *The US National Cancer Institutes natural products collection and development programs. Methods and intellectual property rights; with emphasis on the marine program.*

Gordon M Cragg, M R Grever, T Mays, David J Newman and K M Sander

Development therapeutics program, DCT, NCI; Office of Technology Development, NCI, Bethesda, MD, 20892, USA

INORGANIC/ORGANOMETALLIC SYMPOSIUM

Venue: Medium Lecture Theatre

SESSION 1 Tues 14:50 - 16:50

Chair: Michael Taylor

INO - OR1

14:50 - 15:30 *New Silyl Complexes of Ruthenium and Osmium*

S M Maddock, C E F Rickard, W R Roper, D M Salter and L J Wright

Chemistry Department, University of Auckland, Private Bag 92019, Auckland, New Zealand

INO - OR2

15:30 - 16:10 *New Thiolate-Bridged Complexes of Cadmium (II) and Mercury (II) with Mixed Ligands*

Philip A W Dean, Nicholas C Payne, Jagadeese J Vittal and Yang Wu

Department of Chemistry, University of Western Ontario, London, Ontario N6A 5B7, Canada

INO - OR3

16:10 - 16:30 *Useful New Alternative to 2,2'-Bipyridine*

Gene E Honey, Ian G Phillips, Jonathan Steenwijk and Peter J Steel

Chemistry Department, University of Canterbury, Christchurch, New Zealand

INO - OR4

16:30 - 16:50 *Linked Triosmium Clusters*

Eric W Ainscough, Andrew M Brodie, Richard K Coll, Angelika J A Mair and Joyce M Waters

Department of Chemistry and Biochemistry, Massey University, Palmerston North, New Zealand

SESSION 2 Wed 10:30 12:30

Chair: Warren Roper

INO - OR5

10:30 - 11:10 *Chemistry of Transition Metal Complexes Containing Low Valent Silicon and Germanium Species as Ligands*

Hiroshi Ogino

Department of Chemistry, Faculty of Science, Tohoku University, Sendai 980, Japan

INO - OR6

11:10 - 11:30 *A New Macrocyclic Ligand*

Vickie McKee and Jan Wikaira

Chemistry Department, University of Canterbury, Christchurch, New Zealand

INO - OR7

11:30 - 11:50 *What's New in Photosystem 2: An XAS and ESR Study of the Manganese Cluster*

Dugald J MacLachlan*, Jonathan H A Nugent and Michael C W Evans

Department of Biology, University College London, UK.

* Present address: Research School of Chemistry, The Australian National University, Canberra

INO - OR8

11:50 - 12:10 *Complexes of Mixed Nitrogen Selenium Donor Atom Cages*

Alan P Arnold, Rajumati Bhula and W Gregory Jackson

Chemistry Department, University College, University of New South Wales, The Australian Defence Force Academy, Canberra, ACT 2600, Australia

INO - OR9

12:10 - 12:30 *Manganese Complexes of Biguanide*

Stephen R Cooper^a, Rachel C Squire^b, and

David C Weatherburn^b

^a Chemistry Department, Oxford University, Oxford, UK

^b Chemistry Department, Victoria University of Wellington, Wellington, New Zealand

SESSION 3 Thurs 10:30 - 12:10

Chair: James Wright

INO - OR10

10:30 - 11:10 *Synthetic and Mechanistic Investigations of Sigma-Bond Metathesis Reactions that produce Lanthanide-Silicon Bonds*

Nora S Radu^a and T Don Tilley^a and Arnold L Rheingold^b

^a Department of Chemistry, University of California at San Diego, 9500 Gilman Drive DEPT 0506, La Jolla, CA 92093-0506, USA

^b Department of Chemistry, University of Delaware, Newark, DE 19716, USA

INO - OR11

11:10 - 11:30 *Orthometallation at Dimetallaic Centres: Synthesis and Reactivity of some Orthometallated Dimers of Gold and Platinum*

Suresh K Bhargava^a, Gary Amiet^a, Matthew J Bowyer-Smyth^a, Sue Holden^a, Martin A Bennett^b, Lee L Welling^b

^a Department of Applied Chemistry, Royal Melbourne Institute of Technology, Victoria 3001, Australia

^b Research School of Chemistry, The Australian National University, Canberra, ACT 2601, Australia

INO - OR12

11:30 - 11:50 *Investigations of Borate Complexes with Aminoalcohol or Polyhydroxylic Compounds as Ligands*

Michael J Taylor, John Grigg, Ian Laban, Peter D W Boyd and Clifton E F Rickard

Department of Chemistry, University of Auckland, Private Bag 92019, Auckland, New Zealand

INO - OR13

13:30 - 14:10 *Metallacyclic Complexes of the Platinum Metals*

William Henderson

Department of Chemistry, University of Waikato, Hamilton, New Zealand

INO - OR14

14:10 - 14:30 *Metal Complexes of Conformationally flexible Dithiacyclophanes*

L R Hanton

Department of Chemistry, University of Otago, P O Box 56, Dunedin, New Zealand

SESSION 5 Thurs 15:10 - 16:30

Chair: Andrew Brodie

INO - OR15

15:10 - 15:50 *From Benzyne to Ferrocene and Beyond*

W R Cullen

Chemistry Department, University of British Columbia,
Vancouver, BC, Canada V6T 1Z1

INO - OR16

15:50 - 16:10 *A Study on the Ferrocene Derivatives
containing Arsenic and Tin*

Shujian Shi, Honggang Du and Xinxu Shi

Beijing Institute of Chemical Technology, Beijing 100029,
China

INO - OR17

16:10 - 16:30 *High Oxidation State Diphenylacetylene
Complexes of Tungsten*

P D W Boyd, G R Clark, P A Hunt, J B Metson, A J Nielson,
C E F Rickard and P Schwerdtfeger

Department of Chemistry, The University of Auckland, Private
Bag 92019, Auckland, New Zealand

**ANALYTICAL ENVIRONMENTAL
SYMPOSIUM**

Venue: *Chemistry Seminar Room*

SESSION 1 Wed 10:30 - 12:30 MARINE CHEMISTRY

Chair: S J de Mora

EAC - OR1

10:30 - 11:10 *KEYNOTE ADDRESS: The biogeochemistry
of arsenic in the marine environment*

