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The background of the cover is a photograph of a wine glass filled with red wine. The glass is in the foreground, slightly out of focus. Behind it, a wine label is visible, featuring a portrait of a man and some text. The background is a soft, out-of-focus green.

Featuring

The Chemistry of Post-bottling Sulfides in Wine
Building Innovation through Geopolymer Technology
What do Green Tea, Grapes Seeds, and Docks have
in Common?

Special Interest

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Photo taken by Matt Walters, School of Biological Sciences, University of Canterbury.

Wine kindly supplied by Stonecroft Wines.

The Chemistry of Post-bottling Sulfides in Wine

Dr. Alan Limmer

Stonecroft Wines, Hawke's Bay (e-mail: stonecroft@xtra.co.nz)

There has been a lot of discussion about wine closures of late, including some popular press coverage also. The re-emergence of the screw cap (some of us may recall it's first appearance – especially those of the Cold Duck era) has sparked a lot of interest in the performance of closures. Much has been written in the popular press on various aspects, such as the ability of wine to age under screw caps, the variability of the performance of corks, and the possibility of *reduced* characters under the near anoxic screw cap. Much (most?) of what has been written has little origin in science and more reflects popular beliefs. Further, very little of this material has been subject to any rigorous scrutiny. Consequently, popular opinion has often passed as scientific fact.

The chemistry of post-bottling sulfides in wine is in fact very interesting, at least to a chemist who makes wine! Further, the chemistry is reasonably well known and readily available if you know where to look. The first recorded documentation of the *reduced* character under screw cap was noted by the Australian Wine Research Institute¹ (AWRI) in February of 2003. There was no explanation for the mysterious sulfide character, but it did respond to copper fining. The AWRI seem still to be of the view that this is a winemaking fault to do with residual sulfides left in the wine at bottling despite warnings of a post-bottling reduction (and explanation) published by the author² in February 2002 and earlier popular press articles.

To understand the chemistry responsible for these post-bottling sulfides, we need to revert to redox chemistry. It is generally accepted that the traditional (cork) wine closure and a screw cap inhibit the ingress of oxygen post-bottling. In this regard generally cork is regarded as letting virtually no air into the wine.^{3,4} The screw cap has been adopted on the same basis – as providing a near anaerobic seal.⁵ Two observations have been made since the adoption of the screw cap. Firstly, the wines seem to age more slowly and secondly, there is a notable incidence of sulfides under this closures.¹

If we can accept that the winemaker who doing a good job traditionally under cork (sulfide wise) is also doing an equally good job under screw cap, it is hard to apportion blame for these post-bottling sulfides on the winemaker; all that has changed is the closure. The winemakers who have adopted the screw cap generally have maintained that the cork was also an impermeable closure.^{5,6} However, some permeability data for cork does exist in the form of MOCON (oxygen transmission) measurements as depicted in Fig. 1. It would be dangerous to equate these raw data quantitatively to wine, but they seem to suggest the ability for cork to permit some demonstrable oxygen ingress. If, in fact, cork does have an ability to transmit oxygen at a slightly higher rate than screw caps, then an explanation for the observations regarding ageing rates,

and post-bottling sulfides exists via the differing redox chemistry of the two closures.

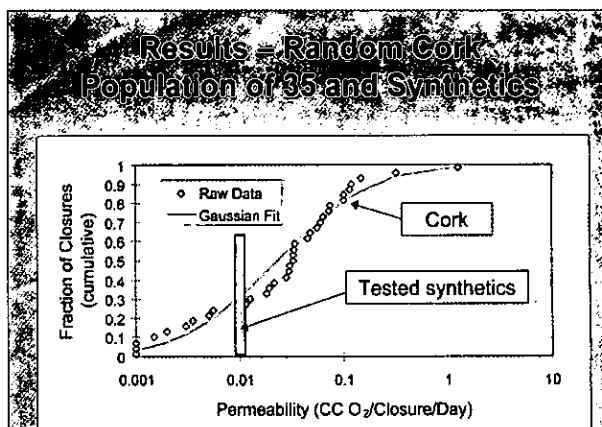


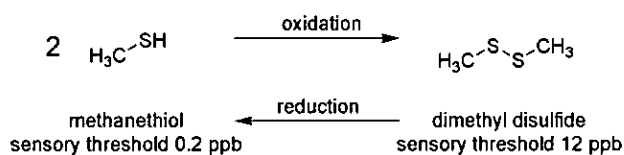
Fig. 1. Oxygen transmission rate for cork (measured by MOCON)

Wine can never be bottled completely free of sulfides. The ferment process leaves a sulfidic fingerprint, the composition of which depends upon the yeast strain and nutrient conditions in the ferment.⁷ Usually, the principal components of these sulfides are the more noticeable H_2S and simple thiols such as methanethiol ($MeSH$). The lesser components tend to be simple dialkyldisulfides (such as dimethyl and diethyl), methyl and ethyl thioacetate ($Me-COSR$; $R = Me$ or Et), and even some trisulfides. Fortunately, H_2S and thiols respond readily to copper fining, depositing as the insoluble sulfides. However, the disulfides and thioacetates do not. As such, these components are commonly found in the bottled wine. Fortunately, these components also have a sensory threshold that is considerably higher than the copper treatable components. Threshold data vary depending on the source of the information, but typical values would be as $MeSH$: 0.2-2 ppb; $DMDS$ 12-50 ppb; $MeSAc$ 40 ppb. Unless a wine has a disproportionate amount of intractable sulfides (disulfides and thioacetates), the sensory effect of these is generally minimal, with typical values in the range of 5-10 ppb.

A common practice in wineries in response to the occurrence of sulfides is to *rack* the wine. This involves an aerative transfer from one vessel to another. Traditionally, this is widely practiced with red wine in barrel with the accompanying observation that the stink reduces. The process is usually repeated at regular intervals up until bottling.

The explanation for the disappearance of the odour can be found in the relatively easy oxidation of thiols to disulfides. Thus, for example, $MeSH$ with a sensory threshold of 0.2 ppb is transformed into $MeSSMe$ with a sensory threshold of 12 ppb. And the stink has gone. Or has it? Like many redox reactions the reaction is reversible. A

common observation is that some months later, the wine needs racking again. Given that sulfides are formed at fermentation, there is no likely source for the formation of new sulfides from wine that is separated from the lees (dead yeast). So the obvious explanation for the recurrence of the stink is the consequent reduction of the disulfide under a suitably low redox potential. This effect is depicted in Scheme 1. The evidence also shows that a typical redox potential scheme for racking is as depicted in Fig. 2.



Scheme 1

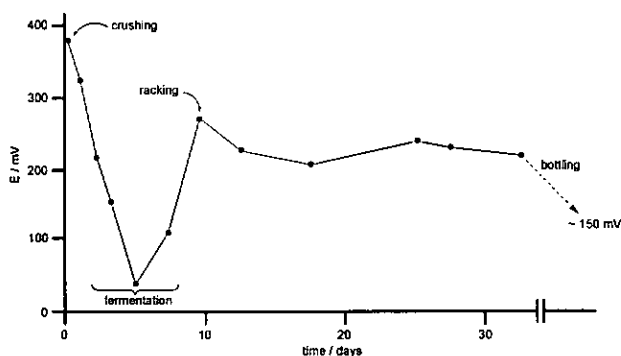
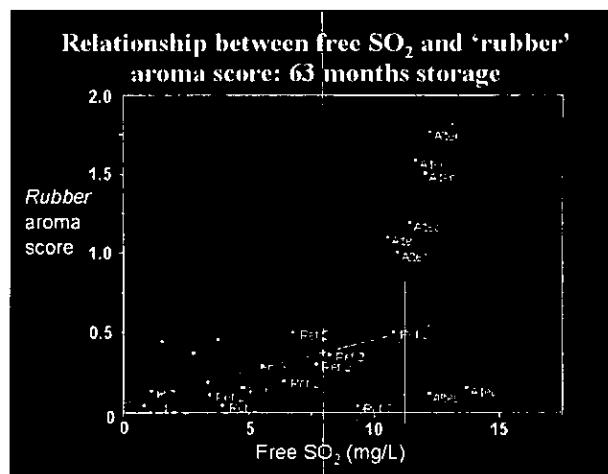


Fig. 2. Evolution of reduction potential during winemaking

So, we have a useful explanation for the occurrence of post-bottling sulfides for otherwise clean wine – *if the redox potential is low enough*. What is now needed is evidence of variation in the redox potential (dissolved oxygen) between the various closures. This can be gleaned from early screw cap development work such as that described by Bergeret *et al.*⁸ These authors found that the redox potential under a tight sealing Al foil drops twice as far as other barriers, and the wine developed a *reduced* character. More recently, the AWRI have instigated a comprehensive assessment of the performance of various closures. This includes sensory analysis as well as basic chemical assays of, *e.g.* SO₂, that is known to interact with the oxidative products in wine, and is widely, but mistakenly, regarded as an antioxidant. It has no direct interaction with oxygen,⁹ and its prime function is to bind with oxidative products such as aldehydes – which have a detrimental sensory effect on wine. In spite of the sometimes complex equilibria of the SO₂ in wine, a comparative measure of the respective levels in a wine gives some indication of the amount of oxidation that has taken place. The AWRI trials have generally focused on the *free* (or molecular) component rather than the total SO₂. The free SO₂ is the chemically active component. Some comparative data for the closures are shown in Fig. 3 and one can see that the screw cap (ROTE) retains higher levels of SO₂ than traditional corks, suggesting a lower amount of oxygen ingress. Altec also is a cork, but is of manufactured origin with an oxygen transmission rate quoted by the manufacturer as equivalent to ROTE. Interestingly, this information also shows a correlation between oxygen ingress and sulfide odour. Typically MeSH is attributed

with a rubber character but there is also a strong relationship between the sulfide odour and SO₂. This is no coincidence, at least according to this author! It should be noted that AWRI claim that there is no causal link between the SO₂ correlation and the sulfide aroma.¹⁰

Fig. 3. Sulfide character related to closure type and SO₂

The kinetics of disulfide reduction have been described by Bobet *et al.*¹¹ and have been found to be first order with respect to disulfide and SO₃²⁻ (the requisite reducing agent for the disulfides), which is a component of the SO₂ equilibria. The time-scale for the complete reduction in a wine-like solution at pH 3.5 was *ca.* 2 years. This explains why these things are more prevalent as post-bottling phenomenon than in the winery, although the observant winemaker often notes that a wine in tank develops sulfide notes after copper fining. There is one further source of post-bottling sulfides via the thioacetate pathway. The hydrolysis of the thioacetates has been described by Rylander *et al.*¹² While the rates are higher for alkaline hydrolysis, acid hydrolysis also can produce measurable MeSH within a matter of weeks.¹³

So, via two independent pathways, one can observe and predict thiol accumulation in wine post-bottling. The reason why this is rarely seen under cork (see Fig. 3) is that the rate of oxygen ingress exceeds that of the thiol accumulation. Analysis of wine sulfide profiles post-bottling typically show an accumulation of disulfides at the expense of thiols and thioacetates.

This explanation of post bottling sulfides is still not generally accepted by those using screw cap closures; they prefer to attribute the problem to poor winemaking and pre-bottling sulfides. However, the chemistry tells us that the nearer we get to anoxia, *i.e.* the lower the rate of oxygen ingress under a closure, the more sulfide we are likely to encounter. This situation is graphically depicted from further AWRI results (Fig. 4). The ampoule could be considered completely anaerobic, with the screw cap near anoxic, and the cork slightly less anoxic.

So, in one of life's serendipitous coincidences, it would appear the humble cork has got the oxygen permeability just about right if we wish to avoid these post-bottling sulfides. Raising the permeability of the screw cap liner would have a similar effect.

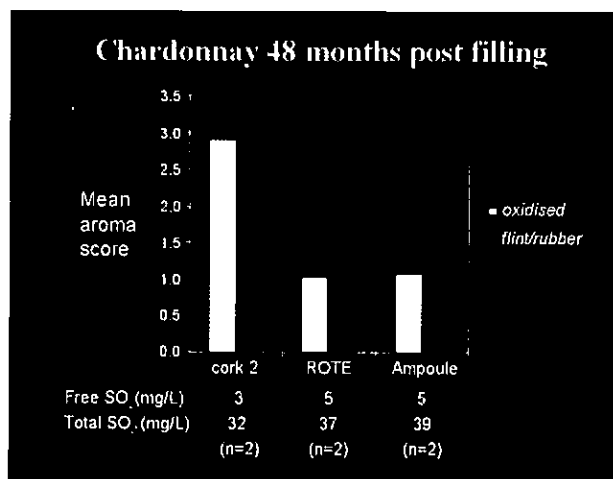


Fig. 4. Sulfide incidence related to closure type

An interesting aside to this discussion is the permeability of cork as depicted in Fig. 1. The data were derived by MOCON-type measurements that involve the headspace under a cork inserted into a bottle being swept into an oxygen-sensitive detector. These results suggest something like a 1000-fold variation in permeability, and some relatively high gaseous exchange rates for a supposedly near-anaerobic closure.³ This variability has been widely reported by the screw cap proponents as evidence of the superiority of the screw cap as a closure. However, it is interesting to look at the data of Fig. 3 where the spread of SO₂ for any given closure type is very similar. Note carefully that 'Ref.2' and 'Ref. 3' that appear in this figure *do not* relate to the citations of this article but to that particular study for visual gradings of cork quality). The figure also tells us that the visual grading of corks has some control over the permeability as they seem to cluster as groups, *i.e.* 1 + 1, ref 2, ref 3, Altec, etc., suggesting a variation in permeability better than 1000-fold, and comparable to the screw cap (ROTE). Further confirmation is found in the statistical data for free SO₂ reported in the 36-month results.¹⁴ The standard deviations for these results are listed below where you will note the difference between ROTE and cork is minimal. Further confirmation of the predictability of the performance of cork is shown in the ability of the AWRI to predict¹⁴ the SO₂ levels at 24-months from the 6-month data with an *r*² value of 0.89.

