VOL 61 NO.6 NOVEMBER/DECEMBER 1997

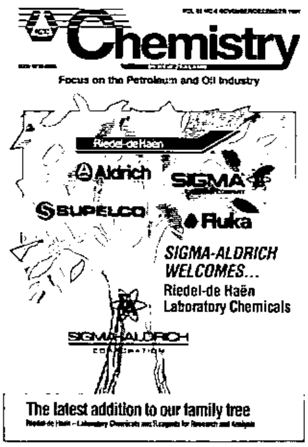
NZIC Chemistry IN NEW ZEALAND

ISSN 0110-5566

Focus on the Petroleum and Oil Industry

UP FRONT ...

As manufacturers of reagents, research and development as well as for quality assurance, and environmental checks, Riedel-de Haën continues to produce chemicals of uniformly high quality and developing new reagents for modern applications.



For further information see the cover story article on page 2

Chemistry IN NEW ZEALAND

Published on behalf of the New Zealand Institute of Chemistry in January, March, May, July, September and November each year.

The New Zealand Institute of Chemistry Incorporated
P O Box 12-347, Wellington, New Zealand
Phone: +64-4-4739444, Fax: +64-4-4732324
Email: nzic@ipenz.org.nz
WWW: http://webtwo.rsnz.govt.nz/www/nzic/nzic.html
President: Dr R S Whitney, Hon Treasurer: D P Karl
General Secretary/Executive Officer: Alan A Turner

Advertising Sales & Publisher:
Robert B Lyon
Ancat Holdings Limited
32 Murvale Drive, Bucklands Beach, Auckland
P O Box 38-546, Howick, Auckland, New Zealand
Phone: +64-9-5353475, Fax: +64-9-5353476
Email: ancat@ihug.co.nz

Managing Editor:
Louanne R McLeay
Ancat Holdings Limited
32 Murvale Drive, Bucklands Beach, Auckland
P O Box 38-546, Howick, Auckland, New Zealand
Phone: +64-9-5353475, Fax: +64-9-5353476
Email: ancat@ihug.co.nz

IN THIS ISSUE ...

COVER STORY ... 2

A POPULAR CHEMICAL GLOSSARY
By David Jones ... 2

OCTANES, AROMATICS AND COMBUSTIBLE CARS
By C L H Stonyer ... 3

INDUSTRY APPLICATION:

Determination of Lead in Unleaded Gasoline on the Liberty Series II ICP-AES with the Axially-Viewed Plasma
By Andrew Ryan ... 9

NEW PRODUCTS ... 13

ORGANOMETALLIC MOLECULAR CATALYSTS, SMALL MOLECULE MACHINES
By Cornelis (Cees) Lensink and Neil B Milestone ... 20

IUPAC-SPONSORED SYMPOSIA IN 1998 ... 25

PATENT PROZE
By Jane Calvert and Greg Lynch ... 26

INTERNATIONAL NEWS ... 27

CONFERENCES & SEMINARS ... 28

A MULTI-TECHNIQUE APPROACH TO SURFACE ANALYSIS. PART 2. SCANNING PROBE MICROSCOPY
By Dr Richard Haverkamp ... 30

NEW LITERATURE & MEDIA ... 33

NZIC NEWS:

MESSAGE FROM THE PRESIDENT ... 34

NZIC COUNCIL NEWS ... 35

NZIC BRANCH NEWS ... 36

NZIC TREASURER'S REPORT AND FINANCIAL STATEMENTS ... 39

ADVERTISERS INDEX ... 42

SOFTWARE REVIEW: CAMBRIDGESOFT CHEMOFFICE PRO ULTRA 4.0 ... 43

COMING UP ...

January 1998 - Environmental Control, Waste Management, Water Analysis
GC, GC-MS

March 1998 - Food and Beverage Manufacturing and Research
HPLC, IC, LC-MS

Deadline for material:
5th of the month of publication

Contributions and enquiries to:
The Editor,
Chemistry In New Zealand,
P O Box 38-546, Howick, Auckland, New Zealand
Phone: +64-9-5353475, Fax: +64-9-5353476
Email: ancat@ihug.co.nz

COVER STORY

SIGMA ALDRICH brings

Riedel-de Haën

Laboratory Chemicals to you

As manufacturers of reagents for research and development as well as for quality assurance and environmental checks, Riedel-de Haën continues to produce chemicals of uniformly high quality and develop new reagents for modern applications. The range of laboratory chemicals includes:

CHROMASOLV: Solvents for chromatography

SPECTRANAL: Solvents for IR and NMR

PESTANAL: Solvents for residual analysis

OEKANAL: Solvents for trace analysis

HYDRANAL: Solvents for Karl Fischer titration

AQUANAL: Water analysis

Many of the chemicals can be manufactured in large quantities and for this reason we also offer these products in large quantities. Please let us know if you require larger quantities of chemicals of special purity.

In addition, Riedel-de Haën has developed the "ELISA-Systems" range. These enzyme immuno-assay kits offer rapid tests for the analysis of foods, animal foodstuffs, and water.

To learn more about the Riedel-de Haën range of products or for a FREE copy of the Riedel-de Haën Catalogue on Disk, contact:

SIGMA ALDRICH PTY LTD
P O Box 12423 Penrose
Auckland, New Zealand
Free Phone: 0800 936666, Fax: 0800 937777
circle number 1 on the reader reply card

A POPULAR CHEMICAL GLOSSARY

David Jones

Additive: a chemical maliciously added to an otherwise natural product. See **Pure**.

Animal: creature with rights. See **Pest**.

Atom: highly explosive and radioactive constituent of bombs, power stations, and nuclear waste. See **Nuclear-free zone**.

Cancer: terminal disease brought on by chemicals. Since 20 percent of us will die of it, this proves how deadly they are.

Chemical: synthetic substance which is bad for you or the environment (*qv*).

Chemical Industry: a large and wicked enterprise dedicated to the production and dispersal of pollutants (*qv*).

Chemist: (a) a friendly figure in a white coat who dispenses drugs. (b) a sinister figure in a white coat who synthesises chemicals.

Drug: (a) a chemical with redeeming features. (b) a chemical with no redeeming features.

Ecology: a discipline for classifying activities, substances, objects and technical operations into their due degrees of goodness or wickedness. See **Green**.

Environment: recently discovered territory in urgent need of protection from pollutants.

Gas: a chemical in vapour form. Requires the adjectives 'poisonous' or 'deadly'.

Green: (of a product) containing fewer chemicals than it might; (general) conducive to feelings of ecological virtue or self-satisfaction.

Health and Safety: bureaucratic form of exorcism for warding off chemicals. See **Permitted level**.

Homeopathic remedy: medicine containing just sufficient chemicals.

Insecticide: chemical deadly to vertebrates and higher forms of life.

Natural: extracted from the environment without the use of chemicals. See **Synthetic**.

Nuclear-free zone: municipal region containing no atoms.

Part per million, part per billion etc: (of chemicals) dangerously excessive concentration.

Permitted level: (of chemicals) dangerously excessive concentration resulting from inadequate application of health and safety regulations.

Pest: creature without rights.

Plastic: subtle chemical which pollutes the environment simply by cluttering it up.

Pollutant: any chemical loose in the environment. See **Chemical Industry**.

Pure: containing no chemicals.

Radiation: form of invisible evil which goes through everything. Requires the adjectives 'dangerous' and 'hazardous'. Given off by atoms (*qv*), and some other technological products.

Radon: form of radiation resulting from atoms getting into houses.

Synthetic: a nasty substitution for something natural.

Vitamin: benevolent non-chemical substance found in natural foodstuffs. Destroyed by boiling.

Waste: mixture of pollutants. Requires the adjective 'toxic'. In a perfectly green world, no activity would produce any waste.

Zinc, selenium, copper gluconate, β-carotene, chromium etc: (a) benevolent ingredients of natural foodstuffs and diet supplements, conducive to health. (b) poisonous synthetic chemicals.

Octanes, Aromatics and Combustible Cars

C L H Stonyer
10 Manly Garden, Paraparaumu

Crisis

In early 1996 two events occurred in New Zealand - there was a fuel leak in the VW engine of a home-made plane, and the change of 96 octane petrol from leaded to lead-free started. With the help of very little information from the oil companies, a lot of poorly investigated reports of trouble in the performance of car engines, and news about "inexplicable" car fires, our electronic media developed a "fuel crisis". Many facts were ignored in the nightly circus we saw on TV, but it soon turned into a classic of Good Guys versus the Bad Guys. The latter were, of course, the oil companies and the Government. Facts such as the Fire Service report that New Zealand usually has 200 or so car fires a month were mentioned and quickly ignored; absurd statements were made that rubber components for use with fuel were guaranteed to be suitable up to an aromatic content of 50%, and were therefore going to fail if the aromatics content were 51%, and would last much longer if they were cut to 49%.

Our Cars and Their Maintenance

With the New Zealand tradition of "do it yourself" it is not surprising that worn parts are often replaced by car owners, especially in the case of older cars, which still make up a high proportion of our fleet. As an example, the author once stopped a car that was dripping flames from under its engine, and encouraged the driver to get out and retreat to a safe distance, rapidly. When he did, the flames died, because he had switched the engine off. It didn't take long to find the culprit: a piece of common plastic tube sold for household use had been used as a fuel pipe. Swelling and leaking, it had dripped petrol on to the exhaust pipe.

A petrol pump attendant's tale is also illustrative: the attention of a young male driver was drawn to a petrol leak coming from somewhere in the engine. The reply was "She'll be right mate - it's only a small leak!"

The quality of imported parts, not those supplied by the retailers who stock the manufacturers' parts, but those that can be bought from a number of retailers who have no connection with car manufacturers, is the subject of the story from a colleague. He had a pre-holiday service done by his usual reliable garage, and was persuaded to have a new fuel hose fitted. Luckily, his car stood in his own garage overnight, because the leaked petrol smell helped him to discover that the brand new hose had failed. Subsequent investigations showed that the entire shipment of hoses was faulty. The aftermarket, as it is called, supplying parts long after the car agents have ceased to do, turned out to be a major source of trouble.

Octane Numbers

Why did we have lead in our fuels? What changed in the fuel when it became lead-free? These questions cannot be answered without reference to octane numbers. What is an octane number? The answer is simple: it is one of a number of parameters used to specify the quality of automotive fuels. Others include: the vapour pressure at various temperatures; the range of boiling points obtained when fuel is distilled in a specified way; the density; the amount and nature of the non-volatiles; the content of lead; the oxidation stability; the hydrocarbons present; the upper and lower flammable limits; and a number of others. Different countries have different requirements, depending on such things as climate, the nature of their vehicle fleet, their Government regulations, distance from a refinery, method of distribution, and of course, cost. To reduce their dependence on imports, some require the addition of locally made alcohol.

Of these parameters, octane number has come to be associated in most motorists' minds with fuel quality - all the other requirements being trusted to the oil companies, and to their observance of Government regulations. (We have more regulations about petrol quality than almost any other country in the world.)

The basic definition of octane number is that it is the percentage of iso-octane by volume in a mixture containing iso-octane and normal heptane that matches the "anti-knock" performance of a given fuel. Simple!

Knocking, a sound like hammering on each complete cycle of a four-stroke engine, was noticed in the very early days of motoring, and since it was clearly not good for an engine, various ways were sought to stop it. On a given fuel, means of doing this included altering the timing (the point in the compression stroke when the spark is initiated): reducing the compression ratio; altering the air-fuel ratio; and simply easing off the throttle (or accelerator in today's language). All these methods are still available to engine manufacturers now, and some of them are done automatically, especially in cars with electronic sensors and rapidly responsive controls.

As more fuels became available, it was found that some were better than others at resisting knocking, and means of testing and quantifying this property were sought. In 1927 fuel suppliers agreed on the design of a test engine. This engine, still in use almost unaltered, is a single-cylinder engine, with a variable compression ratio, spark advance setting, air-fuel ratio, and several other factors. Knocking is measured by an electronic sensor, the result being shown on a dial. CFR engines, as they are called, are located in Auckland, Wellington and New Plymouth, and could possibly be seen if the owning oil company agreed.

A CFR engine is operated in several modes including MOTOR, RESEARCH, LEAN and RICH AVIATION. The figures on petrol pumps are RESEARCH results. To make a measurement of a fuel expected to have an octane rating of say 85, it is tested against 84% iso-octane/16% n-heptane and 86% iso-octane/14% n-heptane, and should give a result between these two blends. Random variables mean that expressing an octane number to the nearest 0.5 is about as good as can be claimed. The writer was at one time a participant in world-wide tests involving all the CFR engines that his employer owned. We all received a seated l-gallon tin of a fuel, and had to test it before a specified date. The variations in octane numbers were startling - some were so far out that they were omitted from the average calculation. We did not look forward with pleasure to the arrival of the next sample! The moral is - don't take too seriously the figures on the petrol pumps!

It is possible to use a real car as a test engine, but as you might guess this is not easy - all sorts of tanks, valves, measuring devices, revolution counters and so on must be fitted, roads must be chosen and drivers trained. It has been done in New Zealand, but to what end I am unsure.

Causes of Knocking

Knocking occurs near the end of the compression stroke of a four-stroke engine, after the spark has been fired. With a good fuel, the flame front spreads evenly through the fuel-air mixture, exerting an even pressure during the downward (power) stroke of the engine. With a poor fuel, the residue of unburnt gases always present in the cylinder can undergo a series of pre-flame reactions, and when the flame front arrives, a violent reaction occurs, which is audible in bad cases. Really bad knocking can destroy an engine.

Some History

The first car was brought into New Zealand in 1898, and, needless to say, a law about motoring was passed - the McLean Motor Car Act. By 1908 we were importing a million gallons of petrol a year, in 4-gallon (18.2 litre) tins. There were more regulations! Price was 36 pence/gallon, about 6.6 cents/litre. Adjusted for inflation, this is $20-$25 per litre today! The octane number was probably not much above 60. During the period 1923-1925, mechanically-operated petrol pumps were installed, the first bulk imports arrived, "pinking" was featured in advertising, and because our octane rating was only 63, imported cars had to have lowered compression ratios, as well as manual spark advance/retard controls.

It was 10 years later, in 1934, that "super" petrol was introduced; 78 octane. At the outbreak of war in 1939, this grade vanished, and there was 70 octane only. Rationing of sales lasted until 1950, but there had been a slight improvement to 72 octane. 1954 saw 79 octane, and by 1960 we had 83 "standard" and 95 "premium". Following the opening of the Marsden Point refinery in 1964, the lead level of both was set at 0.84 g/litre. Twenty years later, 83 became 91 at the same lead level. Refinery upgrading, finished in 1985, enabled the lead content of all petrol to be reduced to 0.45 g/litre, and two years afterwards the 91 fuel became lead-free, because many imported cars were specifying it. Finally, in 1996, Government required 96 octane to become lead-free.

Why High Octane?

To get more power from engines of reasonable size, manufacturers had been steadily raising the compression ratios of cars. Larger vehicles with bigger engines had higher values. The octane-number needs were set by the makers, and by the fuels available in their largest markets. Hence if we wanted to run these cars, we needed the same fuels. Table 1 shows the relationship between compression ratio and the octane number required to avoid knocking. (The numbers are only indicative of the period they were measured, not of our current vehicles.) Many factors affect the correlation between the "road" octane number and the "Research" value. Many years ago, in training oil company sales staff, we claimed that a car could run normally at 50 km/hr on a flat road on zero-octane fuel, and that high-octane was needed only when driving the car hard, at maximum acceleration, up a hill, in top gear. The gap between a modern car's maximum and minimum octane-number needs is probably lower because of the sophisticated controls that work without our interference or knowledge, as well as better design features.

Table 1. *Octane number requirements of automobile engines. Octane number requirements of automobile engines increase as compression ratio increases.*

Engine compression ratio	Typical research octane number required for knock-free operation
4:1	60
5:1	73
6:1	81
7:1	87
8:1	91
9:1	95
10:1	98
11:1	100
12:1	102

Source: B F Greek, 'Gasoline', Chemical and Engineering News, 9 November 1970, p52.

The two basically incompatible requirements, fuel economy and maximum power from a given engine have been met to many people's satisfaction today. Which is the more important? My personal view is that if we could buy 80 octane for half the cost of 91 or 96, manufacturers would soon make cars that a lot of people would buy.

The Use of Lead

A research programme started in 1921 to discover how best the anti-knock properties of fuels might be improved. Midgley, of the Kettering Research Organisation, discovered that organic lead compounds, like tetra-ethyl and tetra-methyl lead, were extremely effective, and were much cheaper than other methods such as using more aromatics in the fuel. The additive used in petrol almost ever since also contains chlorinated and brominated compounds to prevent lead compounds from depositing on the cylinders and in exhausts of engines. These "scavengers", as they are called, can contribute dioxins to the atmosphere. Lead is a well known poison, and it is extraordinary that, 75 years after its initial use, it was still being used in New Zealand petrol. There were many reasons for this apparent lack of concern:

- New Zealand is a long, narrow, windswept country, and exhaust fumes are usually dispersed very quickly.

- The cheapest way of raising octane number is by adding lead.

- Our refinery, built and owned largely by the oil companies, was originally a simple one, and could produce high-octane fuels only if they were present in the crude oil feedstock. Refinery upgrading may have been delayed because of the difficulty of raising the refiner's margin to give an adequate return on the capital. (Refiner's margin is the difference between the cost of crude and the price of the finished product and is carefully watched by Government to ensure that the public is not being overcharged.)
- There was possibly some reluctance on the part of Government to allow the price of petrol to rise to cover the cost of eliminating lead, because the only way of avoiding a price rise was to forego some of the large tax that is applied to petrol.
- Last but not least, the "Green" lobby, and the public perception of the dangers of lead were not strong enough to combat the factors leading to a resistance to change. It is also interesting to note that when our "Regular" i.e. leaded 91, was replaced in 1987 by unleaded 91, sales of that grade dropped from 7% of total petrol sales to 4%. It took extensive advertising and tax rises of 6.6 and then 8 cents per gram of lead in "premium" 96 to raise this figure to nearly 50%, which was not achieved until 1995.

Alternatives to Adding Lead to Hydrocarbons

Among the possibilities are the use of:

CNG/LPG
Methanol/ethanol
Other oxygenates
Hydrogen
Fuel cells
Ammonia
Water

CNG/LPG

CNG is 70-90% methane, 10-20% ethane, and some propane. Methane has octane numbers (Motor-Research) of 120-120, and propane 97-112, so CNG is an excellent fuel. It needs a heavy, pressurised fuel tank, and a converted motor can give only about 85% of its normal maximum power. The cost of conversion, more frequent refuelling stops, and the unavailability of it in the South Island, have steadily reduced the number of users. Under pressure, LPG is liquid at average temperatures, but the vehicle consumes 20% more fuel, unless the compression ratio is raised to say 12:1, not practicable for the ordinary motorist. LPG is mostly propane, with iso-butane and n-butane. With a much higher price for crude oil, and with engines built specifically for them, these fuels may yet be used.

Methanol/ethanol

Methanol has octane numbers 92-106 (Motor-Research), and ethanol, 89-107, putting them into the area of interest. Their other physical properties make them suitable on their own as motor fuels, although the addition of a small amount of light hydrocarbons is desirable to overcome cold-starting problems. Their high cost relative to other fuels is at present a handicap.

With the octane numbers above, it may appear that the use of alcohols as additives, replacing lead, is the answer to the octane-number problem, and in several countries around the world it is done, but not entirely for this reason. In places where hydrocarbon fuels are all imported, addition of alcohol is sometimes mandatory because it is made locally. In New Zealand we produce large amounts of methanol from natural gas [1], most of which is sold, with some being used to make synthetic petrol. In a different political climate, we might have saved the money spent (it's very wasteful in terms of energy in the natural gas compared to that in the petrol) and used the gas in cars. Or we could have used the methanol with, or instead of, petrol.

There are problems with adding alcohols to petrol. A few years ago an extensive trial was done in buses in Auckland with methanol and ethanol at 10% and 15% in petrol. Engine performance was good, but the fact that not much water can be added to alcohol-petrol mixtures before phase separation occurs (with the alcohol going into the aqueous phase) was a real problem. Our petrol distribution system, from the bulk storage tanks to the service stations' underground tanks, is "wet" meaning that water is used for cleaning, and is tolerated in small amounts throughout the system. Other objections were raised, like corrosion of some metals, and unsuitability of some rubber parts, but all these adverse factors can be overcome, as the Brazilians have demonstrated. Higher alcohols, e.g. propanol and butanol will give good octane-number improvement, but have other problems, not the least of which is cost.

Oxygenates

Many compounds containing oxygen have been proposed both as additives or as complete fuels, but most have been rejected. One of the survivors is methyl tertiary butyl ether. As a fuel on its own it has possibilities, but cost is against it. As an additive it is effective, but must compete with the aromatic hydrocarbons that oil refineries make so easily. Propylene oxide (1,2 epoxy propane) has similar properties to high-octane petrols, and has been used in racing cars. Because it needs less air, the volumetric efficiency of the engine is increased. Nitromethane does the same, and also gives dramatic cooling of the inlet fuel. It is often used with methanol.

Increasing the oxygen content of the incoming air, either by membrane filtration or by the use of nitrous oxide (N_2O) is hardly practical for the average motorist, and this method is confined to racing cars.

Hydrogen

Hydrogen may look like the perfect fuel, with only water to worry about in the exhaust pipe. However, when burnt in air, the high combustion temperature gives NO_X emissions as well (due to oxidation of N_2). It was first suggested nearly 100 years ago, when hydrogen-filled airships were sailing the skies, and the vented hydrogen seemed to be such a waste. History books show why helium replaced hydrogen after the explosion of the R101 in 1930. In automotive use, the high flame speed means that flashback can occur through minute valve openings. Water mist and other remedies have been used to stop this, but the use of hydrogen as a fuel in our cars is not imminent.

Books have been written on how to make hydrogen. For example see Professor J Bockris's 1975 book *"Energy - The Solar Hydrogen Alternative"* in which this Melbourne man gave not only a possible production method, but also showed how it could be widely used.

Fuel Cells

Eliminating the internal combustion engine, and oxidising fuel in a fuel cell to make electricity, is an idea whose time may come, even if it destroys the car engine industry. The best fuel is probably hydrogen, but blowing air into methanol, using a platinum catalyst, is an interesting classroom activity. Efficiency is very good - 50% of the calorific value of the fuel can be obtained as electricity. But the useful life of current fuel cells is well below the life of the modern car engine, and the initial cost is very discouraging.

Ammonia

Anhydrous ammonia can be used as a fuel in internal-combustion engines to give about 70% of the power output of iso-octane. Of course, there is no CO_2 to worry about and interestingly, NO_x emissions are less than those from conventional fuels using air. Production and handling are obvious problems [6].

Water

Water can be injected into the cylinder to cool it, and during World War II this was done in fighter aircraft, enabling more fuel to be used, but only in a dire emergency - the engine had to be stripped down afterwards. A Mr Gunnerman has claimed that a mixture of LPG, water and an emulsifier, with a catalyst in the cylinder, will give great fuel economy, with no undesirable exhaust emissions. He claims that the catalyst dissociates the water into H_2 and O_2, but since recombination will give back only the same amount of energy used to dissociate them, other factors must be involved. The Caterpillar Tractor company have become interested, and are said to be doing extensive testing.

Aromatics

With the need for higher-octane-number fuels over the years, and with the lower lead contents permitted, refiners tried to raise the content of the cyclic and branched-chain hydrocarbons. However, with cost limits on how far this could go, even with the best of crudes, they turned to aromatics as the cheapest solution. Aromatics are all toxic, benzene being especially bad. It is alleged that air containing 0.015 g of benzene per cubic metre, if breathed all the time in normal working hours, will at some time cause bone marrow loss and leukaemia. Data on benzene exposure is not easy to get, and, as readers of this publication will have read [2, 3], calculation of such risks is subject to wide uncertainties. Since 1988 when Government imposed detailed petrol specifications on the industry, the benzene content of petrol has been 5% by mass maximum (approximately 4.2% by volume). Benzene content of the exhaust gases is affected by the amount in the fuel, but also by the content of the other aromatics, since some benzene is produced from these other aromatics during combustion. An increase in discharged benzene was anticipated, and the Ministry of Commerce produced an extensive report on this [4]. After the so-called crisis, regulations were introduced limiting the total aromatic content to a maximum of 48% by volume. The oil companies also introduced a voluntary limit of a maximum of 40% of toluene plus xylene.

