A snapshot of Antipodean chemistry: a report on the 2006 Royal Society of Chemistry Australasian Lectureship

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A snapshot of Antipodean Chemistry – a report on the 2006 Royal Society of Chemistry Australasian Lectureship

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When Alan Bond contacted me to enquire if I had a mind to become the 2006 RSC Australasian lecturer I was delighted to accept; the recognition of my peers, the possibility of having a snapshot of Australian and New Zealand chemistry, and the chance to catch up with many friends and colleagues, all at the RSC's expense was too good to miss. Luckily, too, I had just been invited to spend a year's sabbatical at the National Measurement Institute (Australia) as a visiting professor. The absence of university commitments to teaching and administration gave me a clear run at the lectureship (although I spilled over into 2007 for my last trip to Western Australia).
The aim of the lectureship is to provide some benefit to antipodean RSC members who pay the same dues as those in the UK but without access to the plethora of meetings and services provided there.
It is not possible to include every university in the region, but visiting each state or territory in Australia at least once, and the major centres in New Zealand, is obligatory. Table 1 shows the program of lectures. To give the greatest flexibility to the organisers I offered three lectures (the abstracts are in Appendix 1), that covered my current interests. Two concerned my research, one in electroanalytical chemistry ("All that SAMs is not gold"), and the other in chemometrics and metrology in chemistry ("From the Prosecutor's Fallacy to Environmental Protection: Bayes Theorem – matching spectra for oil spills and the heroin signature program"). As I occupy arguably the only (and certainly the oldest), chair of analytical chemistry in Australia, I have found myself as an expert witness in court on a few occasions. This has led to an interest in the process of how courts deal with expert opinion. I gave a submission to the recent Law Reform Commission investigation of expert opinion, and I share the concerns of many that the complexities of modern science and the relative lack of scientific knowledge of members of the public (or some judges for that matter) can lead to courts failing to gain full benefit from experts who appear before them. These concerns were coupled with a recent Australian criminal case in which failings in the analysis of an alleged drug of abuse led to the overturning of a prosecution on appeal, and caused me to write a paper "Scientist v's the Law" [1]. This paper became the basis for a lecture of the same title that was also offered during the RSC tour. Scientist v's the Law is a wider ranging lecture that is suitable for more general audiences, although it does have some serious points to make. Perhaps not surprisingly this was by far the most popular of the three lectures. A common

pattern was to give a research lecture to a chemistry department in a lunchtime slot, then Scientist v's the Law at an evening function.

Table 1: Lectures given during the RSC 2006 Australasian Lectureship

New Zealand

Date	Place	Title
Monday 24th July	University of Auckland, Department of Chemistry	*All that SAMs is not gold*
Monday 24th July	New Zealand Institute of Chemistry/ Royal Society of Chemistry, University of Auckland	*Scientist v the Law*
Tuesday 25 th July	University of Waikato, Department of Chemistry, Hamilton	*Scientist v the Law*
Wednesday 26 th July	Victoria University of Wellington, Wellington, School of Chemical and Physical Sciences	*All that SAMs is not gold*
Wednesday 26 th July	New Zealand Institute of Chemistry/ Royal Society of Chemistry, Victoria University of Wellington, Wellington,	*Scientist v the Law*
Thursday 27 th July	Massey University, Palmerston North, Institute of Fundamental Sciences	*Scientist v the Law*
Thursday 27 th July	Royal Society of New Zealand, Civic Centre, Palmerston North	*From the Prosecutor's Fallacy to Environmental Protection*
Friday 28 th July	Department of Chemistry, University of Otago, Dunedin	*Scientist v the Law*
Monday 31st July	Department of Chemistry, University of Canterbury, Christchurch	*Scientist v the Law*

