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2006 New Zealand Institute of Chemistry Conference

Back to the Basics: From Small Molecules to Biological Systems and Materials

Novotel Convention Centre, Rotorua, 2-6 December 2006

For brief details, programme synopsis, and registration see:
www.nzic.org.nz or www.massey.ac.nz/~nzic



The NZIC conference has been established to disseminate recent research results in the chemical sciences within NZ. It is held every two to three years. This year's chosen theme is **Back to the Basics**. As little funding is currently available for fundamental science in NZ, it was felt that the NZIC conference is an ideal showground for demonstrating that basic science in this country is still thriving. Without basic science we may just delete the word *knowledge* in front of our most widely used phrase, *knowledge economy*. We are also striving to place the conference to a more international level, as reflected in the large number of high profile plenary and invited lecturers from overseas. And last but not least we would like to celebrate the great scientific achievements of one of our most outstanding chemists in the country, Prof. Warren Roper, who will give the opening lecture for the conference.

There will be a special symposium organized by Prof. Jim Metson from Auckland University, entitled **Showcase: Industrial Chemistry in New Zealand**. This will provide an opportunity to get first-hand accounts of Industrial Chemistry in New Zealand. The aim is to foster an understanding of the global nature of the chemical industry

and the challenges and opportunities that will arise in near future. We aim to shed light on the social, economic, and professional development that the chemical industry has gone through with a clear focus on NZ. We plan on covering all players in this market and specifically ask for a good participation in this session. Opportunities for education and training within the chemical industry and the exchange and interaction with academia will be highlighted. It also provides a chance for researchers to establish closer contacts with industry, and to foster and enhance basic science here.

Two poster sessions are planned, the Easterfield Medal lecture will be given, and we offer again a prize for the best student poster in each poster session. As the financial success of this conference crucially depends on the number of participants, you all invited to participate, either in delivering a lecture or presenting a poster. Registration has already opened on the web site.

See you all in Rotorua.

Peter Schwerdtfeger (Conference Chairman)

The Plenary Speakers



Professor Mark A. Barteau (Chairperson, Department of Chemical Engineering, University of Delaware) received his BS degree in Chemical Engineering from Washington University (St. Louis) and his MS and PhD from Stanford, working with Prof. Robert J. Madix. He was

an NSF Postdoctoral fellow at the Technische Universität München, before joining the University of Delaware faculty as an assistant professor and associate director of the Center for Catalytic Science and Technology in 1982; he was promoted to associate professor (1987) and professor (1990). He became director of the Center for Cata-

lytic Science and Technology in 1996 and Chairperson of the Department of Chemical Engineering in July 2000. He has held visiting appointments in at the University of Pennsylvania, and the University of Auckland.

Prof. Barteau's research, presented in more than 200 publications and a similar number of invited lectures, focuses on chemical reactions at solid surfaces, and their applications in heterogeneous catalysis. He was one of the pioneers in demonstrating the application of surface spectroscopies to study the mechanisms of organic relations on single crystal metal oxide surfaces, and such studies remain an important component of his research today. There is a significant applications thrust to his work. He and his students have demonstrated a number of *firsts* in catalysis by metal oxides, including the first example of oxide-catalyzed cyclization of acetylenes to substituted

aromatics, the first heterogeneously catalyzed reductive coupling of carbonyl compounds, and a new oxide-catalyzed process for the environmentally benign synthesis of ketenes. He and his students have also made significant advances in olefin epoxidation catalysis, demonstrating, by experiment and theory, the crucial role of surface oxametallacycle intermediates in this chemistry. He has also investigated mechanisms of a number of other selective oxidation processes, focusing most recently on the utilization of Scanning Tunneling Microscopy to probe redox properties of polyoxometalate catalysts.

The concept of *catalysis by design* has been a dream for decades. To specify the composition and structure of matter to effect a desired catalytic transformation with desired and predicted rate and selectivity remains a monumental challenge, especially in heterogeneous catalysis. With the advent of surface science techniques in decades past, the promise was perceived of turning increased molecular level understanding of reaction mechanisms and surface sites into principles of catalyst design. Surface science alone has not proven to be sufficient for this purpose. Over the past decade the rise of powerful, computationally efficient theoretical methods has shown promise, not just for identifying catalytic intermediates and reaction pathways accessible to experiments, but of providing quantitative predictions of energetics for elementary reaction processes not easily accessed experimentally. Much of Barteau's work is aimed at the rational design of catalysts for direct epoxidation of olefins. This chemistry remains one of the most challenging problems in heterogeneous catalysis and he will be discussing this in Rotorua.

Prof. Barteau is the recipient of numerous awards, some of which include the 2001 Alpha Chi Sigma Award and the 1991 Allan P. Colburn Award, presented by the American Institute of Chemical Engineers; the inaugural International Catalysis Award, presented by the International Association of Catalysis Societies in 1998; the 1995 Ipatieff Prize from the ACS; the Paul H. Emmett Award in Fundamental Catalysis, given by the North American Catalysis Society, and the 1993 Canadian Catalysis Lecture Tour Award of the Catalysis Division of the Chemical Institute of Canada. He has served as associate editor of the *AICHE Journal*, and is on the editorial boards of a number of other journals, including the *Journal of Catalysis*. He was one of the 17 members of the NRC committee that recently produced the report *Beyond the Molecular Frontier: Challenges for Chemistry and Chemical Engineering*.

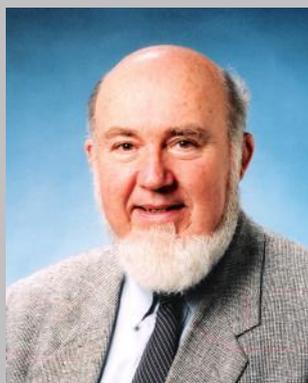


Professor Harry B. Gray (Professor of Chemistry and Founding Director of the Beckman Institute at the California Institute of Technology) began his work in inorganic chemistry at Northwestern University, where he earned a PhD in 1960. After a post-

doctoral year at the University of Copenhagen, he joined the chemistry faculty at Columbia University, where his main interests centered on the electronic structures and reactions of inorganic complexes. In the years 1958-64, he worked on ligand substitution mechanisms, establishing fundamental principles that were published in a book with C. H. Langford in 1966. During this same period, he employed molecular orbital theory to describe the electronic structures of transition metal complexes. After moving to CIT in 1966, he and his coworkers investigated the solar photochemistry of metal complexes, including the construction of donor-acceptor systems that mimic the early events of photosynthesis. He also attacked the problem of electron flow through biological molecules by examining the kinetics of reactions of iron and copper proteins with inorganic complexes. Working with Ru-modified proteins in the early 1980s, he and coworkers demonstrated that electrons can tunnel rapidly over long molecular distances through folded polypeptide structures. In the years following, he and J.R. Winkler developed laser-photochemical methods to investigate the free energy and distance dependences of electron tunneling through proteins and other biological molecules. Very recently, Gray and coworkers have constructed photoactive electron tunneling wires to probe deeply buried active sites in P450s and other redox enzymes. Employing fluorescent probes, he and Winkler have mapped the folding energy landscapes of several heme proteins. He has published over 700 research papers and 17 books.