W R Cullen

Department of Chemistry, University of British Columbia,
Vancouver, BC, Canada

EAC - OR2

11:10 - 11:30 *Trace metals as palaeo-indicators of ocean
chemistry*

K Hunter

Department of Chemistry, University of Otago, Dunedin,
New Zealand

EAC - OR3

11:30 - 11:50 *Chemical Studies of Sediments and Porewaters
from the Otago Harbour and Coastal Areas*

B Peake

Department of Chemistry, University of Otago, Dunedin,
New Zealand

EAC - OR4

11:50 - 12:10 *PAH contamination in the Kitimat Estuary*

C Simpson

Department of Chemistry, University of British Columbia,
Vancouver, BC, Canada

EAC - OR5

12:10 - 12:30 *Laboratory and pilot plant studies of SO₂
absorption in seawater*

M Radojevic

Department of Chemistry, University of Brunei Darussalam,
Gadong 3186, Bandar Seri Begawan, Brunei, Darussalam

SESSION 2 Thurs 10:30 - 12:30 ATMOSPHERIC
CHEMISTRY

Chair: S J de Mora

EAC - OR6

10:30 - 11:10 *KEYNOTE ADDRESS: Ozone in the Southern
Hemisphere Troposphere: Natural processes and global change*

I E Galbally

CSIRO Division of Atmospheric Research, Mordialloc,
Victoria, Australia

EAC - OR7

11:10 - 11:50 *Physical Chemistry of air-sea gas exchange*

L Phillips

Department of Chemistry, University of Canterbury,
Christchurch, New Zealand

EAC - OR8

11:50 - 12:10 *Passive samplers as devices for the
determination of atmospheric trace gases*

D Shooter

Department of Chemistry, University of Auckland, Private Bag
92019, Auckland, New Zealand

SESSION 3 Thurs 13:30 - 14:50 ATMOSPHERIC
CHEMISTRY

Chair: D Shooter

EAC - OR13

13:30 - 14:10 *KEYNOTE ADDRESS: Environmental Dust:
Composition, Sources and Transport*

J E Fergusson

Department of Chemistry, University of Canterbury,
Christchurch, New Zealand

SESSION 4 Thurs 15:20 - 17:00 RIVERINE CHEMISTRY

Chair: K Hunter

EAC - OR10

15:20 - 16:00 *Aqueous geochemistry of natural water systems
in Antarctica*

S J de Mora

Department of Chemistry, University of Auckland, Private Bag
92019, Auckland, New Zealand

EAC - OR11

16:00 - 16:20 *The chemistry of Lake Wilson and ponds of
the Darwin Valley region, Antarctica*

J Webster

Institute of Environmental Health and Forensic Science,
Auckland, New Zealand

EAC - OR12

16:20 - 16:40 *The fate of mercury discharged to the Waikato
River from the Wairakei geothermal power station*

M Timperley

Institute of Environmental Health and Forensic Science,
Auckland, New Zealand

EAC - OR13

16:40 - 17:00 *Resin acids and chlorophenolic compounds
in the upper Waikato River sediments*

M C Judd

New Zealand Forest Institute, Rotorua, New Zealand

SESSION 5 Fri 10:30 - 12:30 ANALYTICAL CHEMISTRY

Chair: P Hauser

ANA - OR1

10:30 - 11:10 **KEYNOTE ADDRESS: Quality in Contract Environmental Testing**

D Clark

Analchem Bioassay Pty Ltd, Lilyfield, Australia

ANA - OR15

11:10 - 11:30 **The photon counting method for the detection of ultraweak biological chemiluminescence**

R N Tilbury

Department of Chemistry, Victoria University, Wellington, New Zealand

ANA - OR16

11:30 - 11:50 **Secondary ion mass spectrometry in the study of element distribution in tree rings**

R R Martin

Department of Chemistry, University of Western Ontario, London, Ontario, Canada

ANA - OR17

11:50 - 12:10 **Effect of tetraiodofluorescein on lactate dehydrogenase**

R Ledger

School of Pharmacy, University of Otago, Dunedin, New Zealand

ANA - OR18

12:10 - 12:30 **A novel micro enzyme sensor with osmium complex for measuring cholesterol and cholesterol ester**

J Motonaka

University of Tokushima, Tokushima, Japan

EDUCATION SYMPOSIUM

Venue: Large Chemistry Lecture Theatre

SESSION 1 Thurs 10:30 - 12:10 THE ROLE OF CHEMICAL INDUSTRY IN SCHOOL CHEMISTRY

Chair: Dr A F Wilson

EDU - OR1

10:30 - 11:30 **The Chemical Industry - a Natural Partner for Chemical Education**

Miranda Mapleoft

Manager, Chemical Industry Education Centre, University of York, United Kingdom

EDU - OR 2

11:30 - 11:50 **The Role of the NZCIC in School Chemical Education**

Tony Petley

President, NZ Chemical Industry Council, United Environmental Ltd, Auckland

EDU - OR3

11:50 - 12:10 **Chemical Processes in New Zealand - getting started on the new edition**

John Packer

Chemistry Department, University of Auckland, Private Bag 92019, Auckland, New Zealand

SESSION 2 Thurs 13:30 - 14:50

Chair: Dr J M Brittain

EDU - OR4

13:30 - 13:50 **Nuts and Bolts of Chemical Communication**

J R Zdysiewicz

Editor, Australian Journal of Chemistry

EDU - OR5

13:50 - 14:10 **The National Technology Curriculum**

Alister Jones

SMER Centre, University of Waikato, Hamilton, New Zealand

EDU - OR6

14:10 - 14:50 **Development, Trial and Evaluation of an Interactive Computer Tutorial for Teaching Quantitative Volumetric Analysis**

Janet Barton, Paul Fritze, Heather Grant, Carmel McNaught, Peter McTigue and Bob Prosser

University of Melbourne, Parkville, Australia

SESSION 3 Thurs 14:50 - 16:50

Chair: Dr J E Packer

EDU - OR7

15:10 - 15:50 **The Curriculum Framework, Unit Standards and the Chemistry Prescriptions**