Australia

Date	Place	Title
Friday 4th August	School of Physical and Chemical Sciences, Queensland University of Technology, Brisbane	*All that SAMs is not gold*
Monday 7th August	Royal Australian Chemical Institute/ Royal Society of Chemistry, University of South Australia, Adelaide	*Scientist v the Law*
Tuesday 8th August	School of Chemistry, Physics and Earth Sciences, Flinders University, Adelaide	*Scientist v the Law*
Tuesday 8th August	School of Chemistry and Physics, University of Adelaide, Adelaide	*All that SAMs is not gold*
Wednesday 9th August	School of Chemistry, Physics and Earth Sciences, Flinders University, Adelaide	*From the Prosecutor's fallacy to Environmental Protection*
Wednesday 6th September	Royal Australian Chemical Institute/ Royal Society of Chemistry, Environmental Research Institute of the Supervising Scientist, Darwin	*Scientist v the Law*
Monday 11th September	Research School of Chemistry, Australian National University	*All that SAMs is not gold*
Wednesday 20th September	Department of Chemistry, University of Tasmania	*All that SAMs is not gold*
Monday 16th October	Royal Australian Chemical Institute/ Molecular Sciences Society, JCU, School of Pharmacy & Molecular Sciences, James Cook University, Townsville	*Scientist v the Law*
Tuesday 14th November	School of Chemistry, Monash University	*All that SAMs is not gold*
Wednesday 15th November	University of Melbourne Chemical Society, Melbourne	*Scientist v the Law*
Wednesday 4th April, 2007	Department of Chemistry, University of Western Australia	*From the Prosecutor's fallacy to Environmental Protection*
Wednesday 4th April, 2007	Royal Australian Chemical Institute/ Royal Society of Chemistry, CSIRO	*Scientist v the Law*
Thursday 5th April, 2007	Department of Applied Chemistry, Curtin University	*All that SAMs is not gold*
2007,TBA	School of Chemistry, University of New South Wales	*TBA*

New Zealand

The New Zealand RSC members have got this trip completely organised. Well in advance I was advised to make my way from north to south with a weekend in Queenstown before the final commitment in Christchurch. Planes, hire cars, buses and a nearly defunct train duly ferried me between the six centres (Auckland, Hamilton, Wellington, Palmerston North, Dunedin, Christchurch). The weather remained fine and the hospitality was excellent. My weekend off in Queenstown was a highlight.
Many departments were concerned about research funding and the application of the Performance-Based Research Fund (PBRF). The partial round in 2006 was hoped to fix several perceived inaccuracies in the inaugural 2003 effort. There had been keen scrutiny of the success or otherwise of competing universities and everyone was well aware of the approaches that appeared to have worked (or not).
Apart from the delight in giving my lectures to six vibrant chemistry departments, I left Auckland with my participation in a Foundation for Research Science & Technology (FRST) application (Sensors and systems for high-density mapping of urban air quality – led by David Williams), found students to help with experimental design in Dunedin and renewed collaborations with Christchurch. Research funding is a problem in New Zealand, but the quality of chemical research is very high, and younger members of staff all appeared keen and focussed.

Australia

There are great differences between the big metropolitan universities and those at the extremities of the country. With very few staff, Charles Darwin University (the university of the Northern Territories) has carved a niche with its Environmental Analytical Chemistry Unit. The unit has several projects with mining companies and in marine ecology. James Cook University, centred in Townsville, has chemistry in a School of Pharmacy and Molecular Sciences. Richard Keene has provided a focus for transition metal chemistry for many years and has shown how to run a world class research effort outside the “group of eight”. My lecture in Townsville was videoed for the benefit of other campuses; I wonder what they made of it. It was good to catch up with Professor Danny Coomans, one of the small, but active, band of chemometricians in Australia. In the capital cities relations between universities range from collegial to downright frosty, and just as my own institution struggles to promote inter-faculty collaborations, we have to make more of opportunities to share facilities, knowledge and possibly teaching. Flinders University, with its Forensic course, took full advantage of my visit. In two days I gave three lectures, in addition to the one at the University of Adelaide and the official RSC lecture organised by the local RACI. My host Stewart Walker was on standby to give evidence about glass fragments at the Norfolk Island murder trial, thus providing an interesting backdrop to Scientist v’s the Law. My time in Brisbane, at QUT, was more restrained with just the one lecture. Again meeting fellow chemometrician Serge Kokot was a delight. Tasmania was a pleasant stay, hosted by Paul Haddad but missing my predecessor, Alan Canty, who was still finishing off the 2005 lectureship. We then happened to meet each other on the street in Melbourne, a somewhat surreal moment. The departments in Monash University and Melbourne University were

