



# Chemistry

IN NEW ZEALAND

■  
**SPECIAL  
FEATURE:  
SPECTROSCOPY**

■  
**CHEMISTRY  
IN THE  
MANAWATU**

■  
**HEALTH AND  
SAFETY IN  
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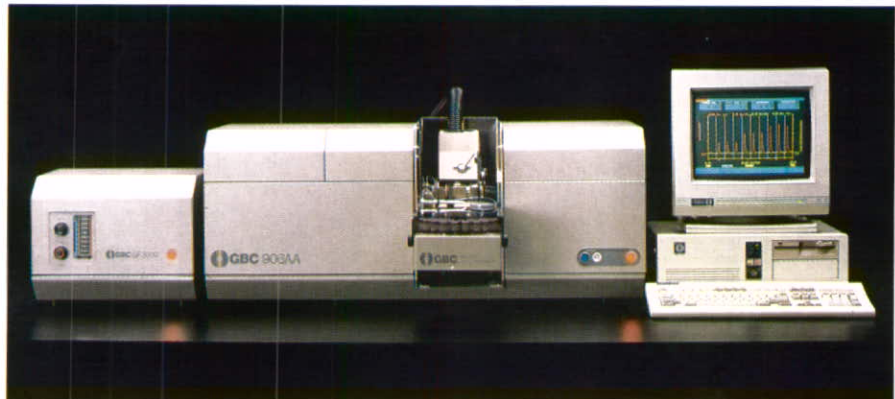


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This issue of Chemistry in New Zealand is brought to you with pride by the Manawatu Branch of the Institute. Manawatu is one of the larger branches, with 174 members and covering the area indicated in our branch logo, including New Plymouth, Napier and Levin. However most of the membership (75%) and most of the Chemistry activity is in or around Palmerston North. In this issue are outlined some of the major chemistry activities in the area. Space did not permit all of the Branch contributions to be included. Manawatu does not accept the current prevalent attitude that the Institute is going downhill, and that the heyday of chemistry and the chemist is over. Far from it!! Nor do we believe that we can or should even contemplate getting into bed with RACI in order to survive. Instead, we believe that the Institute should look very carefully at the changing/changed role of chemistry in the 1990's and what are the needs of chemistry and chemists in these times. We have identified several issues:

#### Changed nature of chemistry:

Chemistry is no longer a discipline to be studied in splendid isolation. Today's science is focused very strongly on useable outputs. Nowhere has this been more clearly signalled than in the structure of the present Crown Research Institutes. There is no special Chemistry Institute. This is a reflection of the times and not necessarily a bad thing. New Zealand's economy is still mostly dependent on the export of what we can grow: dairy, meat, forestry, fishing and horticulture products are what we do best. This production is limited by available land and sea resource, and the thrust today is towards producing more processed products. Improvement of our processing of products is the thrust of much of our science today. In this, chemistry is a major component. Food chemistry, wood chemistry, biochemistry and nutrition are some of the areas of prime importance to the future of New Zealand. In many of the modern areas, the chemistry is applied, mixed with other approaches from other disciplines. Chemistry, and in particular the Institute of Chemistry, needs to not only be aware of these trends, but to actively pursue them. The NZIC must become market-responsive to its wider potential membership. The modern sciences, such as biotechnology, food science and materials science, must be accepted into the wider chemistry fold.

**Poor public image of science:** We are a nation of lawyers and accountants. This is reflected in the boards of most major companies and in our government. Science has become a target for the economists in Treasury, and the Green movement alike. At the moment the public image of a chemist is somewhere between an irrelevant parasite, pursuing his/her own interests at the taxpayer's expense, and a villain, responsible for each and every ecological disaster in the



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world. The NZIC needs an active public relations working group to put before the eyes of the public positive image of chemistry in New Zealand that we in the profession all know.

**Need to recruit top students:** All the signs are pointing to a growth in the need for an increasing number of chemists to work in applied areas. Yet there is a paucity of good students coming through, and very few staying on to postgraduate degrees, where the need will be greatest. A strong message needs to be given to students and careers advisors alike, that chemistry is a career with a real future.

To address these issues the Branch has run several activities:

**Recruitment of local students:** The branch has a student meeting each year, to attract student members, seeing the induction of 30 new members in 1992. Many of the student members are lost to us when they leave university, and are no longer eligible for student membership. Given the large jump in subscription from student member to full member, we should consider a

graded way of making the transition. The \$140 membership fee is quite a sum for a recent graduate to find.

#### A promotion in a local newspaper:

This included a chemistry quiz that highlighted the positive aspects of chemistry. A accompanying editorial article pointed out the all-pervasive positive impact of chemistry on a day in our lives. Local companies put in advertorials, describing their involvement in chemistry.

**Local school activities:** These have included a titrations competition, a chemistry quiz in schools, both run by the Branch, and planned to be repeated in 1993.

**Careers advisory:** The Branch put on a stand at the local careers expo. We fielded hundreds of enquires from interested students and parents. The exercise will be repeated at future careers expos. The Institute has in the past put out a brochure on careers in Chemistry which was very popular, but desperately needs re-doing.

M. Boland

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# SPECTROSCOPY - DEVELOPMENTS IN THE ULTRA-VIOLET AND VISIBLE REGION

By Roger Whiting

The term UV-Visible spectrophotometer can describe a range of devices from humble bench top machines to highly sophisticated research instruments. The simple bench top UV - Vis spectrophotometer is now a standard piece of laboratory equipment but, like all things, it too is undergoing a continuous process of development and improvement.

The recent changes have seen the performance of these machines improve in terms of optical quality, speed and ease of use and versatility of applications.

## SINGLE BEAM GAINS

The use of double beam optics in spectrophotometers has been common for many years and is still the standard in the top level instruments.

Meanwhile the simpler and less expensive instruments for routine work have tended to have single beam optics. The advantage of double beam optics is that the instrument is only measuring the difference in intensity between the sample and the reference beams. This means that any variations in lamp intensity and detector response are cancelled out. With the improvement in lamp stability, variations in light intensity have become less of a problem. This leaves only the variation of detector response with wavelength as the major reason for using double beam optics.

The development of inexpensive electronic memory devices has meant that the spectrophotometer now can store the background spectrum and calculate the absorbance of the sample. This counteracts the variation in detector response so the advantage of double beam optics is reduced.

The use of single beam optics brings certain advantages. The most obvious advantage is simplicity. The use of mirrors to pass the light beams through the sample and reference cells requires optical devices and cells that are matched. This adds to the cost of the instrument and gives possible sources of error. The simpler optics of the single beam system also gives increased light level to the detector.

The double beam system requires the use of choppers and mirrors to split the light beam and take it to the sample and reference cells and then recombine it and pass it to the detector. As there is a slight light loss at every reflection the result of a more complex light path is a reduction in the amount of light reaching the detector. This increases the effect of noise due to increased amplifier gain need to read the signal.

As the industry demands that spectra are recorded more quickly the need move to shorter scan time becomes more acute. At high scan speeds the change in wavelength as each segment of the chopper moves through the light beam becomes significant and the result is an apparent shift of absorption maxima toward shorter wavelengths. Also the maximum absorbance can be significantly reduced.

## DIODE ARRAY DETECTORS

The use of single beam optics makes possible the use of diode array detectors. The diode array detector is a solid state device which consists of a row of light sensitive capacitors. All the light from the source passes through the sample and is then passed through a polychromator which separates the light into its wavelengths and projects them onto the diode array. The more intense the light the more quickly the capacitors discharge and the more current is required to recharge them. This information is read every tenth of a second and the information stored and displayed as a spectrum. Thus scan times of a tenth of a second are possible or averages over several scans can be calculated to improve the signal to noise ratio.

The actual sample spectrum is calculated by comparison to a stored background scan. This background scan is made every time the instrument is switched on.

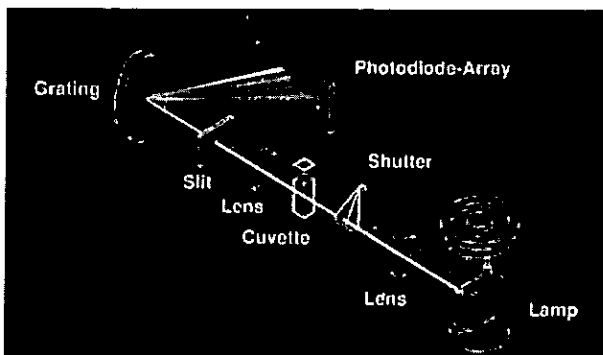


Figure 1 HP 8452A diode-array UV-Visible Spectrophotometer optical diagram

The typical diode array has 316 diodes which, over a scan from 800nm to 200nm, gives a data point every 2nm. Thus the instruments are ideally suited to routine analysis and applications needing rapid identification of species.

## UPGRADING THROUGH SOFTWARE

A great deal of development has been directed towards fitting the instruments to specific tasks. This involves developing methods and display characteristics that will make it difficult for an unskilled operator to perform the task incorrectly. This trend has been countered by the desire to have each instrument perform as many tasks as possible. This conflict has been resolved in such instruments as the Shimadzu 1201. Here programme cards, which can be plugged into the

instrument, programme it to carry out a range of analyses. The programmes step the operator through the procedure and make errors difficult to achieve. Also available are reagent packs which are designed to fit the methods so that all aspects of the analysis are taken care of. This type of development is becoming more common as the computing power needed to store the background and calculate the spectrum becomes less expensive so that there is surplus computing power on board the instrument which can be programmed to perform the necessary steps. Also less expensive electronics is encouraging microprocessor control of the spectrophotometer functions such as wavelength setting which make programming more feasible. It also has the advantage that rough handling of the controls ceases to be a problem.