	1+1	Ref 2	Ref 3	Altec	ROTE	synthetic
SD(mg/l)	2	4	3	2	4	2

Furthermore, note the absolute values of oxygen transmission for the synthetic closures in Fig. 1. These were also under trial by the AWRI, but they ceased being of significance by about 36 months. The oxygen ingress rate was such that the wines had expired by this point. So, we know for sure that corks actually lie to the left of the synthetics in actual permeability, as their performance is still strong as seen by the 63 month data (Fig. 3).

All this information tells us that there is a considerable disparity in the actual performance of cork as a closure compared to the direct permeability measurement data. The reason for this disparity is not clear, but the author suspects it is connected to the various means of gaseous transport and specifically to diffusion kinetics vs pressure

driven gaseous flux. The bottles in the AWRI trial were stored inverted at relatively constant temperature suggesting that the results are strongly driven by diffusion kinetics. It is interesting to note that the ref 3 corks in Fig. 3 are 38 mm while those of ref 2 are 44 mm in length. A longer diffusive pathway seems to indicate a higher degree of impermeability, although there is a grading difference further clouding the issue. The author would be interested in any further explanation readers may have to offer regarding the disparity in these results.

In closing, the closure debate has been a fascinating process for the chemist and winemaker to observe. Clear demarcations have occurred within the industry over choice of closure and writers have devoted miles of column inches to the topic; the winemaker's opinions on the mysteries of the chemistry above have passed as scientific fact. The process has, at times, had more in common with a fanatical religious belief than science. A few paraphrased quotes from a recent supposedly authoritative publication¹⁰ on the subject serves to illustrate the point:

H₂S can be reduced to mercaptans (p. 116).

Thiols can be copper treated but mercaptans are more difficult. (p. 116/117).

There is no SO₃²⁻ in wine (p. 101).

DMS and DMDS are examples of mercaptans (p. 116)

.. the permeation of oxygen thru the closure is negligible, if not zero*

.. Corks have a variable permeability of 1000-fold.*

*These two quotes were by the same author in different publications 3 months apart.

One conclusion from the recent focus on wine closures is that they will never be the same again. Cork manufacturers are for the first time learning about the technical aspects of the performance of cork, synthetic manufacturers are trying to reduce the level of permeability, and the screw cap manufacturers will need to consider a range of permeabilities rather than just focus on highly anoxic closures.

And the wines will be better off.

Acknowledgement

Thanks are extended to Justin Bendall (Fonterra, Palmerston North) for assistance with Scheme 1 and Figure 2.

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4. NZSC Symposium, Nov 2004; NZSCI: www.screwcap.co.nz;

"the quantities of oxygen that normally penetrate into the bottles are negligible if not zero. Oxygen is not the agent of normal bottle maturation".

5. NZ Screw Cap Initiative web site: www.screwcap.co.nz;

"Screw caps are the ideal closures to exclude oxygen from the bottle."

"Q. The wine is a living breathing thing, and it needs to breathe through the cork, doesn't it?"

A. "(In every case) the answer is NO".

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"Hence, it is clear that the oxygen permeability of the screw cap is essentially identical to that of the very best corks, and is in both cases negligible. The screw cap thus accurately replicates the maturation conditions provided by the very best corks."

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About the Author

Alan Limmer gained his PhD in Chemistry from Waikato University in 1982. Currently he is a Director of NZ Winegrowers and Chair of the Research Committee for NZ Winegrowers, and initiated the Hawke's Bay Charity Wine Auction that is now in its 14th year with over \$1M raised for the local hospice. He is the owner and winemaker of Stonecroft Wines. Alan was awarded the ONZM in 2004 for services to winemaking and, in particular for his outstanding efforts in getting the Gimblett Gravels area of Hawke's Bay established.

Personal Story of ANU Explosion



Maria Matveenko shares her personal account of the explosion in early August in the Research School of Chemistry at the Australian National University in Canberra. Maria completed her undergraduate studies at Victoria University and a summer studentship at IRL in Lower Hutt.

I had just loaded my precious newly made tetracyclic alkaloid onto a column when I heard an incredibly loud bang. It could only have been from a big explosion, and luckily blew the door of my lab shut (for some completely scientifically explainable reason which I don't want to hear as I call this a miracle).

I then saw fire through the window in my door, it was coming from the room directly opposite mine. Naturally, I decided to run for my life, hoping that the fire wouldn't trap me in the lab. I ran out, there was blue smoke everywhere, the pipes were blown and water was running, the ceiling looked like it was falling down and there was debris in the air and on me afterwards. The aluminium door of the room that contained the fire was gone, but I didn't really notice that until I was told about

it afterwards. All I could see was fire, and I just ran towards the fire exit, as did everyone else from other parts of the building. Of course, some people didn't realise for a while what was going on, and were just having their lunch outside. It wasn't until we could smell the smoke outside that everyone knew that this was bad. We all just stood at a distance and watched a huge column of smoke rising, at which point some people started crying, especially those that are about to finish their PhDs.

I'm just happy to be in one piece at the moment, everyone was looking for me after the incident, because I was the closest to it and people saw "the student" running out, so from then on I was referred to as "the student", but it has since progressed to "oh, THE Maria".

I guess those of us that do chemistry are always at risk of being in this situation, but I vividly remember thinking that this can't be happening. Although no one was hurt and the fire and water damage was very localised and minimal, we must remember to always be prepared for such incidents, starting from backing up our work over and over, to taking all those annoying fire drills seriously.

Maria Matveenko

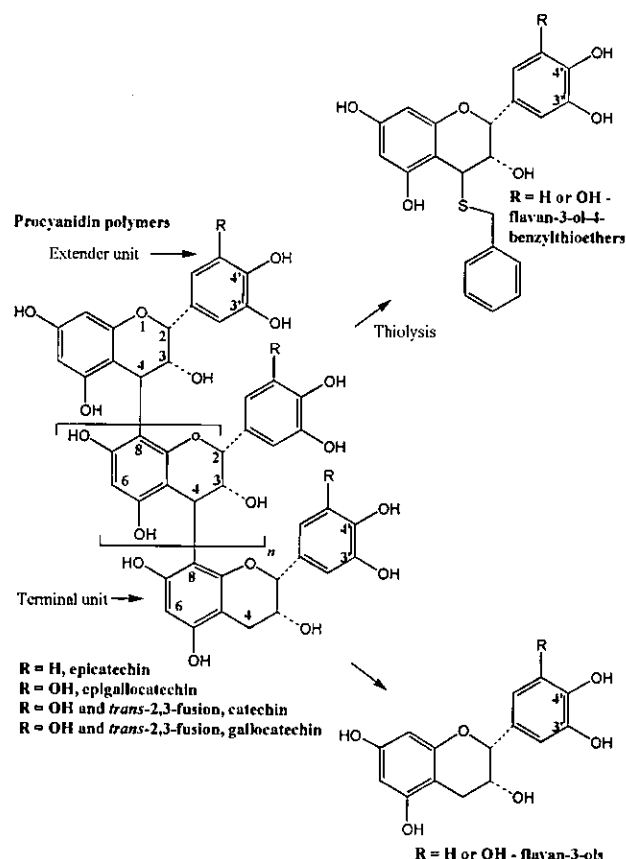
What do Green Tea, Grapes Seeds, and Docks have in Common?

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Introduction

The phenolic constituents of green tea (*Camellia sinensis*) and grape (*Vitis vinifera* L.) seeds have been the focus of much research attention in human health and nutrition. Proanthocyanidins are polymers of flavan-3-ol units found in green tea, grapes and numerous other plants (Scheme 1). The phenolics in green tea are flavan-3-ols and flavan-3-*O*-gallates and the major component - epigallocatechin gallate (EGCg) - is known to have a broad spectrum of biological activities as antioxidant,¹ antibacterial,² and antifungal.³ The efficacy of proanthocyanidins from green tea extracts has not warranted as much attention. The major components extracted from grape seeds, oligomeric and polymeric proanthocyanidins, are widely used, mainly as nutritional supplements and have *in vitro* antioxidant, antibacterial⁴ and antiproliferation⁵ activity. Galloylation, the extent of oligomerization, and stereochemistry strongly influence the observed activity of the compounds.



Scheme 1

Properties of proanthocyanidins

Proanthocyanidins properties depend upon their structure in terms of monomer units (degree of hydroxylation and 2,3-*cis*- or 2,3-*trans*-stereochemistry), their degree

of polymerisation (DP) and the type of linkage between the flavan-3-ols (4,8- as in Scheme 1, or 4,6-branched structures). For the procyanidin (PC)-type polymers with 3',4'-dihydroxy substitution the constituent flavan-3-ol units are either catechin (*trans*) or epicatechin (*cis*) with R = H while prodelphinidin (PD)-type polymers with 3',4',5'-trihydroxy substitution contain either galocatechin (*trans*) or epigallocatechin (*cis*) units with R = OH (Scheme 1). However, the majority of the proanthocyanidin polymers in plants comprise mixtures of the two classes and mixtures of oligomers (DP 5–10) and higher polymeric material (DP >10).

Proanthocyanidins in forage legumes

At Grasslands Research Centre, the search for alternative forage species to supplement pasture and ensure sustainable agriculture has included the evaluation of a wide range of pasture legumes. These species are native to Eurasia and the Mediterranean region and can tolerate arid environmental extremes. Temperate forages such as *Lotus* species containing proanthocyanidins provide nutritional benefits for grazing ruminants including improvements in weight gain, wool growth, milk production and composition, ovulation rate, and increased efficiency of feed utilization. A recent review on the effects of *Lotus* species by Min⁶ suggests they derive from reduced degradation of dietary protein to ammonia by rumen microbes and increased protein outflow from the rumen, which can result in increased absorption of amino acids from the small intestine.

The common weed, referred to as dock (*Rumex obtusifolius*), found growing in many NZ pastures was observed to be an antibloat agent for cattle.⁷ Its phenolic constituents warranted phytochemical investigation given the observed *in vivo* effects and they were identified as a series of oligomeric and polymeric proanthocyanidins with galloyl derivatives, which may explain the observed *in vivo* biological activity of dock.

Extraction and purification of proanthocyanidins

Dock leaves were extracted with acetone-water, the solution fractionated (Sephadex LH-20 chromatography; acetone-water; 7:3 elution - a modification of the method of Foo⁸) to give a fraction containing procyanidin oligomers and polymers. Likewise, proanthocyanidin-containing extracts of green tea were prepared by modification of the method of Degenhardt,⁹ while a grape seed extract was obtained from RMF Nutraceuticals NZ Ltd seed and prepared by extraction with aqueous ethanol (80% v/v) at room temperature. Chemical and spectroscopic methodologies have been applied to characterize and to compare

the structures of the proanthocyanidin oligomer and polymer fractions from these three extracts. The identities of the individual proanthocyanidin polymer units and chain length were estimated by strong acid-catalysed cleavage in the presence of benzyl thiol. This thiolysis releases the terminal units as free flavan-3-ols, while extender units are distinguished as benzylthioether adducts formed from nucleophilic capture of the carbocations generated under the acidic conditions. More recently, mass spectrometry (MS) has been utilised to characterise the oligomeric composition of proanthocyanidins by electrospray injection (ESI).