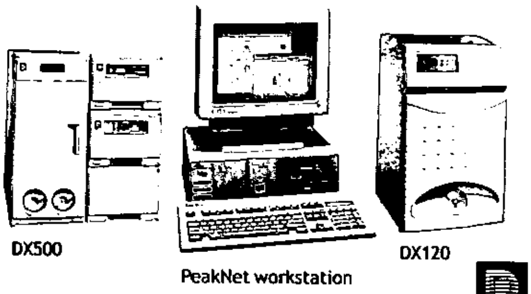
Data on the introduction of lead-free high-octane petrol in other countries, and the general freedom from problems, can be found in the 32-page report issued by the Ministry of Commerce [5].

Besides their toxicity, the other major property of aromatics that can cause trouble is their effect on elastomers, especially some types of rubber. From the tyres, to the brake systems, to the fuel hoses, to the numerous O-rings, seals and gaskets, rubber is essential to motor vehicles. Initially the fires and other troubles were attributed to the new unleaded fuel, but subsequent investigations showed that old and poor quality parts were to blame in the vast majority of cases. (One imported shipment of petrol containing an unusual and excessive aromatic content could have legitimately been blamed for some troubles in the area in which it was distributed, but by the time it became known the "crisis" was over.)

An ironic confirmation of the poor quality of imported parts was the fitting of defective rubber parts in many of the oil companies' own pumps!

Valve Seat Lubrication

Many cars made before 1981 did not have hardened inlet valve seats, and depended on the lubrication properties of the tetra-ethyl lead mixture for their continuing functioning. When lead was eliminated from 91 octane in 1987 few problems arose, because the new cars whose makers recommended 91 had hardened valve seats, and did not need special lubrication. However when lead-free 96 was about to be launched, it was realised that many

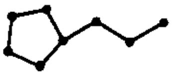
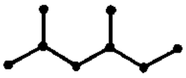
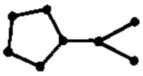
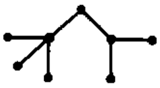
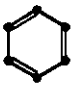
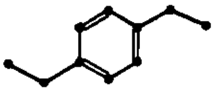
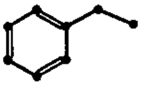
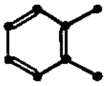
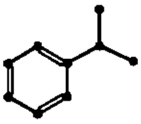
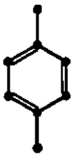
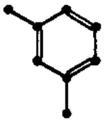
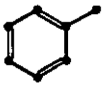


older cars that used the leaded "Super" fuel (possibly in the mistaken belief that "Super" meant "Superior power") might need an added lubricant. (Overseas, some fuel suppliers, when they dropped lead, put a valve-seat lubricant in their product for up to two years afterwards.) The oil companies therefore set up an easily handled supply of lubricant, and recommended that owners of the critical cars should add it to each fill of petrol. Because of the age of most of the cars at risk, it has also been suggested that they would benefit from an engine overhaul, during which hardened valve-seat inserts could be fitted!

Catalytic Converters

In countries where air pollution from car exhausts has been a major problem, even although lead has been eliminated, attempts are being made to stop unburnt fuels, carbon monoxide, and NO_x gases from being discharged, with devices containing expensive metals that act as catalysts, fitted in the exhaust line. Lead will poison these catalysts, and hence leaded fuels must not be used in cars fitted with them. If the Government one day decides that use of catalytic converters is necessary in New Zealand, we are ready!

Table 2. *Structures and research octane numbers of some hydrocarbons.*

Hydrocarbon	Structure	Unleaded research octane number (RON)
n-Octane		-19.0
n-Heptane		0.0
n-Hexane		24.8
n-Propylcyclopentane		31.2
Octene-2, cis-isomer		56.2
n-Pentane		61.7
Isopropylcyclohexane		62.8
2,4-Dimethylhexane		65.2
Octane-4, trans-isomer		73.3
Isopropylcyclopentane		81.1
Cyclohexane		83.0
Pentene-1		90.9
Hexene-2, trans-isomer		92.7
n-Butane		93.8
Propane		97.1
Butene-1		97.4
2,2,4-Trimethylpentane (iso-octane)		100.0
Cyclopentane		101.3
Propylene		102.5
2,4,4-Trimethylpentene-1		102.5
Benzene, technical grade		105.8
1,4-Diethylbenzene		106.0
Ethylbenzene		107.4
o-Xylene		107.4
Isopropylbenzene (cumene)		113.1
p-Xylene		116.4
m-Xylene		117.5
Toluene, technical grade Toluene, chemically pure		117.8 120.1

Source: B F Greek, Gasoline, Chemical and Engineering News, 9 November 1970, p52.

Lessons

Many people should have learnt something from the happenings of early March 1996. TVNZ should have learnt not to generate a "crisis" without better checking their sources of information - although given the ratings-driven nature of our commercial TV, this may be unlikely. Their allegations that there were large increases in the number of fuel-related problems were shown to be untrue [5]. The possibility of increased cancer risks from greater exhaust discharges of benzene has also been discounted [4].

The oil companies might have realised that the make-up of our car fleet, with about 55% of our vehicles being made before 1987, could cause problems, even if overseas experience in dropping lead was usually trouble-free. Retailers of after-market parts may have learnt to be more careful about the quality of the parts they buy. Government may now realise that, despite a mass of regulations about petrol quality, deeper questioning of oil companies is needed before any changes are made.

Acknowledgement

The author received a lot of help from the oil companies, particularly Christopher Reid (Mobil), Barry Blackett (BP), and Shell's Graham Wilson. Also very helpful were Bryce Williamson, University of Canterbury (an editor of *CHEM NZ*), and Alan A Turner (an ex Shell chemist, now General Secretary of our Institute).

Table 2 on octane numbers originally appeared in *Chemical and Engineering News,* November 1970. Reference 5 contains information from many sources, and is recommended to anyone who wants more detail. It is available from the Ministry of Commerce.

References

1. Parker, L; Bibby, D and Milestone, N (1995) The Synthetic Fuels Plant. *CHEM NZ*, **60**:20-24.

2. Mann, J D (1993). Units in Measuring Risk. *CHEM NZ*, **53**:1-2.

3. Roberts, L (1994) Why Study Risks? *CHEM NZ*, **57**:3-6.

4. Biggar, Keven, (1995) A Preliminary Appraisal of the Risk from Benzene with a High Octane Unleaded Petrol. *Chemistry in New Zealand*, **59**, 5:11.

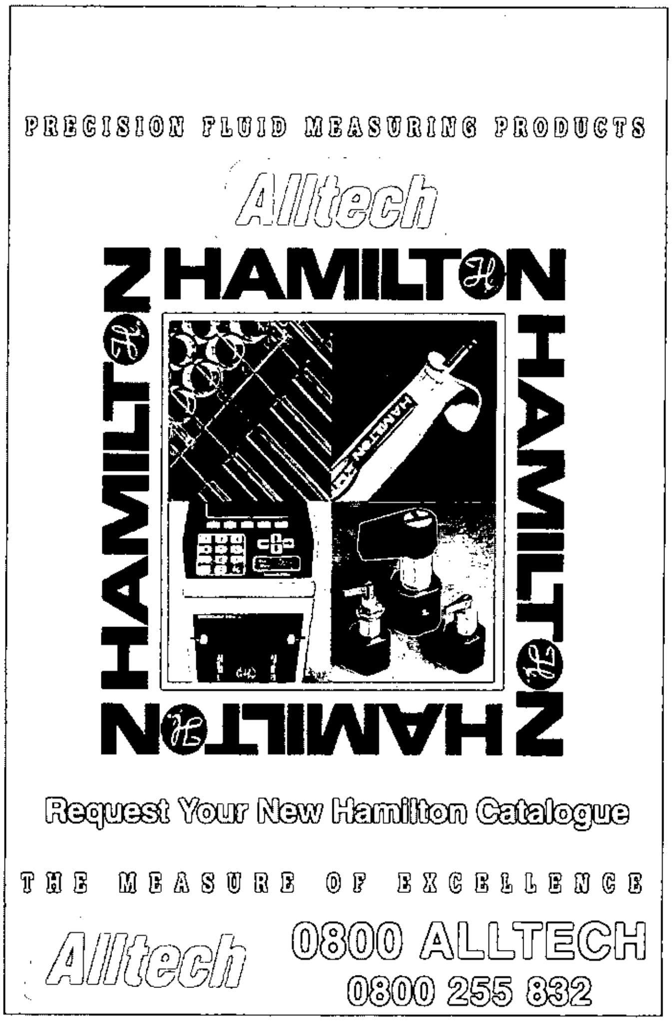
5. Premium Unleaded Petrol: Detailed Report on Investigations Into Fuel System Failures. July 1996: ISBN 0-478-00346-3: Ministry of Commerce, Wellington.

6. Goodger, E M (1980) Alternative Fuels. MacMillan Press (London).

ABOUT THE AUTHOR

Lester Stonyer has 50-plus years of industrial chemistry experience including 15 years in Mobil Oil.

The above article was reprinted with permission from *CHEM NZ* Number **68**, (August 1997).



Industry Application

Determination of Lead in Unleaded Gasoline on the Liberty Series II ICP-AES with the Axially-Viewed Plasma

Andrew Ryan, Varian Australia Pty Ltd, Mulgrave, Victoria, Australia 3170

Introduction

In the past twenty-five years, the determination of lead in unleaded gasoline has become important as various studies have shown that most of the lead released into the environment is from the combustion of gasoline. In 1986, the United States Environment Protection Agency (USEPA) reported that 90% of the total lead released into the environment in the United States was the result of lead emission from gasoline combustion[1].

Due to the widely held belief that ICP-AES with axial-viewing exacerbates problems with molecular band emissions and carbon build-up when analysing organic liquids, it is not often considered for the analysis of organic liquids[2], particularly highly volatile organic liquids such as gasoline. Recent advances in ICP-AES technology have overcome these problems, so that the axially-viewed ICP can be used with confidence for the analysis of organic liquids.

This work describes the determination of lead in unleaded gasoline by ICP-AES with axially-viewed plasma, oxygen accessory and volatile organics kit, to overcome the effects of the gasoline matrix.

The extremely high vapour pressure of gasoline overloads the plasma which destabilises, or may even extinguish, the plasma. Plasma flicker adversely affects the stability of the signal. A cooled spray chamber reduces the solvent load into the plasma and results in a much more stable signal. The Auxiliary Gas Module 1 (AGM-1) oxygen accessory adds a small flow of oxygen to the argon auxiliary gas to reduce molecular band emissions and carbon build-up in the torch injector tube and on the Cooled Cone Interface of the Liberty axially-viewed Series II spectrometer.

This work also shows that in the analysis of gasoline, lower detection limits are attainable for lead using the axially-viewed plasma compared to the radially-viewed plasma[3]. The accuracy of the method has been assessed by the use of National Institute of Standards and Technology (NIST) Standard Reference Material (SRM) 2712 Pb in Reference Fuel, which contains tetraethyl lead.

Experimental

Instrumental

A Varian Liberty Series II ICP-AES with the axially-viewed plasma, AGM-1 oxygen accessory and cooled glass spray chamber were used.

The Liberty Series II ICP features a 40 MHz, free running RF generator, a 0.75 m Czerny-Turner monochromator with a 1800 grooves/mm holographic grating used in up to four orders. The resolution of the optical system ranges from 0.018 nm in 1st order to 0.006 nm in 4th order.

The instrument was controlled with a Digital Equipment Corporation (DEC) Celebris computer with an Intel Pentium processor and Varian's Plasma 96 software running under the Microsoft Windows 95 operating system.

The instrument operating conditions are listed in Table 1.

Table 1. Instrument operating conditions.

Power	1.5 kW
Plasma gas flow	16.5 L/min
Auxiliary gas flow	1.5 L/min
Spray chamber type	Cooled glass spray chamber
Spray chamber temperature	-10 °C
Torch	Demountable torch with an 0.8 mm ID injection tube
Nebuliser	Standard glass concentric nebuliser
Nebuliser pressure	90 kPa
AGM-1 setting	210 mL/min
Pump tube	Inlet - Viton, orange-orange 0.89 mm ID Outlet - Viton, grey-grey 1.30 mm ID
Pump speed	10 rpm
Sample uptake rate	0.5 mL/min
Integration time	5 seconds
Fast pump	Off
Grating order	Pb 261.418 nm - 2nd order Pb 283.306 nm - 2nd order
Background correction	Offpeak Pb 261.418 nm - left 0.010 nm right 0.010 nm Pb 283.306 nm - left 0.010 nm, right 0.010 nm
PMT voltage	650 V

Reagents

Analytical reagent grade organic solvents and chemicals were used:

- Iso-octane, (Unichrom, Ajax Chemicals)

- Toluene, (BDH)
- Dekalin (decahydronaphthalene), (Unilab, Ajax Chemicals)
- Aliquot 336 (tricaprylmethylammonium chloride), (Aldrich Chemicals)
- Iodine, (Univar, Ajax Chemicals)
- 10% v/v Aliquot 336/dekalin solution: dissolve 5 mL (or 4.4 g) of Aliquot 336 into 50 mL
- 3% w/v iodine solution: dissolve 1.5 g of iodine crystals in toluene and dilute to 50 mL.

Premium unleaded gasoline was obtained from a service station.

Dekalin was used as the rinse solution.

Standard preparation

A 10 mg/L Pb secondary standard was prepared by accurately weighing 2 g of a 500 mg/kg Conostan S21 standard in hydrocarbon oil and diluting to 100 mL in iso-octane.

Working standards were then prepared by pipetting 1.25 mL and 2.50 mL of the 10 mg/L Pb standard solution into 25 mL volumetric flasks[3]. Then 20.00 mL of the unleaded gasoline sample was added to each flask, followed immediately by the addition of 0.3 mL of 3% iodine solution.

This was mixed well and allowed to stand for 5 minutes. Then 0.5 mL of the 10% Aliquot 336/dekalin solution was added. It was made up to volume with dekalin and mixed well. The final solutions contained 0.5 mg/L and 1.0 mg/L Pb additions, respectively.

Sample preparation

20.00 mL of the unleaded gasoline sample was transferred to a 25 mL volumetric flask followed immediately by the addition of 0.3 mL of 3% iodine solution.

This was mixed well and allowed to stand for 5 minutes. Then 0.5 mL of the 10% Aliquot 336/dekalin solution was added and made up to volume with dekalin and mixed well.

For the NIST SRM 2712 Pb in Reference Fuel, 3.00 mL of the sample was transferred to a 25 mL volumetric flask. Then 20.00 mL of the unleaded gasoline was added, followed immediately by 0.3 mL of 3% iodine solution. This was mixed well and allowed to stand for 5 minutes. Then 0.5 mL of the 10% Aliquot 336/dekalin solution was added and made up to volume with dekalin and mixed well.

Iodine is added to form iodo lead alkyl anions which are then stabilised by the addition of a quaternary ammonium salt such as Aliquot 336. This treatment ensures that all alkyl lead compounds (tetramethyl lead and tetraethyl lead) in the sample and organometallic lead in the standard give an identical response.

Results and discussion

The standard additions calibration method was used for the determination of lead in unleaded gasoline.

The 261.418 nm and 283.306 nm lead lines were selected for the analysis based upon detection limits and freedom from spectral interference. The more intense 220.353 nm lead line was not used due to spectral interference from the matrix at this wavelength. Care must be taken when using the standard additions calibration method as the presence of spectral interferences, such as from the matrix, will still produce a linear calibration but the determined concentration will be higher than the true value. The mean results of four analyses are listed in Table 2.

Table 2. Results of the analysis.

Sample	Pb measured value at 261.418 nm (mg/L)	Pb measured value at 283.306 nm (mg/L)	Pb certified value (mg/L)
Unleaded gasoline	0.507 ± 0.004	0.525 ± 0.003	-
NIST SRM 2712	7.7 ± 0.2	7.8 ± 0.1	7.9 ± 0.3

The measured values of the standard reference material for the 261.418 nm and 283.306 nm lead lines compare well with the certified value. Similar results were also obtained for both lines for the unleaded gasoline sample confirming the accuracy of the method.

The measured values of the unleaded gasoline sample are well within the specified limits for the lead content in unleaded gasoline.

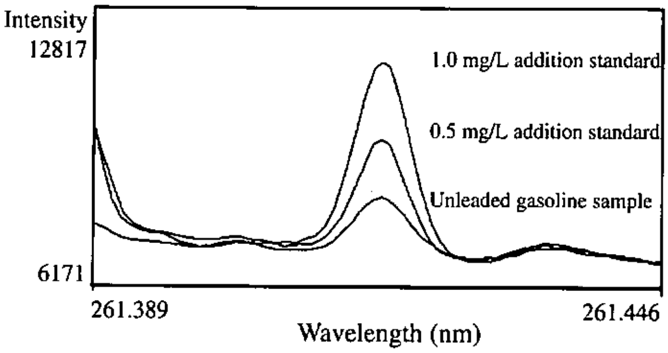


Figure 1. *Wavelength scans of addition standards 1 and 2 and the unleaded gasoline sample at the Pb 261.418 nm line.*

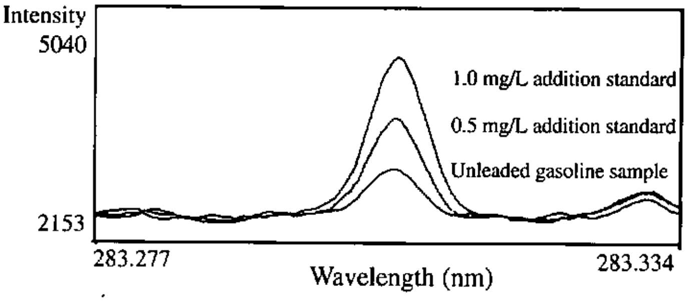


Figure 2. *Wavelength scans of addition standards 1 and 2 and the unleaded gasoline sample at the Pb 283.306 nm line.*

Long term stability

Long term stability was evaluated by performing a calibration and then analysing the unleaded gasoline sample that had been spiked with 1 mg/L of Pb, Cu, Ti, and Zn. The reproducibility of the measurements over one hour ranged from 0.9 to 1.1 %RSD. The long term stability plots are displayed in Figure 3.

Five replicates were measured at an integration time of three seconds for each line. The precision for each measurement ranged from 0.2 to 1.1 %RSD.

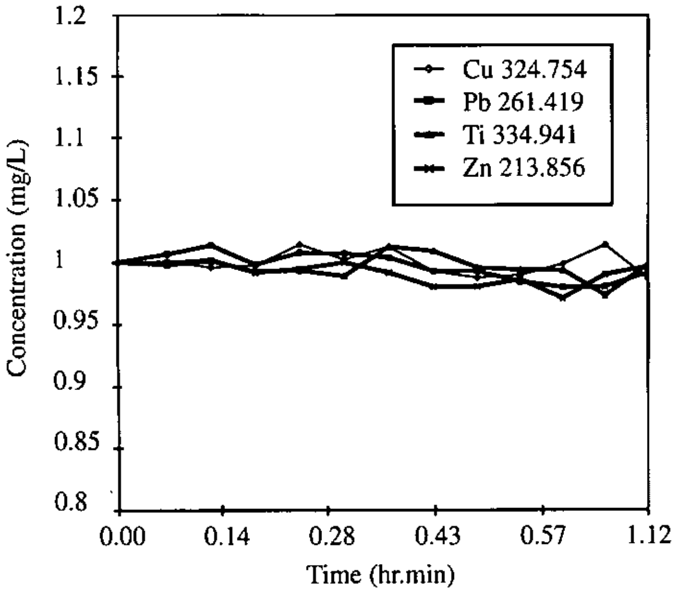


Figure 3. *Signal stability over one hour for 1 mg/L of Cu, Pb, Ti, and Zn spiked in unleaded gasoline.*

Detection limits in iso-octane

The detection limit (3 σ) of lead in iso-octane was determined for the 261.418 nm and 283.306 nm lines using an integration time of 5 seconds and 10 replicates. These are compared with those determined on the ICP-AES with the radially-viewed plasma[3] in Table 3.

Table 3. *Detection limits in iso-octane.*

Element	Wavelength nm	Axial ICP detection limit µg/L	Radial ICP detection limit µg/L
Pb	261.418	11	50
Pb	283.306	12	75

It has also been observed for the analysis of organic solvents on the axially-viewed ICP that using a higher plasma gas flow allows more oxygen to be injected into the plasma. With more oxygen present in the plasma, lower background and therefore improved signal-to-background ratios and detection limits are observed.

Summary

The determination of lead in unleaded gasoline on the Liberty Series II with axially-viewed plasma using the AGM-1 oxygen accessory and volatile organics kit has been described. An improvement in detection limits of a factor of about 5 to 6 compared with the radially-viewed plasma has been observed for the 261.418 nm and 283.306 nm lead lines.

The measured value of lead in NIST SRM 2712 is in good agreement with the certified value and long term stability and short term precision are excellent.

References

1. Air quality criteria for lead. (1986) USEPA, EPA-600/8-83/028, I-IV, US EPA, Triangle Park, North Carolina.

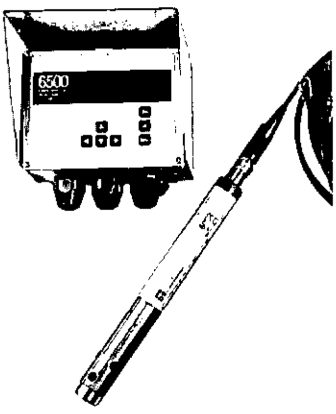
2. Demers, D R (1979) Evaluation of the Axially-viewed (End-on) Inductively-Coupled Argon Plasma Source for Atomic Emission Spectroscopy, *Applied Spectroscopy*, **33**:584-591.

3. Nham, T (1993) Determination of lead in unleaded gasoline by ICP-AES with the use of oxygen and a cooled spray chamber, Varian Australia Pty Ltd, Mulgrave, Victoria 3170, Australia, ICP-AES At Work No. 15, October.

For more information on Varian ICP products,
Contact: A.i. Scientific (NZ) Ltd
P O Box 35579, Browns Bay, Auckland
Phone: (09) 4787954, Fax: (09) 4781360
circle number 51 on the reader reply card

NEW PRODUCTS

ONE OF A KIND ENVIRONMENTAL MONITORING SYSTEM



The YSI 6500 Environmental Monitoring System is a multi-parameter water quality monitoring system designed for continuous, on-line monitoring of municipal and industrial effluent, drinking water intake sources and power utility discharge.

The YSI 6500 system consists of a YSI 6500 and a YSI 600R. The YSI 600R sonde simultaneously monitors any or all of the following parameters, dissolved oxygen, pH, temperature, and conductivity. The YSI 6500 converts the digital output from the YSI 600R to an output compatible with existing plant and process systems.

Contact: John Morris Scientific Ltd
P O Box 6348, Wellesley Street, Auckland
Free Phone: 0800 651700, Fax: (09) 3663060
Email: sales@jms.co.nz
circle number 21 on the reader reply card

PETROCHEMICAL APPLICATIONS FOR ION CHROMATOGRAPHY

The chemical/petrochemical industry is an important market for Dionex. The primary applications (over 80%) are for the analysis of inorganic ions.

Typical application examples include boiler, cooling, and/or wastewater analysis for corrosive anions and organic acids, scale-forming divalent cations, trace level transition metals (e.g. Fe^{3+}, Cu^{2+}, Zn^{2+}), polyphosphates, chelating and anti-scaling agents, and water treatment agents.

Other application areas include:

- anionic tracers, (e.g. SCN^-) and scale-forming cations, (e.g. Ca^{2+}, Ba^{2+}, Sr^{2+}) in oilfield water
- corrosive anions and organic acids in ethanolamine scrubber solutions
- ethanolamines in wastewater
- inorganic ions in chemical reagents, (e.g. trace sulfate in brine, trace calcium, and magnesium in brine)
- salts
- plastics and polymers
- combustion-IC of organic materials such as used motor oils, polymeric catalysts, and solvents, for elemental analysis (e.g. halogens, S, P, Se).