#### **DEVELOPMENTS IN ATOMIC ABSORPTION BACKGROUND CORRECTION IN MANY WAYS**

The use of background correction has become a more common feature of Atomic Absorption Spectrophotometers over recent years. This has been spurred on by the need to reduce detection limits necessitating the use of graphite furnace techniques which need background correction. The interesting developments in background correction are in the various ways in which background correction can be carried out.

The historical method is to use a deuterium continuum source and combine its beam and the hollow cathode lamp beam using a half silvered mirror. The combined beam is shone through the flame and the two separated by modulating them at different frequencies

The Shimadzu 6500 Atomic absorption spectrophotometer uses a background correction based on the line broadening and line reversal that occurs as the lamp current is increased. The modulation cycle of the lamp has three portions. One with the lamp off one with the lamp at its normal operating current and one at a higher current. At the higher current the emission line of the lamp broadens and the cloud of atoms in front of the cathode expands and these two factors combine to give a line shape that consists of two "wings" either side of the normal emission line. This then acts as a continuum source against which the absorbance of the emission line in the normal current portion of the cycle can be compared. The advantages claimed for this system are ease of optical alignment, wide wavelength range, high light levels due to the lack of the half silvered mirror.

The use of Zeeman splitting in Atomic absorption was investigated in the 1970's but its application in the form of a proprietary instrument was delayed until the appearance of the Hitachi 70. Now both Hitachi and Varian have Zeeman based background correction systems.

The principle of Zeeman based background correction is the splitting that occurs in emission and absorption

lines when a magnetic field is applied. If a magnetic field is applied to the atom cloud in the carbon furnace then the absorption lines of the sample are split and are no longer a match for the emission lines of the lamp. At this point the light intensity should be the same as that when no sample is present. Any decrease in intensity is due to background absorbance. This can be compared to the absorbance of the emission line when the magnetic field is turned off and the absorption line matches the emission line. This system has the advantage that the light used to measure the background is the same as that used to measure the sample absorbance. However it has proved expensive to produce and appears on the more expensive instruments.

#### **AUTOMATION**

Most of the developments in the atomic absorption field in recent years have been in the area of automation. Most manufacturers can now supply carousels and samplers which will feed samples to the instrument and most can supply and instrument which will perform calibrations change lamps and make up and dilute standards and or samples to give meaningful results. In the case of the Shimadzu 6501 this has been extended to include changing over to and from carbon furnace atomisation and also burner adjustment to ensure maximum sensitivity.

#### **BURNER ROTATION ON TAP**

An interesting development in the matter of automation and sensitivity is in the latest GBC range where allowance can be made for samples that are out of range. One of the traditional methods for this was to rotate the burner head. This was usually done by hand (or asbestos glove) and required new standards to be made. Now with the GBC when the instrument detect an out of range sample it can automatically rotate the burner to bring the sample inside the optimum absorbance levels (0.1 - 0.8) and then rerun a set of standards to match that approximate concentration. This relieves the analyst of rerunning some samples in the batch because they were out of range.

#### **CONCLUSION**

The developments in the field of spectroscopy are increasingly reducing the need for highly skilled personnel spend time carrying out analyses. The trend seems to point in two ways either simple instruments programmed to step untrained operators through basic tests or to very sophisticated instruments that can be set up and left to perform unattended. Either way the analyst in charge is going to become more a "coordinator" for a variety of processes going on under his or her control and less a bench worker.

**Recent changes  
have seen the  
performance  
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optical quality,  
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# CHEMISTRY IN THE MANAWATU

**Palmerston North, the home of the Manawatu Branch of the NZIC, has the largest group of knowledge-generating and educational organisations in New Zealand.**

In the area of chemistry, we have educational institutions such as Manawatu Polytechnic and Massey University as well as the college of education and a plethora of primary and secondary schools. It is however on the research front that the Palmerston North area stands out. Chemistry based research is carried out at Massey University, not only in the Department of Chemistry and Biochemistry, but also in the Technology Departments, Soil Science, Various Agriculture and Animal Health related departments, and even in the department of Business Studies.

Outside the University, we have the headquarters of the Horticultural Research Institute, as well as major stations of the Pastoral, Crop and Industrial research Institutes. As well we have the Dairy Research Institute, Leather and Shoe Research Institute, and Industries such as Glaxo and New Zealand Pharmaceuticals, all involved in chemistry to a greater or lesser degree.

Papers presented in this issue of the journal all describe work being done in these organisations. A brief description of the main organisations follows:

## **DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY, MASSEY UNIVERSITY:**

This department is the largest in the Faculty of Science at Massey. The combination of disciplines is unique in New Zealand and has allowed the development of significant collaborations in the areas of protein structure and function, protein purification and enzymology. The Department also has active research programmes in synthetic organic chemistry, coordination, organometallic and bioinorganic chemistry, analytical and geochemistry, peptide synthesis, the thermodynamics of biochemical systems, nuclear magnetic resonance spectroscopy and chemical crystallography. The biochemistry research programmes include studies of enzyme structure, function and biosynthesis as well as molecular biology and mammalian and bacterial metabolic biochemistry.

To support its wide range of research, the department houses a range of major instrumentation and facilities. In addition to a range of standard laboratory instrumentation for chemistry and biochemistry, the following facilities are in place: Protein chemistry and biochemistry are served with an Applied Biosystems automated protein sequencer and peptide synthesizer, as well as two amino acid analyzers. Crystallographic data are collected on a Nonius X-ray diffractometer with associated Digital computing facilities, and analyzed on an Evans and Sutherland interactive computer graphics system. The NMR unit houses a JEOL 270 MHz spectrometer with wide-bore superconducting magnet. In addition a Hitachi 60 MHz R-1200 correlation NMR spectrometer is available for research and teaching. Electron spin resonance spectroscopy is carried out on a Varian E-104A spectrometer. A Digilab FT Infrared spectrophotometer, with vacuum bench, services infrared spectroscopy needs.

During the period 1989 to 1991, academic staff, post-doctoral fellows and graduate students have published about 120 articles in the international literature of chemistry and biochemistry. A large part of the research is supported

by grants from agencies external to the University. Over the last three years staff have attracted grants amounting to more than \$2.6 million from such agencies as:

- \* Lottery Science research
- \* Lottery Medical Research
- \* Health Research Council of New Zealand
- \* NZ Dairy Research Institute
- \* US National Institutes of Health
- \* US National Geographic Society
- \* DSIR Grasslands
- \* Ministry of Energy
- \* Palmerston North Medical Foundation
- \* World Health Organisation as well as the Massey University Research Fund.

The Department has recently produced an attractive booklet "Opportunities for Research" which gives detailed information about its research programmes. A copy can be obtained by writing to the Head of Department, Department of Chemistry and Biochemistry, Massey University, Palmerston North.

## **HORT + RESEARCH. THE HORTICULTURE AND FOOD RESEARCH INSTITUTE OF NEW ZEALAND LTD.:**

HortResearch is New Zealand's nationally focused research organisation. It was formed on 1 July 1992 and combines the horticultural research expertise of DSIR Fruit and Trees, DSIR Plant Protection and MAFTechnology.

Horticulture is New Zealand's fastest growing industry. In the early 1980's horticultural exports were just \$156 million. By the year 2000 they are predicted to top \$2 billion. HortResearch is working with this dynamic industry to help further develop and enhance its competitive advantages. The Institute is very much a "one stop shop" for the industry. Its research spans molecular biology, plant breeding and crop production through to food processing, transport and the evaluation of consumer preferences.

Over 500 scientists and support staff are employed by HortResearch. They are situated at 16 regional research centres and orchards throughout New Zealand with the Head Office based in Palmerston North.

HortResearch is a research company owned by the government and run by a board of directors. It undertakes contract research for the Foundation for Research, Science and Technology (FRST) and for commercial clients, and is also able to enter into joint ventures with clients to put new ideas into practice. HortResearch works closely with grower organisations and the marketing boards.

HortResearch has three research divisions:

The **Plant Improvement Division** uses both traditional plant breeding and genetic manipulation to develop new and improved plant varieties. It is seeking to enhance the quality, consumer appeal, yield and disease resistance of a range of horticultural crops.

The ongoing development of new and improved management techniques for the major horticultural crops and for a range of "sunrise" crops is the responsibility of the **Crop Production and Protection Division**.

Scientists in the **Postharvest and Food Science Division** are working to enhance the competitiveness of new Zealand's horticulture-based food industries through improving the quality of fresh and processed fruit.

## **THE NEW ZEALAND DAIRY RESEARCH INSTITUTE:**

The DRI is the hub of the dairy industry's research activity.

It concentrates on the development and manufacture of milk products in order to enhance returns from the export market. As an integral part of the co-operative dairy industry, the Institute enjoys a close relationship with the dairy companies, the New Zealand Dairy Board and the Dairy Board's many offshore marketing and development subsidiaries.