As is well known, aerobic respiration and photosynthesis work in concert with the oxygen that is evolved by photosynthetic organisms being the oxidant that sustains life in aerobic microbes and animals, and, in turn, the end products of aerobic respiratory metabolism, carbon dioxide and water, nourish photosynthetic organisms. Electron flow through proteins and protein assemblies in the respiratory and photosynthetic machinery commonly occurs between metal-containing cofactors that are separated by large molecular distances, often in the 10-25 Å range. Although these cofactors are weakly coupled electronically, the reactions are remarkably rapid and specific. Understanding the underlying physics and chemistry of these distant electron transfer processes is the goal of the Gray's experimental work and progress will be discussed at the conference.

Prof. Harry Gray has received the National Medal of Science from President Ronald Reagan (1986), the Bailar Medal (1984), the Centenary Medal (1985), the Pauling Medal (1986), the Linderstrøm-Lang Prize (1991), the Basolo Medal (1994), the Gibbs Medal (1994), the Chandler Medal (1999), the Harvey Prize (2000), the Nichols Medal (2003), the Wheland Medal (2003), the Grollman Award (2003), the National Academy of Sciences Award in Chemical Sciences (2003), the Benjamin Franklin Medal in Chemistry (2004), the Wolf Prize in Chemistry (2004). He has also received six national awards from the ACS including the Priestley Medal (1991), and sixteen honorary doctorates, five from outside the US.



Prof. Warren Roper, FRS (University of Auckland,) was born in Nelson in 1938. He studied chemistry at the University of Canterbury and completed his Ph.D in 1963 under the supervision of the late C. J. Wilkins. He then undertook postdoctoral research with J.P. Collman at the University of North Carolina, and returned to NZ in

1966 as Lecturer in Chemistry at the University of Auckland. In 1984 he was appointed Professor and, in 1999, Research Professor of Chemistry.

Prof. Roper's research interests are in synthetic and structural inorganic and organometallic chemistry. Special themes in his research have been low oxidation state platinum group metal complexes, oxidative-addition reactions, migratory-insertion reactions, metal-carbon multiple bonds, metallabenzenoids and metallated arenes, stabilization of reactive molecules through coordination, and (more recently) compounds with bonds between platinum group metals and the main group elements, boron, silicon and tin. In 1972 he spent a sabbatical leave in F.G.A. Stone's laboratory at Bristol and it was at this time that he began his studies of metal-carbon multiple bonds. His research has been published in more than 200 research papers and he has served on the Editorial Boards of *Organometallics*, *Inorganic Chemistry*, the *Journal of the Chemical Society-Dalton Transactions*, *Inorganic Syntheses*, and *Inorganica Chimica Acta*.

Prof. Roper has lectured widely and been Visiting Professor at the Universities of Leeds, Rennes, Sydney, and Stanford University. His work was recognized by the RSC through the Organometallic Chemistry award (1983) and by the Centenary Lectureship (1988). He was elected FRSNZ in 1983 and FRS 1989. He has been a Fellow of the Japan Society for the Promotion of Science (1992), the Burrows Lecturer for the Royal Australian Chemical Institute (1992), the H. Willard Davis Lecturer at the University of South Carolina (1994), the Glenn T. Seaborg Lecturer in inorganic chemistry at the University of California-Berkeley (1995), the Dwyer Memorial Lecturer at the University of New South Wales (2000), the Inorganic Foundation Visitor at the University of Sydney (2001), the Stone Lecturer at the University of Bristol (2003), and the Arthur D. Little Lecturer at MIT (2005). He was awarded the degree, Doctor of Science (honoris causa), by the University of Canterbury in 1999.

The Rotorua lecture culminates Warren's career as he is shortly to retire. It will be a personalized retrospective of his 40 years of research in chemistry at The University of Auckland from which he has made contributions to some of the fundamental concepts of organometallic chemistry such as oxidative addition and reductive elimination, migratory insertion reactions, coordinative unsaturation, and metal-carbon multiple bonding. Selected examples of the stabilisation of reactive molecules through coordination

to a metal centre will also be presented with some emphasis on his recent metalla-aromatics and compounds with metal-boron, metal-silicon, and metal-tin bonds.



Professor David W.C. MacMillan (Professor of Chemistry, California Institute of Technology, USA) focuses his research on organic synthesis with specific interests in the development of new reaction methods of broad utility to enantioselective synthesis and the synthesis of natural products and biologically important molecules.

Organocatalysis is a breakthrough technology, invented by him at Caltech, in which small organic molecules are designed and constructed to serve as general catalysts for asymmetric transformations of other substrates. Organocatalysts have been successfully developed by MacMillan for several important reactions including asymmetric variants of Friedel-Crafts alkylations, 1,4-conjugate additions, and Diels-Alder and 1,3-dipolar cycloadditions. These transformations enable an extremely broad range of chiral intermediates to be readily assembled. The broad utility of these new asymmetric reaction technologies has also been demonstrated by the construction of complex natural product targets including Erythronolide B, (S)-Keterolac, Callipeltoside A, Littoralisone and the cytotoxic metabolite Diazonamide A.

The field has grown from a small collection of chemically unique or unusual reactions to a thriving area of general concepts, atypical reactivities, and broadly useful reactions. While the modern era of organocatalysis still remains in its infancy, growth in this new chemical field continues to move at a breathtaking pace as he will illustrate in his presentation with new and valuable transformations based on the paradigms of iminium-activation, enamine-activation, acid catalysis, and translational catalysis. Furthermore, an alternative strategy for natural product synthesis will feature that is hoped to provide the strategic foundations to bypass the *taxol* problem.

Before moving to CIT in 2000, Prof. MacMillan held a position at University of California-Berkeley having completed postdoctoral work with Prof. David Evans at Harvard and PhD studies with Prof. Larry Overman at the University of California-Irvine. His illustrious career has been accompanied by the award of numerous prestigious prizes and honours including the Elias J Corey award for outstanding contribution in organic synthesis, the 2005 RSC Corday-Morgan Medal, the inaugural 2005 Worldwide Tetrahedron Young Investigator Award, the Bristol-Myers Squibb award for organic synthesis, the Pfizer award for excellence in organic synthesis, and awards from Glaxo Smithkline, Eli-Lilly, Novartis, Astra-Zeneca and Boehringer-Ingelheim.



Professor Richard N. Zare (Professor in Natural Science, Stanford University) is a graduate of Harvard University. In 1965 he became an assistant professor at the Massachusetts Institute of Technology, but moved to the University of Colorado in 1966, remaining there until 1969 while holding joint appointments in the departments of chemistry, and physics and astrophysics. In 1969 he was appointed to a full professorship in Chemistry at Columbia University, becoming the Higgins Professor of Natural Science in 1975. In 1977 he moved to Stanford University.

ments of chemistry, and physics and astrophysics. In 1969 he was appointed to a full professorship in Chemistry at Columbia University, becoming the Higgins Professor of Natural Science in 1975. In 1977 he moved to Stanford University.