Contact: Mark Albertson, A.i. Scientific (NZ) Ltd
P O Box 35579, Browns Bay, Auckland
Phone: (09) 4784967, Fax: (09) 4781360
circle number 22 on the reader reply card

FIBRE ANALYSIS WITH FILTER BAG TECHNOLOGY

The ANKOM 220 Fibre Analyser provides accuracy and precision for ADF, NDF, lignin, crude fibre and more. When used in conjunction with Ankom's proprietary Filter Bag Technology, the ANKOM 220 Fibre Analyser allows each sample to be filtered and digested simultaneously during reflux. The system includes automatic heat and agitation cycles, digital timer and temperature gauges.

The use of the ANKOM 220 Fibre Analyser removes many of the variables that cause a loss of precision. Sample transfer is virtually eliminated. There is also no more reliance on operator experience relative to setting vacuum levels or forming the proper filter matter. The ANKOM 220 Fibre Analyser also frees the user from much of the mundane, time consuming and unsafe elements of chemical handling.

Contact: John Morris Scientific Ltd
P O Box 6348, Wellesley Street, Auckland
Free Phone: 0800 651700, Fax: (09) 3663060
Email: sales@jms.co.nz
circle number 23 on the reader reply card

ENVIRONMENTALLY-FRIENDLY BDH VOLASIL SOLVENTS

Volasil is a new generation of versatile, halogen-free, environmentally-friendly, and safe silicone-based solvents. Volasil 244, 344, and 245 are miscible with a wide range of organic solvents, are excellent degreasers, have high boiling points, relatively high flash points and low surface tension.

They are effective replacements for freon, carbon tetrachloride and trichloroethane without damaging the ozone layer.

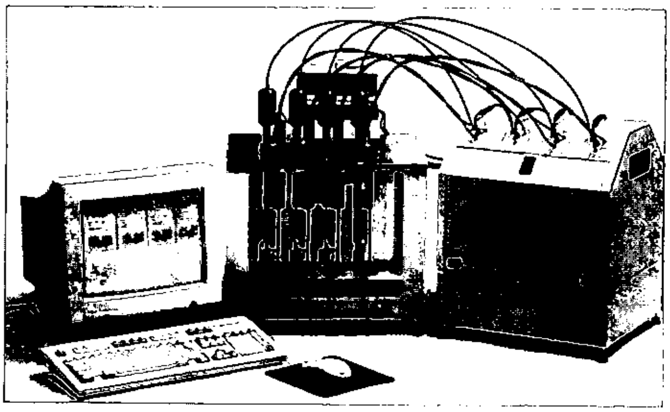
Volasil is available ex-stock in 500 mL and 2.5 litre pack sizes from Biolab Scientific Ltd.

Contact: Neil Bryant or your local branch
Biolab Scientific Ltd
Private Bag 36900, Northcote, Auckland
Free Phone: 0800 807809, Fax: (09) 4803430
Email: neilb@biolab.co.nz
circle number 24 on the reader reply card

NEW RHEOTEK AKV8000 AUTOMATED KINEMATIC VISCOMETER

PSL has recently released the Rheotek AKV 8000 Automated Kinematic Viscometer. It is a fully automated measurement system controlled by a PC capable of up to eight simultaneous kinematic viscosity determinations.

It complies with the standard methods of test ASTM D445 and D446, ISO 3104 and ISO 3105 and IP71 in full. The Rheotek greatly reduces operator time by automatically measuring the flow time of the sample; cleaning the viscometer tube *in situ*, ready for the next sample and calculating the kinematic viscosity. It also improves safety by having a completely self-contained solvent system.



AKV8000 4-head fully automated system with 4 measuring heads, filling stations, vacuum and control module, vacuum pump and solvent container. Also available in 2-head and 8-head models.

A.i. Scientific is currently interfacing their AIM 1250 Autosampler to the Rheotek to allow the automatic introduction of a large number of samples.

Contact: Kevin Moloney, A.i. Scientific (NZ) Ltd
P O Box 35579, Browns Bay, Auckland
Phone: (09) 4787954, Fax: (09) 4781360
circle number 25 on the reader reply card

ORION pH METERS

Orion offers a wide range of high quality benchtop ISE/pH and pH meters, as well as accessories to meet all your measurement needs. Choose from a variety of models, the Advanced, Basic or Speciality meter range.

Advanced ISE/pH and pH Meters
- Superior features for research grade analyses.
- Increased calibration and measurement capabilities.
- Dual- and multi-channel meters allow use of multiple electrodes on one meter.
- RS232 communication provides data transmission of results.
- The GLP doc function provides a hard copy of all calibration and measurement parameters.

Basic ISE/pH and pH Meters
- Fast and accurate measurements at a value price.
- All meter functions are easily identified by colour-coded keys allowing easy operation.
- Large LCD displays provide easy viewing of results and information, including simultaneous display of pH, concentration, mV, and temperature.

Speciality pH Meters
- Orion offers 3 speciality pH meters.
- Non-glass pHuture pH systems provide fast, reliable pH measurements for plant and field analysis or wherever glass electrodes are prohibited.

Contact: Watson Victor Ltd
P O Box 1180, Wellington
Phone: (04) 3857699, Fax: (04) 3844651
circle number 26 on the reader reply card

NEW 70V SERIES ANALYSERS FROM PHASE TECHNOLOGY

Phase Technology has released the new Series 70V laboratory analysers. This series of products includes liquid and air-cooled models. Some of the new features are:

1. Improved cooler capability. The instrument operates on tap water to achieve sample temperatures as low as -68 °C (-90 °F).

2. Fastest analyser available. Analytical time has been significantly improved.

3. Built in graphics display. The behaviour of the sample under test is monitored and displayed to help analysis of problem samples.

4. Run log. Test results are date and time stamped and stored in the computer memory of the analyser.

5. Full data capture of last run. Such information is helpful to support staff to diagnose problems.

Contact: A.i. Scientific (NZ) Ltd
P O Box 35579, Browns Bay, Auckland
Phone: (09) 4787954, Fax: (09) 4781360
circle number 27 on the reader reply card

NEW PRODUCTS

PREP-SEP FROM ALLTECH 96-WELL SOLID PHASE EXTRACTION AND FILTRATION SYSTEM

- Prepares 96 samples simultaneously
- Accelerates Sample Preparation
- Fits Automated Systems
- Eliminates Sample Prep Bottlenecks
- Does not require Volume Extensions

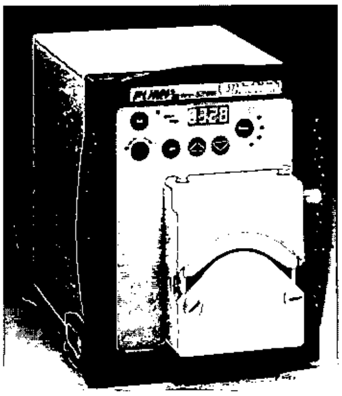
Alltech's Prep-Sep solid-phase extraction and filtration plates are the answer for pharmaceutical, toxicology, clinical, and drug discovery laboratories searching for faster sample preparation methods. Prep-Sep's patented system reproducibly processes up to 96 samples simultaneously, eliminating the sample preparation bottleneck in combinatorial chemistry, immunoassay, receptor binding assay, and other high sample throughput laboratories. Prep-Sep prepares samples quickly to keep up with the fast run times used in LC/MS/MS analyses.

Prep-Sep is at least five times faster than conventional SPE, based on Prep-Sep processing 96 samples simultaneously while the conventional way processes 24 samples simultaneously.

Request your copy of Bulletin #382 for Prep-Sep and Bulletin #324 for the Alltech Filtration Products Mini Catalog.

Contact: Alltech Chromatography Help Desk
Free Phone: 0800 ALLTECH (0800 255832)
Fax: (09) 4442399 or Email: alltech@alltech.co.nz
circle number 28 on the reader reply card

PUMP SYSTEMS - NEW FROM HEIDOLPH



The new range of pump systems from Heidolph includes Peristaltic, Gear, Immersion, Centrifugal and Built-In pumps. In the Peristaltic pump range there are six pumps available with electronic speed control, control accuracy of ± 2% and reversible direction of rotation. The tubing for the pumps is also available with diameters ranging from 0.8 mm id to 7.9 mm id so no matter what flow rate you require there is a pump and tubing to satisfy it.

With the Gear pumps there are three models of pump drives and three models of pump heads to choose from allowing you to design a system right for you. The pump systems have a back-up pressure of up to 7 bar, electronically-controlled speed, and soft starting feature.

There are three Immersion pumps available with depths ranging from 90 mm to 260 mm. Special immersion depths are also available on request. The pump body is made of a special steel or plastic and as there are no seals or valves, there is no wearing parts.

The Centrifugal pumps also have no shaft seals or valves so are also designed for long life. All parts of the six available Centrifugal pumps which come into contact with the medium are made of chemically-resistant materials.

Heidolph also supply pumps for built-in applications, tailored to your specific requirements.

Contact: John Morris Scientific Ltd
P O Box 6348, Wellesley Street, Auckland
Free Phone: 0800 651700, Fax: (09) 3663060
Email: sales@jms.co.nz
circle number 29 on the reader reply card

LANCER: PROFESSIONAL WASHING OF THE HIGHEST ORDER

Lancer has been doing its upmost for 20 years to solve all the problems of professional washing.

Background
From the small built-in washing machine to the tailor-made washing tunnel, Lancer provides a solution for all applications in laboratories, hospitals, or research and industrial sectors. With some 44 different models, of all sizes, Lancer's "standard" range is without doubt the largest, the most extensive and the most complete on the market.

Qualities
Lancer washing machines are designed to ensure a faultless professional service, in robustness and reliability, or ease of operation, washing quality, decontamination or drying.

Functions
The brain of the Lancer washing machine, is its microprocessor based electronic programming unit, an area in which Lancer is a pioneer. In this respect, the feature of the new "UP" unit are particularly noteworthy:

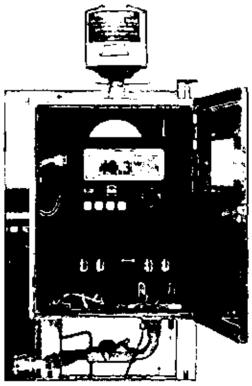
- it can memorise up to 40 programs,
- its numerical control keyboard provides access to all functions, with direct reading,
- each program can be given an individual name to ensure easy identification,
- each user can be designated by name according to the programs that he/she has defined, and according to the type of functions that he/she wants to be performed,
- the quantities of additives can be programmed separately for each function of each program whose different temperatures and durations will be adapted to the specific needs.

Baskets
The baskets supporting the objects being washed are the guarantee of a perfect result. It is essential that they be perfectly suited to the case they will have to deal with, therefore Lancer's

basket range is wide and comprehensive. In the event that a special basket has to be designed for a specific application, Lancer has all that is required for carrying out the design and production.

Contact: Watson Victor Ltd
P O Box 1180, Wellington
Phone: (04) 3857699, Fax: (04) 3844651
circle number 30 on the reader reply card

NEW ON-LINE VAPOUR PRESSURE ANALYSER



On the back of their successful MiniVap range of portable laboratory-based instruments for measuring vapour pressure Grabner Instruments have now released their MiniVap On-line for the automated on-line determination of vapour pressure and vapour-to-liquid ratio temperature of non-viscous liquids such as gasoline and gasoline blends. It is also possible to measure vapour pressure of LPG and NPG with a modified pressure tranducer.

The MiniVap On-line provides accurate determination of Dry Reid-equivalent vapour pressure according to ASTM D5191, absolute vapour pressure, and air saturated vapour pressure. Housed in an explosion-proof enclosure with Class I Type X purging system the MiniVap On-line is a stand-alone instrument and is connected directly to the sample stream via a sample conditioning unit to remove solid particles and entrained water. It can accommodate up to three separate sample streams, has a minimum response time of only five minutes for a vapour pressure measurement and offers fully automated instrument verification testing.

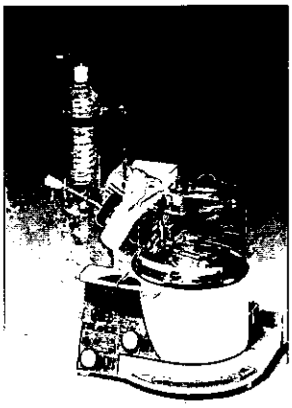
Contact: A.i. Scientific (NZ) Ltd
P O Box 35579, Browns Bay, Auckland
Phone: (09) 4787954, Fax: (09) 4781360
circle number 31 on the reader reply card

ROTARY STARS - THE NEW EVAPORATOR CONCEPT FROM HEIDOLPH

A range of four new Rotary Evaporators from Heidolph produces the complete system for all your laboratory distillation needs. The new Rotary Evaporator range offers a unique environmentally-friendly concept of vacuum control, faster distillation rates, high recovery rates of even low-boiling solvents, and best of all attractive prices.

Five sets of glassware, based on the vapour conveying system, are available to meet the most diverse requirements. All glassware sets are also available with a plastic coating (condensor and collecting flask).

Another new product from Heidolph, specially tailored to the requirements of the Rotary Evaporators, is the unique Rotacool. The Rotacool is a circulating condenser with high control accuracy of the pre-selected coolant temperature and short, directional links between the coolant connections of the circulating condenser and the Rotary Evaporator.



Contact: John Morris Scientific Ltd
P O Box 6348, Wellesley Street, Auckland
Free Phone: 0800 651700, Fax: (09) 3663060
Email: sales@jms.co.nz
circle number 32 on the reader reply card

ALLTECH OXY-TRAPS, SUPERIOR PROTECTION

Alltech OXY-TRAPS with OXY-MAX adsorbent work to remove oxygen to below 1 ppb immediately. Other adsorbents fail to reduce oxygen below 100 ppb or take up to 1 hour to reach their maximum adsorbency which exposes your capillary column to damaging oxygen.

Only the original Alltech OXY-TRAP with OXY-MAX adsorbent is unconditionally guaranteed to be the most efficient oxygen adsorbent available without exception. OXY-MAX has the highest capacity for oxygen so your traps last longer between regenerations.

Only Alltech OXY-TRAPS deliver the superior performance of OXY-MAX for maximum column protection from damaging oxygen.

Contact: Alltech's Chromatography Help Desk
Free Phone: 0800 255832 or Email: alltech@alltech.co.nz
and request Bulletin #255.
circle number 33 on the reader reply card

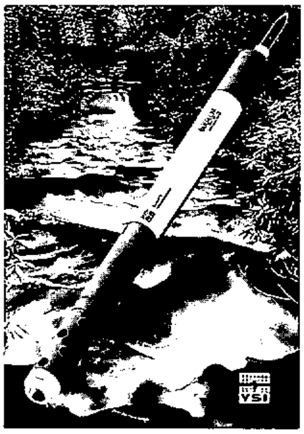
YSI'S MOST COMPACT AND ECONOMICAL LOGGING UNIT

YSI introduces the Model 600XLM Logger. A system which logs any combination of 6 parameters - stirring-independent dissolved oxygen, conductivity, temperature, pH, vented or non-vented level and ORP.

The 600XLM is YSI's first logging instrument that will fit down a 2-inch well. The 600XLM is designed to house 5 field replaceable sensors and offers the option of adding a level-sensor module (vented or non-vented) to the sonde body.

Additional calculated parameters available are specific conductance, salinity, total dissolved solids, and resistivity.

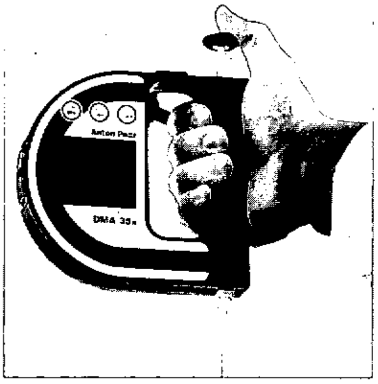
Because the YSI 600XLM has 'on board' battery power, it can be left unattended for weeks at a time with measurement parameters sampled at your setup interval and data securely saved in the units internal memory.



Contact: John Morris Scientific Ltd
P O Box 6348, Wellesley Street, Auckland
Free Phone: 0800 651700, Fax: (09) 3663060
Email: sales@jms.co.nz
circle number 34 on the reader reply card

THE DMA 35N PORTABILITY AND POWER IN ONE SMALL PACKAGE

The new DMA 35N from Anton Paar is a hand-held digital density meter which is also capable of measuring the specific gravity and % concentration of your sample.



The DMA 35N weighs only 270 g so your arm won't get tired no matter how many samples you measure. It is also small enough to fit easily into hard-to-reach places without bending or stretching. The pump is of a pipette-style which gives you better control of the sample flow and the entire pump assembly is easily replaced in less than five seconds.

Measured results can be stored in the instruments memory for later analysis. The memory can store up to 1024 data points which can be transferred to a computer or printed later.

Contact: John Morris Scientific Ltd
P O Box 6348, Wellesley Street, Auckland
Free Phone: 0800 651700, Fax: (09) 3663060
Email: sales@jms.co.nz
circle number 35 on the reader reply card

A NEW STANDARD IN MICROWAVE DIGESTION

A.i. Scientific is pleased to announce the release of a revolutionary new microwave digestion system the MARS 5 (Microwave Accelerated Reaction System) from CEM.

CEM has incorporated 20 years of experience with microwave technology into the system which processes up to 14 high pressure vessels with easy slide-in assembly and rapid cooling. New pop-in sensing line connections eliminate water lines, fibreoptic temperature probes and thermocouples. An infrared sensor closely monitors temperature in all vessels and continuously correlates to the in-vessel temperature sensor to ensure the highest accuracy. The cavity is 52% larger than previous models to allow increased throughput and more room for vessel set-up and sensor connection. New vessel technology allows the highest pressures (1500 psig) and temperatures (300 °C) to ensure complete digestions. The MARS 5 system delivers up to 1200 watts full range continuous power for precise reaction control with additional unpulsed low level power settings (300 W, 600 W) for smaller sample loads. Easy to use operating software provides one-button operation to start methods.

The MARS 5 system establishes a new standard in microwave digestion by simplifying sample preparation, making it faster, safer, with even more throughput than previously possible.

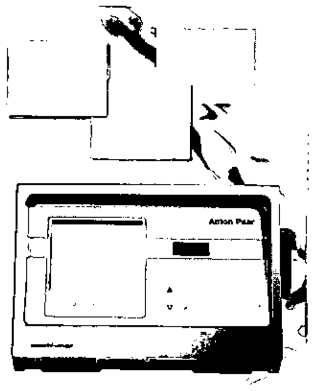
Contact: Kevin Moloney, A.i. Scientific (NZ) Ltd
P O Box 35579 Browns Bay, Auckland
Phone: (09) 4787954, Fax: (09) 4781360
circle number 36 on the reader reply card

THE FASTEST AND EASIEST TO USE DENSITY METER AVAILABLE

The new DMA 5000 from Anton Paar is probably the most accurate, highest precision density meter available and yet it is also the fastest and easiest to use.

The DMA 5000 is user-friendly because you are able to control every measurement it makes. You design every measurement easily, step-by-step with easy to read, easy to understand instructions shown on the display. Once a measurement technique is defined, you are able to save it. Each time you need it, you can recall it with the touch of a button.

The DMA 5000 performs perfectly in even the harshest of environments, thanks to its spill-proof housing and front cover. Internal filters also protect the electronics from spikes and surges.



Contact: John Morris Scientific Ltd
P O Box 6348,Wellesley Street, Auckland
Free Phone: 0800 651700, Fax: (09) 3663060
Email: sales@jms.co.nz
circle number 37 on the reader reply card

KARL FISCHER REAGENTS AVAILABLE EX-STOCK

Biolab Scientific Ltd are able to supply ex-stock both BDH and HYDRANAL Karl Fisher pyridine-free reagents. These 1 litre volumetric reagents are available as either two components or one component, for use with all popular Karl Fischer titrators.

For pricing or more information,

Contact: Neil Bryant or your local branch
Biolab Scientific Ltd
Private Bag 36900, Northcote, Auckland
Free Phone: 0800 807809, Fax: (09) 4803430
Email: neilb@biolab.co.nz
circle number 38 on the reader reply card

UNIQUE CARY 50 PROBE UV-VISIBLE SPECTROPHOTOMETER FOR FAST, ACCURATE, HASSLE-FREE MEASUREMENTS OF LIQUID SAMPLES

A.i. Scientific is proud to introduce the Cary 50 Probe UV-Visible Spectrophotometer from Varian, a new version of the revolutionary Cary 50 instrument providing a dedicated fibre optic dip probe for making fast, accurate and hassle-free measurements of liquid samples.

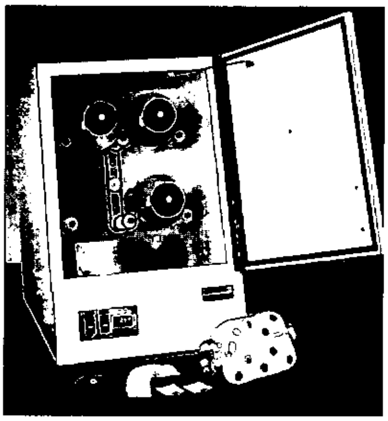
The spectrophotometer is designed for routine quantitative analysis. With the Cary 50 probe, the user simply places the sample vessel up to the standard fibre optic dip probe and presses a built-in Read switch on the probe. Liquid sample measurement is almost instantaneous. By rinsing between samples, carryover is non-existent and sample throughput is improved considerably. The Cary 50 probe provides faster analysis times than is possible with typical sipper systems as no time is wasted pumping samples into a flowcell and the time required for cell contents to equilibrate is eliminated. By taking the light to the sample, as opposed to aspirating the sample to the instrument, all the solution pumping problems inherent in some flowcell systems are eliminated. Bubbles in the flowcell that can block the light beams and destroy measurements are non-existent, as are tubing leaks and degradation. Unlike some conventional spectrophotometers in which room light can effect the quality of measurements, the Cary 50 system is immune.

Key to the performance and reliability of the Cary 50 probe is a single pulsed xenon lamp source that is only on when the spectrophotometer is taking a reading, this prolongs lamp life and saves energy. The intensity of the pulsed xenon lamp provides more effective useful light, which improves the instrument's signal-to-noise performance. This, in turn, increases the accuracy of measurements made by the Cary 50 probe.

Catering for up to 30 standards and up to five replicates, Cary 50 probe users have the maximum flexibility in terms of the level of precision they want in their results. The built-in weight and volume correction enables users to obtain the final result without having to perform additional calculations. The Cary 50 probe is the first true "plug and play" spectrophotometer. All electronics for controlling the Cary 50 probe are contained on a circuit board that plugs into any suitable PC. With few system elements, there is little that can go wrong with the Cary 50 probe.

Contact: Kevin Moloney, A.i. Scientific (NZ) Ltd
P O Box 35579, Browns Bay, Auckland
Phone: (09) 4787954, Fax: (09) 4781360
circle number 39 on the reader reply card

IN VITRO DRY MATTER DISAPPEARANCE STUDIES MADE EASY



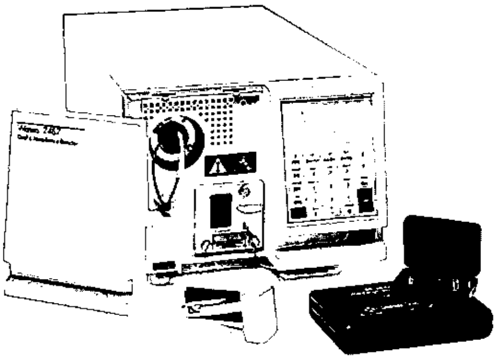
The DAISY II 220 makes *In Vitro* Dry Matter Disappearance (IVDMD) studies easy and efficient. Designed with the user in mind, the Daisy II can digest up to 100 samples at one time. Rumen or enzymatic inoculum needs only to be divided into four vessels, rather than 100 conventional flasks. Batch processing and the removal of the filtration step simplifies the IVDMD assay.

The DAISY II system maintains constant and uniform heat (pre-set for 39.5 °C) and agitation within a controlled chamber. With the DAISY II you can be assured of consistent results regardless of the user.

Contact: John Morris Scientific Ltd
P O Box 6348, Wellesley Street, Auckland
Phone: 0800 651700, Fax: (09) 3663060
Email: sales@jms.co.nz
circle number 40 on the reader reply card

WATERS 2487 DUAL λ ABSORBANCE DETECTOR

Alphatech introduces the new Waters 2487 detector as the most sensitive and versatile absorbance detector available for HPLC. It features advanced programmability, dual wavelength capability, unmatched signal-to-noise performance, reduced optical bandwidth and exceptional linearity. Designed to provide the highest performance in UV/Visible detection for your HPLC analyses, the 2487 detector offers the sensitivity required for detection of minor impurities, with the linear dynamic range to simultaneously quantitate major and minor components. With versatile and easy programmability from the front panel keypad, time-saving qualification derived from the built-in cuvette holder, the ability to view real-time chromatograms or spectral scans via the front panel LCD display, and dual wavelength performance, the 2487 dector will enhance the productivity of any chromatography laboratory.