The Institute employs 300 staff, in many disciplines of science and engineering. Much of its work, particularly in the development of milk products, is funded by the industry and focused on the marketplace. Strategic research into the chemical structure and function of milk components, eg protein tertiary structure investigations, provides an important base for future developments, and adds to the pool of scientific knowledge. Some projects of this nature attract FRST funding.

Services to dairy companies include engineering contracts, specialist help in effluent disposal and water treatment, specialised chemical analyses and access to trained taste panels to evaluate new products.

The processing hall, with its comprehensive range of pilot-scale equipment, provides facilities for training as

well as research. Courses afford an important practical link with the industry, and enable scientists and technologists to transfer expertise directly to dairy factory operators.

The ability to cater for specific customers and offer products of unbeatable quality is critical to New Zealand's success as an exporter of dairy products. The Dairy Research Institute plays a vital role in achieving these aims and hence earning the maximum possible income from milk - one of our most important natural resources.

Chemistry plays an essential role in meeting this challenge. A wide range of sophisticated chemical and biochemical techniques is used to investigate the composition, structure and properties of milk components and products. Chemical analysis is important in testing the final products, to check that flavour and composition meet customers' demands, and to ensure that new Zealand dairy products meet the high standards required to compete in any international market. Chemical research underlies most of the dairy industry's innovative new products such as the "Anchor Spreadable Butter" that has taken Britain by storm, and Flavour Rich Milk powder developed as a food ingredient for chocolate manufacturers.

## The Importance of Flexibility in the Structure and Function of Lactoferrin

*Bryan F. Anderson, Heather M. Baker, Gillian E. Norris, Clyde A. Smith, Sylvia V. Rumball, David H. Thomas and Edward N. Baker. Department of Chemistry and Biochemistry, Massey University, Palmerston North.*

Lactoferrin, together with serum transferrin, ovotransferrin and melanotransferrin is a member of the family of iron binding proteins, the transferrins (1) which play a key role in regulating iron levels in biological fluids. These proteins are monomeric glycoproteins, Mr 80 000 Da, each having the ability to bind very tightly, but reversibly ( $K \sim 10^{20}$ ) two  $Fe^{3+}$  ions. A striking feature of transferrin chemistry is the requirement that a suitable anion must be bound with each metal ion. This relationship is synergistic, in that neither cation or anion is bound significantly in the absence of the other.  $CO_3^{2-}$  is the anion of highest affinity, although some other anions with a carboxylate group such as oxalate or malonate, can be substituted (2).

Likewise other metal ions can be bound in place of  $Fe^{3+}$ , but again only in combination with a suitable anion. Over the past few years, our protein crystallography group, at Massey University has been involved in studying the structure of human lactoferrin using X-ray diffraction techniques. Although lactoferrin is found in a wide variety of human secretions (eg. tears, saliva, bile, cervical fluid), as well as in the white blood cells, the lactoferrin studied was isolated from human colostrum, where it is present in high concentration (up to 4 mg/ml). Because of this distribution in the body, and its ability to tightly bind iron, lactoferrin is thought to act primarily as scavenger of iron, mopping it up to protect the host, both from bacterial invasion (by starving bacteria of iron and preventing growth) and from cell damage (by free radicals generated by the Haber-Weiss reaction). It does, however, have the

ability to kill some bacteria directly, in a way that is not yet fully understood (3).

Lactoferrin (Lf) is a large protein molecule. It consists of 691 amino acids folded in a precise arrangement that is directly responsible for its function. With a view to understanding how metal binding and release are accomplished, and how the protein can accommodate bigger cations and anions, the structures of diferric lactoferrin ( $Fe_2(CO_3)_2(Lf)_2$ ) (4), apo-lactoferrin (apoLf) (5) and a complex in which  $Fe^{3+}$  is replaced by  $Cu^{2+}$  and one of the  $CO_3^{2-}$  ions by oxalate ( $Cu_2(CO_3)(C_2O_4)(Lf)$ ) (6), have all been determined. Further, these have been refined at high resolution (2.2, 2.2 and 2.0Å respectively) which means that it is possible to make meaningful comparisons between the different structures.

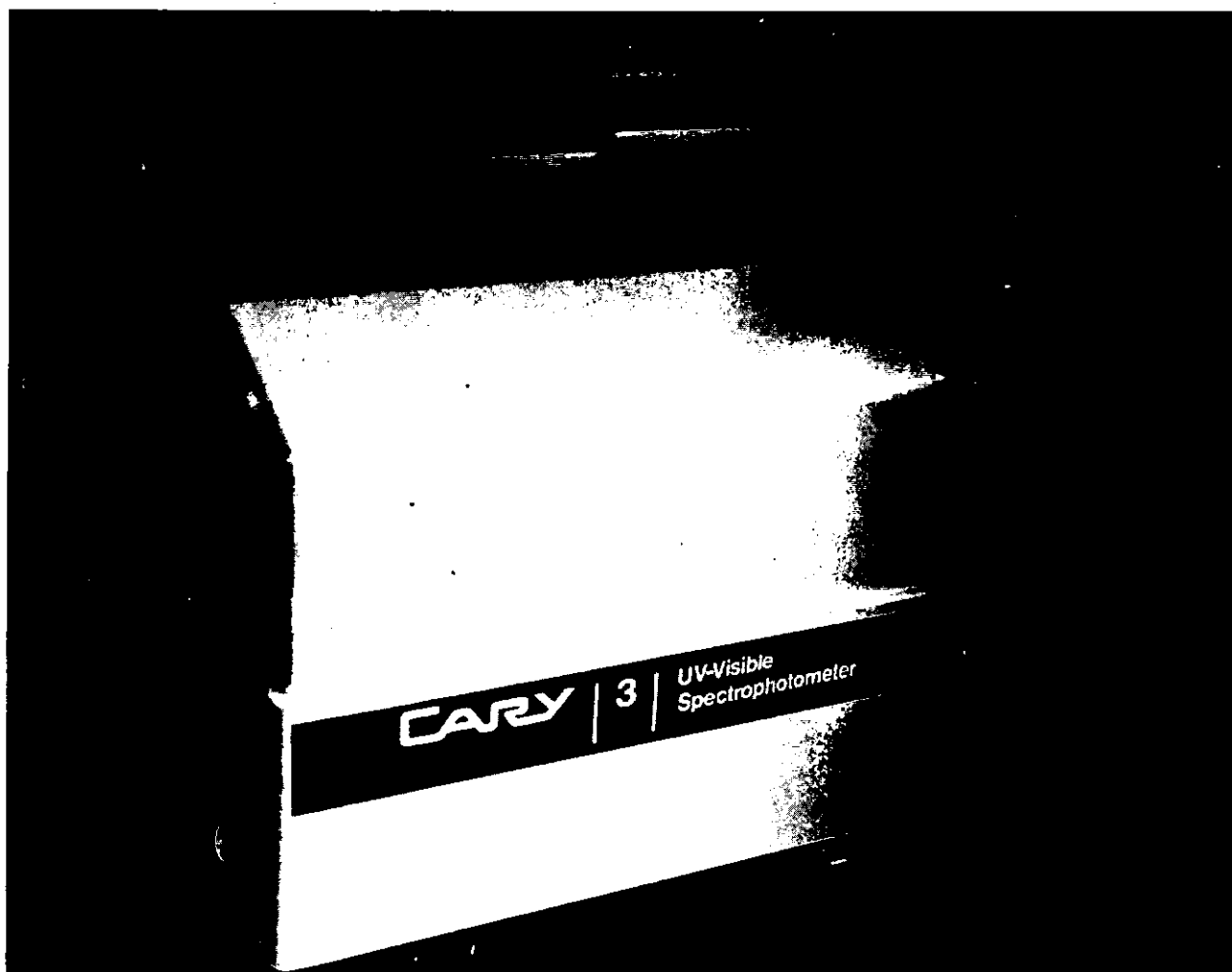
The structure of  $Fe_2Lf$  (Figure 1) shows that the single polypeptide chain is divided into two lobes, (N and C), that are connected by a short  $\alpha$  helix.

Figure 1. Cartoon representation of the  $Fe_2Lf$  structure. Domains are: N2 C1 N1 C2



Each lobe is further divided into two domains, (N1 and N2 in the N-lobe, C1 and C2 in the C-lobe), with the metal binding site of each lobe located deep in the cleft between the domains. Two oligosaccharide attachment sites are located on the outside of each lobe on the N2 and C2 domains, while the region thought to be responsible for killing bacteria (3), is located on the surface of the N1 domain.

The two metal sites are essentially identical, ligands being an aspartic acid, a histidine and two tyrosine residues, as well as the synergistic anion. These have a distorted octahedral geometry. The  $CO_3^{2-}$  ion fits into a pocket between the iron atom and two positively charged regions, an arginine sidechain and a helix N-terminus. The preference for  $CO_3^{2-}$  as the synergistic anion must result from its near perfect fit into this pocket; the two coordinated oxygens also receive hydrogen bonds from two protein NH groups, while the non-coordinated



# What's in a name?

## Correct Answers

Cary UV-Vis spectrophotometers have a tradition of optical, mechanical, and photometric performance; the new Cary 1 and 3 are no exception. With excellent linearity, stability and signal-to-noise performance, the Cary's double beam design with optional dual monochromator allows you to have complete confidence in your results. No other instrument in this class delivers the same level of performance.