Ian Torrie

St Cuthberts College, Auckland

Either (A)

EDU - OR8

15:50 - 16:10 **Training Graduate Students as Teachers in Undergraduate Laboratories**

Louis Brown

University of Alberta, Edmonton, Canada

EDU - OR9

16:10 - 16:30 **Peer Group Learning in the Tertiary Chemistry Laboratory**

John Casey and L M Greenhill

Victoria University of Technology, St Albans, Melbourne, Australia

EDU - OR10

16:30 - 16:50 **Rapid Evaluation of Chemistry Lecturer Performance**

John Orbell, Stephen Bigger, Simon Bennett, Lawrence Ngeh and Mary Milikan

Victoria University of Technology, St Albans, Melbourne, Australia

or (B)

15:50 - 16:50 **General Forum on Teaching School Chemistry**

Time for further discussion on school chemistry matters if required.

POLYMER SYMPOSIUM

Venue: Medium Lecture Theatre 2

SESSION 1 Thurs 10:30 - 12:10

POL - OR1

10:30 - 11:10 *Biodegradable Polymers and Environment: Recent Results and Present State of Development*

C David

Universite Libre de Bruxelles, Belgium

POL - OR2

11:10 - 11:30 *Synthesis and Structure/Property Relationship of Polyurethane Ionomer Dispersions*

B K Kim

Pusan University, Korea

POL - OR3

11:30 - 11:50 *S_mI₂ in Polymer Synthesis*

Yakov S. Vygodskii

Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Science

POL - OR4

11:50 - 12:10 *Properties of water in dextran sulphate solutions*

Philippa Wiggins and Diana Siew

Department of Medicine, University of Auckland, Private Bag

92019, Auckland, New Zealand

SESSION 2 Thurs 13:30 - 14:50

POL - OR5

13:30 - 14:10 *Direct Formation of Polyimide Thin Films by Vapour Deposition Polymerisation*

N Okui and A Kubono

Tokyo Institute of Technology, Tokyo, Japan

POL - OR6

14:10 - 14:30 *Modern Trends in Polyheteroarylenes Chemistry*

Alexander L Rusanov

Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Science

POL - OR7

14:30 - 14:50 *Natural and Artificial Weathering of uPVC*

Neil Trebilco

BRANZ, Wellington, New Zealand

SESSION 3 Thurs 15:10 - 16:10

POL - OR8

15:10 - 15:30 *Effect of Polymer Viscoelasticity on Orientation of Liquid Crystals*

W S Ahn, D Y Kim and C Y Kim

Korea Institute of Science and Technology, Korea

POL - OR9

15:30 - 15:50 *Chemical Embrittlement of Poly (Vinylidene Fluoride)*

Clive Sterling, Veronica Van Tilburg and Neville Miller

Industrial Research, Auckland, New Zealand

POL - OR10

15:50 - 16:10 *Siloxiranes; Aerospace Polymers for Coating Systems*

Neil Edmonds

Auckland Industrial Technologists

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THE POLYMER NETWORK

By Neil Edmonds, Auckland Institute of Technology

Polymer science and technology is an integral part of New Zealand industry. Our economy was founded "on the sheep's back", and wool will always be a major export earner. The other natural polymer of economic importance is wood. For those who have priced timber recently they will appreciate that this is now valued according to the export price; forestry is experiencing an export boom and overseas demand is only likely to increase.

The cry of Government however is for more "added value". Don't export unprocessed materials, process them into more valuable materials first. This requires technology, and such knowledge is provided by the Wool Research Organisation of New Zealand (WRONZ) in Christchurch and the Forest Research Institute (FRI) in Rotorua.

The study of polymer science and technology is usually associated with synthetic polymers rather than naturally occurring macromolecules. There is no industry-funded organisation for the development of synthetic polymers, but the industry sector would form one of the largest blocks outside of those concerned with primary produce.

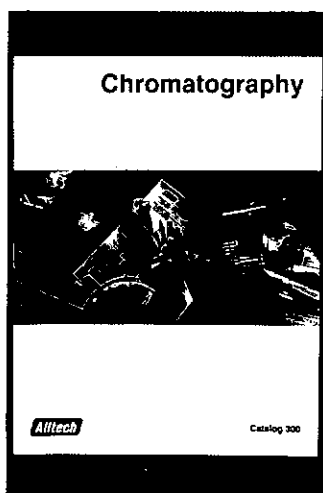
Thermoplastic polymers are, of course, not manufactured in New Zealand, but large quantities are imported for processing into plastic film, tubes, bottles, etc. To date only the film manufacturers (e.g. Trigon, Borden Filmpac, Transpak) and

PVC compounders (e.g. Marley, Chemby Vinyl) employ chemists, the industry being dominated by engineering requirements rather than chemical. This is changing however as the complexity of thermoplastics has increased markedly in recent years and more manufacturers realise their vulnerability through limited knowledge of plastics materials.

The largest sector of the chemical industry however would probably be that covering synthetic resins, surface coatings, inks and adhesives. Companies such as A C Hatricks, Nuplex and Rohm and Haas perform complex operations in large reactors at high temperatures; they must employ numerous chemists, to formulate, monitor and, often sell these products - a marketing degree is not a lot of use if the agent does not understand what they are marketing.

The future is bright for chemists who enter the polymer industries, jobs are plentiful both here and overseas, especially in Australia where the study of polymer science at tertiary level is very strong. The Pacific Polymer Federation is shortly holding its third conference, in Queensland, and it is hoped that many local polymer scientists will be able to attend. For those unable to make the Australian meeting, the Polymer Symposium at the NZIC Conference will provide the opportunity to meet with overseas experts stopping over on their way to PPC-3.

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DR PEAK'S CHROMATOGRAPHY MADE EASY

"STANDARD PRACTICE FOR FUSED-SILICA CAPILLARY COLUMNS"

By Roger Whiting, Auckland Institute of Technology

The ASTM "Standards Practice for Installing and Maintaining Fused-Silica Open-Tubular Capillary Columns in Gas Chromatography" provides a standard practice for laboratories wanting to maintain high standards of quality management. The new standard starts with a simple step by step procedure for installations of fused-silica capillary columns which is an important task for most working analysts. Then it follows with detailed methodologies for a number of aspects of the use of these columns.