Contact: Alphatech Systems
P O Box 37583, Parnell, Auckland
Phone: (09) 3770392, Fax: (09) 3098514
Email: sales@alphatech.co.nz
circle number 41 on the reader reply card

SGE'S BPX1-SimD

BPX1-SimD, from SGE are a new technology high temperature methyl silicone range of capillary columns available for ASTM D2887 and its extended petroleum crude methods (HTSD). The columns feature a new dimensionally stabilised phase chemistry providing increased temperature range and reduced bleed. The BPX1 was designed as a high temperature alternative to the conventional 100% dimethylsilicone stationary phases. With a routine operating temperature of 430 °C, extremely low bleed, and excellent chemical inertness, the column is superior to all "MS" grade columns on the market. The BPX1 column offers two major advantages:

- First, the low bleed at the upper temperatures required for the extended high temperature analysis results in better integration and therefore better quantitation for the higher hydrocarbon numbers. This results in the ability to quantify C110 without background subtraction or column compensation from a blank analysis.

- Second, lower column bleed means less loss of column phase and therefore a smaller decrease in capacity ratios. This is important to the practicing chromatographer as the calibration can be carried out less often because of the greater stability in retention times.

Unique advantages for the BPX1 are:
- Not a silphenylene but a dimensionally stabilised methyl siloxane.
- High temperature capabilities, even with thicker films compared with standard methyl silicone columns.
- Lower bleed.
- Maximum column temperature 430 °C.

Applications:

The BPX1-SimD range of columns are specifically designed for the American Society of Testing and Materials (ASTM) method D2887, their extended methods and the new High Temperature Simulated Distillation (HTSD) method. The new method extends the boiling range distribution requiring a higher temperature - lower bleed capillary column. BPX-SimD offers specifications required for these methods.

Request your copy of PD-0151-C BPX1-SimD.

Contact: Alltech Chromatography Help Desk
Free Phone: 0800 ALLTECH (0800 255832)
Fax: (09) 4442399 or Email: alltech@alltech.co.nz
circle number 42 on the reader reply card

SCALTECH BALANCES
GREAT QUALITY, GREAT PRICES

Well known overseas particularly in Europe for producing high quality, reasonably priced balances, SCALTEC balances are now available in New Zealand through newly appointed distributor SciTech.

Scaltec weighing instruments cover the full range of applications: analytical balances, top pan balances, scales and moisture analysers. With features like great looks, ease of operation, precision, reliability and a down-to-earth price there is a Scaltech for every situation and every budget.

Contact: Andrew Pearce, SciTech
P O Box 663, Dunedin
Phone: (03) 4777860, Fax: (03) 4777870
Email: apearce@scitech.co.nz
circle number 43 on the reader reply card

Organometallic Molecular Catalysts, Small Molecule Machines

Cornelis (Cees) Lensink (and Neil B Milestone)
Industrial Research Ltd, P O Box 31-310, Lower Hutt

Chemists have for centuries sought ways to convert inexpensive raw materials into valuable products. The key to success was often the discovery and development of a catalyst. Allow me to refresh your memory and explain very briefly what catalysis involves.[1,2] In very simple terms, the rate of a chemical reaction may be increased by a substance not appearing in the balanced equation for the net reaction. Such a substance is called a *catalyst*, and the phenomenon is called *catalysis*. It is important to realise that a catalyst increases both the forward and backward reactions but does not shift a thermodynamically determined equilibrium. It only causes that equilibrium to be reached a lot faster. Many industrially important reactions are catalysed by surfaces of solid materials. The catalytic reaction takes place at the solid/gas or solid/liquid interface. Catalysis of this type is called *heterogeneous* catalysis because the catalyst, reactants and substrate are present in different phases. A particular example of heterogeneous catalysis in a New Zealand industrial context is the methanol production and the MTG process operated by Methanex in their plants in Taranaki.[3] Another important application of heterogeneous catalysis is the catalytic converters on modern cars to ensure complete combustion of exhaust gases.

Over the last 30 years, many discoveries were made in the field of organometallic chemistry. The impact of these discoveries on industrial process technology has been enormous. I will illustrate this by discussing some of the exciting discoveries and their successful application in industrial processes.

Organometallic molecular catalysts are quite different from heterogeneous catalysts. One way of looking at them is to use the analogy of a machine or apparatus. According to a dictionary, a machine is a piece of equipment for applying mechanical power. It has several parts, each with definite function. A small molecule machine would therefore be an apparatus (in this case an organometallic complex molecule) for applying chemical power, or better said, to catalyse a chemical reaction. Just like a machine, an organometallic molecular catalyst has several parts with each of those parts having a definite function.

The concept of organometallic molecular catalysis is illustrated in Figure 1. The metal atom M provides the reactive site, the heart of the machine where all the action takes place. The reactivity and selectivity of the reactive site are fine-tuned by the surrounding ligand(s) (L). These ligands can be small molecules such as carbon monoxide as we will see in one of the examples below. Ligands can be more complex organic fragments or as large as a complete enzyme. The catalytic cycle illustrated in Figure 1 shows that the reactant (R) and substrate (S) both coordinate to the metal centre, react and subsequently dissociate from the metal centre as product (P). This complete cycle takes place in one homogeneous and often liquid or solvent phase, hence the term *homogeneous* catalysis. The ligands play an important role in directing the outcome of the catalytic reaction through their steric and electronic influences.

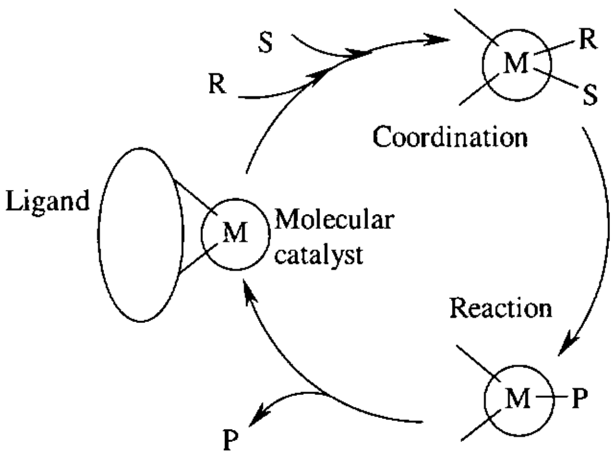


Figure 1. *A schematic representation of a catalytic cycle involving an organometallic molecular catalyst. M = metal, R = reactant, S = substrate, L = ligand and P = product.*

Approximately 85% of all industrial catalytic chemistry (including the processing of mineral oils by the petrochemical industry) is heterogeneous and the other 15 % is homogeneous.[4] There are advantages and disadvantages to both heterogeneous and homogeneous catalytic processes and it is not really surprising that some of the largest industrial processes rely on the easier handling of heterogeneous catalysts. The major differences between heterogeneous and homogeneous catalysts are summarised in Table 1 taken from reference 5. One advantage of homogeneous catalysts is the fact that the molecular structure is generally well defined. This molecular structure can be varied by changing the type and properties of the associated ligands. The variability in structure often results in subtle modification of the catalytic properties such as selectivity and reactivity. Often, the exact steps that make up a catalytic cycle are known. This knowledge allows the catalysis scientist to optimise a particular catalytic process step-by-step. Organometallic chemistry gives us a great deal of control over the catalytic process.

Hydroformylation

Perhaps a good way to illustrate the breadth of homogeneous catalysis is to look at the developments in the oldest and now probably most important industrial homogeneous catalytic process, the 'oxo' synthesis or hydroformylation.[6] Hydroformylation was discovered in 1938 by the German scientist, Otto Roelen, when he passed a mixture of ethylene and synthesis gas (H_2/CO) over a cobalt-containing fixed-bed catalyst. He isolated a small amount of propanal from this reaction. It was subsequently found that this reaction is general

Table 1. The Major Differences Between Homogeneous and Heterogeneous Catalysis.[5]

	Homogeneous Catalysis	Heterogeneous Catalysis
Activity (relative to metal content)	high	variable
Selectivity	high	variable
Reaction conditions	mild	harsh
Service life of catalyst	variable	long
Sensitivity toward catalyst poisons	low	high
Diffusion problems	none	may be important
Catalyst recycling	expensive	not necessary
Variability of steric and electronic properties of catalysts	possible	not possible
Mechanistic understanding	plausible under random conditions	more or less impossible (except for model systems)

for alkenes and it was shown that the nature of the catalyst is homogeneous. The hydroformylation reaction is illustrated in Figure 2. The reaction of an alkene with synthesis gas yields a mixture of linear and branched aldehydes. For example, the hydroformylation of propene yields a mixture of iso-butanal and n-butanal. Research efforts have focused on optimising the product ratio in favour of the desired n-butanal product. The first generation of hydroformylation processes was entirely based on *cobalt* as the catalyst metal. In order to stabilise the catalyst complex ($HCo(CO)_4$) and to prevent the deposition of metallic cobalt the operating conditions need to be harsh with pressures ranging from 200 to 350 bar and temperatures between 150 and 180 °C. An improvement for this reaction was discovered by Shell researchers. Addition of phosphines (PR_3) stabilises the catalytic complex and allows for milder operating conditions.

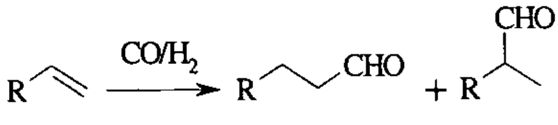


Figure 2. The hydroformylation of terminal alkenes yields both linear and branched aldehydes.

A second generation process was commercialised in 1974 by the former Celanese Corporation. This utilised phosphine modified *rhodium* complexes as the catalyst. The switch of metal from cobalt to rhodium allowed for even milder reaction conditions and a better control of the product distribution in favor of linear n-butanal. This process became known as the low-pressure oxo (LPO) process.

The separation of the catalyst from the products is a general problem in homogeneous catalysis and much of the research and development efforts for the hydroformylation reaction is concentrated on this. Unlike heterogeneous catalysis, where the separation of product from catalyst is often trivial. Homogeneous catalysis is carried out in one homogeneous phase, so special technology needs to be developed in order to recover the expensive catalyst metal. Even the recovery of the ligands must be considered in modern high-tech applications of homogeneous catalysis (*vide infra*). An elegant solution was found by researchers at Rhône-Poulence and commercialised by Ruhrchemie.[7] This third generation process uses water soluble phosphine ligands (Figure 3). The aqueous catalyst solution is easily separated from the organic products phase and can be recycled many times. The rhodium loss in this process is only minimal (ppb). The use of water as a non-corrosive and environmentally-friendly solvent is an added bonus.

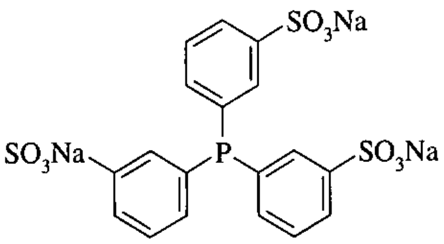


Figure 3. Sulfonated triphenyl phosphine (TPPS), the water-soluble ligand used for the hydroformylation of propene by Ruhr-Chemie.

Asymmetric catalysis

One of the most important achievements of organometallic molecular catalysis is the ability to synthesise chiral molecules with enantiomeric excesses approaching 100%. For the year 1994 the total sales for the world chiral drug market were estimated to be 45.2 billion US dollars. An annual growth of about 9% has been predicted for the near future.[8] There are estimates that by the end of this century 80% of all chiral pharmaceuticals will be produced optically pure.[9] The same development is occurring in the agrochemical sector.

There are just so many examples of asymmetric homogeneous catalysis application that it is not possible to discuss all of these here. The reader is referred to a number of recent review articles and books on the subject.[10-13] What we can do, however, is to look at a few representative examples.

The first commercialisation of an asymmetric homogeneous catalyst was the synthesis of L-DOPA (3,4-dihydroxyphenylalanine). This drug is needed in quantities of ca. 200 tons a year[14] for the treatment of Parkinson's disease. In the early 1970s, Monsanto developed a process to prepare L-DOPA by the enantioselective hydrogenation of dehydroaminoacids.[15] This hydrogenation uses a Wilkinson-type rhodium catalyst with a diphosphine ligand called DIPAMP (Figure 4).

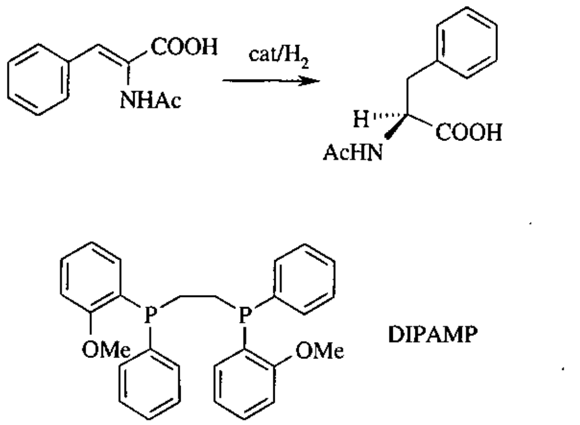


Figure 4. Asymmetric hydrogenation of dehydroamino acids yields optically active amino acids, in this example L-phenylalanine.

Another important application of asymmetric homogeneous catalysis can be found in the production of (-)-menthol. Of the eight possible stereoisomers only the isomer with the (1R,3R,4S) configuration is useful. The estimated worldwide consumption of (-)-menthol is 4500 tons per year. It is widely used in many consumer products such as cigarettes, chewing gum, toothpaste, and pharmaceutical products. Natural (-)-menthol is obtained mostly from *Mentha arvenis* cultivated in China, while synthetic material is produced by several processes. The most interesting of these processes (at least in my opinion) is carried out in Japan by Takasago Perfumeries and produces approximately 2000 ton of (-)-menthol with 94 % enantiomeric excess.[16] The process is illustrated in Figure 5.

The homogeneous catalysed key step in this process is the isomerisation of an allylamine to an enamine using the catalyst $Rh(BINAP)_2^+$. Interestingly, the initial catalyst was a rhodium complex with only one BINAP ligand. This operated with a turnover number (TON) of only 100. Catalyst modification, substrate purification and process quality control lifted this number to 400,000 thereby reducing the cost of the catalyst in this process dramatically.

My personal experience with industrial asymmetric catalysis started when I was employed as a research scientist by DSM in the Netherlands. There we looked at the asymmetric hydrogenation of imines to yield enantiomerically-enriched amines. At that time a water soluble enantioselective imine hydrogenation catalyst was reported to hydrogenate the benzylimine of acetophenone with 99 % enantiomeric excess. This catalyst was a rhodium complex of a bisphosphine ligand (2S,4S)-BDPP (Figure 6).

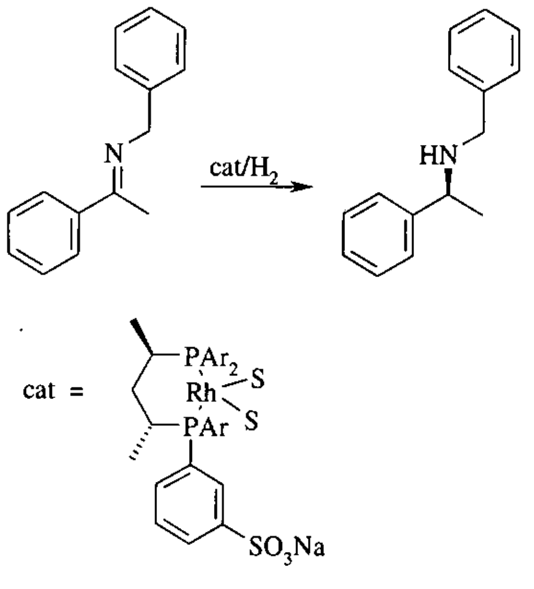


Figure 6. The asymmetric hydrogenation of benzylimines is catalysed by rhodium diphosphine complexes.

The ligand was made water soluble by sulfonation, similar to the water soluble hydroformylation catalysts mentioned above. A closer inspection of this system by the team at DSM revealed that this water soluble catalyst system consisted of multiple components. We successfully isolated and purified the various components. As it turned out only one of the components was an active and selective hydrogenation catalyst for benzylimines.[17-19] Low selectivity and activity for other imine substrates prevented a future development of this system. The hydrogenation of imines has, however, recently been commercialised by Novartis (formerly Ciba-Geigy) for the synthesis of the herbicide (S)-metolachlor (Figure 7). The catalyst for this particular process is based on an iridium complex of a chiral diphosphine ligand with a ferrocene backbone. Imine hydrogenation with this catalyst is reported to occur with a TON of 10^6 and a turnover frequency (TOF) of 200,000 per hour.[20]

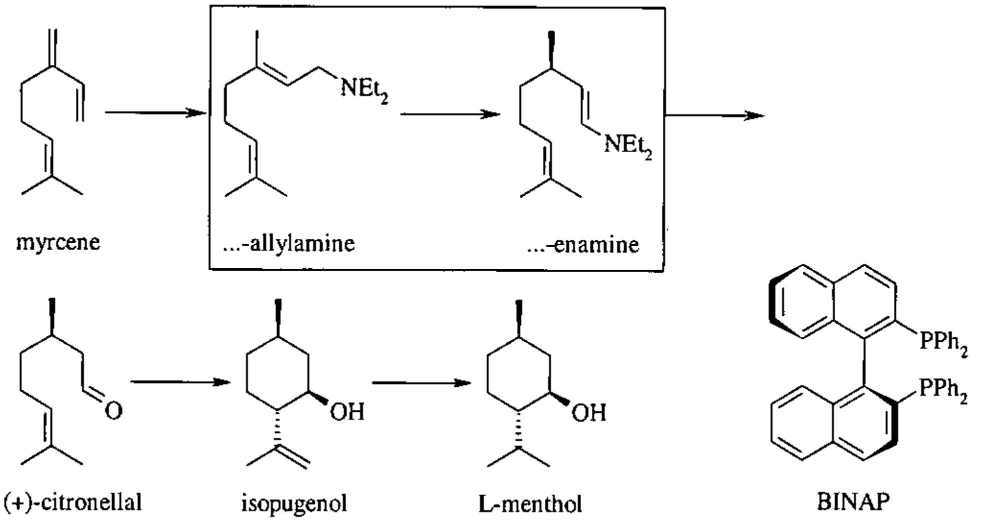


Figure 5. The commercial synthesis of L-menthol by Takasago Perfumeries. The key step is the asymmetric isomerisation of an allylamine to an enamine. This reaction is catalysed by a homogeneous rhodium BINAP catalyst with very high efficiency.

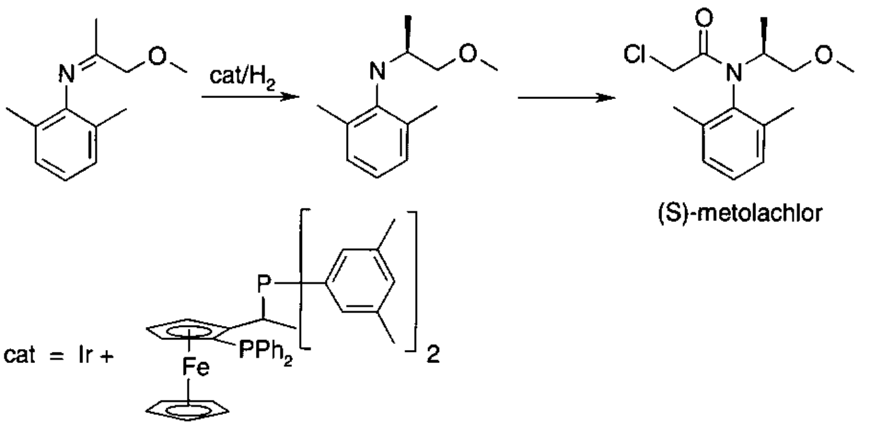


Figure 7. The synthesis of the herbicide (S)-metolachlor. The route involves an asymmetric hydrogenation of an C=N double bond. The catalyst used for this reaction is iridium-based with a chiral ligand with a ferrocene backbone.

Metallocene polymerisation catalysts

A very recent development is the use of metallocene complexes for the polymerisation of olefines such as ethylene and propylene. In this industrial application the adaptability of organometallic catalysts and the machine-like control the chemist can exert on a chemical reaction are clearly shown. Plastics, and in particular polyethylene, polypropylene and other polyolefines, are widely used in everyday life. About 50 million tons of polyolefines are produced each year. Designing a catalyst to control the properties of polymer chains has always been difficult but metallocene catalysts can provide the control necessary to create polymers with properties that are tuned to a particular use. The polymerisation of olefines consists of breaking C=C double bonds and forming C-C single bonds into long carbon chains. Propylene can be polymerised to give polypropylene using a variety of different catalysts. Figure 8 illustrates the different ways the propylene monomers can be assembled into polypropylene depending on the orientation of the side group methyls when propylene polymerises.

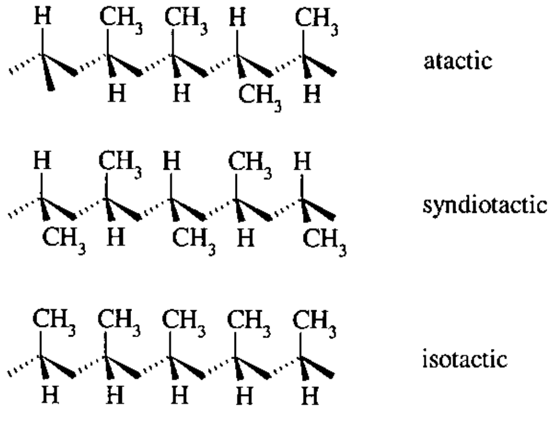


Figure 8. The polymerisation of propene can lead to a number of different polypropylene types. A number of the more important types are shown here.

The major types of polypropylene are:

- *isotactic* polypropylene where all the methyl group bearing carbon atoms have the same stereochemistry.
- *syndiotactic* polypropylene where the stereochemistry alternates regularly.
- *atactic* polypropylene where there is no regular stereochemistry but rather a random stereochemistry.

The mechanism of propylene polymerisation is now well understood and the reader is referred to an excellent review article on the subject.[21] The metallocene organometallic catalysts used are usually based on zirconiun. Because the mechanism of polymerisation was fairly accurately defined, it has been possible to design catalyst complexes that would produce a type of polypropylene virtually on demand. This is illustrated with the next few examples.

The catalyst complexes need to be activated by a large excess of methylaluminoxane (MAO) with Zr to MAO ratios >200. Using bis(cyclopentadienyl)zirconium dichloride and MAO up to 140 kg polypropylene per g Zr per h can be obtained. The polymer that is produced by this catalyst is atactic polypropylene.[22] In order to be able to produce stereospecific polymerisation a chiral catalyst centre is needed. This is depicted in Figure 9. In this particular C_2 symmetric catalyst complex, the central zirconium atom is coordinated by two tetrahydro-indenyl groups that are strapped together by an ethylene bridge. This strapping of the indenyl moieties results in a stereochemically rigid complex. The growing polymer chain end bonds to the zirconium atom in one of the two available coordination sites. The incoming propylene monomer can only coordinate to zirconium in one orientation. The polymer chain is growing via the insertion of propylene into the Zr-polymer chain. The net result is a polymer chain where all methyl groups are oriented in the same way and high quality isotactic propylene is formed.[23]

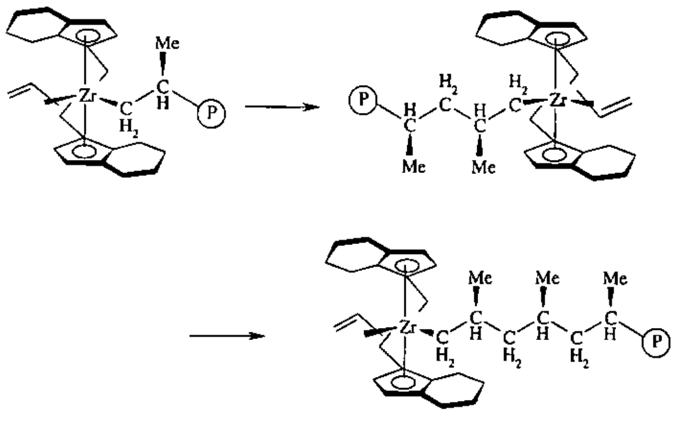


Figure 9. The mechanism of the isotactic polymerisation of propene by a catalyst generated from a C2-symmetric bis(indenyl)zirconocene.