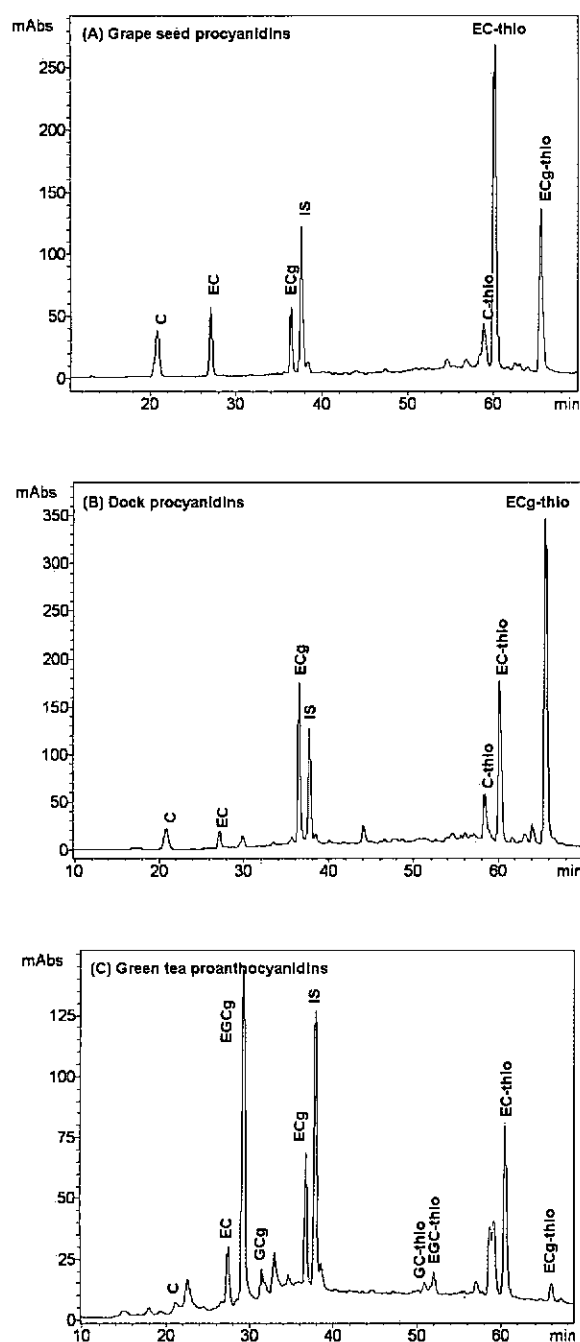


Fig. 1. Reversed phase HPLC chromatograms (280 nm absorbance) of thiolysis products; C, catechin; EC, epicatechin; ECg, epicatechin gallate; GCg, gallocatechin gallate; EGCg, epigallocatechin gallate; IS, internal standard, dihydroquercetin; the suffix - signifies the corresponding benzylthioether.

The chemical degradation of proanthocyanidins by thiolysis

The mean composition and mean DP (mDP) of proanthocyanidins can be determined from total thiolysis and chromatography of the products by HPLC; a variation of Guyot's¹⁰ method was used for the thiolysis (see Scheme 1). Such degradation provides good yields of cleavage products with low levels of degradation and epimerization. The mean composition of the terminal units can be determined from the ratio of the released monomers, that of the extender units in the polymer chain from the ratio of benzylthioether adducts, and the mDP from the monomer to extender unit ratio. Samples were analyzed by the method of Meagher.¹¹ Responses relative to the internal standard, dihydroquercetin, for terminal flavan-3-ol units were 0.30 PC and 0.06 PD while extender flavan-3-ol units had 0.26 PC and 0.06 PD benzylthioethers, both in accord with published values.¹² Gallate terminal flavan-3-ol units were 1.09 for PC and assumed to be 1.09 for the PC gallate extender benzylthioethers. The chromatograms (280 nm monitor; Fig. 1) show the terminal units released as monomers before 30 min and the extender units eluting after 45 min as benzylthioether adducts. The catechin and gallocatechin thioethers appear as two peaks in the chromatograms due to separation of the C-4 epimer pair. The same pattern is not observed for the benzylthioethers from epicatechin and epigallocatechin as there is very little epimerization during thiolysis.

The data obtained show grape seed proanthocyanidins to be gallated procyanidin polymers (mDP 3.5) (Fig. 1A). The terminal units consist predominately of catechin (46%), epicatechin (46%), and a minor epicatechin gallate component of 8%. The cleavage products of the extender units are dominated by epicatechin benzylthioether (77%), and components of catechin and epicatechin gallate benzylthioethers (15 and 8%, respectively). Quantification of epicatechin gallate benzylthioether was achieved from cleavage of an epicatechin gallate homo-dimer. Thus the predominant *cis* (epicatechin) stereochemistry of the extender units differs from the equal portions of *cis* and *trans* terminal units (Table 1). The thiolysis data show dock proanthocyanidins (Fig. 1B) to be gallated procyanidin polymers (mDP 4.3) similar to grape seed and the terminal units to consist of equal proportions of catechin, epicatechin gallate, and epicatechin. As with grape seed, the cleavage products of the extender units are dominated by epicatechin benzylthioether (57%) with components of catechin and epicatechin gallate benzylthioethers (18 and 25%, respectively). The difference between grape seed and dock procyanidins is simply the extent of galloylation (8 vs 27%). Procyanidins from a variety of plant species including apple (mDP 2 to 190),¹² cocoa (mDP 14), brown sorghum bran (mDP 14), lowbush blueberry (mDP 39), and cranberry (mDP 15)¹⁰ have been characterized previously from thiolysis. Thus dock procyanidins are comparable in flavan-3-ol composition to grape seed, which is dominated by catechin terminal units and epicatechin extension units. Dock has greater proportions of epicatechin gallate in both the extender and terminal units. There is apparently different selectivity in the biosynthesis of monomers that form the terminal units to that of precur-

Table 1. Comparison of procyanidin extender and terminal unit contributions from grape seed and dock extracts, mDP and % galloylation by thiolysis.

	mDP	Gallate %	Terminal			Extender		
			C ^a	EC ^b	ECg ^c	C	EC	ECg
Grape seed	3.4	8	0.46	0.46	0.08	0.15	0.77	0.08
Dock	4.3	27	0.39	0.23	0.38	0.18	0.57	0.25

^aCatechin; ^bEpicatechin; ^cEpicatechin gallate

sor units which extend the polymer chain. The molecular species involved in chain extension remains a matter of conjecture.¹³

In contrast to the above, the thiolysis data show green tea proanthocyanidins as a mixture of procyanidin and prodelphinidin units (Fig. 1C). Quantification of the thiolysis products was not possible for the proanthocyanidin polymer due to a lack of standards for the benzylthioethers of gallic acid and epigallocatechin gallates (elution 59 min; Fig. 1C). Compared with grape seed and dock, green tea has contributions from the three gallates epicatechin, gallic acid, and epigallocatechin in the terminal units, but no catechin gallate. The extender units of green tea proanthocyanidins appear less dominated by gallates with a low concentration of epicatechin gallate. However, there maybe a significant contribution from prodelphinidin gallates that were not quantified.

ESI/MS analysis of proanthocyanidin oligomers

Evidence of proanthocyanidin oligomer composition can be provided by ESI-MS. In the negative ion mode, and with weakly acidic conditions for the scan (m/z 250-1400), proanthocyanidin oligomers can be detected as anions because of the acid phenolic protons; the degree of ionisation and numbers of negative charges increase as chain length increases.¹⁴ The weakly acidic conditions inhibit ionisation so that for $DP \leq 3$ singly-charged ions dominate, DP 4-8 have the doubly charged species predominating, and for higher DP triply or higher charges predominate. Although the ions for doubly-charged oligomeric species with an even DP overlap those for the singly charged species, they can be distinguished by the ion masses (odd for singly-charged species, even for doubly-charged species), and the spacing between them (16 and 8 daltons, respectively, for singly and doubly-charged species). The practical upper limit of ion detection comes more from the broad chromatographic peaks of the higher oligomers than the limit of the quadrupole mass spectrometer (2000 amu); molecules of higher mass carry higher charge. Characteristic ions can be used to assign proanthocyanidin oligomers, but without authentic standards the epimers C (catechin) and EC (epicatechin), or GC (epicatechin gallate) and EGC (epigallocatechin) cannot be distinguished. Therefore oligomers were assigned as either PC consisting of C and/or EC, or PD consisting of GC and/or EGC. Mass spectrometry can also provide useful information on the composition of proanthocyanidin oligomer mixtures in the form of ion masses that correspond to sets of oligomers of the same DP and com-

position. Negative ion reverse phase HPLC-ESI-MS has been used to characterise procyanidin gallates in grape products.¹⁴ However, the presence of mixtures of proanthocyanidin oligomer gallates confounds interpretation as the mass of the two galloyl derivative units is the same as a single gallic acid oligomer unit.

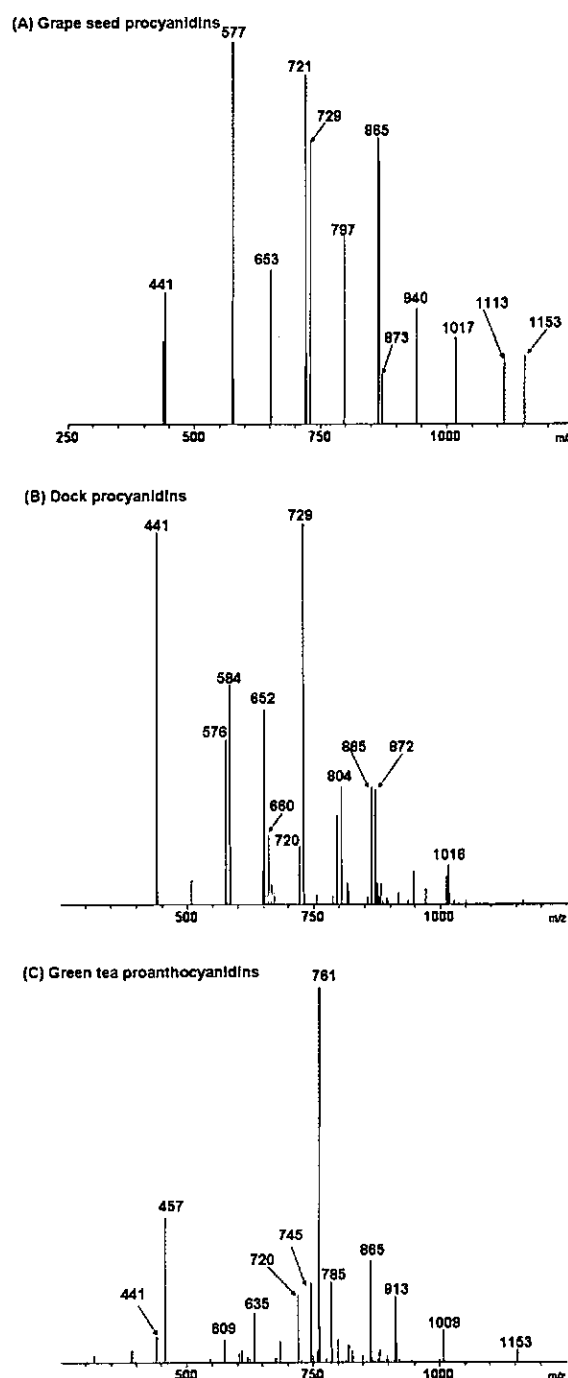


Fig. 2. Mass spectra of the extracts (see text).

The ESI-MS of the proanthocyanidin fractions give ions from oligomers with DP 2-6 (Fig. 2) broadly consistent with the mDP estimated by thiolysis (Table 1). Grape seed (Fig. 2A) and dock (Fig. 2B) extracts were exclusively procyanidin homo-oligomers. A wide mass range was recorded from (singly-charged) dimers to (doubly-charged) hexamers. In each range, the dominant species observed come from procyanidin homo-oligomers, namely a singly charged dimer and a trimer species (m/z 577 and 865), and doubly charged tetramer to hexamer species (m/z 576, 720, and 864). All the major peaks corresponded to molecular ions of procyanidin-type oligomers. The spectra are compounded by the appearance of ions from procyanidin-gallates; singly charged monomer, dimer, and trimer species (m/z 441, 729 and 1016) and doubly charged tetramer to hexamer species (m/z 652, 796, and 940). Proanthocyanidin oligomers with galloyl derivatives were identified in green tea (Fig. 2C).¹⁵ These include a galloyl dimer [m/z 761; (PD)₂-g] as the dominant prodelfphinidin ion in the mass spectrum, a trimer [m/z 913; (PD)₃ or perhaps (PCPD₂g²⁺)], a second trimer [m/z 865 (PC)₃], a tetramer (m/z 1153 (PC)₄], the doubly charged hexamer (PC²⁺)₆ (m/z 1008), and the gallated flavan-3-ols GCg (m/z 457) and ECg (m/z 441). The trimer [PC₃] could also be EAg-(4β-8)-ECg, A (azfelechins; m/z 865), the dimer assigned by Degenhardt.⁹

Conclusion

Surprisingly, the study shows that the common weed dock has more in common with grape seeds than with green tea. While dock (*Rumex obtusifolius*) has been studied in Turkey for its anthraquinone content,¹⁶ the procyanidin gallates identified here may indicate that its extracts have biological activity similar to grape seed procyanidin extracts.