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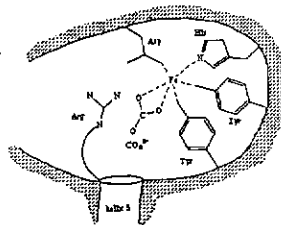
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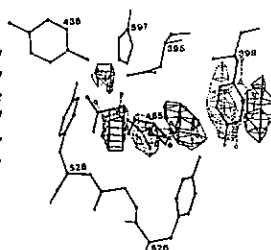
oxygen is involved in two hydrogen bonds (Figure 2).

Figure 2. A schematic diagram of iron and anion binding in human lactoferrin (shown for the N-lobe).



The presence of a large internal cavity near the metal binding site gives it a flexibility which allows room for both bigger metal ions and anions to bind. For example, analysis of the structure of  $\text{Cu}_2(\text{CO}_3)(\text{C}_2\text{O}_4)_2\text{Lf}$  shows that although the protein structure is essentially the same as that for  $\text{Fe}_2(\text{CO}_3)_2\text{Lf}$ , there are differences at the metal and anion sites. In the C-lobe, where the oxalate anion is bound, its extra bulk requires that two neighbouring sidechains, of arginine 465 and tyrosine 398, move approximately 2 Å away from their positions in  $\text{Fe}_2(\text{CO}_3)_2\text{Lf}$ . (Figure 3).

Figure 3. A section of an electron density map showing differences in electron density at the C-terminal anion binding site between  $\text{Fe}_2(\text{CO}_3)_2\text{Lf}$  (thick lines) and  $\text{Cu}_2(\text{CO}_3)(\text{C}_2\text{O}_4)_2\text{Lf}$  (dashed lines). The electron density is represented by thin lines, -ve electron density by clotted lines.



The  $\text{C}_2\text{O}_4^{2-}$  binds in a symmetrical 1,2-bidentate mode, however, similar to the  $\text{CO}_3^{2-}$  in  $\text{Fe}_2(\text{CO}_3)_2\text{Lf}$ . In the N-lobe, the effect of substituting  $\text{Cu}^{2+}$  for  $\text{Fe}^{3+}$  results in a movement of the Cu atom 0.7 Å from the Fe position, which causes the anion to become monodentate, and the copper geometry to be square pyramidal. (Figure 4).

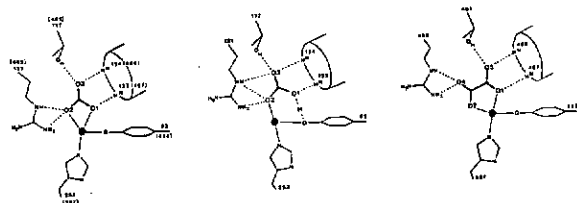
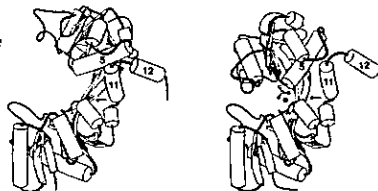


Figure 4. A schematic diagram showing the anion interactions with the protein and the metal ion in (a, left) the bidentate carbonate site in each lobe of  $\text{Fe}_2(\text{CO}_3)_2\text{Lf}$  and the (b, middle) monodentate (b1) carbonate site in the N-lobe of  $\text{Cu}_2(\text{CO}_3)(\text{C}_2\text{O}_4)_2\text{Lf}$  and (c, right) the oxalate site in the C-lobe of  $\text{Cu}_2(\text{CO}_3)(\text{C}_2\text{O}_4)_2\text{Lf}$ .

The structure solution of apo Lf (Figure 5) showed that the binding cleft of the N-lobe is wide open while that of the C-lobe remains closed. Binding of iron to the N-lobe of apoLf is accompanied by a 54° rotation of the N2 domain (and a physical movement of some parts of the structure by up to 30 Å) with the result that the metal ion is buried some 10-14 Å within the protein molecule and so isolated completely from the surrounding medium.

Figure 5. A schematic representation of the N-lobe of human lactoferrin showing the conformation change between the open (left) and closed (right) forms. An arrow marks the approximate hinge point.



Nevertheless superposition of each of the individual  $\text{Fe}_2\text{Lf}$  domains onto their apoLf equivalents indicate that this large conformational change occurs with little disturbance to the polypeptide chain folding, and that the N2 domain moves as a rigid body (rms differences

in and C2 are 0.55 Å, 0.61 Å, 0.45 Å and 0.41 Å respectively.) This conformational change has two elements; a hinge between the two domains and a pivot, where domain N2 moves against N1. The hinge is formed in the two antiparallel strands of beta sheet which lie behind the iron site and connect the two domains. Here residues flex in concert to move the N2 domain. Changes in the torsion angles are small (maximum 45°) and do not move the structure through energetically unfavourable conformations and the interchain hydrogen bonds remain intact. Nevertheless the resulting movement is considerable and emphasises the flexibility inherent in beta sheet structures. The pivot is found in a hydrophobic patch between helix 5 which lies along the length of the moving N2 domain and helix 11 which extends like a post away from the N1 domain. This interface is completely hydrophobic and consequently provides a non-interactive, 'greasy' surface for the two helices to move over while at the same time holding the two domains adjacent. In its apo form, only the C-termini of the two helices are tethered together through hydrogen bonds in apoLf but on iron binding the N-termini of helices 5 and 11 approach each other and two extra hydrogen bonds are formed. This has the appearance of a latch which may contribute to the stability of the closed, metal-bound form. The movement of helix 5 is accompanied by a rotation of 24° in the same sense of helix 12 which is set at right angles to helix 11 and provides the connection between the two lobes. There is thus a tendency to reposition the C-lobe when iron binds to the N-lobe but this is counteracted by a set of hydrogen bonds between the C-terminus of the molecule and residues of the backbone strands of the N-lobe. The final result is that the

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C-lobe undergoes a rotation of  $6^\circ$  and a shift of 1.9Å. The terminating helix moves away from the N1 domain and what were direct hydrogen bonds are now mediated by water molecules. It is possible that these concerted movements enable cooperativity in iron binding at the two sites. The closed C-lobe in the apoLf structure has caused us a lot of debate and has several possible implications (7). It is consistent with a lesser flexibility of the C-lobe, which could make the closed configuration a stable structure (though not necessarily the only stable structure) even without a metal atom bound. The lesser flexibility probably arises, in part, from the presence of an extra disulphide bridge which links the two helices equivalent to helices 5 and 11, and which may thus constrain the movement of the C2 domain. The conformational change seen here has its parallels in other binding proteins. Within the transferrin family, a recent structure analysis of human transferrin with one ferric ion bound shows that the single iron atom is bound within the closed C-lobe, while the empty N-lobe binding cleft is wide open, as in apoLf, with a very similar domain movement. In the bacterial binding proteins specific for sugars, ions and amino acids, two-domain structures very similar in folding to each lobe of Lf are found (8). Both open and closed structures have been characterised for these proteins, and energy calculations analysing the hinge-bending motion indicate that there is little energy difference between the two states (9). This is consistent with what we observe for Lf, and in particular with the unexpected discovery of a closed, but iron-free, C-lobe in apoLf.

### Conclusions

The structural results described here demonstrate several levels of flexibility in the lactoferrin molecule which are important for its function. The complexes in which

$\text{Cu}^{2+}$  and  $\text{C}_2\text{O}_4^{2-}$  are substituted for  $\text{Fe}^{3+}$  and  $\text{CO}_3^{2-}$  demonstrate that there is sufficient flexibility in and around the binding site for other metal ions and anions to be accommodated without any disturbance of the overall protein structure. The rigid body domain movements, seen from the comparison of the apo- and iron structures indicate that the binding of substrates is accompanied by a large conformational change that has very localised effects on the polypeptide chain. The question of iron release, however, remains a puzzle. It is triggered by low pH (below pH 4.0) and influenced by the binding of non-synergistic anions to secondary sites (10) and by ionic strength (11). We speculate that these factors may act to destabilize the "closed" state, perhaps through environmental changes around the hinge region. There is no doubt that flexibility plays a key functional role for lactoferrin and, by analogy, for other members of the transferrin family, and for bacterial binding proteins.

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## A CHEMIST'S VIEW OF BUTTERMAKING

Dr Alastair K H MacGibbon, New Zealand Dairy Research Institute, Palmerston North

### Introduction

This is the basis of a lecture given to the NZIC. The aim is to show how chemistry and knowledge of chemistry contributes to the production of a significant international food product. Chemical principles involved include the biochemistry of milk synthesis and the organic chemistry of fats combined with the physical chemistry of melting, crystallization, and process technology of phase inversion and separation. Buttermaking has played a substantial part in the export returns of New Zealand over many years. Though New Zealand's butter production is not large by world standards, the major proportion of the butter is exported. In contrast, the major proportion of the butter production of other countries is consumed in their local market. This means that in terms of the export markets New Zealand has a significant role. In spite of its economic importance, and the fact that butter is one of the most recognised food items, the details of the buttermaking process are not known by most consumers.

### History of Buttermaking

Records show that the art of buttermaking dates back to very early times, the Indians of Asia using butter as a food prior to 2000 BC. Throughout history there are references to butter as a food, a medicine and its use in religious

ceremonies. It was probably introduced into Europe by the Scandinavians, for whom it became an export item. There are reports that in the twelfth century the Germans were sending cargoes of wine to Norway in exchange for butter and dried fish.