Ewen and co-workers took the concept of stereochemical control over propylene polymerisation even further.[24,25] Figure 10 shows their results obtained with two related catalyst complexes. In one case isotactic propylene was obtained. In the other an atactic polymer was formed. Before this work, syndiotactic polypropylene was available in only tiny amounts in laboratories. Now syndiotactic polypropylene is a preferred plastic for a number of applications in the medical field.

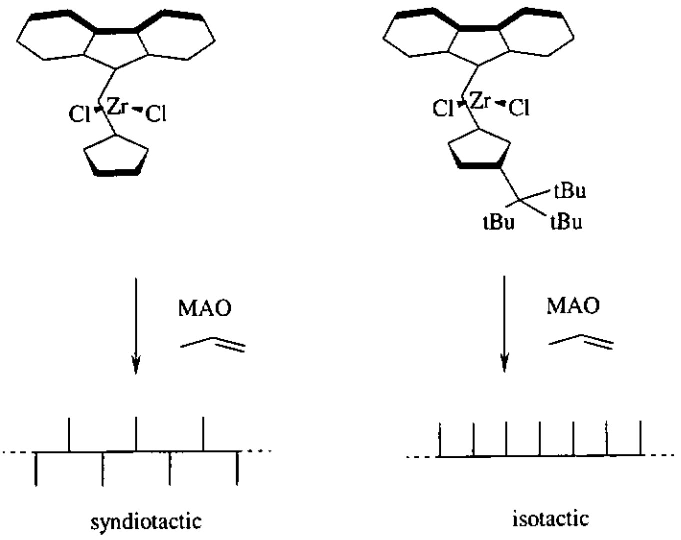


Figure 10. The relationship between the catalyst structure and the stereoselectivity of propene polymerisation.

Conclusion

With the examples discussed in this article I have attempted to illustrate that organometallic small molecule machines are a powerful tool for the industrial chemist. Many more examples could have been mentioned together with detailed discussions of the chemistry and mechanisms. However, I do not believe this is necessary in order to appreciate the simplicity and sometimes incredible efficiency of some of these catalysts. It is important to realise that these catalysts are used in industrial processes and that they are extremely succesful. Much of the development and improvements resulted from a thorough understanding of the mechanisms that play a role in organometallic chemistry. The realisation that the steric and electronic influence of 'ligands' can be used to improve catalyst performance is crucial in this type of work. At Industrial Research Limited the 'Catalysis and Inorganic Materials team' works on a number of different projects that are aiming to utilise both heterogeneous and homogeneous catalysts. These projects range from the conversion of natural feedstock to gaining a more fundamental understanding of organometallic catalysis chemistry of e.g. early transition metals. Organometallic compounds can be made to perform difficult tasks and asking the questions of how and why such catalytic reactions take place will eventually lead to better and more efficient small molecule machines.

When Seebach[26] asked in 1990 the question 'Organic synthesis - Where now?' it prompted the reply by Cornisl and Herrmann[27] that the obvious answer is 'towards organometallic chemistry' and I fully agree with this, of course.

References

1. Thomas, J M (1994) *Angew. Chem. Int. Ed. Engl.* **33**: 913.

2. Parshall, G W and Ittel, S D (1992) *Homogeneous Catalysis*, John Wiley & Sons, Inc.

3. Allum, K G and Williams, A R (1988) *Studies in Surface Science and Catalysis* (Bibby, D M; Chang, C D; Howe, R F and Yurchak, S, eds.), Elsevier, Vol. 36, p761.

4. Parshall, G W and Putscher, R E (1986) *J. Chem. Edu.* **63**:189.

5. Herrmann, W A and Cornils, B (1997) *Angew. Chem. Int. Ed. Engl.* **36**:1048.

6. Frohning, C D and Kohlpaintner, C W (1996) *Applied Homogeneous Catalysis with Organometallic Compounds* (Cornils, B; Herrmann, W A, eds.) VCH Publishers, New York, NY (USA), p27.

7. Kuntz, E G (1987) *CHEMTECH* **17**:570.

8. Stintson, S L (1995) *Chem. Eng. News* **73**:44.

9. Botteghi, C; Paganelli, S; Schionato, A and Marchetti, M (1991) *Chirality* **3**:355.

10. Ojima, I (Editor) (1993) *Catalytic asymmetric synthesis*. VCH Publishers, New York, NY (USA).

11. Noyori, R (1989) *Chem. Soc. Rec.* **18**:187.

12. Berrisford, D; Bolm, C and Sharpless, K B (1995) *Angew. Chem. Int. Ed. Engl.* **34**:1059.

13. Hoveyda, A H and Morken, J P (1996) *Angew. Chem. Int. Ed. Engl.* **35**:1262.

14. Izumi, Y (1971) *Angew. Chem. Int. Ed. Engl.* **10**:87.

15. Knowles, W S (1993) *Acc. Chem. Res.* **16**:106-112.

16. Otsuka, S and Tani, K (1991) *Synthesis* 665.

17. Lensink, C and De Vries, J G (1993) *Tetrahedron: Asymmetry* **4**:215.

18. Lensink, C and De Vries, J G (1992) *Tetrahedron: Asymmetry* **3**:235.

19. Lensink, C; Rijnberg, E and De Vries, J G (1997) *J Mol. Catal. A: Chemical* **116**:199.

20. Spindler, F; Pugin, B; Jalett, H-P; Buser, H-P; Pittelkow, W and Blaser, H-U (1996) in *Catalysis of Organic Reactions* (R E Malz, ed.), Marcel Dekker, New York, p153.

21. Brintzinger, H H; Fisher, D; Muelhaupt, R; Rieger, B and Waymouth, R M (1995) *Angew. Chem. Int. Ed. Engl.* **34**:1143.

22. Kaminsky, W and Miri, M (1986) *Homogeneous and Heterogeneous Catalysis* (Yermakov, Y and Likholobur, W, eds.), VNU-Science Press, Utrecht, p327.

23. Kaminsky, W; Kuelper, R; Brintzinger, H H and Wild, F R W P (1985) *Angew. Chem. Int. Ed. Engl.* **24**:507.

24. Ewen, J A; Jones, R L; Razavi, A and Ferrara, J D (1998) *J. Amer. Chem. Soc.***110**:6255.

25. Ewen, J A (1997) *Scientific American* **276(5)**: 60.

26. Seebach, D (1990) *Angew. Chem. Int. Ed. Engl.* **29**:1320.

27. Frohning, C D and Kohlpaintner, C W (1996) *Applied Homogeneous Catalysis with Organometallic Compounds* (Cornils, B and Herrmann, W A, eds.) VCH Publishers, New York, NY (USA), p14.

ABOUT THE AUTHOR

Cees Lensink, born 1959 in the Netherlands, graduated Cum Laude with a major in inorganic chemistry (cyclic and poly-phosphanzenes) in 1983 at the University of Groningen, the Netherlands. In 1987 he received a PhD with Professor T Chivers at the University of Calgary, Canada. After a one year Post-doctorate with Professor J Verkade at Iowa State University he moved back to the Netherlands in 1989 where he became a scientist with the Fine-Chemicals Research Division of the chemicals producer DSM. At DSM his research became focused on homogeneous catalysis. In 1993 a lifestyle decision was made to emigrate to New Zealand where he is now employed as a Senior Research Scientist within the Manufacturing Division of Industrial Research Limited. He has authored over 25 original publications and been granted one patent. Apart from science he enjoys playing golf, renovating his house and breeding tropical fish.

IUPAC-SPONSORED SYMPOSIA IN 1998

4 - 7 May 1998
1st International Conference on Trace Element Speciation in Biomedical, Nutritional and Environmental Sciences
Venue: Neuherberg/Munich
Federal Republic of Germany

28 June - 2 July 1998
12th International Conference on Organic Synthesis
Venue: Venice, Italy

6 - 10 July 1998
7th International Chemistry Conference in Africa
Venue: Durban, Republic of South Africa

20 - 23 July 1998
18th Discussion Conference on Macromolecules: Mechanical Behaviour of Polymeric Materials
Venue: Prague, Czech Republic

2 - 7 August 1998
9th International Symposium on Novel Aromatic Compounds
Venue: Hong Kong

5 - 8 August 1998
8th International Symposium on Solubility Phenomena
Venue: Niigata, Japan

16 - 21 August 1998
14th International Conference on Physical Organic Chemistry
Venue: Florianópolis, Santa Catarina, Brazil

30 August - 4 September 1998
33rd International Conference on Coordination Chemistry
Venue: Florence, Italy

11 - 16 October 1998
21st IUPAC Symposium on Chemistry of Natural Products
Venue: Beijing, China

For further information, please contact:
The NZIC Secretariat
P O Box 12-347, Wellington
Tel: (+64-4)-4739444, Fax: (+64-4)-4732324
Email: nzic@ipenz.org.nz

Patent Proze

by Jane Calvert and Greg Lynch

In previous issues of Patent Proze, we have focused on some aspects of patent law and procedure. Patents are generally the most relevant form of intellectual property to research scientists. However, there are other forms of intellectual property which are commercially important and which have associated rights that can be enforced, if necessary. We outline some of these other forms below.

INTELLECTUAL PROPERTY

The term "intellectual property" is being used increasingly to cover all forms of knowledge or expertise which are of commercial or cultural value. Some forms of intellectual property require registration whereas others do not. Registration systems are available for patents, trademarks, designs, plant variety rights and geographical indications. Non-registrable forms of intellectual property include copyright and trade secrets.

The patent system is well known to many scientists. This is the principal avenue for the protection of inventions resulting from research. In essence, a patent provides an effective monopoly for an invention which is novel having regard to what is already in the public domain. The period of protection is a maximum of 20 years.

The trade mark registration system provides protection for a sign which includes, among other things, a name or a logo. A trade mark is used to distinguish the goods and/or services of one person from those of another person. A registered trade mark provides monopoly protection for a sign in relation to specific goods and/or services. The protection is theoretically available forever provided the registration is maintained by payment of renewal fees.

Many people are unaware that the symbol R used in conjunction with many names or logos is an indication to the public that a trade mark has been registered. The symbol T is usually used to serve as a warning to the public that a trade mark application has been filed by the owner of the name or logo, but registration has not yet been granted. Until the trade mark is actually registered, the owner cannot sue for trade mark infringement under the Trade Mark Act 1953. However, registration of a trade mark is not essential as other causes of action may be available, such as the common law right of passing off or breach of the Fair Trading Act 1986, but these are generally more difficult and expensive to enforce than an action brought under the Trade Mark Act.

The physical appearance of an article may be protected by way of a registered design. A "design" is defined as the new or original features of shape, configuration, pattern, or ornament applied to an article. For example, a new shape of a bottle may be protected in this way. A feature of shape or configuration which is dictated solely by its function is not protectable by way of a design registration. A registered design has a term of 15 years, subject to payment of renewal fees.

Plant variety rights protect a new cultivated plant variety for a period of 20 years or 23 years depending on the type of plant. The grant of a plant variety gives the holder the exclusive right to sell and produce for sale reproductive material of the variety. Cultivated plant varieties do not include cultivated varieties of bacteria or algae.

The registration of a geographical indication will soon be possible. This will protect a name or description used to indicate the geographical origin of goods, for example, "Marlborough" when used in relation to wines from that area. The Geographical Indications Act 1994, while passed by Parliament, has not yet come into force.

New Zealand's copyright law provides for the automatic subsistence of copyright in original literary, dramatic, musical or artistic works. The period of copyright is generally 50 years from the end of the year in which the author died. However, for copyright works which have been industrially applied, the copyright period is 16 years. This restricted term of protection ensures consistency with the design registration system as copyright generally subsists in works for which design registration may be obtained. For most articles, the term "industrially applied" means the manufacture of 50 or more of the articles.

Jane Calvert

Jane Calvert and Greg Lynch are both employed in the patent department of Baldwin, Son and Carey, Patent and Trademark Attorneys, and Solicitors, where they specialise in chemistry patents. Jane joined Baldwins after completing a PhD in chemistry at the University of Canterbury in 1994. Greg also joined Baldwins in 1994 after three years research at Industrial Research Ltd in Wellington. Following completion of a PhD in chemistry at the University of Otago in 1989, he spent a two year period as a postdoctoral researcher at Oxford University in the United Kingdom.

Greg Lynch

As the above shows, the forms of intellectual property are significantly different. Each has a particular function. A feature common to all is ownership, that is, the rights attaching to intellectual property are owned by a legal entity. The issue of ownership will be high on the agenda of discussions in relation to the WAI 262 Treaty of Waitangi claim currently before the Waitangi Tribunal. This claim is concerned with native flora and fauna and intellectual property rights of Maori. The WAI 262 claim is arguably one of the more significant claims brought before the Waitangi Tribunal. We will report on the significance to existing intellectual property laws of the WAI 262 claim in a future Patent Proze.

INTERNET

The Baldwin, Son and Carey home page contains Patent Proze (including back issues). Information on a variety of topics including trade marks, designs, copyright, plant varieties rights, and other aspects of intellectual property is also available on the home page. The address is www.baldwins.co.nz

Please forward any queries to:
Patent Proze, Baldwin, Son & Carey
P O Box 852, Wellington
Email: email@bscwlg.baldwins.co.nz

International News

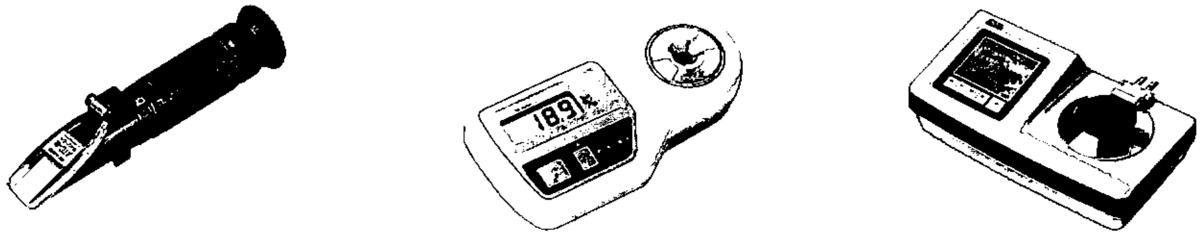
J&W SCIENTIFIC INC. APPOINTS NEW PRESIDENT

J&W Scientific Incorporated, a leading manufacturer of high resolution GC columns worldwide, has announced the appointment of John W (Jack) Frank as President.

Mr Frank, a chemist by training, brings over 20 years of analytical practice to the business, with senior management experience at Varian Instruments, OI Analytical and Valco Instruments. Mr Frank possesses extensive experience in international business, corporate acquisition/joint venture accomplishments, as well as demonstrated successes with R&D, marketing and manufacturing strategic initiatives.

The appointment of Mr Frank supports J&W's corporate growth strategy of increasing its market share in the separation sciences market worldwide by building on innovative technology and expansion through company acquisitions.

You can visit J&W's Web Site at http:/wwwjandw.com



CONFERENCES & SEMINARS

30 November - 5 December 1997
Nature Conservation in Production Environments
Venue: Taupo, New Zealand
Contact: University of Auckland
School of Environmental and Marine Sciences
Tel: (09)-3737599
Fax: (09)-3737042
Email: sems@auckland.ac.nz

2-5 December 1997
13th Symposium on Biological Macromolecules and Ligands: Structure, Interactions and Applications
Venue: Quezon City, Philippines
Contact: Dr Gisela P Concepcion
University of the Philippines
Marine Science Institute
Quezon City 1101
Republic of the Philippines
Tel and Fax: (+63-2)-9213799

6-8 April 1998
Conference on Production and Uses of Starch
Venue: Edinburgh, Scotland, United Kingdom
Contact: Dr C M Duffus
Crop Science and Technology Department
Scottish Agricultural College
West Mains Road
Edinburgh EH9 3JG
Scotland, United Kingdom

15-18 April 1998
Third International Meeting on Esterases Reacting with Organophosphorus Compounds
Venue: Dubrovnik, Croatia
Contact: Dr Elsa Reiner
"Esterase Meeting"
Institute for Medical Research and Occupational Health
P O Box 291, Ksaverska cesta 2
HR-10001 Zagreb, Croatia
Fax: (+385-1)-274572

19-22 April 1998
International Symposium on Stability and Stabilisation of Biocatalysts
Venue: Cordoba, Spain
Contact: Dr F J Plou
Department of Biocatalysis, CSIC
Campus Univ Autonoma
28049 Madrid, Spain
Fax: (+34-1)-5854760

26-29 May 1998
VIIIth International Symposium on Luminescence Spectrometry in Biomedical and Environmental Analysis
Venue: Las Palmas de Gran Canaria, Canary Islands
Contact: J J Santana Rodrigues
University of Las Palmas de GC
35017, Las Palmas de GC
Canary Islands, Spain
Fax: (+34-9)-28452922

24-26 June 1998
Asia-Pacific Society for Neurochemistry: Biennial Conference
Venue: Seoul, Korea
Contact: Peter Dodd
Email: peterD@qimr.edu.au

or full details from:
Professor Yoo-Hun Suh
c/o Organising Secretariat of 4th APSN Meeting
Department of Pharmacology
Seoul National University College of Medicine
28 Yongon-dong, Chongno-gu
Seoul 110-799, Korea

26 June - 2 July 1998
9th Congress of the International Society for Biomedical Research on Alcoholism (ISBRA)
Venue: Copenhagen, Denmark
Contact: Professor Christer Alling
Department of Medical Neurochemistry
Institute of Laboratory Medicine
University Hospital
S-221 85 Lund, Sweden
Fax: (+46-46)-175376

13-17 July 1998
MACRO 98 AUSTRALIA
37th IUPAC International Symposium on Macromolecules
Venue: Gold Coast, Queensland, Australia
This forefront conference will bring together polymer-oriented scientists, technologists, educators and students from all areas of the scientific community: academia, industry and government. It will provide an international forum for the communication and discussion of general and specific contemporary topics of interest to the polymer community.

The conference will embrace both the fundamental and applied aspects of polymer chemistry, polymer physics, materials technology and engineering. The program will focus on a number of broad themes which will incorporate a range of symposia, involving plenary and invited lectures, and contributed verbal and poster presentations. Plenary speakers will be Professor J Economy (USA), Professor J Feast (UK), Professor A Khokhlov (Russia) and Professor Y Tabata (Japan). A special International Symposium will be held in honour of the late Professor Jim O'Donnell.
Contact: MACRO 98 Secretariat
Chemistry Department, University of Queensland
Brisbane, Queensland 4072, Australia
Fax: (+61-7)-33654299
Email: macro98@chem.chemistry.uq.edu.au
Website: http://www.uq.edu.au/~cmawhitt/macro98.html

23-26 July 1998
18th International Machinery and Materials Exhibition for Asia - Mex 98
Venue: Hong Kong International Trade and Exhibition Centre, Hong Kong
Contact: Business and Industrial Trade Fairs Limited
Unit 1223, 12/F

CONFERENCES & SEMINARS

1 Trademart Drive, Kowloon Bay, Hong Kong
Tel: (+852)-28652633
Fax: (+852)-28661770 or (+852)-28662076

2-7 August 1998
The 9th International Symposium on Novel Aromatic Compounds (ISNA-9)
Venue: The Hong Kong Convention and Exhibition Centre, Hong Kong
Contact: Professor B Halton
Chemistry Department
Victoria University
P O Box 600, Wellington, New Zealand
Fax: (+64-4)-4955241
Email: brian.halton@vuw.ac.nz

24-28 August 1998
17th International Cancer Congress
Venue: Rio de Janeiro, Brazil
Contact: Congrex do Brazil
Ruad do Ouvidor, 60 gr 413
20040-030 Rio de Janeiro RG, Brazil
Fax: (+55-21)-2231492

23-25 September 1998
International Symposium on Preparative and Industrial Chromatography and Allied Techniques - SPICA 98
The subject of SPICA 98 will focus on isolation, purification and fractionation of value-added products, e.g. fine chemicals, natural products, pharmaceuticals, biotechnical products, agrochemicals, aroma and food additives, applying chromatographic techniques, membrane technology and electrophoresis. In conjunction with the Symposium, an exhibition of instruments will be held, giving participants the opportunity to meet most of the world's leading suppliers of preparative and industrial separation products and technologies.
Venue: Strasbourg, France
Contact: Secretariat SPICA 98
ENSIC
1, rue Grandville - B.P. 451
F-54001 Nancy Cedex, France
Tel: (+33-383)-175003
Fax: (+33-383)-350811
Email: brionne@ensic.u-nancy.fr

18-22 October 1998
14th International Clean Air and Environment Conference
Venue: Melbourne Hilton on the Park, Melbourne Australia
Contact: PR Conference Consultants Pty Ltd
Tel: (+61-3)-98169111
Fax: (+61-3)-98169287
Email: prcc@labyrinth.net.au
Website: http://www.labyrinth.net.au/~prcc

December 1999
23rd Australian Polymer Symposium
Venue: Geelong, Victoria, Australia
Contact: Dr W D Cook
Department of Materials Engineering
Monash University
Clayton, VIC 3168
Australia
Tel: (+61-3)-99054926
Fax: (+61-3)-99054940
Email: WDCOOK@eng2.monash.edu.au

6-11 February 2000
RACI 11th National Convention
Venue: Canberra, ACT, Australia
Contact: Dr W D Cook
Department of Materials Engineering
Monash University
Clayton, VIC 3168
Australia
Tel: (+61-3)-99054926
Fax: (+61-3)-99054940
Email: WDCOOK@eng2.eng.monash.edu.au

14-19 December 2000
Pacifichem 2000
Venue: Waikiki, Honolulu, Hawaii
Contact: Professor B Halton
Chemistry Department
Victoria University
P O Box 600, Wellington
New Zealand
Fax: (+64-4)-4955241
Email: brian.halton@vuw.ac.nz

A Multi-Technique Approach to Surface Analysis

Part 2. Scanning Probe Microscopy

Dr Richard Haverkamp
Research Centre for Surface and Materials Science, University of Auckland, Private Bag 92019, Auckland

In the previous article (*Chemistry in New Zealand* **61**, 5:22-24) I discussed the importance of surfaces to many properties of materials and described how X-ray photoelectron spectroscopy and Auger electron spectroscopy can be used to provide useful information about surfaces. In this article we discuss the emerging techniques of scanning probe microscopy.

The Range of Techniques Available

Scanning probe microscopy is the generic name for a wide range of techniques each with their own acronym. Most people have heard of scanning tunnelling microscopy (STM) which was developed in 1981 by Binnig and Rohrer[1] (for which they received the Nobel Prize in 1986). However there have been major developments since then. The best known is probably atomic force microscopy (AFM) developed in 1986 by Binnig, Quate and Gerber[2]. Now there are a range of variations on these basic methods, with labels such as TMAFM, LFM, CFM, some of which I describe below.

Atomic Force Microscopy (AFM)

The technique

Atomic force microscopy is, as the name suggests, a form of microscopy where an image is obtained of a surface. This image shows the topographic features on the surface. But what is really amazing about the technique is the resolution that can be achieved - under certain conditions it is possible to see individual atoms!

The AFM works a bit like an obsolete (now replaced by CD's) record player. In the record player a stylus was dragged along a groove in the record and bounced up and down with the bumps in the groove generating a voltage in the pickup. In the AFM the principle is similar although there are some major refinements. The sample goes back and forth and scans from top to bottom (rather than rotating like the record). The tip (in place of the record player stylus) is very sharp and small and is mounted on a microscopic force sensor. The deflection of the cantilever is sensed by a laser reflecting off the back of the cantilever to a photodiode array. In most AFM systems the cantilever holding the tip isn't allowed to bend very much but rather the sample (or cantilever holder) moves up and down attempting to keep the force (the atomic repulsion) of the tip on the sample constant. A feedback system is used to maintain this constant force as the sample is scanned.

As a tip approaches a surface it is initially attracted towards the surface largely due to capillary forces. This attraction is non-localised. However as the tip approached closer it experiences a repulsive force which is very localised.