The basic procedure for installing fused-silica capillary columns is as follows:

- * Cool all heated zones and replace spent oxygen and moisture traps.
- * Clean and deactivate injector and detector sleeves if necessary.
- * Replace critical injector and detector seals.
- * Replace the septum.
- * Set detector and makeup gas flow rates.
- * Carefully inspect the column for damage or breakage.
- * Cut 10 cm from each column end using a ceramic scoring wafer or sapphire scribe.
- * Install a nut and an appropriate sized ferrule on both column ends.
- * Cut an additional 10 cm from both column ends to remove ferrule shards.
- * Mount the capillary column in the oven using a bracket that does not allow the column to become scratched or abraded.
- * Connect the column to the inlet at the distance indicated in the gas chromatograph's instrument manual.
- * Set the approximate column flow rate by adjusting the head pressure (see the column manufacturer's literature)
- * Set split-vent, septum purge, and any other applicable inlet gases according to the instrument specifications.
- * Confirm flow by immersing the column outlet in a vial of solvent such as acetone or dichloromethane.
- * Connect the column to the detector at the distance indicated in the instrument manual.
- * Check for leaks at the inlet and outlet using a thermal conductivity leak detector. Do not use soap or liquid-based leak detectors.
- * Set the injector and detector temperatures and turn on the detector when temperatures have equilibrated. Do not exceed the phase's maximum operating temperature.
- * Inject a nonretained substance to set the proper dead time.
- * Check system integrity by making sure that the dead volume peak does not tail.
- * Condition the column for 2 hrs at the maximum operating temperature to stabilize the baseline. To determine the column's maximum temperature, consult the column manufacturer's literature.
- * Run the test mixtures to confirm proper installation and column performance.
- * Calibrate the instrument and inject samples.

The standard practice also discusses in detail a number of issues related to column installation.

CLEANING AND DEACTIVATING INJECTOR SLEEVES:

To give optimum performance the injector sleeves must be free of particles from the septa and ferrules and of residues from previous samples. If samples with active functional groups are to be analysed then the sleeve must also be deactivated.

If the sleeve is not excessively dirty it can be cleaned with an organic solvent. First the septa particles can be removed by use of solvents such as methanol or iso-propanol which do not swell the rubber. Then solvents such as pentane, dichloromethane or toluene which will solubilize any sample residue should be used to rinse the sleeve. Pipe cleaners can help in this. It is important not to use any soaps, acids or bases for cleaning as these will remove the deactivation layer.

New sleeves can be purchased deactivated or can be deactivated using a procedure given in the new ASTM method.

REPLACING CRITICAL SEALS AND SEPTA

Before reinstalling the inlet sleeve it is important to review the instrument manual and replace the critical seals. In most gas chromatographs the injection ports use a rubber O-ring or graphite ferrule to seal the sleeve inside the injection port body. The seal must fit tightly and prevent carrier gas from leaking around the outside of the sleeve.

A new septum should ideally be installed at the end of each analytical sequence so that it can condition in the injector. If the septum is not replaced regularly then it can leak and degrade which results in particles falling into the inlet sleeve. This can be the cause of ghost peaks and loss of inertness.

FERRULES

Graphite or Vespel-Graphite are the usual material for ferrules to seal the capillary column to the injector and detector. Graphite is soft and will deform to fit different column sizes and configurations. However graphite can flake and fragment on removal leading to particles in the injector or detector. Vespel-graphite ferrules are hard and have to match the column dimensions closely to form a good seal. They will deform on initial heating and so must be tightened after first use. However, they do not flake or fragment so can be reused.

CUTTING COLUMN ENDS

If the capillary column is incorrectly cut it is possible for the glass or the polyimide outer coating to come into contact with the sample stream and reduce system inertness. Poorly cut columns can have a number of effects which degrade the quality of the chromatography. Among these effects are peak broadening (poor resolution), peak tailing and peak splitting. Scratches to the polyimide layer can make the column prone to breakage. To avoid these problems cutting blades are preferred to scribes as they make a squarer cut. These come in the form of silica scoring wafers, sapphire blades and tungsten carbide blades and are available from most column suppliers. The ASTM standard gives detailed instructions on how to achieve good cuts.

INSTALLING THE NUT AND FERRULE

When capillary columns are shipped they usually have the ends flame-sealed or capped with a septum. The recommended procedure is to cut approximately 10 cm off each end then put on the inlet connecting nut and a ferrule as described by the instrument manufacturer. Keep the column pointing down when doing this to stop flakes off the ferrule dropping down the capillary. With the nut and ferrule pushed well along the column cut approximately an extra 10cm from the end to ensure any pieces from the ferrule which have been pushed into the column are removed.

CONNECTING THE COLUMN TO THE INLET

Determine how far the column has to be inserted into the injector, lay the column down and determine where this lies. This point can be marked with a black marker or alternatively the nut and ferrule can be held in place using tweezers or a rubber septum which is put on the column before the nut and ferrule. The column can then be gently inserted into the inlet fitting. Care should be taken that the end is not scraped or crushed against the metal parts of the fitting. Then, maintaining the correct insertion distance, tighten the nut one turn past finger tight until the column is held firmly.

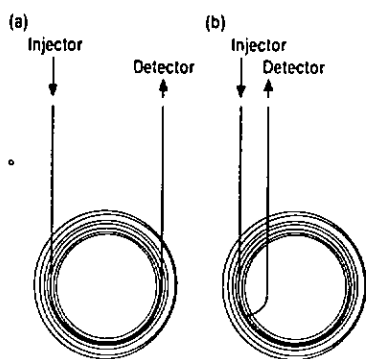


Figure 1: Positioning fused-silica column tubing during installation. Shown are (a) correct, and (b) incorrect, positioning.

Sharp bends in the column can weaken the fused silica and cause spontaneous breaks. Therefore, keep all curves to diameters greater than 15 cm. If sharp bends cannot be avoided then uncoil one turn of the column and repeat the installation procedure.