It was really not until the end of the 19th Century that buttermaking left the farm, due mainly to the development of the centrifugal cream separator. This allowed cream separation to be carried out in central plants, processing large quantities of milk, and led to the mechanisation of buttermaking and large scale production.

### Buttermaking

There are five steps in the buttermaking process (Figure 1). The first is the concentration of the milk (4% fat), into cream of 40% fat using the centrifugal cream separator. The fat in cream is not free but is contained within a globule which ranges in size from 1 to 10  $\mu\text{m}$  diameter. Each of these globules is surrounded by a thin phospholipid membrane which stabilizes the globule as an oil-in-water emulsion. The cream is

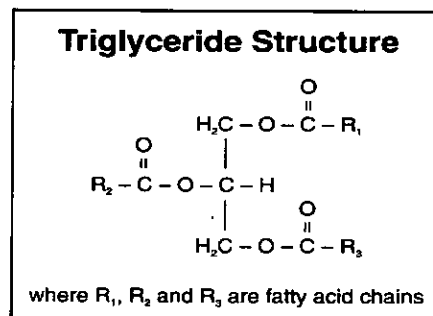


Figure 1. Buttermaking process

then cooled to allow about 40 to 45% of the milkfat to crystallize to provide some rigidity to the globule for optimum buttermaking. If there is too much solid milkfat the butter will be hard and brittle, whereas if it is too low then more fat will be lost in the buttermilk. The crystallization is a slow process and the rate of cooling, final temperature and the chemical composition are important in determining the final texture.

The physical phase inversion occurs during the churning of the cream, which destabilises the fat phase of the cream. Under intense agitation with the incorporation of air, some of the membranes break, releasing fat which bonds together the unbroken globules, forming granules too large to remain in suspension. The fat thus separates and buttermilk is released and drained off, until a stable water-in-fat emulsion is obtained.

The kneading (working) process turns the granules into a pliable plastic mass and excess water is squeezed out, producing the butter texture. Before kneading about 80% of the fat is still within globules, but this is reduced to 8-30% with kneading. There is significantly more free fat and this free fat helps provide the network structure which is characteristic of butter.

The final goal of the kneading is to give an homogenous butter which is finely dispersed water-in-oil emulsion. Salt can be added (as a slurry) and then further kneading disperses the water into small droplets of less than 10 µm. This fine dispersion is important for product quality and shelf life. The final kneading is also under vacuum, which removes air and gives a smooth even texture. A typical composition of butter is about 81.5% milkfat, 15.5% water, 1.5% curd (protein and lactose) and 1.5% salt.

Commercially the butter is made continuously with machines operating at a rate of up to 12 tonnes per hour, but the principles are the same even in a small domestic batch process. The major factors which affect the texture of the butter are the specific chemical composition of the milkfat triglycerides (the combinations of fatty acids) and the processing conditions used in manufacture. Both are very important and it is the combination of these factors which makes buttermaking so fascinating.

#### Chemical Composition

Milkfat contains triglycerides which consist of three fatty acids attached to a glycerol backbone (Figure 2).

Over 500 different fatty acids have been found in milkfat, so a very large number of different triglycerides are possible. Hence milkfat is a complex mixture. Many of the triglycerides are present in very low concentrations, and over 100 have been isolated and identified. Figure 3 shows a typical gas chromatograph trace of milkfat triglycerides, separated simply on the basis of



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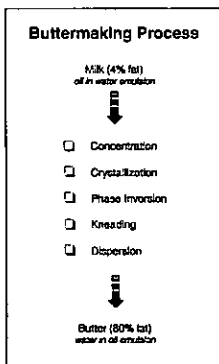
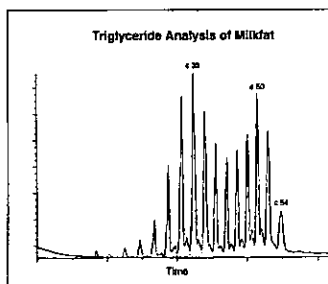


Figure 2. Triglyceride structure

molecular weight. Each peak contains triglycerides of the same carbon number (the sum of the number of carbons on the three fatty acids). For instance, triglyceride peak c50 contains three fatty acids with the carbon atoms summing to 50, e.g. 16 + 16 + 18. The significant triglyceride carbon numbers present in milkfat range from c28 to c54. Because New Zealand dairying is based on efficient pasture production, there are seasonal changes in the milkfat

Figure 3. Triglyceride analysis of milkfat. Non-polar capillary gas chromatography trace using a temperature ramp up to 340°C. The separation of the milkfat triglycerides is simply on the basis of molecular weight.



characteristics influenced by the grass growth. This, together with the lactational effects of the cow produces substantial changes in the composition of the milkfat. In the summer there are more saturated fatty acids in the milkfat and this is reflected in harder butter. The unsaturated fatty acids and the short chain fatty acids contribute to softer fats and hence softer butter, such as occurs in the spring. The changes in the hardness are reflected in the differential scanning calorimeter (DSC) trace (Figure 4).

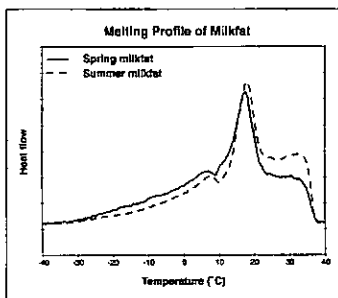


Figure 4. Melting profile of milkfat. Comparison of the DSC melting profile spring and summer milkfat. Heating rate was 5°C/minute.

The DSC records the energy changes in a sample on heating at a constant rate, giving a direct measure of the apparent specific heat as a function of temperature. Figure 4 shows the energy changes as a consequence of the melting characteristics (heat of fusion) of the milkfat. Milkfat melts over a very large temperature range, -4°C to 40°C so most of the properties of milkfat relate to a semisolid, that is partially liquid and partially solid. The spring milkfat contains more low-melting triglycerides (more melting occurring at low temperatures) and the summer milkfat more high-melting triglycerides.

### Manufacturing Effects

The chemical composition is not the only factor affecting butter texture. One intriguing property of pure triglycerides is that they have multiple melting points, due to three distinct crystal forms (polymorphism). These different forms are found in milkfat depending on the method of crystallization, though because there are a huge range of triglycerides polymorphism is not the

major factor in milkfat properties. However it is very important in cocoa butter used in chocolate production where blooming, a slightly grey surface with whitish spots, is a problem. This is due to a transformation from the usual  $\beta 1$ -2 form to the large crystal  $\beta$ -3 form, producing lumps on the surface. Chocolate manufacturers spend a lot of effort trying to stop or slow this transformation. Polymorphism is also important in margarine manufacture where there is less variety of triglycerides than in milkfat. In this case the  $\beta'$  form is preferred as the  $\beta$  form produces large crystals which gives a sandy mouth-feel to the product.

Because milkfat has many different triglycerides, they do not form pure crystals but they tend to crystallize in groups of similar size and structure. So it is not the polymorphic forms which are most important but the composition of these mixed crystals. The presence of mixed crystals means that the melting points are different from the individual pure triglycerides, with a reduced melting range. The triglycerides within the mixed crystal are usually within 6 carbon numbers. Three main groups can be distinguished in milkfat, a low melting group, an intermediate group and a high melting group as can be seen on the DSC trace (Figure 4). For milkfat this mixed crystal formation is very important as the composition of the mixed crystals is affected by the cooling regime. The faster the crystallization the greater the variety of triglycerides that are crystallized together, and the harder the product, because more soft triglycerides are trapped within the crystal. In addition the crystals tend to be small, 1-2  $\mu\text{m}$ . If the crystallisation is slow there is more selectivity, and the crystals tend to be larger. This is important in buttermaking as crystallization procedures can be changed during the dairy season to compensate for changes in the chemical composition of the milkfat so as to reduce the variation in the texture of the butter.

With the importance of the crystallization of the milkfat, it is not surprising that melting and recrystallization under different conditions can produce different properties. As an example, butter which has melted on the picnic table and then is allowed to recrystallize when it is returned to the fridge, is often harder than the original butter. This is due to changes to the structure resulting from the different crystallization conditions. In conclusion, the chemistry of milkfat is a fascinating subject. Even though buttermaking is a very old process there are a lot of chemical interactions involved, and a better understanding of these interactions is essential for the control and improvement of the textural properties of the product.

### Experiment

An entertaining experiment, especially with children, is to make butter in the kitchen mixer. The steps in the process outlined in Figure 1 can be observed. Leave a carton of cream in the fridge overnight, to ensure sufficient of the milkfat has crystallized, and then whisk using a mixer with a chilled bowl. When the granules are formed they can be separated from the buttermilk with a kitchen sieve and washed with cool water. Finally, knead with a rolling pin to make the butter pliable and to remove excess water. At this point it is possible to add 1-2% salt (about 0.5-1.0% of the original cream weight) for flavour and keeping quality. Since it is not possible to develop the fine moisture dispersion found in commercial butter, the keeping life of the butter made will be short.

# HEALTH AND SAFETY IN EMPLOYMENT ACT 1992 AND ITS IMPLICATIONS FOR EMPLOYERS

By Douglas M Hay BSc, BE (Chem), MSc, DIC, MNZIC

Douglas Hay is a Senior Lecturer in Occupational Safety and Health at Massey University. He is currently running courses for New Zealand employers throughout the country on how to implement the new Health and Safety in Employment Act 1992.