To get very high magnification images needs two factors: a sharp tip and a way of very accurately controlling the movement of the sample (or tip). The control of movement is achieved with a piezoelectric tube, on which the sample (or tip) sits, that can be controlled in three dimensions by applying voltages to it. Applying a voltage to a piezoelectric material causes it to expand or contract just as applying pressure to a piezoelectric material causes a voltage to be generated. The accuracy with which motion can be controlled by these piezoelectric devices is quite incredible, it can be as good as 0.1Å.

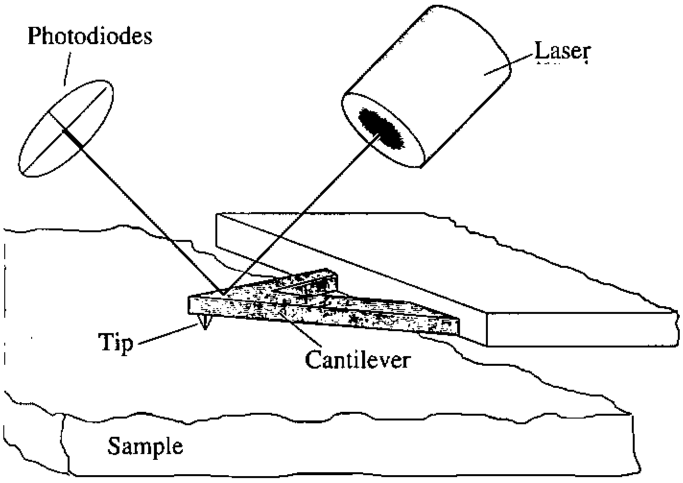


Figure 1. Schematic of atomic force microscope operation.

Advantages

So the AFM is just a microscope that has amazing resolution? Yes but not "just". Even if only using the device as a topographic microscope there is the major advantage that the sample does not have to be in a vacuum but may be examined in air or under a liquid. There are many other uses to which the instrument may be put. Scanning electron microscopy, with which many people will be familiar, requires that the sample is placed in a vacuum and normally requires the sample to be electrically conductive (therefore a coating of carbon or gold is often applied to the sample). With AFM the sample does not have to be conductive and the sample may be imaged in air or in a fluid! Special fluid cells are available to look at samples under the fluid of your choice. Typically this will be water or an electrolyte solution.

Scanning Tunnelling Microscopy (STM)

Because it is restricted to conduction samples, scanning tunnelling microscopy is now a lesser used technique. It differs from AFM in that instead of measuring the force between the tip and the sample a tunnelling current is measured. This is done by applying an electric potential between the tip and the sample. The tunnelling current provides a feedback to control the piezoelectric tube. Typically an image records the sample (tip) displacement needed to maintain a constant current. Some types of atoms on the surface can show up as a depression rather than a protrusion. Although superior to the AFM in terms of resolution, the technique has fallen out of favour as a simple imaging tool but has gained favour with physicists studying surface electronic structure.

Tapping Mode (TMAFM)

Conventional AFM operates in contact mode, that is the tip is dragged along the sample physically in contact with the surface (in the repulsive regime). Tapping Mode™, which is a trademark of Digital Instruments, is a modification of AFM where a piezoelectric crystal in the cantilever assembly holder causes the cantilever to oscillate at or near the cantilever's resonant frequency[3]. The tip is then brought in contact with the sample surface so that it just begins to touch or tap the surface. This enables sample damage to be reduced. In addition it has resulted in the powerful technique of phase imaging.

Phase Imaging

Phase imaging has been used for some time[4] without the phenomenon being well understood. It was observed that surface detail not clearly visible in height images showed up with good contrast in phase images. In addition the elastic modulus of the surface can affect the image so that differences in surface hardness can be detected. Phase imaging works by detecting the phase shift of the cantilever oscillator when it interacts with the sample surface. The theoretical basis of the technique is now well understood[5]. Where small local variations in height are of interest on a sample with larger height variations overall then phase imaging is also a very useful technique. An example of a phase image is shown in Figure 2.

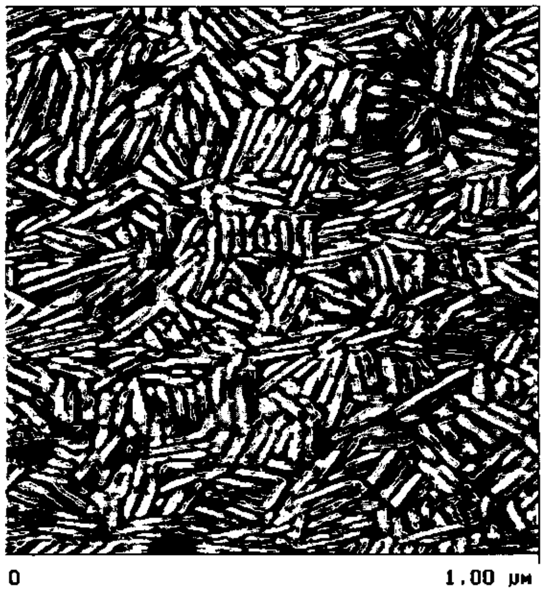


Figure 2. AFM phase image of protein rodlets from Neurospora crassa on mica.

Lateral Force

When a tip is dragged across a sample surface there will be a resistance to the movement of the tip. This resistance to the dragging of the tip, known as the lateral force, can be measured on an SPM[6]. The tip is dragged at right angles to the long axis of the cantilever (in the "y" direction) so that the cantilever will twist as the tip encounters a lateral force. This twisting will cause the laser deflecting off the back of the cantilever to be deflected to one side and this deflection can be measured by a pair of photodiodes. (We need only four photodiodes then to measure height and lateral force simultaneously). This lateral force measurement can tell us about the frictional forces on a microscopic scale or can show up differences on a surface, especially compositional, that are not apparent in height images.

Force Curves

The AFM can also be used to measure the force between the tip and a sample as the tip is brought towards the sample and pulled away from the sample. In this way electrostatic forces between the tip and sample can be measured in air or in liquids[7]. The force is proportional to the tip deflection to a first approximation and an example of a tip-delection verses distance curve is shown in Figure 3. Modifying the surfaces can result in changes to these attractive forces. In air there is often a strong attraction between, for example, a silicon nitride tip and a mica sample due to the capillary attraction from the surface layer of adsorbed water and other contaminants. This interaction can be reduced by immersing the sample in water. Frequently the force between the tip and a surface in a liquid is strongly dependant on the pH of the liquid. This technique can be used to determine isoelectric points. Pioneering work on attaching colloidal particles to AFM cantilevers has been carried out by Dr William Ducker now at the University of Otago[8]. It is then possible to measure the force between the colloid and a surface of interest.

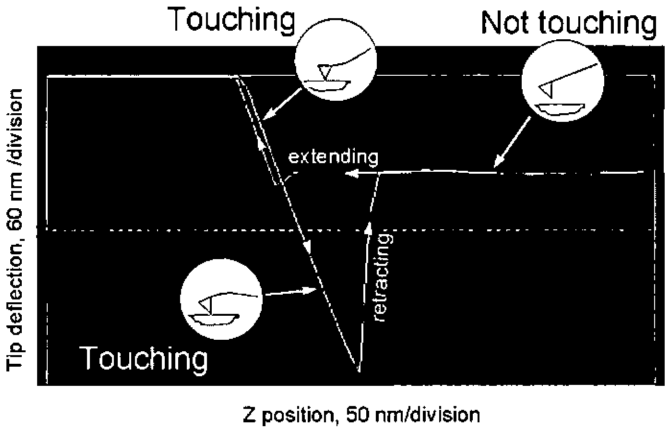


Figure 3. Deflection verses tip-sample distance for a silicon nitride tip on silicon in air.

Magnetic Force (MFM)

If a tip is coated with a magnetic material and a sample is scanned which contains magnetic regions then there will be a magnetic force acting on the tip in addition to the atomic repulsion. But to be able to distinguish between the sample topography and the magnetism of the sample we need to be able to separate these two effects. The atomic forces are very short range and the magnetic forces are longer range so there is an easy way to do this. The tip is scanned across the sample in contact with the surface to get the height data on the first scan and this data stored. On the next scan the tip is scanned over the same area but is lifted so that it follows a path with a fixed height above the surface as determined by the previous scan. In this way any variation in force felt by the tip will be due only to the magnetic forces[9].

Other Techniques

A wide range of new techniques are continually being developed and many more can be expected over the next few years. For example some of the recently reported techniques include scanning capacitance microscopy, scanning near-field optical microscopy, scanning thermal microscopy, surface enhanced raman spectroscopy using scanning near-field optical microscopy and chemical identification by STM photoemission.

Applications

At the Research Centre for Surface and Materials Science in Auckland we have used the basic AFM mode for a range of applications. For example it has been used to investigate amylase proteins, the nucleation and growth of diamond films, fungal hydrophobin protein, wood fibres, fouling on membrane filters and superconducting crystal structure.

Sample Requirements

There are two main sample requirements for AFM for our instrument (Digital Instruments Nanoscope IIIA). They are limitations on size and surface roughness. Height variations (z movement) as low as 0.1Å can be detected but the limit on height variation of the surface is about 5 µm. Samples must be small - about 12 mm maximum diameter and about 5 mm maximum thickness. Other instruments are available that handle larger samples.

References

1. Binnig, G; Rohrer, H; Gerber, C and Weibel, E (1982) "Surface Studies by Scanning Tunnelling Microscopy." *Phys. Rev. Lett.*, **49** **(1)**:57-61.

2. Binnig, G; Quate, C and Gerber, C (1986) "Atomic Force Microscopy." *Phys. Rev. Lett.*, **56** **(9)**:930-933.

3. Hansma, P K; Cleveland, J P; Radmacher, M; Walters, D A; Hillner; Bezanilla, M; Fritz, M; Vie, D; Hansmas, H G; Prater, C B; Massie, J; Fukunga, L; Gurley, J and Elings, V (1994) "Tapping mode atomic force microscopy in liquids." *Appl. Phys. Lett.*, **64** **(13)**:1738-40.

4. Magonov, S N; Elings, V and Whangbo M H (1997) "Phase imaging and stiffness in tapping-mode atomic force microscopy." *Surf. Sci.*, **375** **(2-3)**:L385-L391.

5. Cleveland, J P; Anozykowski, B; Schmid, A E and Elings, V B "Measuring Energy Dissipation with a Tapping-Mode Atomic Force Microscope." *Appl. Phys. Lett.* - submitted.

6. Schwarz, U D; Koster, P and Wiesendanger, R (1996) "Quantitative analysis of lateral force microscopy experiments." *Rev. Sci. Instruments*, **67** **(7)**:2560-2567.

7. Butt, H J; Jaschke, M and Ducker, W A (1995) "Measuring surface forces in aqueous electrolyte solution with the Atomic Force Microscope." *Bioelectrochemistry and Bioenergetics*, **38** **(1)**:191-201.

8. Ducker, W A; Senden, T J and Pashley, R M (1991) "Direct measurement of colloidal forces using an atomic force microscope." *Nature*, **353**:239-241.

9. Rugar, D and Ransma, P (1990) "Atomic Force Microscopy." *Physics Today*, **43** **(10)**:23-30.

Suggested Further Reading

Digital Instruments Web Site: http://www.di.com

Magonov, S G and Whangbo, M-H (1996) Surface analysis with STM and AFM: experimental and theoretical aspects of image analysis VCH. Verlagsgesellschaft mbH, Weinheim.

Acknowledgments

I would like to thank the following for allowing me to use their images in this article; Dr Bryony James for Figure 1, Gabriel Sertsou for Figure 2 and Willium Chiu and Bryony James for Figure 3.

The Research Centre for Surface and Materials Science (RCSMS)

The RCSMS was established in 1987 as a partnership between the Departments of Chemical and Materials Engineering and Chemistry, and is housed within the School of Engineering. Professor Barry Welch and Associate Professor Jim Metson were key in establishing the facility. Funding for the first instrumentation (a Kratos XSAM800) was obtained largely by grants from the University Grants Committee, the New Zealand Lotteries Commission, the University of Auckland Research Committee and New Zealand Steel, with additional funding from BRANZ and New Zealand Aluminium Smelters. Later acquisitions include a Nanoscope IIIA multimode scanning probe microscope (1996) funded by University of Auckland Research Committee, the New Zealand Lotteries Commission and the Research Centre. A merger with the Electron Microscope Facility housed in the Engineering School in 1996 increased the range of techniques available. A major role of the Centre is to operate a surface analysis facility in support of research projects and teaching carried out by academic staff and students of many University departments. The Centre is also active in research projects in conjunction with Crown Research Institutes and short and long term projects for commercial clients. Richard Haverkamp was appointed Technical Director in February 1995.

ABOUT THE AUTHOR

Dr Richard Haverkamp is Technical Director of the Research Centre for Surface and Materials Science and Lecturer in the Department of Chemical and Materials Engineering at the University of Auckland. He has previously worked for Fletcher Challenge, Colgate Palmolive and the DSIR in New Zealand, for the University of Toronto in Canada and SINTEF in Norway and has spent time at Pechiney CRV in France. He has published over 90 scientific papers and technical reports and has been awarded one patent.

NEW LITERATURE & MEDIA

NEW PUBLICATION FROM THE INSTITUTE OF FOOD SCIENCE & TECHNOLOGY

The Institute of Food Science & Technology (IFST) has published a new monograph, *Addition of Micronutrients to Food*. The publication is designed to be a practical working document for both the novice and the experienced scientist working in the field of nutritional enhancement.

Its publication coincided with the distribution of the new European Commission discussion paper, iii/5934/97, *Addition of Vitamins and Minerals to Foods and Food Supplements*, providing a comprehensive review of the legal and technological situation in the United Kingdom with reference to EC directives as applicable.

The document covers the range of permitted additives, the principles to be followed, the effects of processing, the problems associated with excessive enrichment and the changes in the prescribed methods of calculation, all in an easily understandable manner.

The massive increase in the addition of micronutrients, partly as a result of changes in the EC labelling laws, and partly as a result of changes in consumer demands, makes the monograph an essential reference for all working in the food chain, including those in marketing who need to increase the consumer's understanding of the role of nutritional enhancement in a balanced and healthy diet. *Addition of Micronutrients to Food* is available from IFST, price £30. To purchase a copy of the new publication, (cheque with order, please),

Contact: Laura Cole, IFST
5 Cambridge Court, 210 Shepherds Bush Road
London W6 7NJ, United Kingdom
Phone: (+44-171)-6036316, Fax: (+44-171)-6029936
Email: ifst@easynet.co.uk

About IFST: IFST is the professional qualifying body for food scientists and technologists. It is independent of Government, the food industry and any sectorial interest. One of the Institute's objectives is to serve the public interest by furthering the application of science and technology to the supply of safe, wholesome, nutritious and attractive food. For more information on IFST activities, visit our Web Site at: http://www.easynet.uk/ifst/

THE AMERICAN VACUUM SOCIETY INTRODUCES ITS ON-LINE VERSION OF SURFACE SCIENCE SPECTRA

Surface Science Spectra (SSS) will be available in an on-line version at a new subscription rate for individual subscribers. *SSS* Online provides convenient access to the same high-quality, peer-reviewed spectra and related data presented by *SSS* in each quarterly print journal.

Subscribers can access XPS, Auger, and SIMS spectra from a wide range of fields or obtain the most current findings on reference data. Key features of *SSS* Online include a searchable database of all articles - by authors, titles, abstracts, keywords - with links to matching articles. The articles are available in Portable Document Format (PDF), threaded and with thumbnails.

SSS Online will debut with *SSS* Volume 4. Volume 3 is expected to be online by the end of 1997. Online subscriptions will start January 1, 1998, and future issues will be available to subscribers about three weeks prior to the print journal. By the beginning of 1998, *SSS* Online will include more than 80 articles, containing nearly 500 figures representing more than 700 individual spectra, from more than 140 different samples. A portion of the on-line content will be available for review without subscription through December 1997. The subscription rates are as follows:

- **SSS Online Calendar Year Subscriptions** - provides access to all on-line issues for US$100 per year for AVS members or US$150 per year for individual subscribers.
- **SSS Full Subscription** - includes on-line subscription, mail delivery of print journal, and complete digital data (ascii x, y pairs) for all *SSS* articles for US$987 per volume.

For more information, visit the AVS home page at www.vacuum.org, and select *Surface Science Spectra.*

Contact: Surface Science Spectra
150 West Iowa Avenue, Suite 104, Sunnyvale, CA 94086, USA
Phone: (+1-408)-7370285, Fax: (+1-408)-7379529

NEW ZEALAND INSTITUTE OF CHEMISTRY

PRESIDENTS REPORT TO THE 1997 ANNUAL GENERAL MEETING

It is with pleasure that I present the President's report for 1997, an exciting and busy year which I hope will prove to be the start of a successful period of growth for the Institute.

My year in fact started at the end of 1996 at the NZIC conference in Dunedin. My thanks go to Professor Robinson and his team in the Otago Branch for all their efforts in organising this successful conference.

From then on it has been a year of change. Council has been able to build on the ground work of my predecessors, Bill Denny and Nath Pritchard. We have commenced the changes that they identified as necessary to move the Institute forward so that it could become the organisation for New Zealand chemists in the new millennium.

The vision statement (below) summarises Council's aspirations for the Institute over the next few years.

VISION STATEMENT

Membership
An increased active membership that represents the majority of those involved in all aspects of chemical sciences.

Image
Dynamic, modern, respected and publicly recognised, proactive and efficient.

Services
A range of services that provide benefits to members, promote chemical and molecular sciences, and represent those with an interest in chemistry.

Branches
Active Branches that provide a focus for social, networking and service activities.

Specialist Groups
Active specialist groups in chemical sciences that contribute to NZIC and are promoted and supported by NZIC.

Secretariat
A professional service to underpin the above activities. It needs to be business like, proactive, efficient, and have access to modern technologies for good communication with members.

To achieve these goals we have taken several initiatives.

1. Our Vision statement has become part of NZIC's strategic and business plan. It will be the 1st Vice President's responsibility to update this plan each year and then implement it during the presidential term.

2. We have simplified our membership structure. We have now only two grades, members and fellows. Anyone with a genuine interest in chemistry can become a member of the Institute. They need only to be nominated by two members and agree to abide by our code of ethics.

3. Fellowship of the Institute continues to recognise the excellence of a member's contributions to chemical sciences in the broadest context, including service to the Institute. Fellowship of the Institute is an important and unique qualification in that it is an acknowledgement of peer recognition which complements academic and management achievements.

4. The Council has put in place a three year financial plan, which has allowed the Institute to plan for significantly reduced membership subscriptions. Subscription rates were seen as a barrier to achieving our goal of membership growth. Our new membership subscription of $85 is well under the Council's $100 target.

5. Council is also in the process of setting up a new Virtual Secretariat, a service which is based on making maximum use of computerised and electronic facilities to support the Institute's members, branches and council, and to enhance the services NZIC provides.

During the year your Institute has continued to support quality publications, our journal *Chemistry in New Zealand* for our members, and *Chem NZ* for the education sector. My thanks for all their efforts go to the journal editor Robert Lyon and his editorial team from the Auckland Branch, and to Denis Hogan and the *Chem NZ* team from Christchurch Branch.

This year we have sponsored three conferences:
- The 22nd Australasian Polymer Symposium held in Auckland in February 1997,
- The Chemical Education Conference at Massey in July 1997,
- The Oils and Fats Specialist Group conference in November 1997.

We have also continued to support Chemistry in schools by supporting the National Chemical Quiz from Australia, Chem 13 exam from Canada, and the Manawatu Branch Chemistry Quiz.

My presidency has allowed me to visit all the branches, and local branches in Southland, Bay of Plenty and Taranaki. It was great to have this opportunity to meet so many of you. My thanks to those who hosted the meetings and looked after me so well. A highlight of my year was participation in an IUPAC strategic planning meeting in Singapore. This was the first such meeting IUPAC had held in the Asia Pacific region. I would like to acknowledge the financial support for my attendance provided by MoRST through their ISAT (International Science and Technology) scheme.

I am pleased to say that the initiatives that have been taken this year are already leading to growth in our membership numbers. However more work is still necessary. We will need to get our new secretariat up and running next year to achieve our goals. If we are to continue to grow our membership, we will also have to properly integrate our specialist groups into the Institute.

I wish incoming president Alastair MacGibbon all the best as he continues to progress the necessary changes to the Institute. I will be offering my continued support by assuming the responsibilities of Honorary Treasurer for the next two years. In this regard I wish to thank Dennis Karl who is stepping down as Treasurer. He has held this post for eleven years after taking over the position of Registrar from Denis Hogan.

Finally I would like to record my thanks to Alan Turner for his help and guidance during the year. Alan is stepping down as General Secretary and Executive Officer after ten years. He has served the Institute faithfully during this time and knows the membership better than any one else. Members should be grateful for his untiring efforts of their behalf.

Rob Whitney

R S Whitney
President, NZIC

NZIC COUNCIL NEWS

The Council met in Wellington on 25 September 1997 and the following are the highlights from the meeting.

Membership Brochure
All Members will have received a copy of the "Invitation to Membership" brochure - with your subscription invoice! This was created by Otago Branch and thanks were given to the Branch and Dr E W Tan in particular for their fine efforts.

Business Plan
The 1st Vice President (Dr MacGibbon) presented the 1998 Business Plan. It included the setting up of the "Virtual Secretariat" (see below) and the promotion of Fellowship of the Institute to current members.

Membership
Council admitted and welcomed 50 new members to the Institute, and this bodes well for the future. Included were a large number of secondary school teachers who were recruited at the very successful "CHEM ED 97" conference held in Palmerston North. The full list is published elsewhere in this issue of *Chemistry in New Zealand.*

Council also admitted five new Fellows. A photo and pen portrait of each Fellow will be published in the January 1998 issue of *Chemistry in New Zealand.*

Financial
As can be seen from the Financial Report there was an operating deficit for the financial year. With plans for increasing membership it is anticipated that this will be eliminated quite soon. However as an interim measure, grants to Branches would be halved and student travel grants eliminated for the 1997/98 year.

This year also saw the introduction of reduced membership fees with an incentive for prompt payment - a large number of members responded very well to this incentive.

Virtual Secretariat
Council has sought and received several submissions from organisations interested in operating a "Virtual Secretariat" for the Institute. A short list has been prepared and we are now waiting for more detailed submissions to be considered by a sub- committee of the President and Vice Presidents. It is hoped to have the "Virtual Secretariat" operating by the beginning of 1998.

In the process of developing a specification for the "Virtual Secretariat" Council "brain stormed" the concept and it was recognised that there were a whole host of activities in which the Secretariat is engaged. It may not be possible to have all these undertaken by the new Secretariat.

Conferences
It is planned to hold an Institute Conference in Wellington in 1999 to coincide with the 100th Anniversary of the Chemistry Department at Victoria University of Wellington.

1999 will also see the IC'99 Conference in Wellington.

IUPAC
The President tabled a report following his attendance at an IUPAC sponsored meeting in Singapore. IUPAC headquarters have now shifted from Oxford, United Kingdom to North Carolina, USA and the meeting was called as to how IUPAC might better serve its constituents, particularly with respect to the strong economies emerging in the Asia/Pacific Region.

Copies of the report are available from the Secretariat in Wellington.

MEMBERSHIP

The following were accepted by Council at its meeting in September:

FELLOWS

Auckland	DALZELL	Kerry W
Manawatu	WALKER	Neil W
Wellington	MURRAY	Graham J
Canterbury	OUGHTON	Timothy J
Otago	WALLAART	Johannes C

MEMBERS

Auckland	ATOTOTA	Ngarima
	ATTAR-BASHO	Moryad T
	BLACKBURN	Jade
	CHI	Zhang
	CLARK	Mey
	COCKSEY	Brian J

	DAVIES	Rhys
	GIFFNEY	Jan
	HORE	Nathan
	IDRISS	Hicham
	LI	Kwong-Chi
	MAKIN	Miranda
	MILLBANK	Jared
	OLIVER	Christine
	SALTER	David
	SIEGERS	Jan
	SPICER	Julie
	TRAVAS-SEYDIC	Jadranka
Waikato	BONNINGTON	Lea S
	COOPER	Beverley
	DEPREE	Craig
	DINGER	Maarten
	FINCH	Sarah
	HAHSEN	Richard
	MATHIESON	Trevor
	McCAFFREY	Louise J
	SHILLINGTON	David P
	THOMPSON	Dion
	VANDERVEEN	Claudine
Manawatu	COOLBEAR	Kate P
	JULL	Adrian C
	KEER-KEER	Lynda
	KING	Colin
	WIJESEKERA	Swarnapali
Wellington	CROWLEY	James
	JOHNSON	Rosalie
	KEMMITT	Timothy
	LU	Yinrong
	MACHIRAJU	Vekata R
	WATT	Karyn
Canterbury	BEER	David
	BREHAUT	Elizabeth
	HOSKIN	Kristin
	WRIGHT	Kerryann J
Otago	BLACKMAN	Allan
	BROOKER	Sally
	GORDON	Keith
	HAZLE	Richard J
	TAN	Eng W

ANNUAL GENERAL MEETING

Notice is given that the NZIC Annual General meeting will be held on Wednesday 3 December 1997 at 12.30 pm in Room 206, Easterfield Building, Victoria University of Wellington. The Annual General Meeting is being held prior to the December meeting of the Wellington Branch.