Prof. Zare is renowned for his research in the area of laser chemistry that has led to a greater understanding of chemical reactions at the molecular level. By experimental and theoretical studies he has made seminal contributions to our knowledge of molecular collision processes and contributed very significantly to solving a variety of problems in chemical analysis. His development of laser induced fluorescence as a method for studying reaction dynamics has been widely adopted in other laboratories.

The ability to examine individual proteins inside a single cell has been reported but it is limited to special cases where the environment of the cell does not cause changes in the fluorescence of the reporter molecules, and where quenching and endogenous fluorescence does not interfere with measurements. Additionally, *in vivo* approaches are restricted to viewing one or perhaps a few species at the same time. Zare and his group are pioneering a different approach based on manipulating, capturing, and lysing an individual cell followed by the analysis of the single cell lysate using electrokinetic separations. They have developed a microfluidics device that can quantify the low-copy-number protein or protein complexes in a single cell using single-molecule counting and this will be explained in his plenary lecture.

Prof. Zare has received numerous honors and awards that date to the mid-1970s. More recently these include NASA Exceptional Scientific Achievement Award (1997), National Science Board's Distinguished Service Award (1998), the ACS Award in Analytical Chemistry (1998), the Centennial Medal, Graduate School of Arts and Sciences, Harvard University (1998), the ACS E. Bright Wilson Award in Spectroscopy (1999), the Welch Award in Chemistry (1999), the ACS Nobel Laureate Signature Award for Graduate Education (2000), the Royal Society of Chemistry Faraday Medal (2001), the ACS (Sierra Nevada Section) Distinguished Chemist Award (2002), and the ACS (New York Section) Nichols Medal (2004).

Prof. Zare holds honorary degrees from: the University of Arizona (1990), Northwestern University (1993), Eidgenössische Technische Hochschule Zürich (1993), Uppsala University (2000), Columbia University (2000), the

University of York (2001), the State University of West Georgia (2001), Hunan University (2002), and Université Paul Sabatier (2003). He has given named lectures at numerous universities, has authored and co-authored over 700 publications and more than 50 patents, and he has published four books.

Summary:

Preliminary Conference Program:

Other than for the plenary lectures three concurrent sessions will operate as per: Organic/Medicinal/Biochemistry, Inorganic/Organometallic/Physical/Theoretical Chemistry, and Material/Surface/Industrial Chemistry.

Invited Speakers (incomplete at copy date):

Vickery Arcus (AgResearch, Auckland, NZ), Polly Arnold (University of Nottingham), Masakazu Anpo (Osaka Prefecture University), Peter Boyd (University of Auckland), Andrew Brodie (Massey University), Sally Brooker (University of Otago), Owen Curnow (University of Canterbury), Paul Curmi (University of New South Wales), Chris Easton (Australian National University), Bruce C. Garrett (Pacific Northwest National Laboratory, USA), Keith Gordon (University of Otago), Peter Gill (Australian National University), Alain Kiennemann (Ecole de Chimie Polymers et Matériaux, France), Warren Lawrance (Flinders University), Joel Mackay (University of Sydney), Markus Meuwly (University of Basel), Emily Parker (University of Canterbury), Pierre Pichat (Ecole Centrale de Lyon, France), Barry Scott (Molecular BioSciences, Massey University), Rob Smith (University of Otago), Cathy Stampfl (University of Sydney), Richard Taylor (University of York, UK), Geoff Thornton (University College London), Michael G. Ramsey (Karl-Franzens Universität Graz), Veronica Vaida (University of Colorado), Jürgen Vogt (University of Ulm), Natalja Vogt (University of Ulm), David Williams (University of Auckland), Christof Wöel (Ruhr-Universität Bochum), Sotiris S. Xantheas (Pacific Northwest, USA)

Conference Committee:

Peter Schwerdtfeger (Chair), Vesna Davidovic-Alexander (Secretary), Matthias Lein, Jim Metson, Alastair Nielson, Gordon Rewcastle, Tilo Söhnel.

Session Chairs:

Margaret Brimble (Organic and Medicinal Chemistry), Hicham Idriss, (Materials and Surfaces), Geoff Jameson (Biochemistry and Molecular Biology), Henrik Kjaergaard, (Physical and Theoretical Chemistry), Jim Metson, (Showcase - Industrial Chemistry in New Zealand), John Spencer (Inorganic and Organometallic Chemistry).

Investigating Scientific Literacy: Scientist's Habits of Mind as Evidenced by Their Rationale of Science and Religious Beliefs[†]

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[†]A publication from the NZIC Chemical Education Special Interest Group

Science and Scientific Literacy

Science and technology have been incredibly successful in purely technical terms. For instance, international air travel, space flight, and curing of hitherto untreatable medical illnesses all are now routine events. One feature of the incredible (and seemingly ever increasing) advance of science and technology is a sense of unease amongst the general population of science's potential of to change our lives, in sometimes unpredictable and alarming ways. Public understanding of science, or scientific literacy, is of increasing concern worldwide according to much recent literature.^{1,2} The term *scientific literacy* represents a diversity of views.^{3,4} However, a common theme in the scientific literacy literature is that of being *learned* or knowledgeable about some science content, and being able to critique scientific debates. According to Laugksch² a scientifically literate person does not accept opinion about a contentious scientific matter uncritically. Rather, he or she wants to see logic or evidence for any stance taken on the issue (see also Miller³). Some authors argue that the success or otherwise of a science education system can be evaluated by reference to the literacy of the citizens.⁵

It is interesting that many societal scientific debates are characterised by suspicion of scientists and their motives.⁶ Thus Reiss⁷ (p. 154) suggests that *the topics on which scientists work – and so the subject matter of science itself – to some extent reflect the interest, motivations and aspirations both of the scientists that carry out such work and of those who fund them*. In other words, the current rate of technological change is perceived as being driven by the motives, interests, and values of the science and technology community.⁶⁻⁸ This may be one reason that scientists are now seen somewhat as *tainted witnesses* with a vested interest, captured by personal interests, or unduly influenced by funding providers such as central government or multinational corporations.⁹

That the science and technology community has such a large impact on technological change would likely be less problematic if the values and culture (and indeed the demographics) of the science community were considered to be reasonably representative of society as whole.⁷ However, in general this is not the case. For example, women are underrepresented in higher education science and technology faculty posts and other science-related occupations. In the UK only 12% of science professors are women,¹⁰ and a similar under-representation apparently applies to many ethnic minorities. Thus indigenous peoples are underrepresented in post-compulsory science education and science professions, purportedly as a result of perceived conflicts between indigenous worldviews and the worldviews of so-called *Western science*.¹¹

It is hard to overestimate the importance of scientific literacy in the modern era. Carson¹ says (p. 1007) we need to *teach about the physical world, in order to share the achievements of science with our students, and in order to equip students to be good, informed citizens capable of participating in public discourse concerning matters of science*. Important and topical issues relate to matters such as the appropriate use of cloning technologies or genetic modification or engineering.¹² Oftentimes the *right answer* is not obvious for such scientific debates, and the public are faced with trying to decide who is credible. Such debates are hampered by a litany of scientific disasters such as the uncritical use of pesticides like DDT,¹³ and medical mishaps such as with thalidomide.¹⁴ Perhaps the most dramatic recent example of public debate in which scientists were discredited is that of the UK government's *scientifically-based* claims that the so-called *mad cow* disease could not cross the food chain from animals to humans.¹³ This proved patently incorrect, and made the British public very wary about later scientifically-backed claims of GM crops and the like. Carson¹ provides a strong case for the importance of scientific literacy as a focus for science education. He comments (p. 1011) that *science has become far more than an esoteric body of facts about the natural world*.