Acknowledgements

We are grateful to Dr G. Waghorn (Dexcel, Hamilton) and Dr. Y. Foo (IRL, Lower Hutt) for sparking our interest in novel plants such as the pasture weed, dock, and for help-

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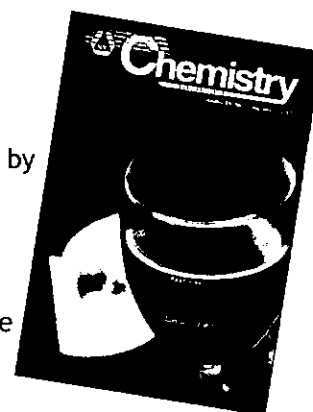
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Building Innovation through Geopolymer Technology

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Introduction

Geopolymer materials are inorganic polymers synthesised by reaction of a strongly alkaline silicate solution and an aluminosilicate source at near-ambient temperature.^{1,2} The low energy process results in a fast-setting material that exhibits exceptional hardness and strength and, in this respect, geopolymers are similar to cements. The focus of our current research is to determine the potential of geopolymers as an alternative cementing system for high-value products.

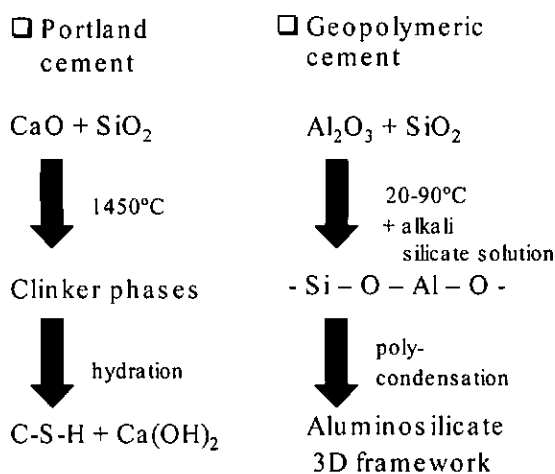


Fig. 1. Comparison of conventional and geopolymer-based cements.

A simple comparison of conventional and geopolymer cements is shown in Fig. 1. While traditional cements are composed of portlandite [Ca(OH)₂] and calcium silicate hydrate (C-S-H) phases, geopolymer cement is based on an aluminosilicate framework. This difference is important in two respects. Firstly, aluminosilicate materials are much more resistant to chemical attack, e.g. by acids, than calcium-rich Portland cement and secondly there is no calcination step (heating to 1450 °C) in the synthesis, thus avoiding the release of CO₂. The former aspect means that geopolymer technology offers new opportunities for entering markets currently inaccessible to traditional cements while the latter illustrates that geopolymers offer significant environmental benefits, a fact important for the future. Geopolymers also possess physical and chemical properties that make them potentially suited for use in refractory applications and as waste immobilisation matrices.^{3,4}

Synthesis and structure of geopolymers

Interest has centred on the types of aluminosilicate sources that can be successfully used in the geopolymerisation

reaction. Naturally occurring clays and pumice as well as industrial wastes such as flyash and slag have been investigated. Particular emphasis has been placed on the waste materials with a view to developing geopolymers synthesised from the flyash obtained as a by-product of coal combustion in power stations. Our efforts have concentrated on locally-sourced aluminosilicate materials, including pumice, allophane, and bentonite, as well as the flyash produced at the Huntly power station. Flyash is extremely useful as it produces geopolymers with very high strengths. However, the composition of the flyash varies from batch to batch, depending on the composition of the coal being burnt in the power station at any given time.

Structural characterisation of geopolymers reveals that these materials are X-ray amorphous. Aluminium is mainly in tetrahedral coordination and silicon has a variety of coordination geometries. A cation, commonly Na⁺ or K⁺, provides charge balance. A structural model proposed by Barbosa *et al.*⁵ is shown in Fig. 2.

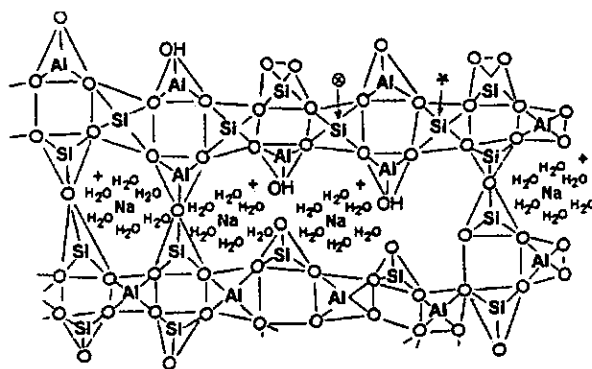


Fig. 2. Proposed geopolymer structure [5].

Characterisation

Any investigation of geopolymers requires characterisation methods applicable to amorphous materials and solid state nuclear magnetic resonance (NMR) spectroscopy and scanning electron microscopy (SEM) are particularly powerful. NMR is used routinely in our own work to determine whether a new product exhibits the chemical characteristics of geopolymers and to investigate on-going reactions within the solid state matrix over time. The nuclides of most interest are ²³Na, ²⁷Al and ²⁹Si; ¹¹B and ³¹P may be used also for studies of boroaluminosilicate and phosphoaluminosilicate geopolymers, respectively.

For electron microscopy, sample preparation is critical in obtaining reliable SEM data. Standard polishing techniques are unsatisfactory for young, relatively soft samples, and for these resin impregnation or an examination of fresh fracture surfaces is preferable. Older samples

may have increased significantly in hardness on ageing and a standard polished section may be prepared.

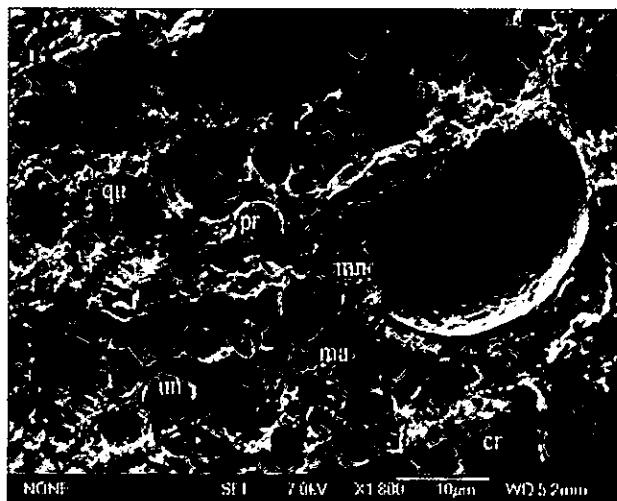


Fig. 3. SEM micrograph of geopolymer product - qu - quartz crystals; un - unreacted fly ash particle; pr - partially reacted fly ash particle, ma - geopolymer matrix; mn - mullite needles; cr - completely reacted fly ash particle.

An annotated SEM micrograph of a flyash geopolymer (Fig. 3) shows a highly complex product morphology that consists of unreacted, partially reacted, and completely reacted flyash spheres that are surrounded by a matrix which also includes quartz crystals and mullite needles originating from the flyash. Energy dispersive X-ray analysis (EDX) shows that the material is extremely inhomogeneous. Of particular interest is the observation that products obtained using the Huntly flyash appear to contain two types of matrix (Fig. 4). A phase rich in sodium, aluminium, and silicon has a characteristic *dense* appearance and is an expected aluminosilicate geopolymer binder phase, while the second *spongy* phase is rich in calcium, sodium, aluminium, and silicon, reminiscent of the C-S-H phase of Portland cement. In fact, at higher magnification this dense phase is found to be quite porous, but the porosity is on a much finer scale in comparison with the spongy phase. These observations suggest the co-existence of aluminosilicate and cementitious binder phases in geopolymers synthesised from starting materials containing the high levels of calcium that Huntly flyash has.

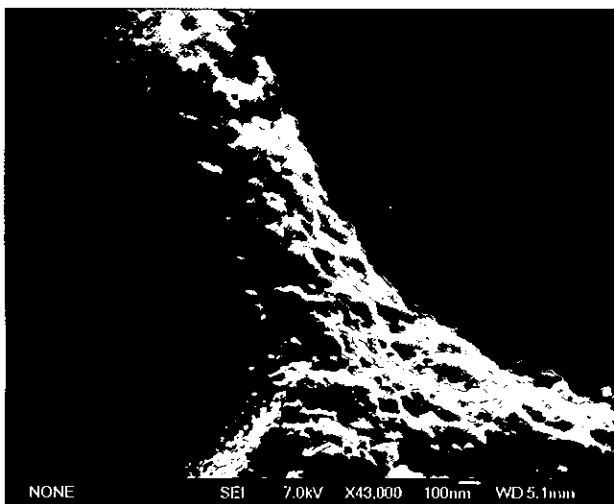


Fig. 4. SEM micrograph showing two types of geopolymer matrix.

Challenges in geopolymer chemistry

Relatively little is known about the chemistry of geopolymers such that a number of challenges present themselves to researchers. Two recent examples are in obtaining a desirable setting time, and in understanding the effect of processing variables.

Control of setting time

NZ flyash geopolymers show considerable promise in a wide range of industrial applications. However, Huntly flyash is *Class C* flyash due to its high lime content and it has extremely short setting times on activation by alkaline silicate solution. This limits the commercial exploitation of this and other *Class C* flyash as a raw material for geopolymers.

Our work has shown that addition of inorganic boron to the activator solution not only significantly extend setting times, but also allows a predefined setting time to be achieved by varying the amount and source of boron added. Subsequent characterisation of the products indicate that the boron is structurally incorporated in the matrix, giving rise to a novel class of borosilicate geopolymers. This work forms the basis of a patent application for commercial exploitation of Huntly flyash and other sources of *Class C* flyash worldwide.⁶

Effect of cure regime

The effects of processing conditions, particularly cure temperature and cure time, on the flexural properties of geopolymers synthesised from Huntly flyash have been investigated and the results are shown in Fig. 5. The most notable feature concerns the bend strength as there are the marked difference from low and high temperature cures. It appears that two different cure mechanisms may operate and on-going work is expected to elucidate the reasons for this.

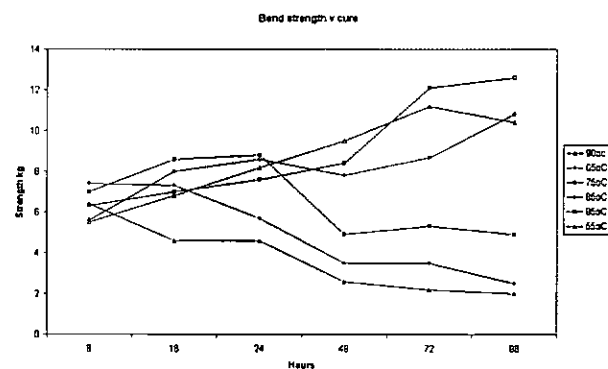


Fig. 5. Effect of cure regime on geopolymer tensile strength.

Future directions

In advancing our understanding of the chemistry and materials science of geopolymers, knowledge will be applied in the key areas of geopolymer composite materials synthesis and prediction of long-term durability.

Geopolymer composite materials

The building sector has signalled a need for reinforcement options for geopolymers, specifically through the design and fabrication of new fibre composites and structures.

This will permit increases in their strength, toughness, and elastic modulus, and generate a wider range of opportunities for new industrial products and applications.

The effects of incorporating solid pultruded rods as reinforcement in a flyash-based geopolymer are being investigated. Three different pultruded rods are currently under investigation, namely polyester resin, vinylester resin, and polyurethane resin with glass fibre as the rod reinforcement.

Durability and performance monitoring of geopolymers

In comparison with conventional cement and concrete systems, geopolymers are very new materials completely lacking the long service history that would enable robust prediction and control of structural deterioration. Performance requirements, drivers for deterioration, and means of predicting and characterising changes that will ultimately result in failure need to be assessed.

Electrochemical techniques such as the measurement of linear polarisation resistance and electrical impedance spectroscopy have been used by us to study the corrosion behaviour of steel and other representative engineering metals in flyash geopolymers for periods in excess of a year. In general terms, carbon steel, 316 stainless steel, and copper appear to perform well in flyash geopolymers. Each metal forms a reasonable bond with the geopolymer and does not undergo excessive corrosion. Zinc appears to suffer accelerated corrosion initially because of the high pH, but the reaction stabilises as the geopolymer sets. The vigorous reaction of aluminium in contact with liquid geopolymer damages the interface between it and the geopolymer, and prevents effective bonding.

As expected, carbon steel electrodes appear to form a protective film in high pH conditions. Corrosion potentials vary which may be a result of local breakdown of the pro-

TECTIVE iron hydroxide film at pH > 14. Copper and 316 stainless steel also appear to have only low corrosion rates after more than a year.