Agenda

1. Welcome
2. Apologies
3. Minutes of 1996 Annual General Meeting
4. Matters Arising
5. Annual Report
6. Financial Report
7. Officers for 1998
8. Prizes
9. General Business

NZIC BRANCH NEWS

MANAWATU

Dr Rob Whitney, Director of the Coal Research Association of New Zealand and founding General Manager of CRL Energy Research and Testing, gave the NZIC Presidential address to the Branch at the New Plymouth Power Station on 1 October 1997. This particular venue was chosen to allow a brief meeting to establish a Taranaki sub-group of the Manawatu Branch. Twenty people met with Rob Whitney for dinner followed by his talk on "Coal fired generation without CO_2". The dinner and meeting was ably organised by Lawrence Scott as the initial meeting to reactivate the Taranaki sub-branch. Chemists from many occupations discussed and shared their problems and solutions during dinner and after the meeting. These discussions showed that the value of the NZIC lies with its members and the valuable contacts they bring. Thanks to Lawrence the Taranaki sub-branch is off to a good start and will continue to be a vibrant forum for chemists around the region.

The 1997 Manawatu Schools Chemistry Quiz was held on 28 August and a record 1460 students from 43 schools entered. A quarter of the entries were from outside the Manawatu region ranging from Glenfield College and Westlake Girls' High School in Auckland to Dunstan High School in Central Otago. We hope to extend the quiz to a full nationwide competition in the next few years. The most entries were received from Taradale High School, followed by Central Hawkes Bay College, then Wanganui Collegiate School. The standard of entries were high, with the average Junior mark being 22/30 and the average Senior mark 17/30. The top students were: Senior (29/30): Aparna Krishnan (Hamilton Girls High School), Junior (30/30): Graeme Bolland, Edward Willis, Rachel Ramsay, Eliot von Hartitzsch (Central Hawke's Bay College); Derryn Bicknell (Freyberg High School); Marion Wilson, Alia Cederman (Hamilton Girls' High School); Brendan Sue (Horowhenua College), Andrew McIver, Ryan Astle, Callum Grayson, Brendon Joe, Nick Rowe (Palmerston North Boys' High School); Romilla Franks (Samuel Marsden Collegiate); Michael Morrison (Tararua College); Seamus Jolly (Wairarapa College); Richard Holberton, Sam Khanbhai, Guy Johnston, Andrew Armstrong (Wanganui Collegiate School); Corrina Thompson (Wanganui High School).

Professor Ted Baker, Department of Biochemistry, Massey University, has moved to the University of Auckland with his wife and fellow team member Heather Baker where he will establish a new structural biology laboratory, additional to the one at Massey (previously reported in the July/August 1997 issue of *Chemistry in New Zealand*). Before coming to Massey, Ted completed his doctorate at the University of Auckland and then spent three years in Oxford as a postdoctoral fellow working with Nobel Prize winner Professor Dorothy Hodgkin investigating the structure of proteins using x-ray crystallography. At Massey Ted began establishing the first protein x-ray crystallography laboratory in New Zealand, which now involves about 20 people and has attracted millions of dollars to the University through research funding. Highlights for Ted and his research group during the past quarter of a century include cracking the structure of a kiwifruit enzyme, actinidin, in 1977. Ten years later and work with a human milk protein, lactoferrin, marked another research turning point. Once again, the work's importance was recognised internationally. The group was still relatively small at this stage, made up of Professor Baker, his wife and colleague Heather Baker, Dr Bryan Anderson, Professor Sylvia Rumble and Dr Gillian Norris. The lactoferrin breakthrough attracted funding from the National Institute of Health in the United States, and that funding has continued for the past ten years. The Howard Hughes Medical Institute in the United States has also contributed more than $1 million towards Massey-based research during the past five years. New Zealand support includes the Health Research Council and the New Zealand Dairy Research Institute. The growth of Massey's structural biology laboratory has led to the solving of more than a dozen new protein structures in the past three years. The research has implications in a huge number of fields, especially medicine and biotechnology, with a growing importance for drug design.

The research team of Dr Tony Burrell and Dr David Officer in the Department of Chemistry at Massey University developing a dye capable of imitating photosynthesis for commercial use in producing a cheap electricity source (previously reported in the July/August 1997 issue of *Chemistry in New Zealand*) have been granted $70,000 from RITE in Japan to assist in the technology development collaboration with an Australian company which is producing solar panels to which the dyes would be attached. This is the first RITE grant awarded to New Zealand scientists. RITE, the Research Institute for Innovative Technology for the Earth, is a Japanese Government agency which currently provides nine worldwide grants for fundamental research into the reduction of CO_2 emissions. RITE representative Mr Hiroshi Ikuno visited Massey University recently to meet the Massey chemists regarding their research proposal on artificial photosynthesis and to discuss funding procedures with the University. It is in the making of synthetic equivalents of chlorophyll that the Massey team has an international advantage. Chlorophyll is made up of arrays of more than 200 porphyrin molecules which individually harvest light. While synthetic porphyrins are easy to make in the laboratory, arrays of these synthetic porphyrins are extremely difficult to construct. However, new synthetic methodology developed by the research team has led to the making of the largest porphyrin array in the world, containing 12 porphyrins, and the methods allow this size to be readily doubled or tripled. The use of these arrays as dyes in new photovoltaic solar cells could revolutionise electricity generation.

In the latest round of the Marsden fund bidding, Dr Benny Theng, Landcare Research New Zealand, was awarded $275,000 for a three-year project 'Survival of fullerenes in geological environments'. Fullerenes, a class of pure-carbon cluster compounds with a cage-like structure, were discovered only a little more than a decade ago. There is recent evidence for the occurrence of fullerenes in ancient clay seams in New Zealand. Because of the ability of clays to protect carbon compounds against chemical and microbial decomposition, it is proposed that the long-term survival of fullerenes in geological environments is due to their close association with clay surfaces. The objective of the research is to find out if clays can adsorb/intercalate fullerenes and, if so, to assess the structural integrity and stability of the surface species.

The Chemistry Department, Massey University is farewelling several of its students who are also members of the Branch. Andrew Gilbert has been awarded a prestigious Cambridge Commonwealth Trust Prince of Wales Scholarship to study for a PhD degree in the Chemistry Department at Cambridge University. He will be working in the area of computational quantum chemistry with Dr Peter Gill. Dr Jeremy Dombroski has accepted a postdoctoral position at Q-Chem Inc. in Pittsburgh working with Q-Chem President, Dr Benny Johnson. He will commence by acting as a coordinator for Q-Chem's multi-site collaborative efforts and as resource manager for the many Unix platforms at Q-Chem headquarters. Dr Mark Smales is to take up a postdoctoral position with Dr David James at the University of Kent and will be working on therapeutic blood products. This will involve some organic synthesis, protein chemistry, peptide synthesis, various types of mass spectrometry, NMR and glycosylation studies. Mark Smales was the Branch Secretary and was farewelled by Branch Committee members at a convivial dinner at the new 'Mr India' restaurant in Palmerston North. The farewell included Dr Clyde Smith, Biochemistry Department, who was the Branch Treasurer and who is joining Professor Ted Baker's newly established protein crystallography group at the University of Auckland .

Alastair MacGibbon from the New Zealand Dairy Research Institute, and current NZIC 1st Vice-President, has been travelling recently. He presented a paper at the Conjugated Linoleic Acid Forum held on the 13-14 August 1997 at the University of Wisconsin, USA, and also a poster at the Functional Foods/Designer Foods for the Future forum held 30 September - 2 October 1997 in Cork, Ireland.

Harry Percival

WAIKATO

NIWA WAIKATO SCIENCE FAIR 1997

Congratulations are extended to Nuwan Rohitha and Katie Martin who won respectively the junior and senior New Zealand Institute of Chemistry Prizes for projects related to Chemistry in the NIWA Waikato Science Fair. Nuwan presented a project on sap stain fungi, and Katie a project on lead in roadside dust.

CHEMQUEST 97

On the evening of Wednesday 29th October 1997, the University of Waikato hosted the inaugural Chemquest, a chemistry quiz for 6th form students. A total of 46 teams (each of three, occasionally four students) participated in the event, which was held in the Coopers and Lybrand Lecture Theatre. The students represented a total of 22 schools from the greater Waikato region, with the team travelling from Opotiki being awarded a special prize for travelling the greatest distance to participate!

The questions (a total of 50) were divided into 5 sections, and covered a wide range. The first section was centred around the Periodic Table, and each student was provided with a New Zealand Institute of Chemistry Periodic Table poster, as part of an information pack, which also contained general University of Waikato and chemistry information. The second section of questions was based around chemical demonstrations, with students required to write equations and identify products of reactions. Section three really got to grips with the senses with a series of questions where students were required to identify the smells of various chemicals (all non-toxic, well-known smells such as violets and aniseed). This was followed up by a series of music questions, which covered various occurrences of chemistry in music, such as the song "Lithium" by Nirvana. Section four involved the identification of famous scientists (one of whom was Margaret Thatcher - appropriately enough known as the "Iron Lady"- who has a track record, albeit short, of publishing papers in chemistry journals). Section five, entitled the Wide Wide World of Chemistry, covered general areas of chemistry, in particular how chemistry covers all aspects of modern day life.

First prize winners were the team from Tauranga Boys' College A, who received a cash prize of $150, gold medals, together with a trophy generously donated by James and Wells Intellectual Property Agents of Hamilton. Second Prize (silver medals and $90) went to a team B from St Paul's Collegiate School (Hamilton), third prize (bronze medals and $60) to St. Paul's Collegiate A, while shared 4th prize (total $75) went to three teams Hamilton Boys' High School A, Hillcrest High School C and John Paul College (Rotorua) A. There was also a draw for Exscite Science Centre tickets at the end of each section, and questions about the displays provided by the various sponsors ensured that many teams went away with a "prize in hand".

The organisers are very grateful to the sponsors: James & Wells, New Zealand Institute of Chemistry, NIWA, Convex Plastics, Hill Laboratories, and the Exscite Science Centre. The input of the following Chemistry Department staff who helped make the event a success is greatly appreciated: Annie Barker, Jenny Chapman, Natalie Curnow, Pat Gread, Wendy Jackson, Jannine Sims, Richard Coll, Lyndsay Main, Brian Nicholson, and Michele Prinsep. Thanks also go to Anne Hume (Hamilton Girls' High School) for her invaluable input, to Nick Kim for designing the Chemquest logo, Cathie Shaw for the certificates, and to Tim Foy (Huntly College), Shirley Brown (Hamilton Girls' High School) and Sue Scahill (Matamata College) for assistance with the judging.

Bill Henderson
Department of Chemistry, University of Waikato

WELLINGTON

Dr Gerald Smith of Industrial Research Limited presented a popular talk at our September meeting, entitled "The Electron in Chemical Reactions" celebrating the centenial of the discovery of the electron. J J Thomson announced his discovery in April 1897 at the Royal Institution. Gerald has worked with Lord George Porter at the Institution's Davy-Faraday Laboratory so chose to present with a number of demonstrations in the spirit of the Faraday Christmas Lectures.

Gerald's talk traced the development of the exploitation and understanding of electron transfer reactions from the earliest technologies; through Faraday's work, which linked electrical charge to chemical changes; through Thomson's discovery of the electron; to present-day chemistry. There was an emphasis on dyes. A familiar blue one made in Nimes, France was shown, the place of discovery lending its name to the popular blue jeans colour - denim! This was an entertaining talk, with the names of many of chemistry's pioneers popping up throughout the evening. It was a very successful meeting with over 70 people in attendance including families and high school students.

In October a number of members took the opportunity of visiting the sewage treatment facilities that are nearing completion at Moa Point. This meeting was organised by the Wellington Branch of the ACA (Australasian Corrosion Association) with very good timing - lots of the chambers which were part of the tour will have an intolerable stench within a couple of months. There were plenty of statistics to back claims of how well the plant will handle all the contributions that will be made, but more importantly one gets a good feeling knowing that the Wellington South coast is getting a chance to recover from the years of biological onslaught.

The October AGM, despite beginning with a complimentary selection of cheeses (to entice more members' participation), still had the lowest attendance of any of our meetings for the year. The Wellington Branch has recently reached an agreement to become affiliated with Science Wellington as the Chemistry Section of that body, while still remaining autonomous. Under the agreement, all our members receive the Science Wellington Newsletter and our meetings are advertised in it, giving us wider publicity in the region and making our Institute known to more potential members. It was also noted that attendance at our monthly meetings had increased significantly this year (by about 80%!), partly due to our above affiliation, although we have not (yet!) had a corresponding increase in new members. The National NZIC Conference to be held in Wellington in 1999 was also discussed. This Conference will mark both the centenary of Victoria University and the appointment of Professor Easterfield as Foundation Professor of Chemistry and Physics. It was suggested that the Conference be moved to December 1999 (February 1999 was originally proposed) and the Committee is in the process of appointing an organising committee.

After the AGM, members were treated to a fascinating talk by Dr George Slim of Industrial Research Limited entitled "Fringe Chemistry". George spoke of his team's research on GAGs - glycosaminoglycans. The talk covered the biosynthesis and biological function of GAGs as well as their role in some of the 'new' natural health remedies, such as the use of shark cartilage to prevent cancer. His group has worked on the isolation and chemical modification of GAGs from various sources and have been testing their bioactivity, recently discovering that one of the major bioactive compounds in shark cartilage is not a true GAG after all!

The Analytical Chemistry Competition, which is a very successful annual event promoting our Institute in the local secondary schools, was held in September. The winners were: Peter Luk and Nick Woodward (both from Hutt Valley High School). The competition was once again successfully run by Dr David Weatherburn and Izabela Pomer of the School of Chemical and Physical Sciences at Victoria University. Their hard work and effort in bringing this to fruition each year is gratefully acknowledged.

Committee members elected for 1997/98 are:

Chairperson:
Graham Murray, Secondary School Chemistry Teacher

Secretary:
Sue Freitag, Central Laboratories, Works Consultancy

Treasurer:
Alan Turner, Executive Officer, NZIC

Members:
Dr Vince Gray, Consultant
Mr Paul Pilotto, Victoria University Postgraduate Representative
Professor John Spencer, Victoria University
Dr Rod Tilbury, Victoria University

VICTORIA UNIVERSITY NEWS

Dr Peter Northcote, who returned to New Zealand in 1994 after working in Tonga and the USA, has recently been promoted to Senior Lecturer. Peter has been instrumental in setting up the new second year Spectroscopy course and is a popular lecturer, particularly at the first year level. His research interests are in natural product chemistry with one of his main projects being the isolation and testing of medicinal compounds from marine sponges.

Professor Robin Ferrier will be retiring as Professor of Organic Chemistry at the end of January 1998 after many years at the helm. A comprehensive article on Robin and his research will appear in the next issue of *Chemistry in New Zealand.*

NEWS FROM IRL

Six of the recent Royal Society RS&T Medals were awarded to IRL scientists, four of which went to chemists:

Tony Woolhouse - Advances in Synthetic Organic Chemistry
Ken Markham - Understanding the Chemistry of Flower Colour
Rodger Newman - Applications of NMR to Chemistry
Ken MacKenzie - Research on Minerals and Ceramics.

TREASURER'S REPORT

FINANCIAL YEAR 1996/1997

The annual Financial Statement of accounts of the Institute for the financial year 1996/1997 is presented.

The accounts show an operating deficit of just under $30,000 for the year. Once adjustments are made for the effects of the cross over of the financial operating years of the Chemical Olympiad and the ANC Quiz the true operating deficit of the Institute is about $10,000. This is in line with the expected results for the financial year.

Subscription income shows a decrease of about $11,000 while the net income shows a decrease of about $5,000. Total expenditure showed a small increase.

In order to make the accounts clearer the Institute accountants have suggested a mechanism to identifiy and isolate the sums attributable to the Olympiad and ANC Quiz activities from the main body of the accounts. This recommendation will be passed on to the incoming treasurer.

Two other significant changes to the financial outlook of the Institute for the coming year are the decision to proceed with the reduced subscription rate proposal together with the decision to make the Institute financial year coincide with the calendar year.

These are significant steps taken to assist in the process of change to the Institute that commenced with the Bill Denny led investigation and report reflecting on the needs and suggestions of you the Institute members.

Dennis Karl
Honorary Treasurer

NOTES TO THE FINANCIAL STATEMENTS FOR THE YEAR ENDED 30TH APRIL 1997

STATEMENT OF ACCOUNTING POLICIES

1. REPORTING ENTITY

New Zealand Institute of Chemistry (Inc.) is a reporting entity registered under the Incorporated Societies Act 1908. The financial statements of the Institute have been prepared in accordance with generally accepted accounting practice and the Framework for Differential Reporting 1993.

2. MEASUREMENT BASE

The accounting principles recognised as appropriate for the measurement and reporting of earnings and financial position on a historical cost basis are followed by the Institute.

3. SPECIFIC ACCOUNTING POLICIES

The following specific accounting policies which materially effect the measurement of financial performance and financial position have been applied:

NEW ZEALAND INSTITUTE OF CHEMISTRY INC.

STATEMENT OF FINANCIAL PERFORMANCE FOR THE YEAR ENDED 30TH APRIL 1997

			1996
REVENUE			
Subscriptions from Members		75,817	84,979
Chem NZ-RSC Subs		12,070	8,750
Publication Sales		992	1,457
Conference Surplus		2,309	817
Chem 13 Exam Fees		3,258	3,402
Chem Education Subscriptions		-	277
IUPAC		30	(441)
Chem 13 News		30	570
Equiticorp Capital Repayment		-	3,676
Fees ANC Quiz		6,897	1,788
Conference Fees – IMM		-	158
		101,403	105,433
Chemical Olympiad Donations	39,252		43,314
Chemical Olympiad Expenses	50,900		24,128
		(11,648)	19,186
Gross Revenue from Operation		89,755	124,619
EXPENDITURE			
Accountancy & Audit Fees	2,057		2,649
Accommodation Expenses	4,239		1,171
ANC Quiz Expenses	10,275		-
Branch Expenses – Capitation Fees	11,341		11,411
Branch Expenses – Student Travel	3,000		3,000
Chem NZ Expenses	5,035		12,115
Chem 13 Expenses	502		1,907
Conference Expenses	950		140
Donation	640		-
Depreciation	18		30
Goods & Services Tax	2,637		3,978
Interest & Bank Charges	528		990
Legal Costs	1,350		-
Journal – Publisher	10,033		10,150
Sundry Publications for Resale	2,795		1,757
Overseas Visitors Expenses	-		500
Printing, Stationery, & Postage	5,731		7,341
Prizes	650		400
Rent to IPENZ	2,565		2,565
Secretarial Services	42,313		41,883
Secretarial – Audit	-		2,656
Subscriptions	2,175		1,516
Telephone & Fax Charges	1,439		457
Travelling Expenses	13,248		12,079
		123,521	118,695
		33,766	(5,924)
OTHER INCOME			
Interest - BNZ	4,116		4,313
Interest - Local Body Stock	(188)		31
		3,928	4,344
Operating Deficit		29,838	(10,268)

NEW ZEALAND INSTITUTE OF CHEMISTRY INC.

BALANCE SHEET
AS AT 30TH APRIL 1997

				1996
CAPITAL FUNDS				
Chemical Olympiad Reserve			3,923	-
Easterfield Reserve			-	567
General Reserve			43,343	46,699
Balance at the Beginning of the Year			15,962	5,694
Plus Net Surplus (Deficit) for Year			(29,838)	10,268
			33,390	63,228
REPRESENTED BY:				
CURRENT ASSETS				
Accounts Receivable		17,472		6,714
BNZ Current Account		3,889		1,912
BNZ Autocall Account		362		17,131
BNZ Term Deposits		16,152		38,878
			37,875	64,635
FIXED ASSETS				
Office Equipment	582			582
Less Accumulated Depreciation	508			490
		74		92
Presidential Chain		360		360
			434	452
INVESTMENTS				
Equiticorp $21,000 Debenture		1		1
Lyttleton Harbour Board Stock 6.25% 1998		500		500
			501	501
TOTAL ASSETS			38,810	65,588
CURRENT LIABILITIES				
Accounts Payable	5,420			2,360
		5,420		2,360
TOTAL LIABILITIES			5,420	2,360
NET ASSETS			33,390	63,228

The accompanying notes form part of these financial statements.

- Accounts Receivable are stated at their net realisable value after allowing for all bad debts.

- Fixed assets are stated at cost less aggregate depreciation. Depreciation has been calculated using the maximum rates permitted by the Income Tax Act 1994.

- Investments are valued at cost value at balance date.

- The financial statements have been prepared on a GST inclusive basis. Accounts Payable and Accounts Receivable are stated inclusive of GST. All other assets and liabilities have been stated GST exclusive.

- The Institute qualifies for differential reporting as it is not publicly accountable and it is not large. Total revenue is less than $2.5 million, assets are less than $1.5 million and there are less than 20 employees. The entity has taken advantage of all available differential reporting exemptions.

4. CHANGES IN ACCOUNTING POLICY

There have been no changes in accounting policies. All policies have been applied on bases consistent with those used in previous years.

AUDITORS REPORT
NEW ZEALAND INSTITUTE OF CHEMISTRY INC.

Audit Report:

We have audited the financial report attached. The financial report provides information about the past financial performance of the Institute and its financial position as at 30 April 1997. This information is stated in accordance with the accounting policies above.

Executive Council's Responsibilities:

The executive council is responsible for the preparation of a financial report which gives a true and fair view of the financial position of the Institute as at 30 April 1997 and of the results of operations for the year ended on that date.

Auditor's Responsibilities:

It is our responsibility to express an independent opinion of the financial report presented by the Board and report our opinion to you.

Basis of Opinion:

An audit includes examining, on a test basis, evidence relevant to the amounts and disclosures in the financial report. It also includes assessing:

- the significant estimates and judgements made by the Executive in the preparation of the financial report, and

- whether the accounting policies are appropriate to the Institute's circumstances, consistently applied and adequately disclosed.

We conducted our audit in accordance with generally accepted auditing standards in New Zealand. We planned and performed our audit so as to obtain all the information and explanations we considered necessary. We obtained sufficient evidence to give reasonable assurance that the financial report is free from material misstatements, whether caused by fraud or error. In forming our opinion we also evaluated the overall adequacy of the presentation of information in the financial report. In common with other organisations of a smiliar nature, control over revenue prior to it being recorded is limited and there are no practical audit procedures to determine the effect of this limited control, and our audit opinion below is subject to this comment.

Unqualified Opinion:

We have obtained all the information and explanations we have required.

In our opinion:

- proper accounting records have been kept by the Institute as far as appears from our examination of those records and

- the financial report attached:
  - complies with generally accepted accounting practice;
  - gives a true and fair view of the financial position of the Institute as at 30 April 1997 and the result of its operation for the year ended on that date.

Our audit was completed on 30 October 1997 and our unqualified opinion is expressed as at the date.