Scientific Literacy and Religious Beliefs

Scientific literacy impacts upon schooling, and sometimes conflicts surface between scientific and religious viewpoints. Because of the variation in scientific literacy in the broader community, conflicts about scientific matters can impact upon the management of schools, especially in highly religious communities. Thus, with devolution of school management in some countries debates about what should be included in school science curriculum can become quite heated as characterized by creationism vs. evolution debates,^{15,16} and the emerging controversy over the inclusion of the *intelligent design* concept.¹⁷ The basis of such debates may lie in view that there is a rather contentious relationship between an individual's religious belief, and scientific knowledge and training.¹⁸⁻²¹ This relationship and its consequences in terms of education are often hotly debated by social scientists and science education researchers. For example, the literature is replete with lengthy discussion about the conflict between scientific and creationist views of the origins of humans.¹⁶ These reports have largely focused on the issue of whether cognitive dissonance occurs in areas for which religious beliefs and scientific thinking are potentially in opposition. Furthermore, many of the studies in the science education literature are confined to issues concerned with Christian religions, particularly those described as fundamentalist,

i.e. in which adherents believe in the literal or near-literal interpretation of the Bible. However, little is known about non-fundamentalist or non-Christian educational contexts.^{15,22,23} Despite considerable rhetoric in the science education literature about such conflicts, little data about scientists' views of such matters has been presented. Indeed, scientists are typically portrayed as sceptics and objective seekers after truth, and are assumed to hold certain viewpoints in religion-science debates, *e.g.* typically, they are assumed to favour of the teaching of evolution and omit creation.²⁴

The current investigation adopts a different approach to that of most previous studies on scientific literacy, by attempting to determine how scientists from different faiths judge claims from within science and their own particular religions. In other words, do they exhibit scientific literacy as defined by Laugksch² and only accept opinion about contentious matters critically seeking logic and evidence for any particular stance? This is of particular interest given the public perception of scientists as *objective seekers of truth* and the view that science has largely demystified or even disproved religious beliefs.^{19,22,25}

Nature of Science and the *Scientific Mind*

An important aspect of scientific literacy is familiarity with the nature of science. To engage in debate about scientific issues necessitates some understanding of the nature of science. Much of the success of science has been attributed to the so-called scientific method,²⁶ and high standards of evidence for claims and theories. But how does science work? How do scientists obtain good data? What are good data? What are the *rules of the game* in science? Much has been written about the nature of science, and much research into students' understanding of the nature of science has been performed. It seems students often see science as a codified body of knowledge that is essentially unable to be challenged.²⁷ Much constructivist writings and constructivist-based pedagogies have sought to overcome such notions. Constructivists see scientific knowledge as mentally constructed personally, based on personal experiences and influenced to a greater or lesser degree by the social context in which knowledge construction occurs.²⁸

It seems from the literature that students ascribe scientists fairly stereotypical stances and beliefs, much as do the general public in seeing them as objective seekers of truth, inevitably ascribing to experimentalist methods of inquiry in their scientific search.²⁹ Scientists are, however, humans and like all humans hold views and biases, *e.g.* seeing some things worthy of inquiry and others not.² However, like technology,³⁰ science is increasingly presented in the science education literature as contextualized and value-laden, and to possess a *sociological agenda*.³¹ Carson¹ argues (p. 1012) that science education should not *leave students vulnerable to the occasional dogmatism of the scientists, but able to appreciate and yet criticise the enterprise of science*. Guisasola, Almudí and Furió³² point out that students, in physics at least, are likely to see science as codified knowledge for which textbooks present a very simplified version of the nature of science, one in

which science knowledge is seen to be accumulated in (p. 333) *non-problematic, non-historical, 'linear' accumulation*. Likewise, recent work by Dagher and Ford³³ suggests that science biographies written for children provide insights about scientific experiments and procedures used by scientists, but speak little of how scientists make connections between theory and evidence.

Gauld³⁴ in a seminal paper summarizes much research into the scientific mind and scientists' views of the nature of science. This is presented in terms of the *scientific attitude* (attributed to Gauld & Hukins³⁵), and *habits of mind*. According to Gauld's³⁶ analysis habits of mind for scientists can include: open-mindedness, scepticism, rationality, objectivity, mistrust of arguments from authority, suspension of belief, and curiosity. A number of these habits of mind at first sight seem incompatible, *e.g.* open-mindedness and scepticism. However, according to Gauld³⁴ it is the interplay of these habits of mind that results in the *scientific attitude*, in which (p. 110) *no idea, conclusion, decision or solution is accepted just because a particular person makes a claim but is treated sceptically and critically until its soundness can be judged according to the weight of evidence which is relevant to it*. According to Zinman,³⁷ a key feature of evidence claims, is that scientists have (p. 79) *very high internal critical standards*.

Herron³⁸ comments (p. 105) that with respect to the understanding of the nature of science presented in the literature we *'talk' a much more impressive procedure than we actually do*, pointing to a need for further research in this area. This resonates nicely with Reif's³⁹ view that to understand science involves more than content knowledge, it also involves (p. 281) understanding of the *requisite thought process* of science.

The literature is replete with commentary and rhetoric about what scientists are purported to think: their epistemological beliefs,²¹ their views about the nature of science,⁴⁰ conflicts between science and religion,^{19,20,34} and superstitious/pseudoscientific beliefs.⁵ But according to Coll and Taylor⁴¹ there are few data reported from contextualized and detailed research studies about scientists' views of the nature of science, and conflicts between scientific and everyday thinking.

Objectives of the Inquiry

Previous work within our research group found that many scientists could be considered to hold superstitious or *New Age* beliefs.⁴¹ It became evident during our inquiry that some participants also held religious views that were in conflict with current scientific theories, *e.g.* ostensibly some believed in, or were not prepared to discount the existence of, spirits/ghosts. The present study examined the relationship between an individual scientist's religious belief and his/her scientific thinking. Gauld³⁴ points out that scientists may hold two positions: a rationalist stance, which is that presented in the public domain (of their community of practice), and the private idiosyncratic views more accessible by interpretivist, ethnographic educational research approaches. The issue of scientific literacy in this work is thus explored by investigation of scientists' views of scientific evidence. Specifically, the present

work addressed the following broad question: “*How do scientists judge evidence claims?*” and is investigated using the vehicle of scientific theories and religious views.