very impressive. They probably now contain the strongest concentration of chemists in Australia (with due deference to Sydney and Canberra). The ANU talk went well, and the tour of John White's latest experiments showed there are still clever thinkers who can follow their ideas. Our self assembled monolayer research found some interested colleagues and we hope to follow possible collaborations. My final visit was to Western Australia where the forensic group at Curtin University led by John Watling (who in fact gave evidence on the glass fragments in the Norfolk Island case), also had the benefit of very interesting discussions on the application of Bayes theorem. I have since received real data from the group to play with; life and blood for a chemometrician. The lecture at the University of Western Australia was the only one at which I had any problems with the technology, the old PowerPoint presentations finally ran out of steam, but to be able to turn up with a USB drive with megabytes of presentation is certainly an improvement on older forms of technology. Western Australia possibly boasts the best university club, and my last outing in my visit was to attend, as a guest of Stewart Bailey, a wine tasting of a dozen 1998 reds. This was before being poured onto the midnight flight back to Sydney.

Epilogue

Both in Australia and New Zealand I came across many retired or quasi-retired professors who were still active in research and sometimes teaching. It was not clear what would happen when they finally depart. The next generation did not seem numerous enough to have this many mentors. As expertise disappears there will be inevitable gaps in our coverage of the subject. This is exacerbated by the tendency to concentrate research in high-powered groups that are obviously working in the very latest area of chemistry/ biochemistry/ materials science. However we have seen the coming and going of many new fields, and the lone academic who pursues their own eclectic research is increasingly a thing of the past (John White notwithstanding).

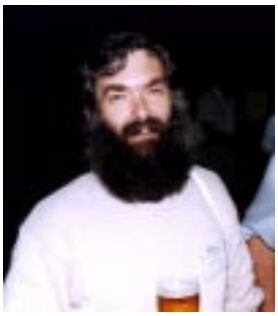
This was an excellent year; not only professionally but the renewing of many old friendships, having splendid dinners, looking at rather nice vintages (including Stewart Bailey's own 2007 Shiraz), were all, as the advertisement says, 'priceless'.

References

1. D. B. Hibbert, *Accred. Qual. Assur.*, 2003, **8**, 179-183.

2006 Royal Society of Chemistry Australasian lecturer

Professor D Brynn Hibbert



Professor Hibbert occupies the Chair of Analytical Chemistry at the University of New South Wales in Sydney. He is the second incumbent and arrived in Australia from England in 1987.
His research interests are in electroanalytical chemistry and chemometrics and metrology in chemistry, but he also does a sideline in expert opinion, scientific fraud and presenting science to the public.
He has published around 200 papers, 5 books and 2 patents. His most recent book, *Data Analysis for Chemistry: An Introductory Guide for Students and Laboratory Scientists* (Oxford University Press, New York, 192 pp) written with Justin Gooding, has just been published at US$19.95. Look out too for Quality Assurance in the Analytical Chemistry Laboratory out early 2007.

He is past Chair of the Analytical Division of the RACI, a titular member of the IUPAC Analytical Division and was co-chair of Interact 2002.