MARKHAMS, Auckland

ADVERTISERS INDEX

A.i. SCIENTIFIC (NZ) LTD Inside Front, 6
ALLTECH ASSOCIATES 8
ANCAT HOLDINGS LTD 24
BIOLAB SCIENTIFIC LTD Inside Front Cover
GBC-AEC 29
HOARE RESEARCH SOFTWARE Inside Back Cover
JOHN MORRIS SCIENTIFIC LTD 27
LABSPEC 24, 32
LABSUPPLY PIERCE Back Cover
MAF QUALITY MANAGEMENT
- National Chemical Residue Laboratory 11
SCI TECH 33
SHIMADZU NEW ZEALAND 12
SIGMA ALDRICH PTY LTD Front Cover

Software Review: CambridgeSoft ChemOffice Pro Ultra 4.0

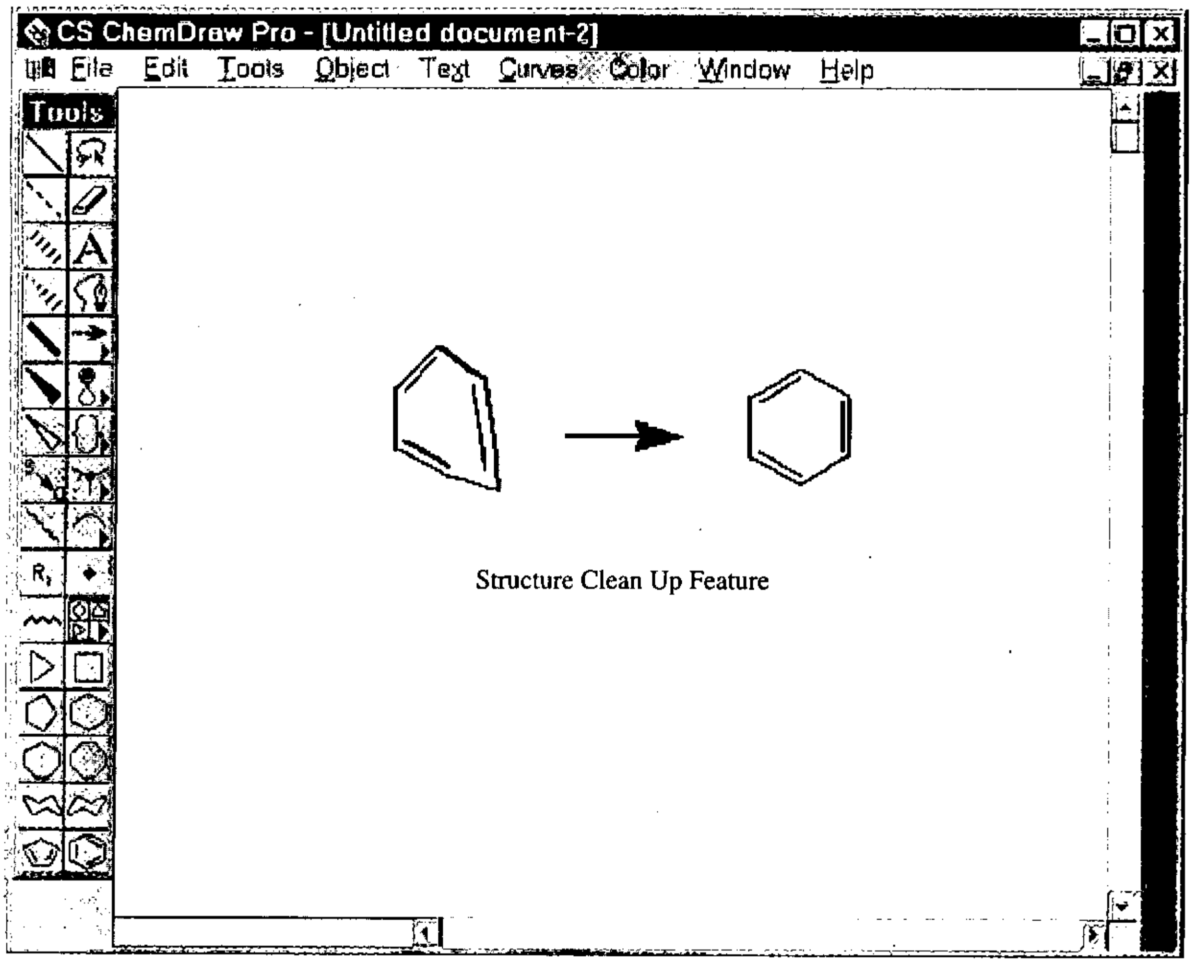
Peter D W Boyd
Chemistry Department, University of Auckland, Private Bag 92019, Auckland

---

The *ChemOffice Pro Ultra Ver 4.0* from CambridgeSoft consists of a suite three programs; *ChemDraw Pro*, *Chem3D Pro*, *ChemFinder Pro*, and the *ChemInfo Pro* database. It is designed to run on either Windows-based personal computers (3.11,95, and NT all in 32 bit mode) or on Apple Macintosh computers. Each of the modules is a stand-alone application with good integration with its partners.

ChemDraw 4.0 is a comprehensive chemical structure drawing program with many extra features that integrate with the two other modules of the *ChemOffice* Suite. It is a well known program originally developed for Apple Macintosh computers. *ChemDraw* like several other available drawing programs provides an easy entrance into sophisticated chemical drawing. The basic drawing features of this package are available from a tools palette in the graphical interface. A wide range of bond and ring tools are available and chemical structures are easily labelled and annotated using a text tool. A set of tutorials are provided which rapidly familiarise a new user with most of the drawing techniques. These range over the construction of reaction schemes, drawing of intermediates, using complex structures with fused rings, Fischer projections, Newman projections and techniques for the perspective drawing of molecules. Although, like many such drawing programs, the prime aim is the depiction of organic molecules and their reactions, inorganic and organometallic complexes are readily drawn. A special feature in this version is the Clean Up command which regularises bond lengths and angles.

ChemDraw has many methods of sharing information (molecular structures) with other programs and applications. Simple copy, cut and paste, and drag and drop features are all well supported as well as Object Linking and Embedding (OLE) protocols. We found that this worked well with both *Microsoft Word 97* and *Corel WordPerfect 8* word processors. Further it is possible to export structures as SMILES strings which are used in several database-property applications. A variety of other formats are possible (e.g. Postscript, ISIS/SKC). GIF format files may be generated for inclusion in internet HTML documents. *ChemDraw* structures may be written as *Molecular Design* MolFiles (*.mol) and *Molecular Simulations* MolFiles. These allow the transition from line drawings to three-dimensional structure. For example *.mol files may be read into the *Chem3D* program for modelling or into a viewing program such as *Molecular Simulations* WebLab viewer or Rasmol. This provides a link between the drawing of complex



Structure Clean Up Feature

structures and the generation of a three-dimensional molecular structure of this drawing. Using *Chem3D* it is then possible to export back a particular view of such a molecule to *ChemDraw* where an appropriate line drawing of this orientation is displayed.

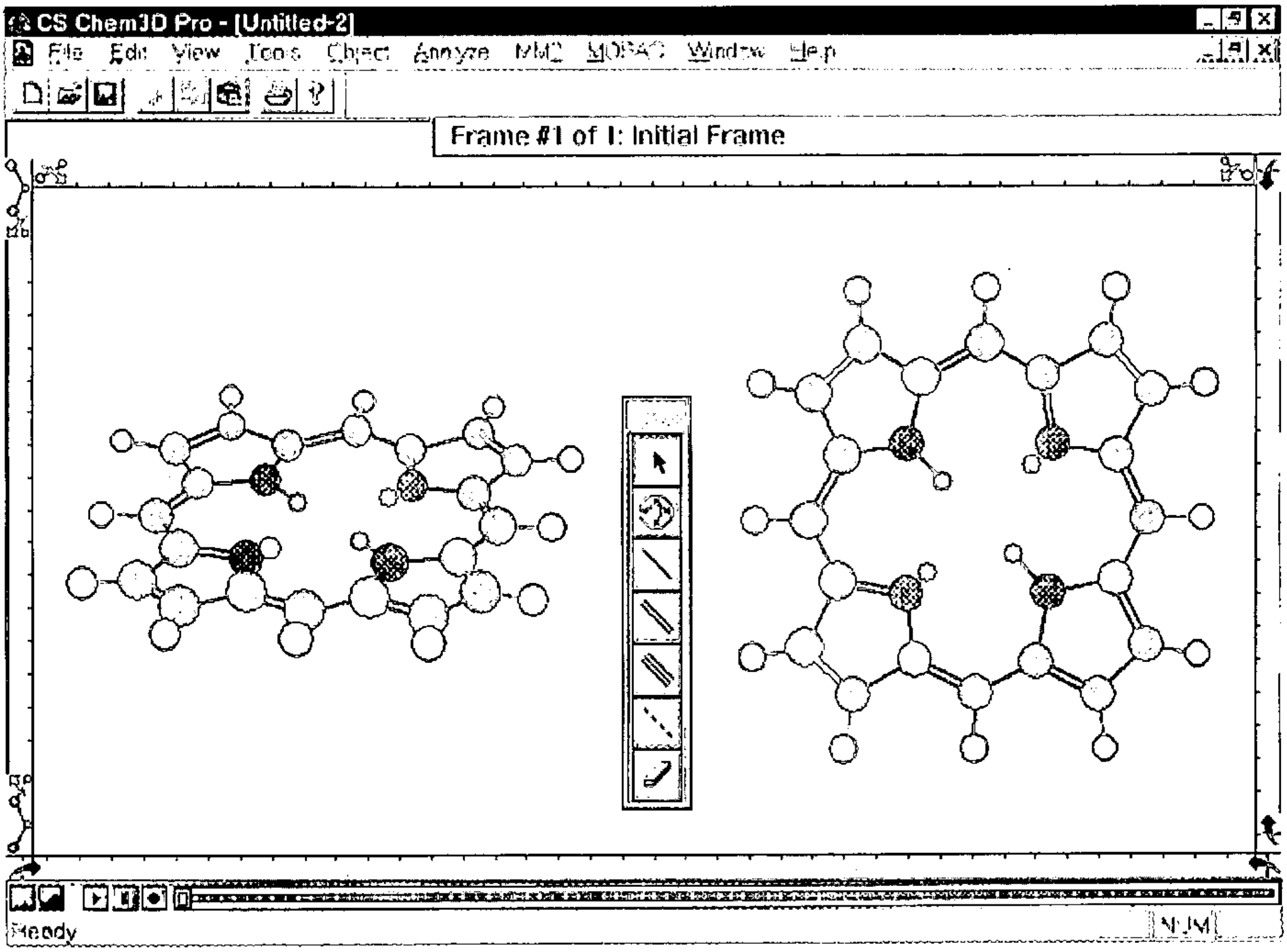
Chem3D Pro is a stand-alone molecular modelling package. Structures may be imported from other building programs in a large variety of formats including all of the most popular such as Protein Data Bank, Molecular Design, Cambridge Crystal Data Base and MOPAC files. Three-dimensional models may also be constructed and modified within the program. There is a very useful tool for the use of substructures in molecular building. A large number of these are available in a database. Substructures may also defined by users and added to this database.

There are two computational tools for the optimisation of molecular structures. The first of these is based on the MM2 molecular mechanics model of Allinger. Force field parameters for MM2 are known for a wide variety of organic molecular atom types. There are extensions to the force field for other elements including transition metals. Some care should be used with these as not all force field parameters are available for these situations. However it is easy to monitor this either by examining the force field tables directly using the *Table Editor* or by a detailed examination of the outputs of a molecular mechanics calculation. There is a clear indication of the quality of the parameters used. Limited conformational searching is available in the Windows version (tested here) but the Apple version also has a dihedral driver option for more systematic searches. The second computational tool, an implementation of the well known semi-empirical molecular orbital program MOPAC is also available. This is based on the most recent version MOPAC 93 and contains all features contained in the original version. MOPAC will compute optimised molecular geometries, heats of formation solvation energies, reaction paths and transition states for closed and open shell molecules.

ChemFinder Pro is a database management system. It allows the storage of information in the form of chemical structures from *ChemDraw* and *Chem3D*, molecular properties, tables of data, text and images. Databases may be designed and created along with forms to display data. *ChemFinder* allows searching by a large variety of textual and structural identifiers. The release reviewed here contained examples of several databases and the *ChemInfo Pro* database was accessible on the CDROM. This contains forms and databases from several chemical catalogues and the NCI archive of compounds. There are now many commercially available chemical databases that may be interrogated by *ChemFinder* such as Index Chemicus (ISI), ChemReact and ChemSelect(InfoChem).

The CDs provided with the *ChemOffice* suite provided both Macintosh and Windows versions. We tried installing the suite on both a 66 Mhz 486 PC (Windows 3.11) and a 200 Mhz Pentium Pro PC (Windows NT 4.0). Both installations worked easily to give a full running version of the software. There are some memory requirements for some parts of these programs and it is probably best to run this software on a PC with at least 16MB of RAM.

In conclusion this suite of software provides a large range of drawing, modelling and informational procedures. We found it easy to get started in *ChemDraw* and *Chem3D*. Once basic tasks are mastered there is a rich collection of features to be discovered.



ChemOffice® 97

NEW Office Ultra

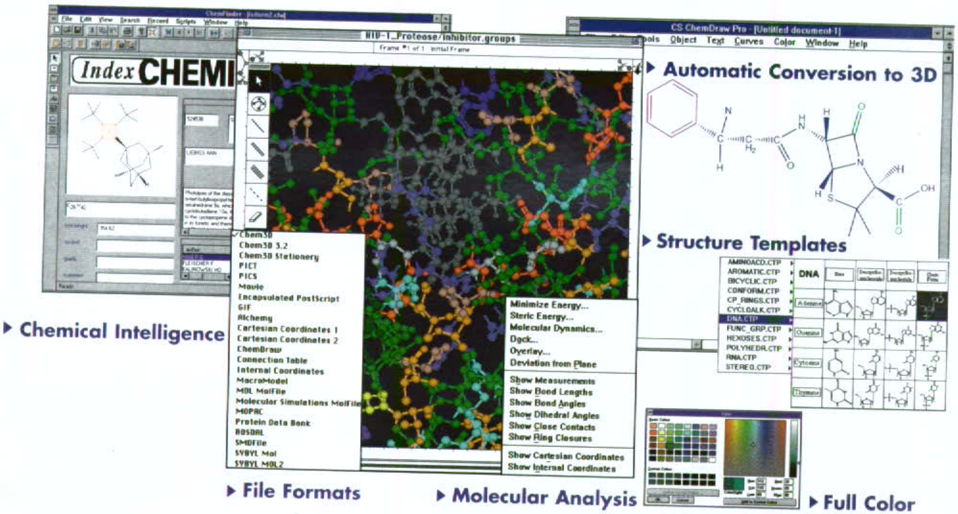
Drawing, Modeling and Information

The *ultimate* software suite for chemists

ChemOffice Pro combines *ChemDraw Pro*, *Chem3D Pro*, and *ChemFinder Pro* into one complete suite for molecule drawing, 3D visualization and computation, chemical database management, and full Internet client/server capability.

Draw reaction mechanisms for publication, visualize 3D molecules and macromolecules, compare conformational isomers and protein surfaces. Perform semi-empirical quantum mechanics calculations with optional *CS MOPAC Pro*. Store molecules for fast retrieval and connect to external chemical databases.

ChemOffice Ultra includes it all, adding *CS ClipArt Pro*, *CS MOPAC Pro*, *ChemInfo Pro*, and more to *ChemOffice Pro*. With *ChemOffice*, the world of chemistry is only a few clicks away!



HRS

Call Today!

Ask about edu prices & competitive upgrades.

Hoare Research Software 0800 HRS PRO (477 776)

CS ChemOffice Std $2350
Pro $2850
Ultra $3295

Also Available:

CS ChemDraw 4.0

With more than 100,000 users around the world, *ChemDraw* is the standard chemical structure drawing software.

ChemDraw Std $895
Pro $1395
Ultra $1850

CS Chem3D 3.5

Advanced visualization and computation. Includes semi-empirical methods, mechanics, protein ribbon views, and more. Output your model to Postscript or GIF (for WWW publishing).
Chem3D Ultra includes *CS MOPAC Pro*.

Chem3D Ultra $1850

CS ChemInfo 4.0

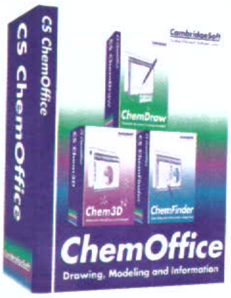
Complete chemical supplier and reference data on CD–ROM. *ChemINDEX*, *ChemRXN*, *ChemACD* and *ChemMSDS* provide easy access to catalogs from Aldrich, Fisher, Acros, and others, as well as up-to-the minute reaction and molecule data from ISI, the NCI, and the WWW. Visit the world's chemical index, the *ChemFinder WebServer*, at www.camsoft.com

ChemInfo Ultra $1850

All prices are in $NZ, include shipping, and exclude GST.

ChemOffice System:
Windows: 3.1, '95, NT   Macintosh, Power Macintosh

circle number 2 on the reader reply card



☑ ***Yes!*** Please send me my **FREE CD-ROM**

Name ______________________________
Firm ______________________________
Street ______________________________
City ______________________ State ______________
Zip ______________________ Country ______________
Phone, Fax ______________________ Email ______________

ChemFinder WWW Chemical Index www.camsoft.com

TEL 0800 HRS PRO (477 776)
EMAIL info@hrs.co.nz **FAX** (07) 8399 103 **WWW** www.hrs.co.nz
MAIL Hoare Research Software P.O. Box 4153 Hamilton East NEW ZEALAND

Microsoft Windows Compatible 32-Bit Application   R&D Elite   Macworld ★★★★   Scientific Computing & Instrumentation Reader's Choice '97   N

CambridgeSoft
Desktop Chemistry Software Leader

NEW ZEALAND'S TECHNICAL SOFTWARE SOURCE

NO PAIN YET GAIN.

Whatman GD/X Syringe Filters are specifically designed to ease filtration of even the most difficult samples. Using state-of-art technology, Whatman Multigrade 150 (10:1 µm) is meshed with Grade GF/F (0.7 µm) without the use of adhesives to constitute the unique prefilter. A wide choice of filter media of different pore sizes is available to meet all your needs. Both 13mm and 25mm syringe filters are available both sterile and non-sterile.

4mm Syringe Filter

- Allows maximum filtrate recovery from a sample of 2ml or less
- Available with tube tip to facilitate transfer of sample into small vials
- Autoclavable, also available sterile

13mm Syringe Filter

- Provides clean filtrate from small volumes up to 10ml
- Wide variety of filter media of different pore sizes
- Autoclavable, also available sterile

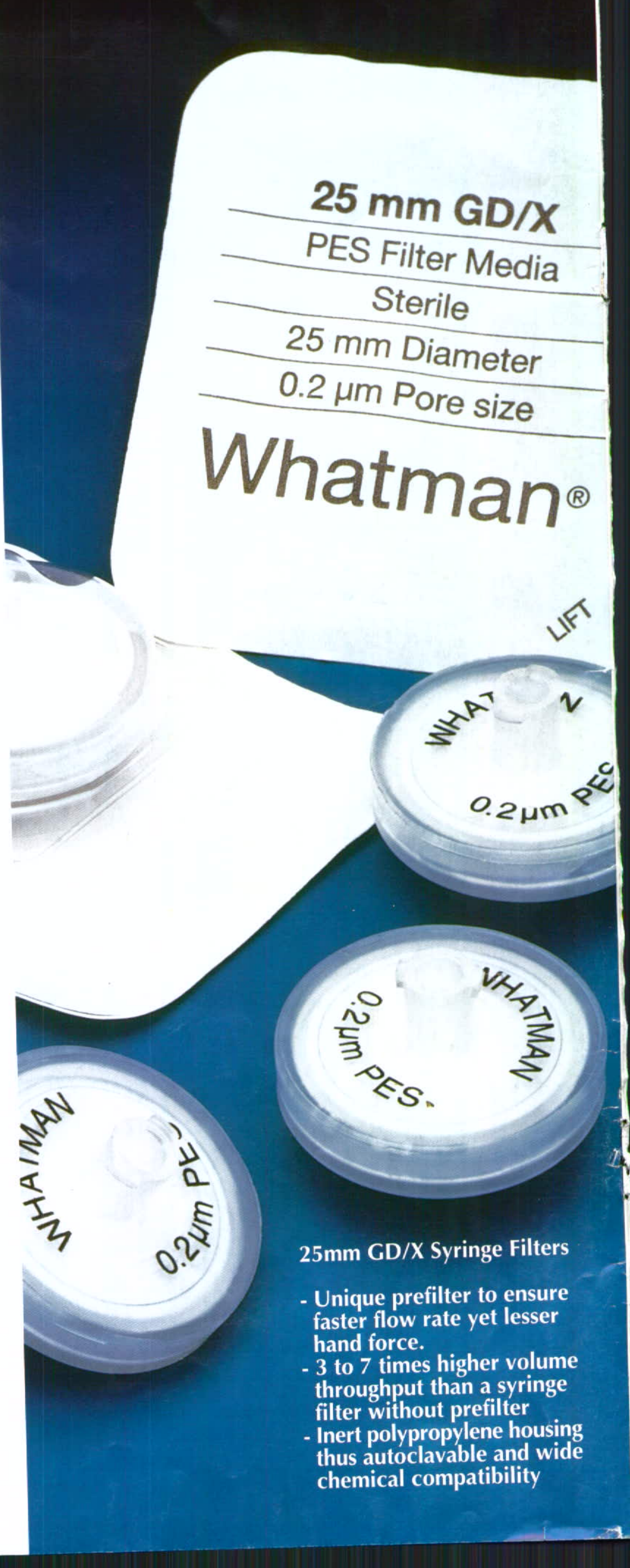
Puradisc 25 Syringe Filter

- Filters samples of more than 10ml
- Faster flow rate, higher volume throughput
- Wide variety of filter media of different pore sizes
- Autoclavable
- Available sterile & non-sterile

Whatman®

Lab Supply Pierce (NZ) Ltd
127 Sunnybrae Road
Glenfield, P.O.Box 34-234
Birkenhead, Auckland 10
New Zealand
Tel: (09) 443 5867 Fax: (09) 444 7314

circle number 3 on the reader reply card



25mm GD/X Syringe Filters

- **Unique prefilter to ensure faster flow rate yet lesser hand force.**
- **3 to 7 times higher volume throughput than a syringe filter without prefilter**
- **Inert polypropylene housing thus autoclavable and wide chemical compatibility**

BUSINESS REPLY POST
Authority No. 90144

POST
PAID

Postage Paid if
posted in NZ

ANCAT HOLDINGS LTD
P O BOX 38546
HOWICK
AUCKLAND 1730

1. SURNAME: INITIALS: TITLE:
INSTITUTION OR COMPANY:
DEPARTMENT:
ADDRESS:
TEL: FAX:
EMAIL:

2. YOUR FUNCTION (please tick)
- MANAGEMENT ☐
- RESEARCH/DEVELOPMENT ☐
- PRODUCTION ☐
- QA/QC ☐
- TEACHING ☐
- PURCHASING ☐
- CONSULTING/ADVISORY ☐
- OTHER (please specify) ☐

3. WHAT EQUIPMENT/TECHNIQUES DO YOU USE? (please tick)
- GC/GC-MS ☐
- UV/VISIBLE SPECTROSCOPY ☐
- AA SPECTROSCOPY ☐
- NMR ☐
- THERMAL ANALYSIS ☐
- MICROSCOPY ☐
- pH/ELECTROCHEMISTRY ☐
- CENTRIFUGES ☐
- XRF or XRD ☐
- HPLC/LC ☐
- FLUORESCENCE SPECTROSCOPY ☐
- ICP, ICP-MS ☐
- POLYMERASE CHAIN REACTION ☐
- FTIR/IR SPECTROSCOPY ☐
- ELEMENTAL ANALYSIS ☐
- PARTICLE SIZE ANALYSIS ☐
- MASS SPECTROSCOPY ☐
- OTHER (please specify)

4. I WOULD LIKE TO KNOW MORE ABOUT BECOMING A MEMBER OF THE NEW ZEALAND INSTITUTE OF CHEMISTRY. PLEASE SEND ME DETAILS.

Please tick ☐

5. I AM INTERESTED IN FURTHER INFORMATION ON THE FOLLOWING NUMBERED PRODUCTS.
(CIRCLE THE CORRESPONDING NUMBER FROM THE BASE OF THE ADVERTISEMENT OR ARTICLE)

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
31	32	33	34	35	36	37	38	39	40	41	42	43	44	45
46	47	48	49	50	51	52	53	54	55	56	57	58	59	60

Chemistry in New Zealand November/December 1997

READER REPLY PRODUCT INFORMATION REQUEST CARD

Dear Reader

This postage paid card is provided so that you can request further information on the products and services featured in this publication.

Please answer all questions on the card. Alternatively you may wish to contact the supplier(s) directly.

Please tell your supplier you saw their product in *Chemistry in New Zealand.*