Theoretical Underpinnings

The inquiry has been conducted within an interpretivist paradigm with a social-constructivist view of learning.²⁸ The authors believe that an individual’s constructs are influenced by his/her environment and subject to influence by prior knowledge, peers, learning experiences, social interactions, and context.⁴² We consider that religious beliefs and scientific thinking are personal in nature and that mental construction of beliefs is a personal cognitive process. However, we feel that previous work has not addressed adequately the sociocultural component of knowledge and belief construction. We wish to develop an understanding of the religious beliefs and scientific thinking of the participants in this study, *e.g.* their views about specific scientific theories like evolution. We recognize that we need to situate our research findings within the context in which the study was conducted, and hence place emphasis on the social aspect of social-constructivism. To develop our approach with a social-constructivist framework, we have drawn on current thinking from sociocultural views of learning. Sociocultural views of learning suggest that past research has not paid adequate attention to the social mediation of mental construction, even in social-constructivist-based studies. Wertsch⁴³ summarizes (p. 86): *The basic tenet of a sociocultural approach to mind is that human mental functioning is inherently situated in social interactional, cultural, institutional, and historical context. Such a tenet contrasts with approaches that assume, implicitly or explicitly, that it is possible to examine mental processes such as thinking or memory independently of the sociocultural setting in which individuals and groups function.*

Methodology

The methodology derived from the social-constructivist-based theoretical framework described above comprised an approach in which individual constructions were elicited by interactive dialogue between the researchers and the participants.²⁸ This dialogue recognized the social nature of knowledge acquisition and personal beliefs,⁴⁴ and so it was conducted on neutral ground in order to reduce the influence of investigator bias.⁴⁵ In practical terms this consisted of the interviewers constantly working to ensure undistorted communication took place: words and beliefs that hold an *established* meaning, *e.g.* a specific religious belief or *established* scientific theory, were only ascribed the meaning imparted to them in the conversation of the interviews (see below, terms like *higher power*, *spirit* and *soul*). A purpose designed instrument was used as the basis for interviews. The instrument[†] contains 18 assertions or propositions that were deemed to consist of potential conflicts between religious beliefs and scientific theories by a panel of experts. Other items were derived from literature reports of pseudoscientific beliefs held by students⁴⁶ – a strategy found useful in our study of scientists’ superstitious beliefs.⁴¹ The panel of experts consisted of scientists from a range of disciplines (see below) that examined each item statement and asserted that it was in conflict

with current scientific thinking in that discipline. These individuals had no contractual interest in the study⁴⁷ and were participants only in this advisory capacity.

Sample items included:

- People can be cured of serious ill health by petition to a higher spiritual power.
- The age of the earth is no more than 10,000 years old.
- After death the soul/spirit of a person returns in a subsequent life form, and
- Human conception can occur by spiritual not physical means.

Participants were asked to respond to a four-point scale ranging from *I believe that this is almost certainly true* to *I believe that this is almost certainly untrue* with two in-between responses qualified by replacing *almost certainly* with *quite likely*. Propositions were chosen to access beliefs purported to come from several religious faiths and denominations: Catholic, Fundamentalist Christian (Christians who believe in the literal interpretation of the Bible), Islam, Judaism, Buddhism, Hinduism, and Bahá’í (based on religious writings and informal interviews with ministers and faith adherents for each of the above named religions).

The sample of 23 scientists (Table 1) was chosen carefully to obtain several cohorts for the reasons detailed below. Firstly, we sought participants who were raised in a faith, practiced that faith as children and young persons, and who now described themselves as *non-practicing*. The intention was to see if these individuals drifted away from their beliefs and religious practices for no particular reason, or if this occurred because they encountered conflict between religious beliefs as they became acculturated into science and if this, in turn, had impacted upon how they assessed evidence. Secondly, we sought participants who were strong faith-adherents and strongly practicing in their faith (as identified by the participants, *i.e.* they reported that they were currently practicing their faith in terms of religious observance and rituals. Thirdly, the participants for interview were chosen purposively to provide a reasonably even gender balance and a range of scientific disciplines (chemistry, earth and biological sciences, physics, *etc.*). The intention was to see if gender or scientific discipline influenced the relationship between religious beliefs and scientific thinking — since discipline of expertise influenced the relationship between individual’s beliefs about superstitions.⁴¹ Fourthly, we sought a variety of religious affiliation/backgrounds. The intention was to see if, for example, a strong Christian was more inclined to *accept* Christian beliefs that were in conflict with scientific theories than they were about say Hinduism or Bahá’í beliefs that were in similar conflict, and vice versa.

Typically, the participants were educated to the doctoral level, or were engaged in doctoral level study (almost exclusively in science), and employed as faculty in their disciplines (mostly full-time but in some cases part-time). The participants ranged from recent appointments with little experience to senior academics with departmental and school management responsibilities. The participants

[†]Available from the authors upon request

were asked to complete the instrument in advance of interviews, such that the interviews addressed their responses along with other topics not presented in the instrument that arose during discourse. The interviewers strove to ascertain the basis on which the scientists had arrived at their views about the propositions contained in the instrument and any other beliefs or views respondents introduced during the interviews.

Table 1. Demographics of Research Participants.

Pseudonym	Religion	Occupation/ Discipline	Qualification
Gerrad	Church of England	Lecturer in Biology	PhD
William	Presbyterian	Lecturer in Biology	PhD
Bob	Hindu	Lecturer in Physics	PhD
Mary	Catholic	Lecturer in Biology	PhD
Arnie	Methodist	Lecturer in Agrosience	PhD
Susan	Agnostic	Lecturer in Agrosience	PhD
Phil	Agnostic	Lecturer in Agrosience	PhD
Iman	Muslin	PhD student - Agrosience	MSc
Perry	Methodist	Lecturer in Science Education	PhD
Tom	Catholic	Lecturer in Science Education	PhD
Jack	Catholic	Lecturer in Biology	PhD
Allan	Bahá'í	Resource Consent Manager	MSc ^a
Celia	Hindu	Earth Scientist	MPhil
Anne	Hindu	PhD student - MAPE	MSc
Brian	Bahá'í	Pharmacist	BPharm
Lyle	Bahá'í	Marine Biologist/Evolutionary Theory	PhD
Liam	Christian	Chemist	PhD student
Kevin	Christian	Earth Sciences	PhD student
Sandy	Hindu	Biology Teacher	MSc/MEd
Patty	Buddhist	Chemist	MSc
John	Buddhist	Chemist	MSc
Rachel	Buddhist	Physicist	MSc
James	Buddhist	Physicist	MSc

^aEnvironmental Science

All interviews were audio-taped and transcribed, transcripts were examined for statements about the scientists' views in an iterative process based on a phenomenographic approach allowing pools of meaning, and subsequent categories of description, to arise from the data.⁴⁸ Portions

of transcripts are used to illustrate the process of analysis and interpretation and pseudonyms are used throughout. These have undergone light and minor editing, e.g. removal of repeated words, changes of tense, in some case to make them more readable. In accord with an interpretive approach, the research findings reported here cannot be directly generalized to other settings. An alternative, and that applicable here, is the notion of transferability⁴⁷ in which the reader evaluates the significance of the findings in his or her own educational context. The provision of descriptive findings (see below), the so-called *thick description*, is intended to facilitate this process.⁴⁹

Research Findings

The findings are summarized in Table 2 and illustrated below. Some of the themes stem from reasons given by the scientist for supporting the instrument propositions, others from reasons for disbelieving them. These differences are detailed under the individual headings that follow.