ESTABLISHING THE GAS FLOW

With the column connected to the inlet turn on the carrier gas and set the column head pressure, split-vent flow and septum purge to the values indicated in tables I and II. Use the values here - optimisation is carried out later. It is important to ensure that the carrier gas is flowing as operating the column without it can cause irreparable damage. The easiest way is to put the detector end of the column in a solvent such as acetone or dichloromethane and look for bubbles. Run the carrier gas for about 15 minutes before connecting the column to the detector.

TABLE I: Column Head Pressure*

COLUMN LENGTH	COLUMN INTERNAL DIAMETER (mm)					
	0.10	0.20	0.25	0.32	0.53	0.75
(m)						
10	15	12	6	3	2	2
15	15	12	6	4	2	2
25	30	30	12	8	4	5
30	30	30	12	8	4	5
50	-	60	24	15	8	10
60	-	60	24	16	8	10
100	-	90	40	30	20	15
150	-	-	60	50	-	-

* helium or hydrogen carrier gas (psig).

TABLE II: Typical Splitter Vent Flow Rates*

Carrier Gas	Column Internal Diameter (mm)		
	0.25	0.32	0.53
Helium	35	80	125
Hydrogen	70	160	250

* For a 50:1 split ratio (cm³/min); 2-5cm³/min septum purge

CONNECTING THE COLUMN TO THE DETECTOR

Before connecting the column ensure that the detector fuel, makeup gas and oxidant flow rates are set according to the instrument manual. In connecting the column to the detector the distance is as critical as when connecting it to the inlet so the same procedure should be used.

OPTIMISING THE FLOW RATE

The column flow rate and dead time are best set by injecting a nonretained substance. The pressure can then be adjusted to give the optimum linear velocity. It is not recommended to measure the flow rate at the column outlet as column to column variations can make this imprecise. About 2 microlitres of a nonretained substance that is compatible with the detector (see table III) should be injected. When using headspace vapours

use a 10 microliter sample. Accurately mark the injection start and elution times. The column head pressure should be adjusted until the correct dead time t_m is obtained for the column length and carrier gas used. This is derived from the following formula:

$$t_m = L / \dot{u}_{opt}$$

Where L is the column length in centimetres and u is the optimum linear velocity in centimetres per second. This is 40, 20 and 10 cm/sec for hydrogen, helium and nitrogen respectively.

TABLE III: Recommended Dead-Volume Compounds for Common Detectors*

Detector Type	Recommended Dead-Volume Compound
Flame ionization	Methane, propane, butane
Thermal conductivity	Air, methane, butane
Nitrogen-phosphorus	Acetonitrile headspace vapours
Electron capture	Methylene chloride headspace vapours
Electrolytic conductivity	Dichlorodifluoromethane headspace vapour
Mass spectrometer	Air, methane, propane, butane, argon

* These compounds may be slightly retained on thick-film phases (1.0-7.0 μm), thereby yielding erroneous dead-volume times; however they are reproducible for similar column types.

It is critical to set the linear velocity with the oven temperature set to the temperature that is to be used for the analysis. This is because capillary columns are used in a pressure controlled mode and thus the flow is affected by temperature. If a temperature programme is being used then choose a temperature that corresponds to the temperature at which a critical or hard to resolve peak is eluted. Alternatively choose a temperature in the middle of the programme. Record the temperature and the compound being used to determine the linear velocity so that the process can be repeated by other workers.

DEAD-VOLUME PEAK-SHAPE

The peak obtained from the dead volume test should be examined. It should be a sharp narrow peak as in figure 2b without signs of tailing as in figure 2a. Tailing indicates problems in column installation which needs attention before the system can be used analytically.

OTHER ISSUES

The ASTM standard method covers a range of other aspects of column operating and optimisation and should provide a solid basis for development of quality operating systems.

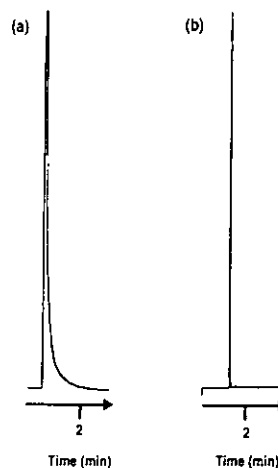


Figure 2: GC analysis of nonretained compounds indicating (a) incorrect and (b) correct column installation. Column: 30m x 0.32 mm, 0.25- μm df 5% diphenyl-95% dimethyl polysiloxane; carrier gas: hydrogen; linear velocity: 40 cm/s; temperature program: 40°C (isothermal); injector temperature: 325°C; detection: flame ionization, 325°C; detector sensitivity: 4×10^{-11} AFS; split ratio: 35:1; vent flow: 80 cm³/min; sample: methane (2.0 μL injection).

Adapted from:
G C Troubleshooting: "A New Standard Practice for Installing and Maintaining Fused-Silica Capillary Columns" by Paul H Silvis, LG•GC Volume 10, Number 5 (May 1992). For Subscription Details of LC•GC Magazine contact:

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Conferences and Seminars

7-10 December, 1993, NZIC Conference

Venue: University of Auckland,
Auckland, New Zealand.

See Conference Programme on page 29

5-8 December, 1993, RACI - Organometallic Meeting

Venue: University of New England, Armidale,
New South Wales, Australia.

For further information contact:

Dr. Mark Humphrey,
Department of Chemistry,
University of New England,
Armidale, N.S.W. 2351, Australia.
Ph. 61-67-732 872
Fax 61-67-711 563

6-10 December, 1993, Australian Conference on Optics, Lasers and Spectroscopy.

Venue: University of Melbourne, Melbourne, Australia.

For further information contact:

Dr. R. J. McLean,
ACOLS '93 Conference Secretary,
CSIRO Materials Science and Technology,
Locked Bag 33,
CLAYTON,
Victoria 3168, Australia.
Ph. 64-3-5422875
Fax 64-3-5441128.