**INTRODUCTION:** On the 1st April 1993 the Health and Safety Employment Act 1992 (HASE Act) comes into force and with it major responsibilities on employers, to manage hazards in their workplaces. It will require management to put in place systems by which hazards can be recognised, assessed with respect to significance, and then controlled so that employees do not suffer any 'serious harm'. Employers who do not put such systems in place will be liable to fines up to \$25,000; a fine of up to \$50,000 where death or serious injury occurs and the employer did not know the condition; and a fine of up to \$100,000 and/or up to a year in prison where a condition is knowingly left that could cause serious harm.

**STRICT LIABILITY:** The HASE Act is based in the concept of Strict Liability as distinct from Absolute Liability. The old Factory and Commercial Premises Act 1981 in New Zealand worked on principle of absolute liability and under it an employer could be prosecuted if a breach occurred regardless of the degree of training etc he/she had in place to alert employees to the dangers. Under strict liability, if the employer can show that he/she has in place a safety system (training, safety devices available for use, auditing, inspections, etc), ie that "due diligence" was being taken, then it would be highly unlikely that a prosecution would result if harm occurred to an employee in that workplace.

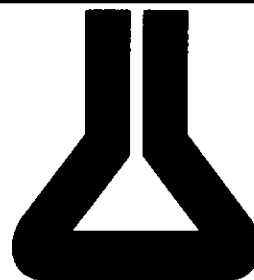
**HAZARD IDENTIFICATION:** Under the new Act the identification of all hazards and assessing their significance is a responsibility of the employer - whether there are regulations governing them or not. Furthermore the employers responsibilities extend to dealing with the hazards, ie - Eliminating them or, if that is not possible - Isolating them or at the very least - Minimising them and also - Educating and informing all employees on the hazards to which they are likely to be exposed.

**RESPONSIBILITIES:** It is the responsibility of the employer to ensure that all practicable steps have been taken to ensure the safety of employees while at work. The chief executive would appoint a safety manager to take control of this function who in turn would most likely establish a safety committee for the organisation. Section heads will be responsible for employees under their control and employees will be responsible for their own safety and that their action or inaction does not harm others.

**PRINCIPALS:** The Act defines a principal as 'a person who or that engages any person (otherwise than as any employee) to do work for gain or reward'. The duties of a principal are wide reaching in that they must take all practicable steps to ensure no employee of a contractor or subcontractor is harmed while doing work for that principal. This means that if a contractor is retained to do work on a site then the principal of that site must ensure they or their employees are not harmed. It will be in the principal's interest to retain only those

contractors who work in a safe manner or introduce a clause into any contract which will protect the principal in situations where a contractor is not working in a manner that pays due regard to the safety of employees.

**ALL PRACTICABLE STEPS:** This is the key to the Act and for the purposes of this Act mean steps that can be taken with regard to current knowledge and invention, taking into consideration the cost of taking those steps and the severity of the harm that could arise if they were not taken. It is worth quoting the definition as given on page 2 of the Act, it is: All practicable steps means all steps to achieve the result that it is reasonably practicable to take in the circumstances, having regard to (a) The nature and severity of the harm that may be suffered if the result is not achieved; and (b) The current state of knowledge about the likelihood that harm of that nature and severity will be suffered if the result is not achieved; and (c) The current state of knowledge about harm of that nature; and (d) the current state of knowledge about the means available to achieve the result, and about the likely efficacy of each; and (e) The availability and cost of each of those means. So if an employer has done 'everything' to reduce the likelihood of harm to an employee then they have nothing to fear. It means that any employer (a person with authority) must keep abreast of current knowledge and implement appropriate counter measures if or when they become available to reduce the likelihood of harm. In a research laboratory this would mean keeping up to date on the likely effect of chemicals on individuals, ie from material safety data sheets and relevant publications in the field. This is no small task considering the number of chemicals there are. It also means that a task analysis should be carried out in all operations to highlight possible problem areas.



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**SIGNIFICANT HAZARDS:** "Significant hazard means a hazard that is an actual or potential cause or source of" (a) Serious harm; or (b) Harm (being harm that is more than trivial). The severity of whose effects on any person depend (entirely or among other things) on the extent or frequency of the person's exposure to the hazard; or (c) Harm that does not usually occur, or usually is not easily detectable, until a significant time after the exposure". The Act focuses on 'hazards' (and 'significant hazards' in particular) because it is the existence of these which trigger action by employers. Section 7 of the Act requires all hazards to be identified and an assessment made of their significance. Two factors must be taken into account in determining 'significance'; Risk and nature (ie seriousness) of the public harm. Paragraph (a) above includes all things which may result in serious harm and are listed in Schedule 1 of the Act and the extent to which it should be controlled depends on whether or not it is practicable to do so. It may well be that the hazard can be easily eliminated or isolated, in which case this must be done. In most cases, all that may be necessary will be to minimise the likelihood of employees being harmed. Paragraph (b) above does include an element of risk, in that greater exposure to the hazard increases the likelihood of harm. Paragraph (c) reflects that the consequences of exposure to the hazard cannot be predicted with certainty at the time of exposure because of the limitations of knowledge. It is the employers responsibility to assess the significance of a hazard and if an OSH inspector considers that this has not been adequately done, an "improvement notice" may be issued and/or legal proceedings for a "breach of duty" initiated. Also an employee could complain to the Department of Labour if he/she considered that the employers assess-

ment was inadequate.

**CODES OF PRACTICE - REGULATIONS:** Part III of the Act (Sc 20-24). These give very precise guidance on what would be regarded as appropriate levels of "care" with regard to: - types and quality of equipment etc, and - standards of competence of particular categories of persons engaged in particular work or activities. An employer who failed to comply with a code or a standard would run the risk of being deemed to be not taking "all practicable steps" if he/she did not have a good reason for not complying. Approved codes of practice will be produced covering noise; material safety data sheets; lead; substances hazardous to health; VDU and a variety of industry specific codes. Regulations will be produced covering; general workplace; forestry and agriculture; tractor and farm safety; construction; substances hazardous to health; machines and industrial major accident hazard appraisal. **HOW TO COMPLY:** The Act is very comprehensive and puts the responsibility on management. There are twelve major steps that an employer must address and these are: (1) Assign responsibilities (2) Become familiar with legislation (3) Involve employees in the development of health and safety procedures (4) Discharge duties to non-employees (ie visitors) (5) Identify hazards (6) Assess significance of hazards (7) Eliminate hazards where possible (8) Isolate remaining hazards where possible (9) Minimise exposure (10) Inform employees (11) Implement training and supervision (12) Establish system for recording and reporting accidents Employers will need to establish an effective safety management system. There are a number of organisations which will be able to provide assistance and these include: (a) Department of Labour - Occupational Safety and Health Division (b) New Zealand Employers Federation (c) Universities with specialist section on Occupational Safety and Health (d) Private consultants; and (e) Regional employer organisations **CONCLUSION** Employers already have in place systems to optimise production, systems for quality control and management systems that give order to an enterprise. These systems can be used in the development of occupational safety and health procedures. The benefits of such a system will be a workplace where employees feel involved - using their detailed knowledge of the process to ensure a better working environment. Also from the 1st July 1992 the new ACC Act has provision for a discount or loading which is dependent on claims history. The prudent employer will have much to gain by introducing an occupational safety and health system.

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University of Waikato School of Science and Technology seeks contact with past students. In 1969, the first staff to teach in the School of Science were appointed, and in 1970 the doors were opened to students. In 1988, the name of the School was changed to The School of Science & Technology. It is felt that the first 25 years should be commemorated in a Jubilee, so that past and present staff and students can renew old acquaintances and memories. Please contact Mrs Emma Sammes, School of Science & Technology, fax 07 8364218 or phone 07 838 4053 so that information can be sent to you. The level of interest will dictate whether or not a Jubilee will be held.

# BRANCH NEWS

## OTAGO BRANCH NEWS

Dr. David Fenby of the Chemistry Department, University of Otago, left New Zealand at the end of November to begin study leave. Initially he will work at Pierre and Marie Curie University, Paris, where he intends using spectroscopic and quantum mechanic studies to examine hydrogen bonding and Van der Waals dimers, his particular interest. This field of work will take him to the Centre for Nuclear Studies Grenoble, the Rutherford Appleton Laboratory near Oxford, and finally to the Chemistry Department, University of Exeter. Dr. Fenby intends returning to the University of Otago early February 1994.

**New appointments in Chemistry:** Dr Keith Gordon takes up an appointment as Lecturer in Chemistry on 1 February 1993. He is a graduate of Queens University, Belfast, where he also completed a Ph.D. in Physical Chemistry under Professor McGarvey on excited state spectroscopy and the dynamics of some copper complexes which are photocatalysts. These interests were extended by work on time-resolved infrared and raman spectroscopy while at Los Alamos as a Post-doctoral Fellow. At Otago, he will study light induced electron transfer reactions related to photosynthesis, develop time resolved spectroscopic methods and begin collaborative work with Los Alamos and Queens.

Mr Paul Orange, a graduate in Chemical Engineering from Canterbury, has been appointed an Assistant Lecturer in Chemical Technology for one year. Apart from contributing to the Chemical Process Science courses he will be associated with an exciting research programme.