Personal Experiences

Personal experience emerged as a reason for believing some propositions with, for example, some scientists reporting friends and colleagues being cured of significant illness, e.g. cancer, by *petition to a higher power*. This was in some cases seen as resulting from what Bob called '*the mere act of petition*' and in other cases from the actual intervention of a higher power as seen in Phil's comment that '*I know that in the intervention of God, there is clear evidence in healing*'.

Those who opposed God-like interventions generally felt that the notion of mind over matter was overriding as seen in Steve's comment that '*pointing the bone, that sort of thing in [Australian] Aboriginal or African culture, if you believe you've done something wrong, it could be because a higher power intervened, or it could be because of a belief that was self-fulfilling*'. Personal experiences reported included Bob's experience of physical encounter with a native bird species which he considered as potential evidence for item 13 *some animals have a special spiritual status* and Jim's personal links and affinity with things Russian which he appeared to consider as potential evidence for having lived a past life: '*One of the other things is that my birthday is on the day of the Russian Revolution*'.

As was seen in our study of scientist views about superstitions and New Age beliefs,⁴¹ some personal experiences reported in the present work were dramatic and strongly influential. Thus a strongly-practising Hindu participant talked of a dramatic personal experience involving *spirits*. Celia said:

I totally believe in it, i.e. 'the spirit or soul of a person lives on after death', because I have had certain experiences. When my grandfather died I was a little girl at the time my mother was looking after him at the hospital and he said wanted to see me ... my mum took holidays for me from the school and I went with my mother to visit him in hospital and he died at the hospital – but the second it really happened that spirit got into me and maybe three or four months later everyday at 12 o'clock afternoon midday I used to get fits. They thought it was fits but it wasn't, it was the spirit in me.

Similar reasoning was used by Celia to explain the com-

Table 2. Summary of Research Findings.

Classification	Basis	Comment
Personal experience/Personal beliefs	The scientists had undergone or knew intimately of some personal experience of the type discussed/The scientists held strong personal beliefs about the topic.	Reports of personal experiences were deemed reliable/Personal beliefs had no foundation other than religious upbringing.
Testimony from other scientists	The scientists rated personal testimony of other scientists as credible	This did not necessarily take the form of direct testimony but included the fact that another scientific discipline existed and inquiry was presumed to be reliable.
Potential theoretical basis/Related evidence	The scientists perceived a potential theoretical basis to the belief/The scientists held domain specific knowledge which they felt was relevant and supportive of the belief.	Commonly related to scientists' own discipline or area of expertise. Virgin birth was at least technically feasible since non-sexual reproduction in other supposedly sexual species was well established.
Don't know enough	The scientists felt current evidence about the belief was inadequate to either support or dismiss the belief.	Related to vagueness of terms such as 'spirit' and 'soul' and notions of cosmology.

mon Hindu support for destiny matters (item 4: *what happens in a persons life is set at the beginning of their life*) which she interpreted as being astrologically-related:

What happens in a person's life except at the beginning of life? Its more like fate isn't it?...The planetary positions and all that ... Even now everyone, *i.e.* in India, decides when you get married, or where you go. We were seven students and he (a pundit-astrologer) said you should be married at 29 and you'll be very rich and be owning a car at that time. I never believed it at that time, but definitely next time. I brought a car here, *i.e.* in NZ, and I think back to him, and I said, you know what he was correct ... There should be some sort of power, control, over your fate, that's what I believe.

The converse also was true in that lack of, or non-fulfilling personal experiences were deemed to be evidence *against* some propositions. To illustrate, apparently Celia did not accept that *a person can be affected in their personal life by petition to a higher spiritual power* (item 5, appendix) as the result of failed petition: *'I was once thinking that if I pray to God I get good marks, it never happens, I have to study to get good marks. So I slowly understand that it doesn't happen'*.

Participants who believed that evil spiritual forces caused evil behaviour tended to point to their experience of human behaviour to explain this: *Well, I've just seen the evidence...I see it as spiritual evil, in that power corrupts and absolute power corrupts absolutely. There are so many people who have brought untold misery to themselves and the world and to others and they are still doing it.*

Personal Beliefs

Personal beliefs based in religion, with no supporting evidence or indeed any need for evidence was used as a basis for acceptance of some of the propositions in the item statements used in the interviews. Jack, a biologist, was firmly of the belief that the soul or spirit of a person continues to exist after death. This was grounded in a dualist material and supernatural view of reality:

It's pretty apparent to me that reality comprises both the material and the non-material...the natural and the supernatural and they are different spheres altogether...you see I'm quite happy with the existence of the supernatural and the recognition that the material world is completely different from that...one is material and other is non-material...and when

you are dealing with the non-material...dealing with the human soul, you are dealing with spirits, you are dealing with God, angels, the devil all those sorts of things...no there has never been a conflict there...I can clearly see that science is a way of knowing which relates specifically to the material...it just that it takes a little time for the truth from one sphere to merge seamlessly with the truth of the other.

While Jack claimed no evidence or personal experience to support his belief in the non-material/supernatural concept, his view of material concepts was strongly grounded in scientific evidence. Thus, when asked why he believed that the world was more than 10,000 years old he responded: *'It is simply the accumulated scientific evidence from geology, palaeontology, physics, chemistry...I think the scientific evidence is overwhelming in this'*. Furthermore, he was also a strong believer in evolution based on the current scientific evidence.

There doesn't seem to be any satisfactory substitute as an explanation for the diversity of the world's living things and eh I know...I'm acquainted with a number of other alternative theories that have arisen in the past and evolution explains things in a purely natural way and em although there are some outstanding details 't's to be crossed and 'i's to be dotted the paradigm is pretty well constructed I think.

However, while individuals were often prepared to accept aspects of their own particular faiths *on trust*, they were often sceptical about the beliefs held by adherents of other faiths. Alan, a Bahá'í, was rather dismissive of Hindu-based beliefs in reincarnation and the special status of some animals: *'I guess the evidence for reincarnation is flawed in that there's not much point to the exercise...why come back as a cow as a punishment?'*

As might be expected, although most participants were more accepting of their own religious beliefs, when they conflicted with science this was not universally accepted. For example, Annie was brought up and remained a practising Hindu. However, when probed about reincarnation (item 3) she commented: *'In Hinduism there is a thing called reincarnation...when people ask if I believe in reincarnation, no I don't, but I believe the soul lives on'*.