10-12 December, 1993, 17th National Meeting of the Australian Society for Biophysics (ASB-93)

Venue: ANU, Canberra, Australia

For further information contact:

Dr Ron Pace,
Department of Chemistry,
ANU, Canberra, Australia
Fax. 61-6-249 0760

13-15 December, 1993, Inorganic Reaction Mechanisms Meeting 93

Venue: Wilhelm-Kempf Congress Centre,
Wiesbaden-Naurod, Germany

For further information contact:

Professor Horst Elias,
Anorganische Chemie III,
Technische Hochschule Darmstadt,
D64289 Darmstadt,
Germany
Ph. 49-6151-162425
Fax. 49-6151-164073

13-17 December, 1993, 3rd Pacific Polymer Conference

Venue: Gold Coast, Australia.

For further information contact:

PPC-3 Secretariat,
Department of Chemistry,
University of Queensland,
Queensland 4072, Australia.
Ph. 61-7-3653511
Fax 61-7-3653628.

10-21 January, 1994, The 27th General Assembly of the International Association of Seismology and Physics of the Earth's Interior (IASPEI 94)

Venue: Victoria University, Wellington, New Zealand.

For further information contact:

The Secretary, IASPEI 94,
Institute of Geological & Nuclear Sciences,
P.O. Box 1320,
Wellington, New Zealand.
Ph. 64-4-4738208
Fax 64-4-4710977

3-4 February, 1994, NZIC Chromatography Group "Supercritical Fluid Extraction, Solid Phase Extraction and other Advances in Chromatographic Analysis"

Venue: Rotorua, New Zealand.

For further information contact:

Dr. Peter Robinson,
R. J. Hill Laboratories Ltd,
P.O. Box 4048,
Hamilton East, New Zealand.
Ph. 64-7-8552266
Fax 64-7-8549886

8-9 February, 1994, Second New Zealand Symposium on Biosensors and Chemical Sensors.

Venue: Bishop Julius Hall,
University of Canterbury,
Christchurch, NZ

For further information contact:

Wendy Collier,
AgResearch Grasslands,
Private Bag,
Palmerston North, New Zealand.
Ph. 64-6-3568019
Fax 64-6-3561130.

13-18 February, 1994, 8th International Conference on Surface and Colloid Science.

Venue: Adelaide Convention Centre,
Adelaide,
South Australia.

For further information contact:

The Secretariat,
Techsearch Incorporated,
GPO Box 2471,
Adelaide,
South Australia 5001.
Ph. 61-8-2671755
Fax 61-8-2674031.

20-22 February, 1994, Australian Chemical Industry Council (ACIC) Convention 1994

Venue: Fairmont Resort,
Lewa, Blue Mountains,
NSW, Australia

28 April - 1 May, 1994. 4th Joint Conference of the Australian and New Zealand Societies of Cosmetic Chemists

Venue: Conrad Jupiters Hotel,
Gold Coast, Australia

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Mt Ommoney,
Queensland 4074,
Australia
Ph. 61-7-376 6700
Fax. 61-7-376 6532

3-8 July, 1994. RACI Division of Organic Chemistry 14th National Conference

Venue: University of Wollongong,
Wollongong, Australia

For further information contact:
Professor John Brenner (Chairman),
University of Wollongong,
Department of Chemistry,
Locked Bag 8844,
South Coast Mail Centre,
NSW 2521, Australia
Ph. 61-42-214 255
Fax. 61-42-214 287

24-29 July, 1994. 30th International Conference on Co-ordination Chemistry.

Venue: Kyoto International Conference Hall,
Kyoto, Japan.

For further information contact:
Professor Koji Taraka,
Secretary of XXX ICCO,
Coordination Chemistry Laboratories,
Institute of Molecular Science,
Myodaiji, Okazaki, 444
Japan.
Ph. 81-564-55-7252
Fax. 81-564-54-2254

1-4 August, 1994. 9th International Drying Symposium (IDS '94)

Venue: Gold Coast, Australia

The NZIC is co-sponsoring this conference and further information can be obtained from:

Alan Turner,
General Secretary/Executive Officer NZIC,
P O Box 12 347,
Wellington
Ph. 04-473 9444
Fax. 04-473 2324

17-22 December, 1995. Pacificchem '95.

Venue: Honolulu, Hawaii, U.S.A.

Were you there in '89? If you did not attend Pacificchem '89 in Honolulu then you should start planning now for the 1995 meeting, because you won't get another chance until 2000! If you *were* there then you'll need little encouragement to return in 1995.

Pacificchem, the International Congress of Pacific Basic Chemical Societies, 17-22 December 1995, provides the only forum for Pacific Basin chemists and biochemists to meet centrally, exchange information and assess the state of their discipline. The Congress opens on Sunday 17 December, the scientific session runs until lunch time on Friday 22 December, and you can get home for Christmas if you wish!

The Congress will operate with something in excess of 400 different half-day sessions grouped into some 130 symposium topics ranging through all major modern aspects of chemistry and much biochemistry. For those interested, the Branch Secretaries and the Victoria University Chemistry and Biochemistry Departments have a list of these. Planning is now well under way and some 48 meeting rooms and accommodations in the Sheraton and Hilton properties on Waikiki beach have been booked. From the symposia already proposed some 25 NZIC members appear to be involved even at this early stage. The presentation of work will be by both invitation and submission. In addition to the many specialised symposia, general sessions will be held in each of the ten broad subject areas.

Sponsorship to the Congress of 30 'Young Scholars' from the emerging nations of the Pacific Basin has been agreed to. If you know of anyone in South America, South East Asia etc, likely to be interested please have them contact:

The Pacificchem Office
American Chemical Society,
1155 16th Street, NW,
Washington DC 20036, USA.

For New Zealand PhD student members (Chemistry and Biochemistry), we now advise that one among you will receive sponsorship from the Ministry of Science and Technology and the NZIC to present a poster for the Student Poster Presentation Award of Merit (the actual presentation will be within the selected congress symposium). Details for application/selection will be available from the NZIC Office and Heads of Departments early in 1994.

Deadlines:

Abstracts for contributed/invited papers: 31 March 1995.
Registration: \$US 275.00 by 1 November 1995.

NZIC BRANCH NEWS

OTAGO BRANCH

The new sixth floor of the University of Otago, School of Pharmacy is now complete and the pharmaceutical chemistry staff, including Institute members Dr Rob Ledger and Dr Paul Fawcett, have moved into new offices and research laboratories.