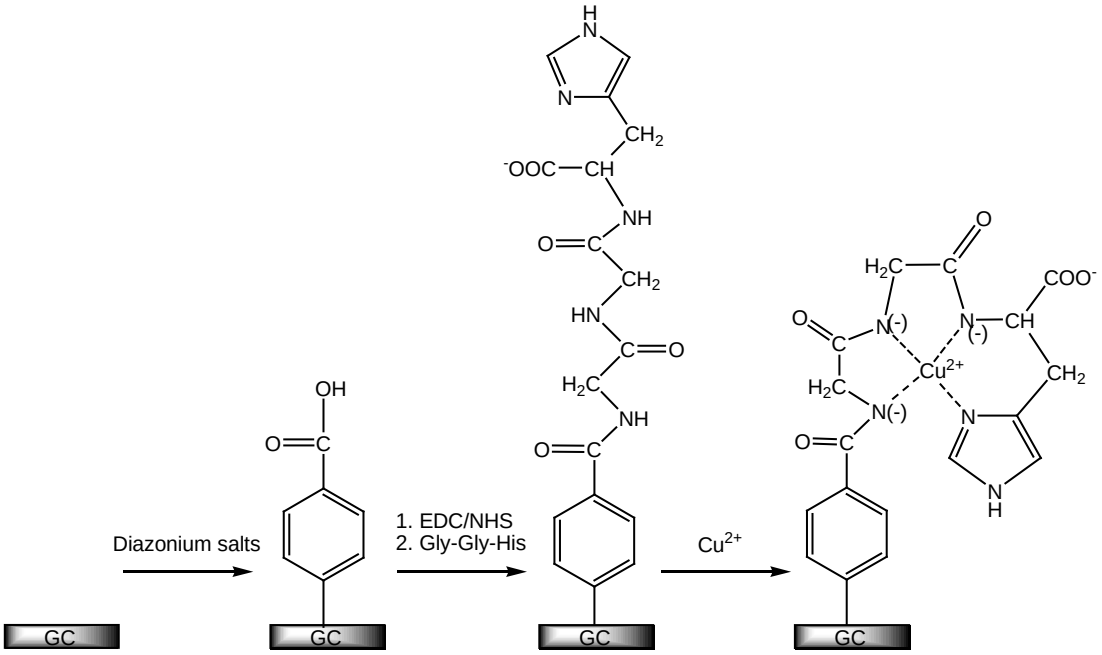
(Portraits © 1997, 2000 Hua Hue Xie – finalists in the Doug Moran prize)

All that SAMs is not gold – biosensor electrodes

In a long standing collaboration with Justin Gooding, the Sensors group at UNSW has been interested in a variety of ways of modifying electrodes to allow the transduction of a recognition event and thus the sensing of ions, and small and large molecules.
This lecture will focus on two projects: a recently completed study of peptides to complex metal ions, and studies of the replacement of gold as a substrate by glassy carbon.

The archetypal modified electrochemical system is the use of immobilised glucose oxidase covalently attached to a thiol self assembled monolayer (SAM) on gold. The fruit fly of this field, this system has been investigated to death, but is a good way of introducing the technology. The flexibility and ease of forming an amide bond led us to look at building up peptides on a gold SAM that were particularly good at complexing with metal ions in solution. Once captured near a conducting electrode (here gold) voltammetry is used in a conventional stripping experiment. We have claimed very low detection limits for copper on Gly-Gly-His, and will report other peptides for cadmium and lead. It is even possible to put these together and use multivariate analysis on the resulting voltammograms.

The thiol bond with gold is thought to oxidise, possibly with trace ozone in the air, and so a more robust substrate/SAM was considered a requirement for long term storage of devices. Glassy carbon can be activated using diazonium salts and if a carboxylic acid is attached to the para position it can be subsequently activated and the usual suspects attached to it. Results on the stability of sensors on gold or carbon will be given and discussed.



From the Prosecutor's Fallacy to Environmental Protection: Bayes' Theorem – matching spectra for oil spills and the heroin signature program

Although the discrete form of Bayes' theorem may be derived in three lines from the laws of probability, it has remained one of the more controversial methodologies in science. Indeed the Reverend Thomas Bayes himself was so concerned with the use of prior probabilities that he could not bring himself to publish during his life and the manuscript of his paper *An Essay towards solving a problem in the doctrine of chances* was not published until after his death in 1763. Modern interest in Bayes' theorem comes from the mid-20th century where a number of branches of science have espoused its approach. The 'harder' sciences of chemistry and physics have resisted the apparent subjective element of Bayesian statistics, but recently in analytical chemistry the move towards estimation of measurement uncertainty following the *Guide to the expression of uncertainty in measurement* has been recognised to have Bayesian elements.