Testimony

A number of the scientists felt that whilst they themselves were not sure of the details of the evidence against some

of the propositions, negative testimony from other scientists meant such propositions could not be taken seriously. This was most typically the case for the age of the Earth proposition with, for example, Keith a biologist commenting that *'the scientific evidence of fossils and dinosaurs and all that sort of stuff, the age of the stars'* and Jane another biologist saying *'you would have to throw out so many theories to believe that one'*. This occurred irrespective of religious faiths with, for example, Annie, a Hindu, commenting *'I know a little bit about carbon dating and I know it is definitely older than 10,000 years because I believe in the carbon dating technique and the research that has been done in terms of prehistoric creatures and the evolution of man'*. When asked why she believed in carbon dating she replied *'because the half life of carbon-13 decays and produces isotopes of carbon, it has been scientifically proven, that decay kills off [sic] carbon'*.

Other participants pointed to things such as near death experiences for which in their minds there were now sufficient reports to support the religious propositions presented in items 2 and 3. Alan comments: *'Our consciousness is not affected by sleep or injury to the person's brain or whatever, there have been far too many cases of people remembering to dismiss...there are studies currently being conducted into near death experiences to the point where enough scientist are taking them seriously to warrant belief'*.

One Earth scientist and fundamentalist Christian ostensibly did think that the Earth was less than 10,000 years old. This he reasoned was a matter of data interpretation: *'There is fossil and dating evidence, facts that suggests the Earth is millions of years old, these are facts...but you can interpret this in other ways'*. When questioned he talked about a theory to do with changes in the speed of light which ostensibly meant that radio-chemical dating experiments were unreliable: *'The speed of light is constant, but it may not always have been constant...this would affect the reliability of the carbon-dating data'*.

However, for other scientists, the testimony of non-scientists could be considered to credible evidence. Thus Jack had no personal experience of *petition to a higher spiritual power* impacting on his own life, but he believed that prayers could be answered based largely upon the experiences of others. *'I know from friends, many of them Protestants, that they believe and that they have experienced the answer to prayers and I wouldn't deny the reality of their experience.'*

One participant, who grew up in the West, but had worked in rural Africa for a number of years, recognised the strong cultural influence in evaluating testimony:

In the village I lived in, in Botswana, we had one of the most powerful witchdoctors...and the stories people would tell about things he was capable of doing...you'd hear from a range of people including university educated people that I worked with in the school, they would tell stories...and you've got no basis for dismissing them, you're not really being very objective if you dismiss it purely because you bring your own beliefs to the situation and there are some really quite strange things.

Implicit in this statement is also the sense that university education adds to the credibility of testimony.

Theoretical Basis to Beliefs

Again similar themes emerged from the religion and science study. To illustrate, for most of these scientists human conception, by spiritual rather than physical means, was deemed impossible. Celia, a Hindu, said: *'It's ridiculous, it will never happen, I totally believe it is due to physical means, because I am not a Christian I have never tried too understand that'*. Similar views were expressed by Annie another Hindu: *'Conception was like a gift that was handed to virgin mums, they were born into a normal family'*. However, some strong Christian adherents used their discipline-specific scientific knowledge to propose reasons as to why this might be possible. For example, human conception was seen as at least technically feasible since non-sexual reproduction in other species was well established as seen in Bill's comment: *'It's a possibility that if we have an all loving God, who constructed these processes in the first place using the natural things anyway, why can't you have as amictic cell, i.e. that can give rise to offspring without fertilization, in the ovary in the womb of a woman turn itself into an embryo? It happens in plants all the time'*. Those that discounted this proposition attributed the belief to something deemed socially acceptable at the time with, for example, Keith commenting *'that way she, i.e. the mother of Christ, can't have been soiled in any way, something that has a basis in belief and trying to fit into a particular framework'*.

It was noteworthy that some scientists reworked original statements, thinking on their feet and seeking alternative explanations. Alan, was dismissive of Hindu beliefs in reincarnation, but upon probing he looked for alternative explanations that might be seen or interpreted as *evidence* at least consistent with such beliefs. He said of reincarnation *'the fact that genetic material is passed from one person to another as generations proceed, one after another, that is 'reincarnation' so to speak'*.

We Don't Know Enough

The notion that we simply don't know enough about many spiritual things meant that some of the participants in the study likewise felt that *we need to keep an open mind*. This occurred particularly in relation to things such as spirits and souls living on after physical death, and cosmological notions of pre-determinism and order in the universe or its creatures. Mary indicated that she thought that order in the universe was almost certainly due to a higher spiritual power: *'You're looking at some structure, let's say a fly or a spider, now what are the chances the probability that something like that can construct itself?'*. This was universal across the religious denominations with Annie (a Hindu) commenting that the reason she was prepared to believe the notion that after death a spirit could continue to exist was because *'I think that there is a lot yet to be discovered, there's a lot yet unknown that we don't know about and it could be prove...even if science has not proved it now, who know what might happen in the next 1000 years?'*. She held similar views about people being cured by petition to a higher power: *'People diagnosed with cancer found other ways and means, not in terms of cures like alterative medicines, but in terms of believing, having faith and praying or taking up religion that they*

have been healed', although she went on to comment that this was likely due to 'a belief that they can destroy it if people believe in something it gives them the ability to fight something better'.

Implications for Science Teaching and Learning

Some authors have argued that an outcome of good science education is improvement in scientific and technological literacy^{2,18-20} and argue that religion and superstition are antiscience.²¹ Modern citizens constantly confront scientific and technological issues and science/religious conflicts. Given that scientists are generally seen as (sometimes *tainted*) authority figures with respect to science claims, it is of interest for science educators to understand what beliefs scientists hold, and on what basis, they hold such beliefs. A more liberal approach to science teaching might, as Matthews²¹ posits (p. 91), *maintain that science instruction should be more than merely the conveyance of factual knowledge*. Quite so! In other words, science is value-laden as many authors working in the area of the nature of science have long maintained.⁵⁰ Others like Oga-wa⁵¹ argue that science needs to move beyond the Western view and take cognisance of *indigenous science*.

One feature of scientific literacy is the ability to make credibility judgements of peoples' and scientists' testimony. Scientific literacy is important in modern society as people encounter debates and issues of a scientific and technological nature, including science curriculum matters. This study provides a window into some scientists' thinking, in this case with respect to potential conflicts between science and religion. The research findings provide evidence for dissonance for many of these participants, but others have, in contrast, rationalized such dissonance in variety of ways. It is our view that these data point to a more open-minded attitude than is commonly ascribed to scientists. This suggests that scientists are not automatically dismissive of non-scientific beliefs (including religious beliefs) and points to a human dimension of scientific thinking.