* * * * *

Sadly MED NZ is losing the services of Dr Don Ferry who is moving to Auckland where he will join W Grayson and Associates.

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New Literature and Media

Further details from the Editor, *Chemistry in New Zealand*

(i) FROM DATABASE TO BOOK

Near infrared (NIR) spectroscopic data, previously available to chemists only as a database, are now obtainable in book form. The new series "SpecBook" is the joint product of the scientific publishers VCH and Chemical Concepts, experts in spectroscopic information systems who have access to the world's largest commercially available collection of spectra and structures.

The first book of the series, the "FT-NIR Atlas", authored by Michael Buback and Hans Peter Vögele, has just been published. It is a well-timed response to the growing interest in NIR spectroscopy, a technique which has become widespread with the recent introduction of commercial NIR instrumentation. Using NIR, scientists can easily obtain a characteristic "fingerprint" of chemical substances. The quantitative analysis of agricultural, pharmaceutical, biochemical and synthetic polymer materials can be performed much more rapidly, conveniently and efficiently. With almost 4000 spectra of 1900 common organic chemicals, the "FT-NIR Atlas" gives scientists an extraordinarily broad basis for the analysis of their samples.

(ii) Olivier Kahn

MOLECULAR MAGNETISM

Molecular magnetism occupies a crossing point between two fields of research - materials science and metal biochemistry - and plays an important role in the emerging field of molecular electronics.

Molecular Magnetism comprehensively addresses both the experimental and theoretical aspects of this new field of research. It introduces the basic concepts concerning magnetization and magnetic susceptibility, establishes the fundamental equations of molecular magnetism, and examines molecules containing a unique magnetic centre, including the high-spin low-spin transition compounds. The book highlights polymetallic species, reviews the phenomenon of interaction between spin carriers from a theoretical point of view, and includes numerous examples throughout to illustrate the topics discussed.

(iii) George J Kavarnos

FUNDAMENTALS OF PHOTOINDUCED ELECTRON TRANSFER

Devoted exclusively to the basic theories, concepts and applications of light-initiated electron-transfer processes, *Fundamentals of Photoinduced Electron Transfer* is the first book to deliver an introductory level account of this highly active research area in a concise and easy-to-follow manner. No prior knowledge of photochemistry is assumed or required to gain a solid understanding of the subject.

The author introduces essential background information on photochemistry and electrochemistry and presents a systematic account of the photoinduced electron transfer process. He carefully explains the fundamental thermodynamic equation governing the photoinduced electron, explores the diverse realms of electron-transfer reactions and provides a survey of today's most important applications. Novel applications such as solar energy conversion, artificial photosynthesis, semiconductor technology, organised assemblies and molecular electronic devices are described in appropriate detail.



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BOOK REVIEW

BASIC ONE AND TWO-DIMENSIONAL NMR SPECTROSCOPY

Second Edition by Horst Friebolin. Translated by Jack K Becconsall.

An understanding of NMR spectroscopy is of fundamental importance to the student of chemistry and the modern chemist, who needs to determine molecular structure or dynamics. Available books about NMR are not all of the same quality, nor indeed do they cover the topic in the same manner. The rapid evolution in NMR spectroscopy has meant that some are now out of date. Others, because they describe in too much physical and mathematical detail the basis of NMR spectroscopy, are unsuitable for the chemist needing only to interpret spectra to confirm a molecular structure. Introductory texts for chemistry students need to be up to date and cover topics of relevance to the chemist, some of which may now be unfashionable to the NMR spectroscopist. A student after reading an introductory text should have some understanding of the basis for NMR spectroscopy, and the knowledge to interpret NMR spectra in terms of possible molecular structures. At a more advanced level, the ability to select a particular NMR experiment to solve a molecular problem, may be required. The text should also assist the educator to explain difficult concepts to the student. Professor Friebolin's book "Basic One and Two Dimensional NMR spectroscopy" fulfils all these roles and more.

The book is thoughtfully composed. The layout includes a wide margin, leaving space for ample and relevant diagrams that enhance the clear explanations encountered throughout. The book starts with a chapter on basic NMR principles and then follows, in more detail, chapters on the chemical shift and indirect spin-spin coupling. Other chapters are on a variety of topics, including relaxation, one dimensional NMR experiments, two dimensional NMR spectroscopy, NOE's, dynamic NMR spectroscopy and finally a chapter on NMR spectroscopy in biochemistry and medicine. What is surprising about this book is the wealth of detail in the text which though presented at a fundamental level, is nevertheless very comprehensive. For instance the chapter on the indirect spin-spin coupling contains about 20 sections on such topics as geminal couplings, vicinal couplings and substituent effects for both ^1H - ^1H and ^{13}C - ^1H couplings. Some are necessarily brief, but most include tabulated values or ranges for representative couplings. This allows the student at the very least a chance to become familiar with typical spin-spin coupling values.

Little else could be identified that should have been included in this book. Perhaps, as this book is written mainly for the chemist, the chapter on "NMR Spectroscopy in Biochemistry and Medicine", and especially the section on magnetic resonance imaging, may seem irrelevant. It could have been replaced by a chapter introducing solid-state NMR. But neither topic can be adequately covered in a single chapter, so that the vignettes that Professor Friebolin has included in this, the last chapter, at least illustrate well the considerable utility NMR

has in these fields, and are consistent with the solution-state angle of the rest of the book.

A book that is closest in style and content to Friebolin's, is "Modern NMR Techniques for Chemistry Research" by Andrew Derome. Both texts are clearly written, although Derome's book tends to be a little lighter in style, and both cover some of the same topics. But Derome's book, containing sections such as those on shimming, ADC resolution, and pulse imperfections, is written primarily from the point of view of the NMR experimentalist. Discussion on these topics are absent from Friebolin's book, but instead there are a wealth of other carefully considered topics, for instance, the sections on empirical correlations for predicting chemical shift correlations, on relationships between T1 and the chemical structure, and on the three spin system. Friebolin's text is more for the chemist.