## MANAWATU BRANCH NEWS.



Dr Gill Norris is the chairperson of the Manawatu Branch for 1993. Gill is well known for her work in X-ray crystallography. Gill's PhD in crystallography was obtained from Massey University in 1982, for thesis work done while at the same time bringing up two daughters. Gill's special interest is X-ray crystallography of proteins, as a means of looking at structure and function. She has worked with Prof Ted Baker since 1982,

and has been involved in structure determination azurin, and more recently of lactoferrin. Her current proteins of interest are endoglycosidases and nitrite reductase.

**Congratulations** to Margaret Brimble (Massey University) for being awarded the Hamilton Memorial Prize. Farewell also to Margaret and Mark Brimble as they leave us for Auckland.

**Congratulations** to Andrew Brodie who has been appointed to a new chair in Chemistry, and to the headship of the Department of Chemistry and Biochemistry at Massey University. Professor Brodie is a PhD from Canterbury University and came to Massey after a Postdoc in London. Andrew has been with the department since 1970. His research interests are in inorganic chemistry, in which he has had a distinguished career.

## BIOGRAPHY - KEVIN MARSHALL

Dr K R Marshall graduated from the Chemical Engineering Department of the University of Canterbury in 1963. He was employed as a Research Officer in the Engineering Department on the New Zealand Dairy Research Institute, and granted an Institute Fellowship to study biotechnology at Birmingham University, England.

Dr Marshall returned to the Whey Products Section of the Institute. He was involved in research on fermentation of whey and the earlier research on the then new technology of ultrafiltration. During this time Dr Marshall completed his PhD at Massey, researching the production of lactic acid from whey. Dr Marshall served as Head of the Whey Products Section of the Institute and, later of the newly-formed Effluent Technology Section.

After a period as Assistant Director of the Institute, Dr Marshall moved to the New Zealand Dairy Board in 1983, initially as Executive Manager, Technical and, for the last two years as the Board's Corporate R & D Manager.

As part of his R & D coordination role, Dr Marshall has had a major involvement with the industry's R & D centres overseas and in dairy companies, as well as with the Institute. Dr Marshall took office as Chief Executive of New Zealand Dairy Research Institute at the beginning of August 1992.

## CONFERENCES

### NZIC CONFERENCE:

In conjunction with the Medicinal and Agriculture Division of the Royal Australian Chemical Institute.

University of Auckland 7 - 10 December 1993

Plenary lectures, Symposia: Medicinal and agricultural chemistry; Natural products; Organic synthesis; Inorganic/organometallic; Analytical/environmental; Surface science; Education in chemistry; Reaction mechanisms; Food, flavours and colours; Forensic science; Physical/theoretical chemistry. Poster sessions, Student paper competition, Instrument and equipment exhibition, Social events.

Contact Dr Allan Easteal, Conference Secretary, Chemistry Department, University of Auckland, Private Bag 92019, Auckland Telephone: 64-9-3737599, Extensions 8963/8343 Fax: 64-9-3737422.

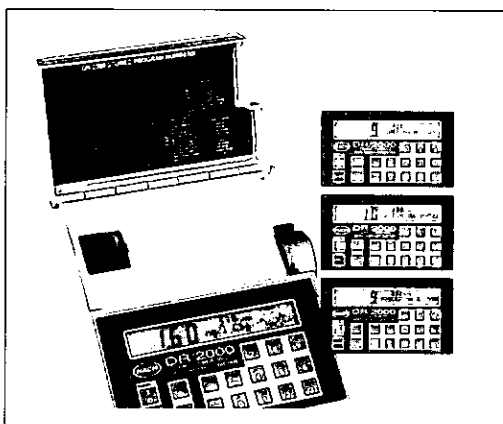
### COAL RESEARCH

Fifth New Zealand Coal Conference 20 - 22 October 1993 Parkroyal Hotel Wellington. The New Zealand Coal Conference is a most significant forum for all those involved in this premium energy resource. This conference also marks the 25th Anniversary of Coal Research Association of New Zealand Inc. The conference provides a unique opportunity for the exchange of ideas, information and concepts. Authoritative overseas speakers will be invited to present keynote addresses and specialist papers. New Zealand Coal Conference 1993 is an extremely valuable opportunity to join with others who share your commitment to the future of this vital energy sector. The Conference Secretary Fifth New Zealand Coal Conference Coal Research PO Box 31-244 Lower Hutt New Zealand

# PRODUCT NEWS

## WILTON INSTRUMENTS Hach DR/2000 spectrophotometer...

Combines microprocessor technology, sophisticated optics and complete system support to make colorimetric analysis easier than ever before. Using the convenient, premeasured reagents will save time. You'll appreciate the economy of ready-to-use solutions, single-dose powder pillows and error-free ampuls. More than 120 preprogrammed calibrations for over 120 commonly performed analyses are permanently stored in the DR/2000's ROM (read-only memory), eliminating manual conversion of absorbance data to concentration values. That means you won't have to prepare calibration curves. Enter the three-digit program



number of the test you want to perform, insert the sample and read the results in concentration units on the digital display. Customize the DR/2000 by adding up to 50 of your own calibrations to the instrument's permanent memory. Update capability A few simple keystrokes is all it takes to add new Hach methods. As new Hach tests become available, you can add new testing procedures to your DR/2000. Extensive prompting in 14 languages Liquid crystal display messages guide the operator through proper control key sequences for each testing and programming procedure. Choose

from 14 languages: English, French, Italian, Spanish, Portuguese, German, Dutch, Norwegian, Swedish, Danish, Finnish, Turkish, Greek and Japanese.

## THE HACH DR/3000 Combines micro- processor technology with advanced, single- beam optics

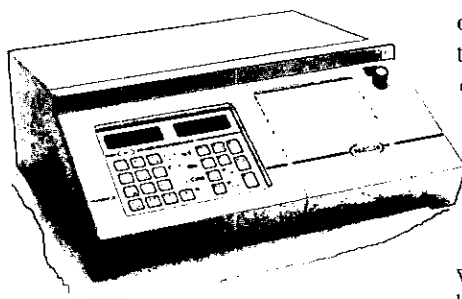


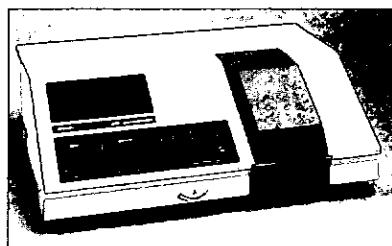
table optics provide precision testing. The DR/3000's unique, double-pass optical system ensures a monochromatic light beam: after a single beam is passed over a grating bar (1200 grooves/mm), the diffracted beam is reflected back onto the grating for a second pass. With this double-pass grating monochromator system, the DR/3000's optical advantages include a full 340-1000 nm wavelength range,  $\pm 1$  nm accuracy, 9-nm spectral bandwidth and less than 0.1% stray light. Samples of up to 3.0 absorbance units can be measured with excellent linearity and reproducibility. DR/3000 Optical Path Diagram

## JENWAY MODEL 6100 - VISIBLE RANGE

### Features

- \* Wavelength 320-920 nm
- \* Bandwidth 5 nm
- \* Microprocessor Controlled
- \* LED Displays of Data & Wavelength
- \* Auto Zero/Auto Calibrate
- \* Sealed Membrane Keypad
- \* %T, Abs and Concentration Modes
- \* Versatile Sampling System

- \* Full Interfacing Capability
- \* Economically Priced



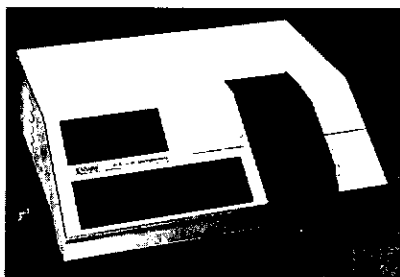
The Jenway Model 6100 Visible Range Spectrophotometer has been designed as a high quality, low cost instrument operating over the range of 320 to 930nm. The unit combines the latest microprocessor technology and a superb optical system with a wide range of sampling accessories. Mode selection and calibration are performed at the touch of a button and critical calibration values are retained, even when the unit is switched off. Combined with a mechanically rigid structure the 6100 provides a system with fast warm-up, low drift and high reliability. Designed for a long, troublefree life to meet the needs of today and in the future.