Conclusions

The cementing properties of geopolymer materials have been known for more than twenty years but key elements of their fundamental materials science remain unknown, undeveloped and unexploited. From an industrial perspective, geopolymer technology can only progress to successful commercialisation when the underlying science is fully understood. Our goal is to develop the knowledge, capability, and intellectual property in geopolymer materials ultimately to build a new technology platform from which commercial processes and products may be exploited for the benefit of NZ.

Acknowledgements

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The Move Towards Electronic Lab Notebooks

By John Landells and Helen Palmer

Have you ever considered discarding that well-worn old lab notebook, and making the move to an electronic version?

Lab notebooks are of course a vital part of any research project. All researchers are well aware of the need to keep full and detailed records of their experimental work for future reference, and so that experiments can be repeated by their colleagues. Such records can also become very important in disputes over patent rights. In most countries, the "winner" in the race for patent rights will be the "first to file" a patent application. However, the current law in the United States is such that the "first to invent" has the right to obtain patent protection for an invention. (Although there are indications that this situation may change in the future.) Therefore, if there is any dispute between two parties, for example over when a particular compound was made and characterised, it may be vital to show that the compound was in fact made on a particular date. Many organisations therefore recognise the importance of adopting standard procedures whereby the researcher signs and dates his or her lab book, and the entry is then read, signed and dated by a witness.

As an alternative to the old-style handwritten lab book, some organisations are now moving to the use of electronic lab notebooks. There are a number of commercial products available, which endeavour to incorporate enough checks and safeguards to satisfy even the most pedantic patent attorney.

There are some obvious advantages to using electronic lab books over the traditional handwritten versions. One of these is the potential for an increase in knowledge transfer, as electronic notebooks allow results to be readily shared with collaborators and colleagues. In addition, because the format is electronic, it can be easier to search through the data and information contained within. Experimental data and text can be easily integrated together and, once entered, cannot be modified. This can assist in preventing possible transgressions by the record-keeper. The researcher can then electronically sign off each piece of work, and the software provides a permanent date and

time record of that piece of work. Such electronic records could form part of any evidence used in a future patent dispute.

Other advantages include the fact that electronic notebooks can be backed up electronically, thereby minimising the possibility of losing vital data, and providing a permanent stored record. However, this does highlight a potential issue for the future - whether or not, with advances in technology, this stored information will be able to be easily retrieved and read ten or even twenty years in the future. One way of dealing with this may be to retain paper printouts from the electronic notebook, together with any other original data - although this somewhat defeats the purpose of storing the information electronically.

Academia may be slower to adopt electronic lab notebooks than industry organisations. Cost could be a factor for academic organisations, particularly if the lab notebook software needs to be tailored to suit individual lab situations and needs. Developing and maintaining such software would require significant input and ongoing maintenance from an IT support team.

Nevertheless, it is easy to see that there will come a time when the potential benefits of electronic lab notebooks will outweigh the disadvantages. Perhaps the "paperless lab" is just around the corner.

A reminder: if you have any queries regarding patents, or indeed any form of intellectual property, please direct them to:

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Helen Palmer and John Landells of Baldwins specialise in chemistry and biotechnology patents. Helen joined Baldwins in 2000. She has a PhD in chemistry from The University of Auckland and postdoctoral research experience. John joined Baldwins in 2003. He has a PhD in chemistry from the University of Otago and is in the final stages of completing an LLB at Victoria University of Wellington.



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The Halton Retirement Symposium: Novel Molecules, New Materials and Small Rings

Brendan Burkett and Joanne Harvey

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Prof. Brian Halton retired on 31 March 2004 after some 36 years of continuous service at Victoria University of Wellington (VUW). During this time he supervised almost 50 graduate students including 11 PhD and 2 Postdoctoral students, published some 140 research papers and review articles, edited 10 books, and co-authored two editions of a classic organic photochemistry text. Brian is an internationally recognised scientist of the highest calibre who has dedicated more than 37 years to providing excellence in research and teaching in organic chemistry, and the promotion of, and service to, chemistry. To mark the occasion of his retirement VUW appointed him Emeritus Professor and the School of Chemical and Physical Sciences hosted a symposium *Novel Molecules, New Materials, and Small Rings* on 29-30 June 2005 to celebrate the enormous contributions made by Brian both to the university and to his discipline.

The symposium, a truly international event, was attended by some of Brian's collaborators and associates, including the current IUPAC President, Prof. Leiv Sydnes (Bergen, Norway), and representatives from the Chemical Society of Japan, Profs. Yoshito Tobe (Osaka) and Jun Nishimura (Gunma). Prof. Klaus Müllen (Max Planck Institute for Polymer Research, Mainz) was represented by Dr. Andrew Grimsdale (now at the Bio21 Institute, University of Melbourne). Many of Brian's former students were also in attendance. Most fittingly, perhaps, was the presence of the first PhD and last Honours student supervised by Brian at VUW – Tony Woolhouse, now a manager at Biopharm (Industrial Research Ltd), and Jarrod Ward, a PhD student at Auckland University. Many of New Zealand's top organic chemists were also present, including Rob Smith (Otago), Jim Coxon (Canterbury), David Officer (Massey), and Margaret Brimble (Auckland), as was the current NZIC President Prof. Graham Bowmaker.

Following the opening of the symposium by VUW Vice-Chancellor Pat Walsh, Prof. Bowmaker presented Brian with the highest honour that NZIC can bestow – an Honorary Fellowship – in acknowledgement of his services to the Institute and the profession of chemistry. At the symposium dinner, held at the university staff club, Brian was further honoured with the presentation of a commemorative plaque acknowledging his services to Pacific Basin Chemistry by Prof. Yoshito Tobe on behalf of the Chemical Society of Japan.

From a scientific perspective attendees were treated to a number of stimulating presentations. Prof. Martin Bannell, one of Brian's early PhD students and now senior organic chemist at ANU, gave an inspirational talk *En-*

abling Methodologies for Natural Product Synthesis, the complex syntheses of biologically active molecules undertaken by his research group in Canberra that have their origins in his PhD studies. Another of Brian's former students, Prof. David Officer (Massey University) gave an account of *Designing Aromatic Molecules for Light Harvesting* and outlined their use in solar cells. From then, the topics ranged from the synthesis of large polycyclic molecules and their properties – *Generation, Characterization, and Reactions of Highly Reactive Cyclic Polyynes* (Yoshito Tobe) – to the behaviour of minute highly strained compounds – *Cyclopropanes I have met since 1972* (Leiv Sydnes); from *Cataract Research at Canterbury* (Jim Coxon) and potential cancer treatments from *Designer Chemicals for Targeting Mitochondria* (Rob Smith) to *Syntheses Directed at Complex Shellfish Toxins* (Margaret Brimble). *Phenylene-based Materials for Nano-Technology* from the Max Planck Polymerforschung were described by Andrew Grimsdale and *Cyclobutane-connected Cyclophanes* from Gunma by Jun Nishimura.

The final word was left to Brian himself, who spoke on *Life in the Strain Lane*, and his work with highly strained organic molecules, and especially cyclopropenes. For the younger chemists, this lecture was a fascinating tour through Brian's life as a researcher, and for former students and collaborators a chance to see their work in the broader context of a research career as opposed to a research project. Tracing back to his PhD studies with methylideneaziridines at Southampton University and his postdoctoral work at the University of Florida where he was involved with cyclopropene rearrangements, he outlined his research at VUW where he has cemented his reputation as a world leader in his field.

Brian's contributions to chemistry cannot be overstated as evidenced by the sheer breadth of chemistry covered by the speakers at the symposium. It is important for the younger generation of chemists now rising through the ranks to realise that contribution to science is not measured merely in publications or the size of a group but also from the integrity of the students we train and the quality of the work they subsequently produce. Brian's continuing contribution to the world of chemistry through his former students was certainly well displayed by those who presented research at this symposium.

Equally important in terms of contribution to science is Halton's involvement in the scientific community. In this respect Brian has been very active through his promotion of the discipline and profession of chemistry. He has



IUPAC President Leiv Sydnes (right) with Andy Kay



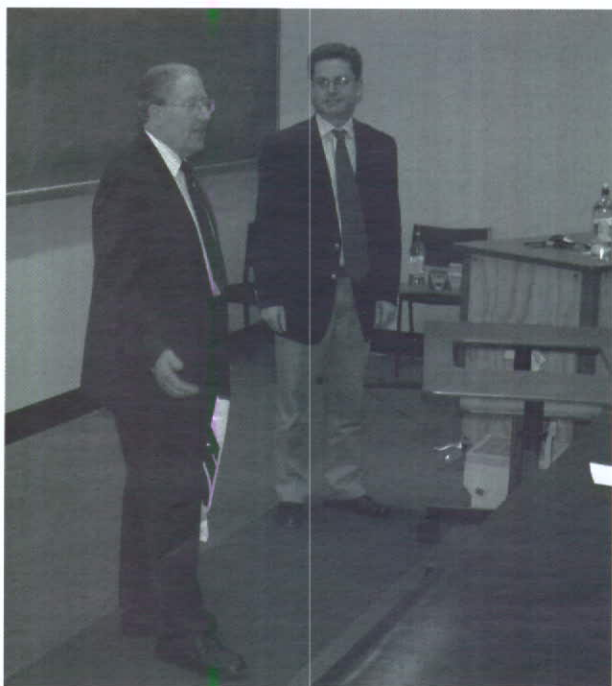
L-R: Roger Brown, Brian Halton, Martin Banwell



L-R: Roger Brown, Brian Halton, Jun Nishimura, Yoshito Tobe



L-R: Andrew Grimsdale, Graham Bowmaker and Jim Johnston



The Last Word!

held the office of NZIC President, served numerous terms as a Council Member, and held many other positions of responsibility in the Institute at local and national level over many years. He has been Editor of *Chemistry in New Zealand* since 2001 and the Institute's representative on the organising committee for The International Chemical Congress of Pacific Basin Societies (*Pacificchem*) for the 1989, 1995, 2000, and 2005 events where he has contributed substantially to the organisation and smooth running of these very large international meetings. He has also

been instrumental in facilitating financial support to enable young chemistry professionals from the developing areas of the Pacific Basin to attend the congress, and in soliciting funds for NZ graduate students to attend, especially in the earlier times. That Australasia is formally involved in this major event is due entirely to his efforts in the late 1980's. In addition, Brian served the wider university and student community as the Victoria University Newman Trustee for some 23 years and was a member of the Trinity-Newman Board that facilitated improved student accommodation at VUW.

Finally, we take this opportunity to join with chemists throughout NZ, Australia, and internationally, in thanking Brian Halton for his many contributions to chemistry and the chemical community, and to wish him the very best in his retirement: here's to many more years of fruitful chemistry Brian!

Norman Trevor Clare – 1912-2005

Norman Trevor Clare was born at Waitara, Taranaki, in 1912 and educated at New Plymouth Boys' High School, where he gained a Taranaki Scholarship in 1930. This took him to Victoria University College, with lodgings at the then newly established mens' hostel - Weir House. He was in residence for its first day, attended its first lunch, and lived-in for two years.

As a Scholar he was expected to be a full-time student although he often doubted that that was advantageous. He expressed the opinion that part-timers, like the cadets in the Agricultural Department such as Brian Shorland, had the advantage. Despite this he did very well at chemistry, becoming Professor PW Robertson's 'lab boy', Departmental demonstrator, and his personal assistant; Norman graduated MSc (Hons.) in Chemistry in 1934. During his course, which overlapped that of Brian, Norman wanted to establish a Victoria Harrier Club. He and Brian Shorland became the inaugural President and Secretary, respectively, and remained involved in an honorary capacity until the club amalgamated with the Athletics Club.

After two years on the university staff, Norman decided to leave academia, preferring in 1936 to join Brian Shorland at the Agricultural Department's chemistry section in Sydney Street (opposite Parliament Buildings in Wellington) because of its interestingly wide range of investigations using chemistry. The Agricultural Chemistry laboratory had been established in 1903 by Barney Aston to investigate problems associated with farming and agriculture, and the last scientist he appointed to the staff before retiring was Norman Clare.

Norman became particularly involved in the problem of facial eczema, and in 1938 transferred from the city laboratory to Wallaceville Animal Research Station in Upper Hutt where much of that work was centred. This interest led him into other diseases involving photosensitivity, the chemistry and metabolism of porphyrins and other animal pigments, and the metabolism of phenothiazines (anti-worming drugs) with which photosensitivity was associated. Norman authored some 40 papers on these subjects and was commissioned by the Commonwealth Agricultural Bureau to publish a review on *Photosensitisation in Diseases of Domestic Animals* (Commonwealth Agricultural Bureau Review Series, No.3, 1952), still cited as a reference veterinary text and which established his worldwide reputation. He had intended to extend this review and submit it for a doctorate, but never quite got around to doing so; undoubtedly it was a work well deserving of such recognition.