In essence, Bayes theorem is

$$\Pr(\mathrm{H}|E) \propto \Pr(E|\mathrm{H}) \times \Pr(\mathrm{H}) \qquad (1)$$

which reads that the probability of a hypothesis, H, given evidence, *E* (i.e. some experimental data), is proportional to the probability of finding the evidence given the hypothesis multiplied by the probability of the hypothesis before any evidence is gathered. The latter probability is known as the *prior* probability and is the source of much of the angst. $\Pr(E|\mathrm{H})$ is the *likelihood* and is the probability often determined using traditional frequentist statistics, in which the null hypothesis is assumed and the probability of finding a particular test statistic (e.g. a Student-t value) is computed.

After an introduction to the prosecutor's fallacy (confusing $\Pr(E|\mathrm{H})$ with $\Pr(\mathrm{H}|E)$ and then inferring guilt) some famous cases will be reviewed – OJ Simpson, Sally Clark (SIDS), two areas of interest to the author will be described.

In some work funded by the NSW Environment Trust, Bayes' theorem was used to match spectra to give evidence of source of an environmental oil spill. A matching parameter is calculated, for example the correlation coefficient between the spectra (IR, fluorescence, mass), and the probability of a match and of no match calculated from a knowledge of the distributions of the parameter for spectra from the same and different oils. The method is powerful but does need a good database of known spectra to generate the distributions of the parameter for matched and unmatched spectra.

Recently the author has joined the National Measurement Institute to help in the heroin signature program to profile seized drugs to establish their origin. The Pong Su, a North Korean registered vessel was the recent source of a large haul of heroin. The profiles and analysis has allowed the identification of a new processing laboratory.

Scientist versus the Law

A largely anecdotal review of the author's work in the courts, including bogus health products, unsuccessful defences of murderers and racehorse trainers, and highly lucrative patent cases.

Notices in judgments include:

Supreme Court of New South Wales, Equity Division Construction List, 55059/97 Optus Networks Pty Limited & Ors -V- Leighton Contractors Pty Limited & Ors, Hunter J, April 2002
"Professor Hibbert was an extremely impressive witness whom I found reliable, responsive in cross-examination and without any apparent bias in his answers which were given promptly and with authority."

"There was no semblance of self interest, or bias in Professor Hibbert's evidence …"

"With that last answer I would find myself in agreement with Professor Hibbert who had, in my view, extraordinarily high qualifications in electro-chemical analyses so important in the dispute in these proceedings"

Ion mobility spectrometry, embodied in instruments such as the Ion Scan is used at airports detect drugs or explosives at trace levels. The author has given evidence in trials of drug importation in which an Ion Scan has revealed presence of a drug with subsequent seizure of substantive amounts. In an early trial, during the author's evidence the "invisible hand" defence was coined when the trial judge misheard a question from counsel and caused the following conversation Judge: "Did you say the hand that touched the cocaine was invisible?". Counsel: "No your honour, I said the cocaine that the hand touched was invisible".

The Ion Mat sold for around $3,000 and apart from claiming to improve your sex life, it cured cancers (various) and ameliorated bad breath. The mattress did this by creating "beneficial negative ions" despite the author's opinion that the electric field was about the same as a toaster and whereas we do not expect our household appliances to make us better, this would not either. The prosecution by the ACCC was a success, but at the end of the trial the principals of the company fled with, it is said, $12 million.

There will be some discussion of statistics (Lies, damned lies and …), dendrites and fractals, stolen wine, contaminated beer and defunct batteries. This will lead to a reflection on expert opinion and the role of professional societies in maintaining standards of professionalism.