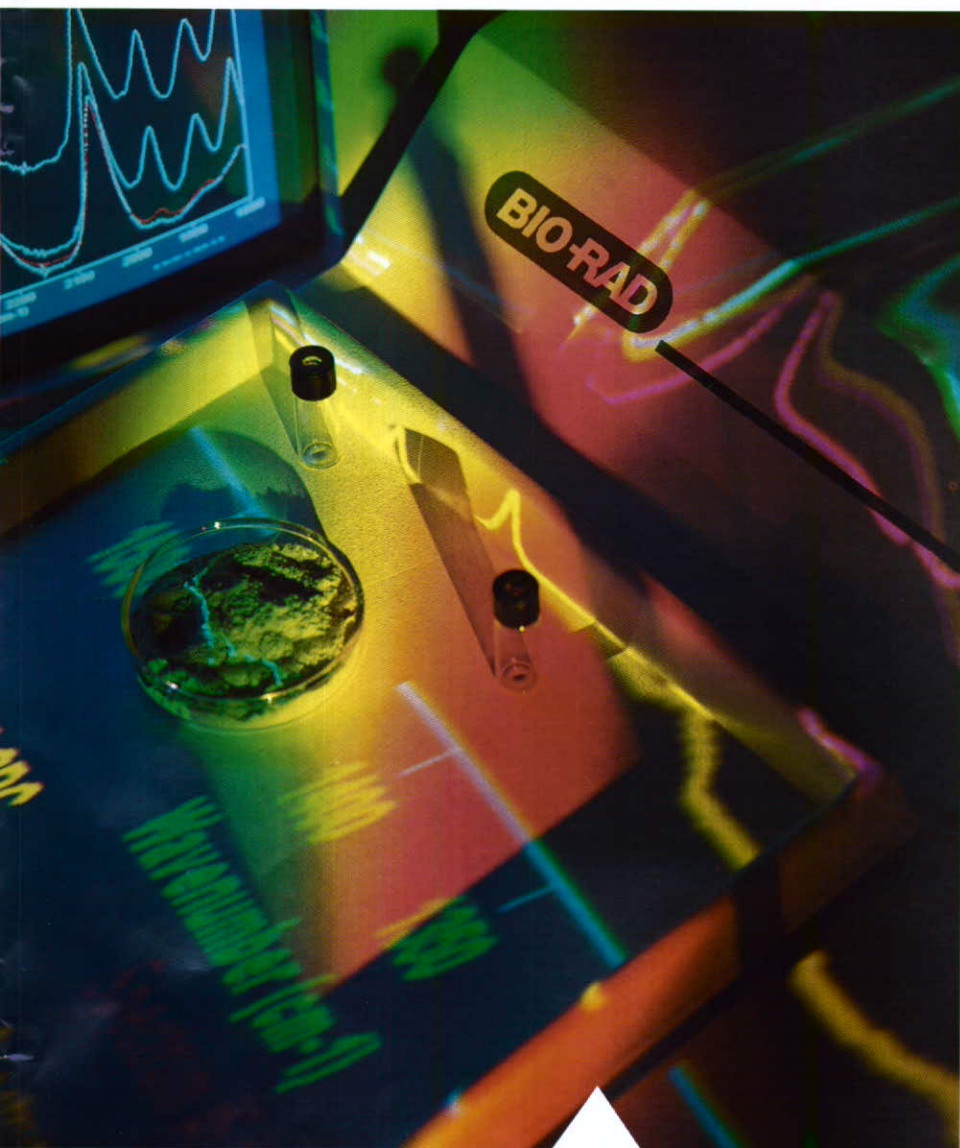
Professor Friebolin's book is an excellent "basic" NMR text, both for the student, the chemist needing to revise his NMR knowledge, and the educator. It should be read by any one interested in obtaining a good "basic" knowledge about NMR spectroscopy and its application to chemistry.

Keith Morgan, *Industrial Research Limited and Victoria University of Wellington*

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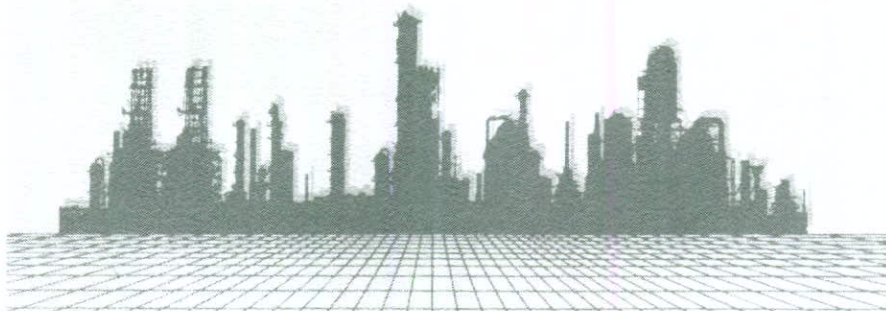
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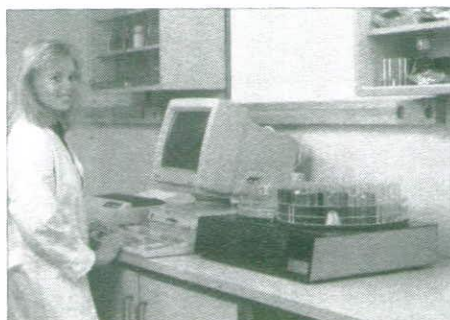
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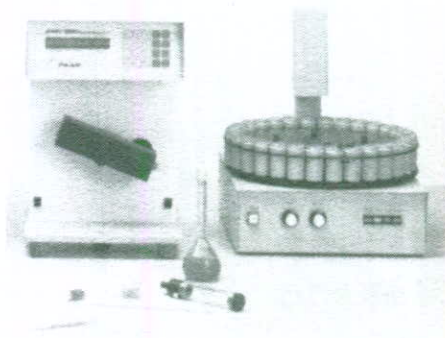
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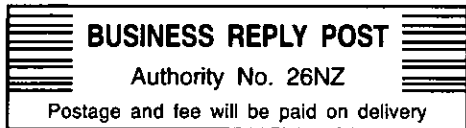
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