In 1947 he was appointed Chief Biochemist at the newly established Ruakura Animal Research Station in Hamilton. Norman then visited research establishments in South Africa, United Kingdom and the USA as his role was to oversee the chemical analyses for a wide range of projects in animal breeding, nutrition and management. However, he continued his work on facial eczema that ultimately led to the isolation of the fungal toxin, sporodesmin, by Singe and White. From 1965 to 1967 he was seconded to

the UN Food and Agricultural Organisation to work on their sheep diseases project at Pendick (Turkey) where he established chemical facilities, trained Turkish scientists, and guided research on copper deficiency around the Black Sea and selenium deficiency in Anatolia.

Norman Clare played a significant role in NZIC affairs since becoming a 1934 member of the Wellington Branch; he served on the National Editorial Committee, the Examinations Committee, and the Wellington and Waikato Branch Committees. He was elected to Fellowship in 1947, and was instrumental in establishing the Waikato Branch in 1952 of which he became its Chairman. He was Journal Editor 1961-62 and organized and chaired several conferences during his time at Ruakura.

He married Eunice Wall, another member of the scientific staff, in 1941. She was much involved in the studies on bush sickness (ultimately found to be due to cobalt deficiency) and other trace element investigations. They had two sons, John - who follows in their analytical interests - and David; sadly, Eunice pre-deceased Norman in 1970.

Norman retired in 1972 and cultivated his interests in trout fishing, bird watching, poetry, and the history of Richard Pierce's first flying machine in NZ; he was working on material for its celebration this year. He was one of nature's real gentlemen maintaining pleasant and successful relationships with individuals whom most others found difficult. He was a life-long friend of Brian Shorland appreciating his peculiar sense of humour and his habit of switching the basis of his argument to taking the role of devil's advocate when he could see he was not going to win. Others found this disturbing; Norman understood what was going on, and was amused by it! He was kind and thoughtful with a keen sense of humour and a love of poetry and literature. His most loved possession was the copy of Professor PW Robertson's own publication *In Search of Beauty* which PW had presented to him when he left for the Agricultural Chemistry laboratory. Norman himself produced delightful poems for celebrations at the Harrier Club and for special NZIC activities.

I first met Norman Clare when I took over editorship of the NZIC Journal from him in 1962. We renewed acquaintance during the last four years of his life when he became a mine of information with stories of Victoria University College in the 1930s, the Chemistry Department, Professor PW Robertson, and Brian Shorland, whose biography I have been constructing.

For the last several years of his life Norman was in a wheelchair, in a rest home across the road from the shore in New Plymouth on the paddocks where he had played among the gorse as a child. He was partly deaf but his mind and memory were active and working well. He died in New Plymouth in June 2005.

I am already missing his contributions to our memories of those early days of the NZIC and its personalities.

Joan Mattingley

Jack Austin – 1927- 2005



Retired chemistry reader Dr. Jack Austin died at the age of 77 on April 14. His adult life was centred on the University of Canterbury. Jack spent four years as a student graduating with an MSc, met his wife Margaret (later a Labour MP and Cabinet Minister) when she was a science student, completed his doctorate while a junior lecturer, and taught chemistry for 41 years. Dr. Austin was known by the wider University community as *the man who did the timetable*.

John Maurice Austin was born and raised in South Canterbury, attending Timaru Boys' High School before coming to what was then Canterbury University College. He studied mathematics, physics, and chemistry, but it was the distinctive lecturing style of Hugh Parton that persuaded him to continue with physical chemistry. In 1949, after finishing his MSc, Jack was appointed as a junior lecturer and enrolled as a PhD student. This was a significant departure from tradition, with the Chemistry Department leading the University in having junior lectureships. The four-year term was conditional on the holder enrolling as PhD student and dividing their time between doctoral study and department duties.

Dr. Austin became the second PhD graduate from the Department. He worked on the thermodynamics of reactions using electrochemical techniques in a primitive basement laboratory where he designed and built a sensitive calorimetric system to measure the heats of associations of ions. Upon completion of his doctorate in 1954 he was appointed to a lectureship, was promoted to Senior Lecturer in 1962, and to a Readership in 1967.

Head of Chemistry Dr. Bryce Williamson said Dr. Austin was a very clear and precise lecturer who was very fair *with students and paid sympathetic attention to their problems and added that he will be remembered for his great organising ability and attention to detail which served the Department, as well as the wider University, very well.* After retirement, Jack remained a cherished and respected member of the Department. He was a regular attendee of seminars and often joined the Department for morning tea up to within a few weeks before his death. Retired colleague Emeritus Professor Michael Hartshorn said that the Department Dr. Austin entered as a student in 1945 was a very different place than that today, having just five teaching staff. During his PhD years Jack held a sequence of temporary assistant lectureships, often as replacements for others heading off overseas, and had a heavy load of teaching duties, including running the first-year laboratories and giving the lab talks on the second floor in C5 of the Old Chemistry Building. *I understand that in honour of his first lab talk he bought a new sports coat*, said Prof. Hartshorn who also described his friend as *a good servant of the University who would be remembered with fondness as an academic, colleague and friend.*

He was also known as an *expert timetabler*. He assumed the responsibility in the early 1960s and one of his last duties before retiring in August 1990 was to complete the 1991 timetable. The heavy dependence of the University on his expertise became quite evident over a period of study leave he took during 1967. In his absence two people undertook to produce the timetable but, on his return, he declared their efforts unworkable and proceeded to make critical amendments. Dr. Austin was involved extensively in administration, serving as Acting Head of Department, on the Professorial Board, and as Chairman of the Timetable Committee. He also served as a University representative on the Burnside High School Board of Governors from 1966 to 1976. Outside of the University, he was a keen cricketer, badminton player, gardener, and tramper.

Dr. Austin is survived by his wife, Margaret, and their three children.



New Zealander Takes Highest Award

A sixth New Zealander has won the American Dairy Science Association's highest research and development award.

Dr Peter Munro is the General Manager planning and integration for the Fonterra Dairy Cooperative. He was presented with the 2005 Danisco (formally called Marschall Rhodia) International Dairy Science Award in Ohio, USA for his contribution to the industry.

Fonterra's Director of Innovation Bob Major said the award was a tribute to Dr Munro's outstanding contribution to the New Zealand dairy industry and to dairy science internationally.

The award was established in 1980. It recognises outstanding accomplishments in research and development outside the USA and Canada in chemistry, biochemistry, microbiology, technology or engineering in the dairy foods industries.

Previous winners from New Zealand include one of the youngest ever recipients, Professor Harjinder Singh from Massey University who won the award in 2001.

Auckland University Announces Professor of Food Chemistry

A Professor of Food Chemistry has been appointed at the University of Auckland.

Professor Laurie Melton has been appointed to the position. He brings many years of experience as a researcher and a lecturer both within New Zealand and overseas.

Professor Melton started the Food Science programme for postgraduate students at The University of Auckland in 1996. The Food Science Group includes programmes for undergraduate students as well as a strong group of researchers and is based within the Department of Chemistry.

Dean of Science Professor Dick Bellamy said "The appointment of a researcher and lecturer of Professor Melton's calibre to this important position is significant. Professor Melton is recognised internationally in the food sciences field and is also the founder of the Food Science programme at this University."

Professor Melton has published over a hundred scientific and technical papers. He is recognised internationally for determining the chemical structure of xanthan gum used in toothpastes for that clean mouth feeling and also as a thickening agent in gravies and soups.

New Business Splits from CRI

Plant Protection Chemistry NZ Ltd is the new independent research and development company to be formed from a long standing science group in Scion.

PPC NZ has been functioning for many years specialis-

ing in the formulation and application of Agrichemicals within the Rotorua based Crown Research Institute, now known as the Scion Group.

Scion Group Ceo, Dr Tom Richardson said "Due to the vision and commitment of core staff, PPC NZ are now recognised as world-leaders in agrichemical application, formulation and efficacy, and it is appropriate for them to forge ahead as a standalone business."

PPCNZ started in 1975 searching for better gorse herbicides for use in forestry. Within five years they had developed a novel organosilicone additive that made the herbicide "Roundup" very effective against gorse, bracken and broom.

In 1998 the group shifted their focus from forest herbicides to horticulture. They have since developed specialised formulations of insecticides and fungicides for use with various fruit crops including apples, kiwifruit and persimmon as well as developing designer additives for other crops.

The standalone company was made possible by a management buy-out by three senior staff; Jerzy Zabkiewicz, Robyn Gaskin and Alison Forster.

Changing Mix of Academics

The gender balance among academics is now equal but women are still under represented in all ranks above lecturer.

This finding was recently released as part of a case study report into gender and promotion in a New Zealand university. The report did not find significant differences between the work done by male and female academics that could explain the discrepancy in seniority.

It was also found on average full time academics spent forty-nine hours a week on their work. Half of the respondents in the case study were dissatisfied with salary levels relative to peers in other organizations and the demands of their job. The main sources for job satisfaction were the teaching or research the academic staff were involved in as well as the support received from colleagues.

Massey University hosted the research carried out by an independent organization, the New Zealand Council for Educational Research.

Oils and Fats Update

The reasons why people should buy pristine oils in dark glass or tin were given in a short talk by Dr Rufus Turner at the recent AGM for the Oils and Fats Specialist Group of the NZIC. Changes to the committee saw David Illingworth resigning and Helen Tervit joining.

There are also plans for a book on lipids in Australasia if author support is found.

Excellence in Polymer Research Rewarded

University of Auckland's expertise in polymer research has got another funding boost.

The Government has awarded up to \$5 million in funding for the Centre for Plastics Innovation and Technology, a collaborative initiative between the University and Plastics New Zealand.

The project will provide a centre for developing advanced polymeric materials, industry specific research, graduate and industry training as well as application of new technologies in plastics processing and manufacturing.

The centre will be located at the University's Tamaki Campus and work in association with the Centre for Advanced Composite Materials. It will not only involve University of Auckland researchers but also collaboration with researchers from other tertiary institutions, Crown Research Institutes and industry.

Fellowship for Organic Chemist

Organic chemistry study has been made easier for Masters student Hemi Cumming who has commenced his thesis research with the support of a Tuapapa Pūtaiao Māori Fellowship. Administered by the Foundation for Research, Science and Technology, the Fellowships are awarded to top Māori students enrolled in postgraduate courses in science, technology and engineering.

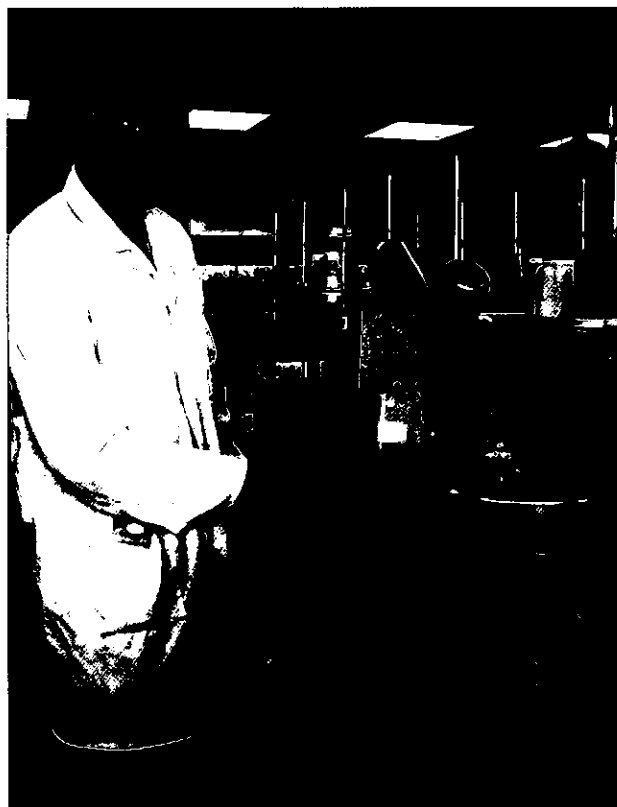


Photo: Hemi Cumming

Mr Cumming, of Ngāti Raukawa and Ngāti Toa Rangatira descent, completed both chemistry and biochemistry majors at an undergraduate level, and decided to advance in organic chemistry. Under the supervision of Dr Emily

Parker in the Institute of Fundamental Sciences, he will investigate the mechanism of two important biosynthetic enzymes for his Masters thesis. The enzymes, DAH7P synthase and KDO8P synthase, have essential roles in plants and bacteria, are not present in animals, and catalyse similar but mechanistically different reactions. Mr Cumming will harvest the enzymes from a variety of bacterial sources, and the results of the research will form the design of inhibitors for these enzymes with the aim of making new and effective antibiotics.

Mr Cumming says he is keen to see more Māori students continue from secondary to tertiary education, especially in the sciences. He says scientists are often directly involved in decision-making in planning, managerial or consultancy roles.

Chem-E-Car Grand Final for University of Canterbury Students

The Warriors may not have made it to the Grand Final this year but University of Canterbury chemical and process engineering students will once again be up against the best in Australasia in the Grand Final of the Chem-E-Car competition in Brisbane at the end of September.