## MODEL 6105 - UV/ VISIBLE RANGE

### Features

- \* Wavelength 190-920 nm
- \* Bandwidth 5 nm
- \* Low Stray Light
- \* Excellent Stability
- \* Microprocessor Controlled
- \* Auto Zero/Auto Calibrate
- \* %T, Abs and Concentration Modes
- \* Automatic Lamp Change
- \* Full Interfacing Capability
- \* Minimal Maintenance /Easy Access

The Model 6105 is a single beam Spectrophotometer which offers all the features of the Model 6100 Spectrophotometer, but operates over an extended wavelength range of 190-920nm. This ensures full access to the many determinations normally carried out in the ultraviolet (UV) part of the spectrum. Particular care has been taken during the design



stages of the Model 6105 to provide superior optical performance; the results of which can be seen in the excellent stray light characteristics and stability rarely found

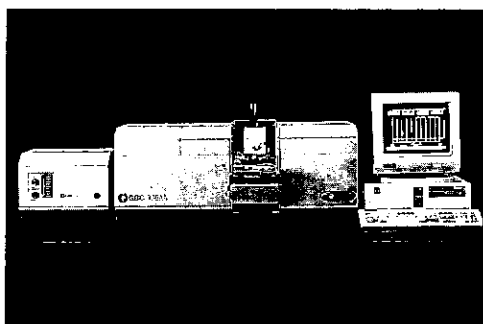
in a single beam spectro-photometer. The Monochromator used in both the Model 6100 and the Model 6105 is of modified Czerny Turner design, incorporating a cam driven 1200 lines/mm holographic diffraction grating and features automatic second order response suppression. The optical system is an independently enclosed unit to give maximum protection from environmental contamination. Careful design of the system has minimised heat transfer to the sample, thus enabling precise measurements to be performed on temperature dependant tests. The light source on the Model 6100 is an efficient Tungsten Halogen Lamp which is easily accessible for replacement. The Model 6100 uses low noise, high stability solid state detector for accurate, reproducible results.

**For further information on Hach Jenway & Turner Spectrophotometers contact Wilton Instruments PO Box 31044 Lower Hutt Ph 0-4 569 7099 Fax 0-4 569 7240**

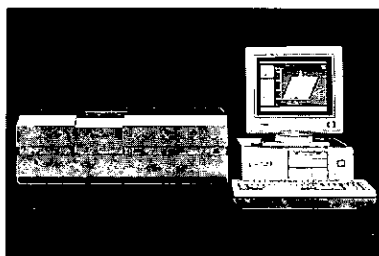
## **ATOMIC, ABSORPTION SPECTROPHOTOMETERS ICI INSTRUMENTS GBC 908 & 909 AA SPECTROPHOTOMETERS**

GBC have also released the new 908/909 Series Atomic Absorption Spectrophotometers. This series covers the full range of AA requirements from low-cost models to an automatic rotating turret multi-

element model. All models feature automatic wavelength and slit setting and are controlled by an external colour computer. The standard interlocked flame control system has been upgraded to include error lights. If the flame fails to ignite because of one of interlocks is not satisfied, these lights indicate where the fault lies. Options include single or double beam optics, background correction, four lamp turret, programmable flame control (B, BT, PBT), automatic burner rotation and up to four super lamp power supply. The top-of-the-range 908PBMT has a motorised lamp turret and is capable of



sequential multi-element analysis. A complete range of accessories, including graphite furnace, flame and furnace autosamplers, flame or electric hydride, hydride generator, high solids analyser and atom trap is also available. All models feature advanced AA software with central control of all accessories, hard disk storage of applications, results and graphics, and comprehensive report



generation.

### **GBC 906**

The GBC 906 will continue as the top-of-the-line GBC AA Spectrophotometer. It is still the most advanced AA Spectrophotometer on the market. Compared to the new 908 series, it offers the following advantages:

1. Automatic eight-lamp turret.
2. Automatic lamp peaking with

each lamp being automatically aligned as it rotates into its operational position for maximum light throughput.

3. Cast optical housing.
4. Easier installation or removal of spray chamber without handling gas lines.

### **ELITE AAS OPERATING SOFTWARE**

This "Elite" software is not supplied with new GBC AAS's but is available as an extra cost option on all computer controlled models. The full benefits are realised when the package is purchased with the unique and very popular

Automatic Burner Rotation accessory. The main features of the "Elite" software are: - Includes Intelligent Quality Control to ensure valid results. It will automatically analyse a check sample and compare the measured result with the expected result. If the measured result is outside pre-defined limits, the IQC system will take the specified error action. It may be used

to validate results with flame, furnace and hydride systems. - When used with a Graphite Furnace, can automatically perform spike recovery to validate results. - Allows a separate blank solution other than normal calibration blank to be used for samples, ensuring best possible accuracy.

**For further information contact ICI Instruments PO Box 68-330, Newton, Auckland 1 Ph 0-9 373 5765 Fax 0-9 360 0683.**

## **WILTON INSTRUMENTS VARIAN ATOMIC ABSORPTION SPECTROPHOTOMETERS**

Spectraa - 5 Single beam with optional background correction. Integrated touch pad keyboard and digital display. High sample throughput For laboratories with a heavy workload INTEGRATE REPEAT analyses hundreds of samplers per hour. Excellence in optics The single beam optical layout gives high energy throughput and excellent



signal-to-noise ratios. Economical Combine high sample throughput with low purchase price and running costs for economical operation. Wide range photomultiplier The multi-alkali PMT enables all elements to be determined, from arsenic at 189.0 nm to cesium at 852.2 nm. High performance flame atomization The highly efficient Mark VI Spray Chamber/Nebulizer system guarantees sensitivity and precision, with excellent performance for high dissolved solids solutions. Low detection limits The efficient design of the monochromator, light sources and atomization system provides excellent detection limits. Direct concentration readout Calibrate on up to 3 standards, directly, without the need to plot calibration graphs. Hard copy of results Automatic print out of results from the optical printer, saves time and eliminates transcription errors. Spectraa 10 plus Single beam with optional background correction, interlocked or automatic gas control, single or four lamp turret. On board computer control with keyboard and VDU. Spectraa 20 plus Double beam models as per Spectraa 10 plus. Spectraa 300 Automatic or programmable, double beam with manual four lamp turret and background correction. Controlled by P.C. Spectraa 400 Automatic or programmable, double beam with manual eight lamp turret and background correction.

- Central control
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- Advanced automatization
- Automatic sample handling
- Built-in SpectraAA reporting power
- Extensive method and data storage
- Flame safety

• Flexibility for expansion Spectraa 300 and 400 Zeeman - Automated systems with Zeeman graphite tube atomizer and programmable sample dispenser.

**For further information contact Wilton Instruments PO Box 31044 Lower Hutt Ph 0-4 569 7099 Fax 0-4 569 7240**

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**For further information contact Douglas Scientific Ph: 0-9 837 5447, Fax 0-9 837 5446. PO Box 45-027 Auckland 8.**

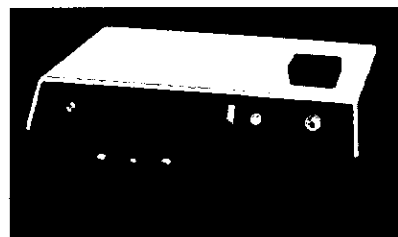
## WATSON VICTOR Turner Spectrophotometers

Turner Spectrophotometers use a plane diffraction grating monochromator with sine bar mechanism in an f7 Ebert mounting with first surface reflective optics. A unique solid state photodetector with a very wide wavelength range (330-1000nm) eliminates the need to change the detector. A narrow bandwidth of 8 nm provides high resolution. The digital displays retain



their resolution over the full photometric range. These important features and Turner's reputation for reliability are not found in similarly priced instruments from other manufacturers.

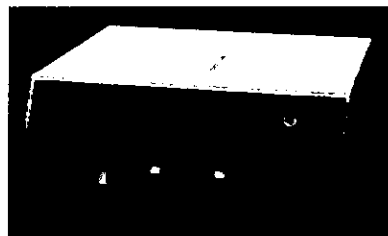
The Model 690 has an advanced microprocessor design for increased ease of use and accuracy. It automatically sets wavelength, inserts the proper stray light blocking filter, blanks instrument and calibrates on standard.



The Model 390 has an 8 nm bandwidth; 3 1/2 digit LED readout over full range; simple operation; Absorbance, Transmittance, Concentration, and Factor modes. It's easy to use and it helps eliminate computation errors.



The Model 340 features 8 nm bandwidth, three controls for simple operation and a large 3 1/2 digit, full range LED display for easy readability.

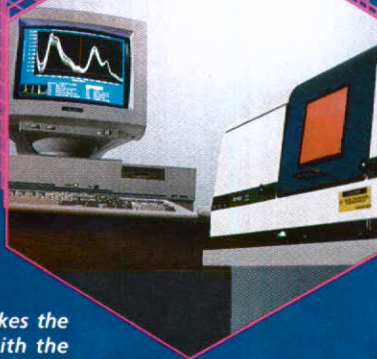


The Model 690-200 Far-UV Source converts Model 690, 390 and 340 Spectrophotometers to full 200nm to 1000 nm UV-Vis Instruments.

**For further information contact Watson Victor Auckland PO Box 1216 Ph: 0-9 579 3039 Fax: 0-9 525 0951. Wellington PO Box 1180 Ph: 0-4 385 7699 Fax: 0-4 384 4651. Christchurch PO Box 706 Ph: 0-3 366 9282 Fax: 0-3 366 2537. Dunedin PO Box 921 Ph: 0-3 477 7291 Fax: 0-3 477 8720**

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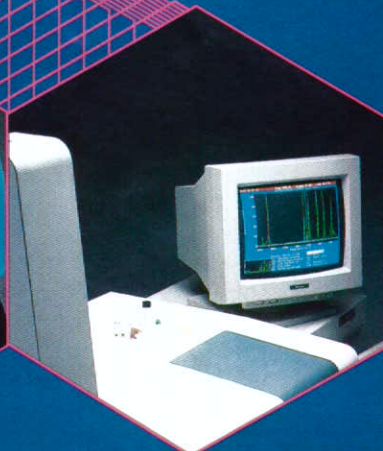
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