The objective of the competition is to design and construct a car that uses a chemical reaction to power it. The competitors also need to control the distance the car travels carrying a specified load.

The winning car from the local performance competitions has been designed by a team of five undergraduate students; Yana Abdul-Hamid, Li Liu, Eryn Md-Saleh, Pingting Lu and Ke Xu. The method of propulsion is a copper-magnesium electrolytic cell that powers an electric motor.

An hour before the running of the competition, the teams are given the distance their car is to travel as well as the load it must carry. The cars must stop as close to the finish line as possible.

It is likely a second Canterbury team may attend this year's competition, if funding can be found. This team won the poster section of the local competition and were a very close second in the performance competition. Their car uses an aluminium-air cell that powers an electric motor. It is stopped by limiting the air supply. This design was only possible because recently very pure aluminium became available from the aluminium smelter.

The competition will be held as part of the Chemeca 2005 Conference. It began as part of the 6th World Congress of Chemical Engineering in Melbourne in 2001. Canterbury has had two winning teams in previous years and is confident of picking up another award this year.

NZIC - supporting chemical sciences

September News

New Honorary Fellow

The Institute's highest honour - *Honorary Fellowship* - has been bestowed on **Prof. Brian Halton**. The framed certificate was presented to Brian in Wellington by President **Graham Bowmaker** at the Halton Retirement Symposium on June 29 (see elsewhere in this issue).



Photo Credit: Brian Halton receiving Honorary Fellowship

IUPAC President Visits

IUPAC President **Prof. Leiv Sydnes** visited NZ in late June and met with RSNZ officials and **Dr. Pat Holland** (Cawthron Institute) who is Secretary of the IUPAC Division for Chemistry & the Environment. The meeting was scheduled to fit with the Halton Retirement Symposium and provided an excellent opportunity for NZ matters to be appropriately raised. **Prof. Laurie Melton** (Auckland) was recently elected as Titular Member to the new Divisional Committee for 2006-2010 while **Prof. Kip Powell** (Canterbury) continues as President of the Analytical Chemistry Division.

BRANCH NEWS

AUCKLAND

Prof. Graham Bowmaker gave the last of his NZIC Presidential addresses *Shedding Light on Molecular Structure: Applications of Spectroscopy in Structural and Materials Chemistry* to the Auckland Branch on July 7. He noted that Auckland University has a long association with research of this type as of NZ's earliest DSc degrees was awarded to **James McLaurin** in 1897 who proved that oxygen was necessary for the complexation of gold by cyanide ligands. This process

was important for the economic extraction of gold from crushed ore. He described his long-standing interest in the structure of the infinite chain complexes of CuCN, AuCN and AgCN and recent studies with use of ^{63}Cu nmr, far infra-red, and powder neutron diffraction (at Sydney University) to appraise the order or disorder of the cyanide bonding.

Chemistry Department UA

Our congratulations to **Jim Metson** who was recently promoted to Professor and to long-serving Committee member **Anna Yee** on receiving her PhD. **Dr. Andrew Dingley** has accepted a post as senior lecturer in NMR spectroscopy and will arrive in February 2006.

The Department has hosted visitors **Dr. J Murray Gibson** - *Nanosciences at the Advanced Photon Source* (Argonne National Lab. USA), **Prof. Jun Nishimura** - *Cyclophanes from Vinylarenes* (Gunma University, Japan), **Dr. David Chen** - *Total Synthesis of Azaspiracid* (Biopolis Chemical Synthesis Lab., Singapore), **Prof. Leiv Sydnes** - *From Halogenated Cyclopropanes to Carbohydrate Analogues* (University of Bergen, Norway), and **Prof. Abhik Ghosh** - *An Organometallic View of Metalloporphyrin-NO bonding* (University of Tromsø, Norway).

CANTERBURY

The June meeting took the form of three short research talks by **Michael Edmonds** (CPIT), **Axel Neffe**, and **Matthew Polson** (both UC postdoctoral fellows). It was a very stimulating evening.

July, a highlight of the year, was the 4th annual *Trivia and Truffles* evening. A record number of 17 teams entered with the winners: 1st The Ruthenates (**William Lewis**, **John Slater** and **Matt Polson**), 2nd Dipolar Disorder (**Andrew Muscroft-Taylor**, **Kim van Berkel**, and **Charles Wright** - Crop and Food) and 3rd Tuskerane (**Bill Swallow**, **Bryce Williamson**, and **Cassandra Hinton** - ESR). The

best-name prize was shared between *Ionic Bond (Taken not shared)*, *Truffles* and *Periodic Success*. Once again **Michael Edmonds** and **Rebecca Hurrell** wrote the questions and compered the evening.

Chemistry Department UC

Leon Phillips has been awarded funding from the RSNZ International Science and Technology Linkages Fund for work with the Chemistry Department at Trinity University, San Antonio, Texas. **Jeremy Harrison**, working with recent Visiting Erskine Fellow, **John Brown**, has been awarded the Millard and Lee Alexander Postdoctoral Fellowship at Christ Church College, Oxford.

Prof. Peter Slade (University College, Fraser Valley, British Columbia) is spending his sabbatical leave working with **Jim Coxon**. **Prof. Bob Pipal** has completed his sabbatical and returned home, while **Richard Gammon** has left after several months in the Department. **Richard Keene** (James Cook University and Adjunct UC Professor) made a two-week visit.

MANAWATU

Massey University

University VC **Judith Kinnear**, has announced the appointment of **Prof. David Parry** as one of 4 Distinguished Professors, the highest recognition that the University bestows on a member of its academic staff; there are to be no more than 10 Distinguished Professors at any one time. David Parry is a leading authority in the field of fibrous proteins and an outstanding academic, internationally recognised for his work in connective tissue, muscle and intermediate filaments, and the 2000 RSNZ Sir Charles Hercus Medal. Also the University has signed an agreement with Peking University to foster academic cooperation that includes teaching and research exchanges. As part of this agreement a science symposium is being held in Beijing in October with a view to initiating ongoing

research collaboration; **Peter Schwedtfeger**, **Geoff Jameson** and **David Officer** will be taking part.

The 700 MHz Bruker NMR has had a CryoProbe installed. **Geoff Jameson** (Centre for Structural Biology), says the cooling function will significantly increase the sensitivity of the spectrometer and allow better quality data to be obtained faster. Worth more than \$500,000, the CryoProbe (the first in NZ) operates in tandem with a 700-MHz magnet, making it the country's most powerful NMR spectrometer. Stage 2 of the Bio-NMR Research Laboratory is just complete seeing an Horizontal Wide Bore Magnet in place but yet to be re-energised. **Paul Callaghan** (VUW) has gifted a console unit to Massey University for use with the this and also offered assistance to **Jason Hindmarsh** in learning the consoles intricacies.

Scott Walker, a 2nd-year PhD student with **Emily Parker**, was jointly awarded the runner-up prize at the *MacDiarmid Young Scientist of the Year* awards in Auckland. His poster *Molecular Design: Progress Towards a New Class of Antibacterial Agents* presented challenges in creating new drugs that work as inhibitors through cellular interruption processes blocking the activity of certain enzymes without causing side-effects. **Emily Parker** is the recipient of the Massey University Womens' Award that will allow her teaching commitments to be reduced and energies focused on research. Her MSc student **Hemi Cumming**, has been awarded a Tuapapa Putaiao Maori Fellowship by FoRST. Hemi, is to investigate the mechanisms of DAH7P synthase and KDO8P synthase.

Karl Shaffer, an Honours student with **Carol Taylor**, was recently awarded a Freemasons University Scholarship while **Nicolas Uhlich** (Ecole Européenne Chimie Polymères Matériaux, Strasbourg) has joined Carol's group for 3-months. Carol recently returned from the US where she visited the Los Alamos National Laboratory and caught up with former Massey colleagues and attended the 39th ACS National Organic meeting in Salt Lake City. She is now on her first sabbatical leave in more than 10 years having attended the

Fall ACS National Meeting and now working with **Dan Kahne** (Harvard University), her former postdoctoral adviser, until early 2006; she synthesing of glycopeptide antibiotics.

Dave Harding's lab has seen the departure of visitor **Simon Burton** and arrival of **Libei Bateman**. **Karen Bang**, **Carl Otter**, and **Steve Kirk** attended the 12th RACI National Convention in Sydney. Karen presented a poster on her combinatorial synthesis of γ -lactones as potential flavour compounds, while Carl and Steve presented posters titled *Coordination chemistry of cyclophosphazene ligands* and *Ligand coordination for potentially metal rich phosphazene scaffolds*, respectively. RSNZ Travel Grants have been awarded to PhD students **Celia Webby**, **Amy Pietersma**, **Scott Walker**, and **Ben Mulchin**, mostly to attend Pacificchem 2005.

Andrew Brodie has received a grant-in-aid to develop linkages in polyphosphazene chemistry between **Harry Allcock** (Penn. State) and the **Brodie-Ainscough** research group. The funding will also allow Allcock to make brief visits to other selected centres in New Zealand.

Fonterra

Dr. Peter Munro, Fonterra Dairy Cooperative Group's general manager planning and integration, has become the sixth NZer to win the American Dairy Science Association's highest research and development award for his contribution to the industry. He was presented with the 2005 *Danisco International Dairy Science Award* in Ohio in July. The award is a tribute to his outstanding contribution to the NZ dairy industry and to dairy science internationally.

WAIKATO

The Branch congratulates its Secretary **Kitty Lee** and **Michael Ellwood** on the recent birth of their first child; a healthy boy - Jamie.

Waikato University

Paul Lu was presented with the Branch-sponsored J E Allan Memorial Prize by NZIC President Graham Bowmaker (top 2nd-year chemistry major in 2004). The prize commemorates the work of Eric Allan

who pioneered the development of atomic absorption spectroscopy in the 1950's at Rukahia Soil Research Centre in Hamilton. **John Mitchell** recently completed his PhD from a project involving **Dr. Yinqui Wu** (AgResearch) and **Lyndsay Main** that developed new chemical sensor methods; John gave an excellent talk on his work at the August Branch meeting.



Photo Credit: Paul Lu receiving the Allan Memorial Prize

New PhD student **Carol Goss** has a TIF-funded project with **Merilyn Manley-Harris**, **Alistair Wilkins**, and **Terry Braggins** (Hill Labs) as commercial partner, while **Jacob Babu's** TIF-project is with **Alistair Wilkins** and **Chris Miles** (HortResearch). **Maryka Gaudio**, an Adelaide University PhD student, is visiting the Department to work on mass spectrometry of organometallic compounds using the recently commissioned high resolution Bruker MicroTOF electrospray mass spectrometer.

Bill Henderson has returned from a period of study leave to once more take up the role of CoD Chemistry, while **Richard Coll** presented an invited paper at the USA-based NSF conference of *Gold Standard Quality Research in Science Literacy*. It is an extraordinary reality that despite living in the most scientific and technologically-advanced era, there is growing superstition and pseudoscience. Richard's programme is based on the premise that the greatest challenge facing compulsory and advanced level educators is to enhance scientific literacy for meaningful debate.

NIWA

Craig Depree has shown that the levels of PAHs present in roadside soils require remediation if international guidelines are to be followed. A clear

link was established from source-to-sink, viz. from coal tar, to roadside soils, to gutter particulates, to stream sediments. The results were presented at the South Pacific Stormwater Conference in Auckland in May.

WELLINGTON

The last three Branch meetings have attracted large attendances. June saw some 50 of us treated to a feast of cinematographic chemistry with *Chemistry and The Lord of the Rings* presented in a lecture demonstration by Auckland MSc graduate **Norman Cates** (Weta Workshops). We were given a tour through the ways that practical chemistry was used in the *Lord of the Rings*TM; from polymers to plasters were shown the many applications for chemistry in the film industry. The audience delighted especially in having an opportunity to handle the props that Norman and his colleagues had made – Norman was responsible for all the elf ears on the films! July provided contrast with **John Emsley** (Cambridge University) attracting large numbers for *Elements of Murder*. The presentation, based on his newly released book of the same name, addressed lead, arsenic, antimony, mercury and thallium. The history of the poisons was charted from alchemical days and interwoven with anecdotes on the ways they have been used through the ages. Each element was documented for its beneficial uses, its unfortunate side-effects that often lead to tragic accidents, and its exploitation by those intent on murder. Mysteries surrounding the deaths or demise of famous people such as Napoleon, Mozart, Newton, Charles II, and George III were explored using modern forensic analysis and our growing understanding of chemistry.

August provided the opportunity for a winter social event. Some 35 members and guests partook of dinner at Curry Heaven in Petone. The restaurant's owner, **Ranjit Sarker**, was our after-dinner speaker. Apart from being a successful businessman, Ranjit is a qualified chemist, having gained his BSc (Hons.) and MSc degrees from the University of Dhaka. Unable to gain employment as a chemist after his arrival in NZ in 1996, he subsequently opened

his first Curry Heaven restaurant in Newtown and in 2003 expanded to his current premises in Petone. Ranjit described his love of chemistry, his disappointment in being unable to continue with his chosen profession here, and his philosophy of enjoying what one does- and his delight in providing great curry! We welcome him as a member of the Institute.

The month of August is a busy one for the Branch with the Regional Science Fair, Titration Competition and Quiz Night. The winners of the Science Fair NZIC Prizes were **Junior: Acid or Alkali?** - **Kimberley Wake** (Samuel Marsden Collegiate) and **Senior: Vitamin C in Broccoli** - **Timothy Leaf-Wright** (Hutt International). The titration competition consisted of determining the amount of MnO₂ in a sample of pyrolusite by standardising a solution of permanganate with potassium oxalate, reacting the pyrolusite with excess oxalate, and titrating the excess. A record of 49 Year 12 and 13 students participated. One 1st and three equal 2nd prizes were awarded to: **1st Prize: Liam Milne** (Wellington College) with **2nd Equal to: Hana Christenson** (Wellington Girls), **Carlton Downey** (Newlands College), **David Isaccs** (Wellington College). The Branch is extremely grateful to **Teresa Gen** and **Jackie King**, the technicians who set up the laboratory and prepared the chemicals for this event. Hana Christenson had a good fortnight in that she also won the major prize at the Wellington Science Fair.

The same evening saw the 7th Annual Years 12-13 Wellington Secondary Schools Chemistry Quiz. Students and teachers from a record 20 schools descended on VUW for what was to be the biggest attendance to date. The teachers were whisked away for a session with VUW Dean of Science **Prof. David Bibby** and **Suzanne Boniface** (Queen Margaret's College) while about 196 16- and 17-year olds (in almost 50 teams) made their way to the Student Union to compete. Quiz masters **Wendy Poplewell** and **John Ryan** led the teams through 8 rounds of general knowledge chemistry brainteasers to the delight of all involved. The end saw a clear first with the **Newlands Col-**

lege Quantum Quacks winning individual prizes and a textbook for their school. Second and third place-getters were allotted by a sudden-death question from which *The Chemistry Set of Wellington Girls'* came out on top leaving *Dilligaf* from **St Patrick's College** third. Spot prizes for best team name (*Hadron Lepton the Valence Electron*, **Newlands College**), loudest team (*The Chemistry Set*, **Wellington Girls'**), best table decorations (*Chemical Ali's Legitimate Chemists*, **Wellington College**), quietest team (*Enthalpy*, **St Oran's College**), most scientific costume (*Pinky and the Brain*, **Queen Margaret's College**), most inventive costume (*Winnie and the Poos*, **Hutt International Boys'**), biggest suck-ups (*Quantum Quacks*, **Newlands College**) and most decorated answer sheets (*Ester Bunnies*, **Wellington Girls' College**) seemed appreciated!.

The evening, had much appreciated help from the VUW Events Coordination Team and sponsorship from Whitcoulls Ltd., Hoyts Ltd., McDonalds (Newtown), Coca Cola Ltd., and funding from VUW Science Faculty, SPCS, and the Wellington Branch. As always the evening owes much for its success to the infamous Happy Helpers – **Kathryn Allan**, **Lynton Baird**, **Rhys Batchelor**, **Mathew Cairns**, **Brendan Casey**, **Shivali Gulab**, **Duncan Henry**, **Fern Kelly**, **Birthe Kortner**, **Teck Hok Lim**, **Andy McFarlane**, **Chris Munro**, **Cat Patchett**, **Mina Razzak**, **Jonathan Singh**, **Emma Turner**, and **Joanna Wojnar**.



Photo caption: Wellington Science Quiz night.

Victoria University

Delivery, installation, and commissioning of the new Varian 600 and 500 MHz NMR instruments took place over the June-August period with the larger instrument housed in a

converted area of the School's lower floor.

Shivali Gulab attended (with Branch support) the Sydney RACI *Connect 2005* conference presenting her PhD work *Towards the Synthesis of Peloruside A and its Analogues*. **Dr. Peter Northcote** and his students **Joanne Wojnar** and **Wendy Popplewell** attended the 4th European Conference on Marine Natural Products in Paris in mid-September. Peter described *The Production of Peloruside A by Aquaculture* while the students, both supported with Branch grants, gave papers *The chemical characteristics of selected New Zealand nudibranchs* and *Novel compounds isolated from the New Zealand marine red alga Phacelocarpus labillardieri*, respectively. **Dr. Kate McGrath** was an invited attendee at a two-week summer school on *Stereochemistry of Novel Materials* at the International Centre for Materials Research (of UC - Santa Barbara) in August. **Dr. Ken MacKenzie** spent a month in Oxford on high-field NMR work, with one week in Paris at the 4th World Congress on Geopolymer Science presenting papers in collaboration with in colleagues from IRL. In recognition of Ken's work he was invited to join a joint EU-US team to contribute NMR spectroscopy to testing the Davidovits theory of how the Pyramids of Egypt were built. This is, in essence, that the pyramid blocks were cast *in situ* from reconstituted limestone powder, held together by a cement which he termed a *geopolymer*. Thus it was suggested that the raw components (readily available Egyptian desert minerals) were carried into position in sacks, mixed with water, cast, and allowed to solidify in a wooden formwork. The pyramid samples and materials from the reputed source quarries are now in Wellington and currently undergoing NMR analysis.

Conferences and Seminars

International Conference on Sensing Technology November 21-23 2005, Palmerston North

ICST 2005 is intended to provide a common forum for researchers, scientists, engineers and practitioners throughout the world to present their latest research findings, ideas, developments and applications in the area of sensing technology.

<http://icst.massey.ac.nz/>

8th Japan Australia Colloid & Interface Gakkai 27 - 30 November 2005, Terrigal, New South Wales

This Conference aims to promote collaboration between scientists from Japan, Australia and other countries in the region, working in the field of Colloid and Interface Science.

www.colloid-oz.org.au

PACIFICHEM 15-20 December 2005, Honolulu

Pacificchem 2005 will promote collaborations among Pacific Basin chemical scientists that improve the quality of life throughout the world and will feature a broadly based scientific programme.

www.pacificchem.org

INTERACT 2006 September 24-28, 2006, Perth, Western Australia

Incorporating the 13th Australasian Electrochemistry Conference (13AEC), and meetings of the RACI Analytical Chemistry and Environment Divisions, and the Australasian Society for Ecotoxicology.

www.promaco.com.au/conference/2006/raci/

4th ISE Spring Meeting 17-20 April 2006, Singapore

Our theme is Electrochemical Materials Science: Fabrications, Characterisation and Applications with the following sub-themes: hybrid and composite materials, molecular tailoring and engineering, supramolecular chemistry, MEMS/NEMS, scanning probe microscopy, nanoelectronics/nanodevices and nanobiotechnology.

www.ise2006.org

19th International Conference on Chemical Education 12-17 August 2006, Seoul, Korea

The 19th ICCE has adopted a theme of "Chemistry and Chemical Education for Humanity". Accordingly, this conference will provide an ideal opportunity for chemistry-related professionals to gather together to share and exchange their experiences and expertise related to such subjects as recent trends in chemistry and chemical-related education, dissemination of chemistry/chemicals information, innovative instrumental methods, the latest research findings, and the benefits of the chemistry/chemicals for humanity and society.

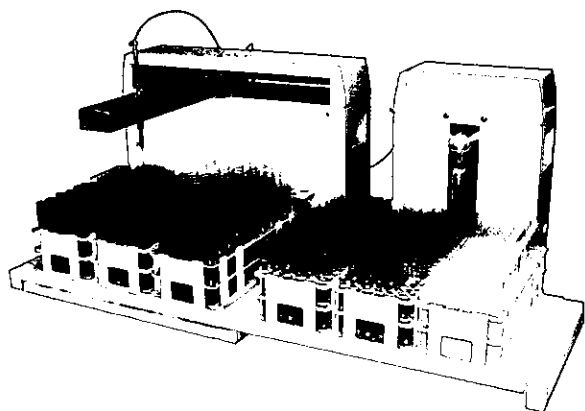
www.19icce.org

37th International Conference of Coordination Chemistry 13-18 August, Cape Town, South Africa

The scientific programme envisaged for the 37th ICCC will consist of modern advances in the field of Coordination Chemistry in general, with specific focus on advancements in areas such as new materials, catalysis, bioinorganic applications, supramolecular chemistry as well as extractive metallurgy.

http://webhost.sun.ac.za/pgm_group/index.htm

New automated dilution station



Ai Scientific introduces the new AccuLute, automatic stand alone dilution station. The AccuLute will prepare up to 135 diluted samples in a single run while the AccuLute Plus doubles this capacity to 270. Each run can carry out up to three separate dilutions allowing multiple dilutions from the same source tube or serial dilutions. The AccuLute brings the benefits of accuracy, speed, and flexible sample types to automated dilutions.

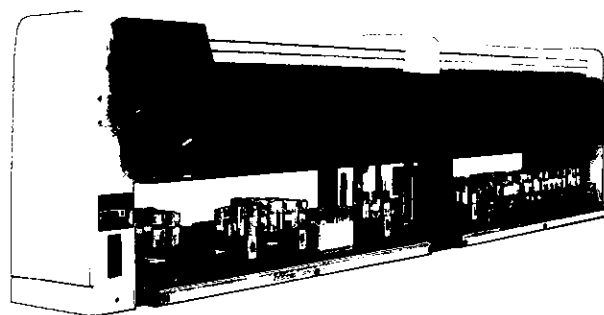
All Ai Scientific products undergo vigorous testing before market release and are manufactured under ISO9001 certification. For further information please send an email to aimail@aiscientific or contact us on 1300 133 063 AU | 0800 95 10 10NZ

New automated tube sorter increases productivity

Growing test workloads are forcing laboratories to constantly improve throughput without sacrificing surety, safety or quality of service. These pressures make it difficult to continue with a manual method of sorting specimens after analysis as it is a function which is labor intensive and difficult to manage. To address these concerns Ai Scientific developed the PathFinder S Sorter.

The PathFinder S is an automated sorter for use with pre- and post-analysis applications. Specimen tubes are placed on the PathFinder S which automatically identifies and sorts the specimen tubes into storage racks or analyser racks for testing. The specimen location is then transferred to the laboratories information system for tube tracking.

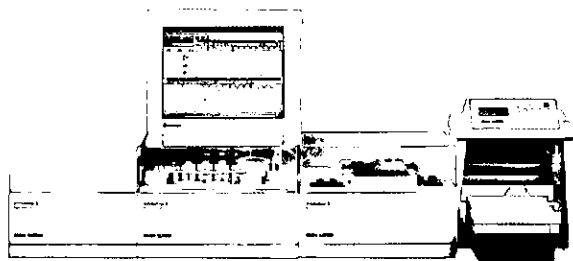
The PathFinder S Sorter is designed to be easy to install, easy to learn and easy to use on a day to day basis. With simple, robust functionality the PathFinder S can help laboratories address many of the challenges associated with patient sample management including turnaround



time and tracking.

As with all Ai Scientific systems, the PathFinder S will undergo vigorous testing before market release and is manufactured in accordance with ISO9001 quality certification. Email aimail@aiscientific or phone 1300 133 063 AU | 0800 95 10 10 NZ today for further information on the PathFinder S.

Ai Scientific & Bran+Luebbe announce partnership in Australia and New Zealand



Ai Scientific is proud to announce its partnership with the creator of continuous flow analysis, Bran+Luebbe. Pioneering innovations and comprehensive know-how in the industry have made Bran+Luebbe the worldwide leader in metering, analysing and processing liquids for more than 70 years. Together, Ai Scientific and Bran+Luebbe will draw on this experience and bring the

very best in analysing equipment to Australia and New Zealand. Ai Scientific has a strong flow analysis knowledge base with over 20 years experience in servicing CFA analysers. Our service engineers are factory trained to help users maintain maximum instrument up time. For further information on Ai Scientific's new Bran+Luebbe instrument range please phone 1300 133 063 AU | 0800 95 10 10 NZ or email aimail@aiscientific

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Chemistry Show Popular



Chemistry won the popularity contest at the recent Incredible Science festival at the University of Auckland.

The Chemistry Magic show was one of the most popular events in the annual one-day festival for primary school children, held on 11 July.

More than 6000 children and parents from across Auckland and the wider districts came to the event organised by the University's faculty of Science.

Faculty of Science Dean, Dick Bellamy said the festival was an effective way of interesting children in science from an early age.

Many children already have an interest in technology

through computer games. The challenge of the festival for the staff and volunteers was to show the region's school children the other areas of science are equally exciting he said.



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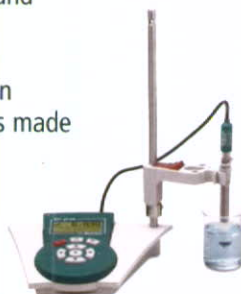
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