A second issue is the impact, if any, of scientists' beliefs on their teaching of scientific content, especially in the case of religious beliefs that conflict with science theories. A scientist's research is screened in that if he or she wishes to publish research in a scientific journal peer-review likely *screens out* views that are widely disparate from those held consensually by the particular community, such as chemists, earth scientists, and so on (insofar as there is consensual agreement). The fact that many of the scientists in the present study held beliefs that were in direct conflict with *normal science* is not necessarily of concern in this context. Tertiary level teachers arguably have more autonomy over specific course content, *e.g.* they are not constrained by external curricula, although course offerings may be subject to some peer review and scrutiny, *e.g.* accreditation programs exist for many professions, and course structure and content in tertiary level science are often externally moderated especially at advanced levels. But what of say an earth scientist or biologist that is required to teach current scientific theories

that conflict with their personal religious beliefs? Several such individuals were identified in this work. There are several possible explanations or responses to such an issue. First, many religious beliefs (spirits, destiny, special status of animals, *etc.*) are topics unlikely to arise during teaching. McGeorge⁵² points out that in the school system sometimes this also is avoided when the topic evolution is not expressly presented in curriculum documents. Second, such individuals might seek to avoid occupations, including tertiary level teaching, that results in such encounters.

Mahner and Bunge¹⁸ assert (p. 112) that *consistency in one's belief system is hard to come by*. This seems to be borne out in the present work. However, their addendum that this is *particularly [so] in the midst of a society where religion wields a formidable cultural and political power*, seems to us to be unjustified and somewhat overstating the case.

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Introduction

Biosensors have been described as the offspring of an arranged marriage between biology and electronics. The first commercially successful biosensors were developed in the 1960s as enzyme-based devices primarily for medical diagnostics. Currently, the fastest growth area involves affinity-based, label-free biosensors that yield real-time information on biomolecular interactions, as well as analyte concentrations in food, agricultural, nutraceutical, or environmental samples.

As illustrated schematically in Fig. 1, an affinity biosensor is essentially comprised of two distinct components: a biological recognition element, *e.g.* antibody, enzyme, lectin, receptor, nucleic acid or microbial cell, and (in close contact) a signal transducer, *e.g.* optical, acoustic, piezoelectric or electrochemical, connected to a detector for data acquisition and processing. The signal from the interaction of analyte with the biological element is converted to a quantifiable signal.

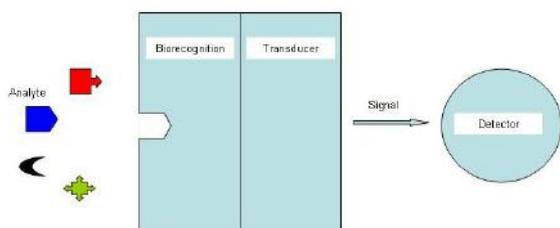


Fig. 1. Schematic of a biosensor.

Several transducer techniques are used in biosensor devices as indicated in Fig. 2. The most commonly reported optical transducer techniques include the variants fibre optic, surface plasmon resonance (SPR), optical grating coupler, *e.g.* optical waveguide light mode spectroscopy, and evanescent wave. Amongst these the SPR-based biosensors are currently the most commonly applied.

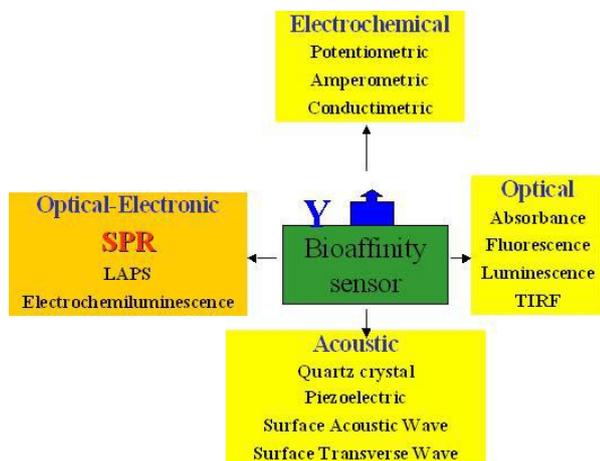


Fig. 2. Overview of transducer alternatives for affinity-based biosensors.

An SPR system generally requires a laser light source, detector, glass prism, and gold surface, (Fig. 3). In an angle-shift instrument, total internal reflection of incident polarised light is configured at the interface of the gold-covered glass and a continuously flowing liquid medium. The electromagnetic field component penetrates the metal and transfers some energy to the valence electrons thereby producing charge density waves known as *surface plasmons* at the interface. The resonance conditions that produce a reflected light intensity minimum are influenced by changes in refractive index at the interface. Thus, any mass changes due to association and dissociation events with immobilised probes at the sensor surface are monitored in the form of a continuous plot of refractive index against time. The significant advantages inherent to such systems are that the transduced signal is acquired both in real-time and label-free.

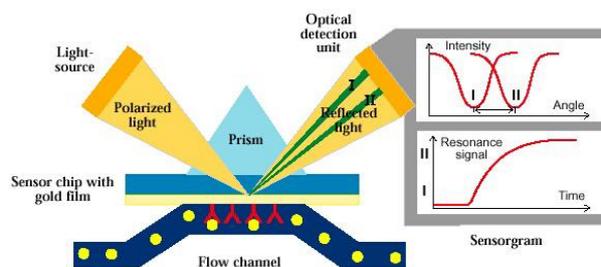


Fig. 3. Schematic of integration of Surface Plasmon Resonance (SPR) optics, sensor surface, and flowcell in a Biacore instrument, reproduced with permission from Biacore®.

The continuous output is in the form of a sensorgram that follows the association and dissociation events within the evanescent field between analyte in solution and the immobilised ligand on the sensor surface. In a typical schematic sensorgram (Fig. 4) the SPR response [in resonance units (RU)] is monitored against time. Unless dissociation is very rapid, a regeneration step is needed to re-establish a fully functional immobilised surface for subsequent cycles.

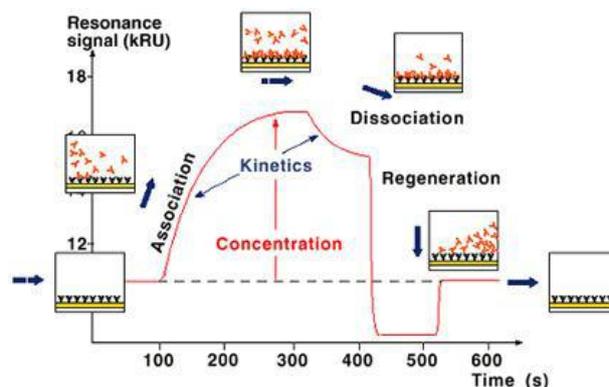


Fig. 4. Schematic SPR-generated sensorgram, illustrating both events and extractable information over time, reproduced with permission from Biacore®.

The information-rich sensorgram, dependent upon the experimental conditions under which it is generated, can yield data related to:

- *Specificity* – the extent to which different molecules interact with a single partner immobilized on a sensor surface.
- *Kinetics* – the rates of a biological interaction, both of complex formation (k_a) and dissociation (k_d).
- *Affinity* – the binding strength (K_D) that can be determined either from the level of binding at equilibrium as a function of sample concentration, or from the ratio of the kinetic rate constants (k_d/k_a) under defined conditions.
- *Concentration* – determined by monitoring the interaction of either a pure analyte or one in a complex mixture, e.g. serum and food samples, over a prepared sensor surface. Direct, sandwich, or indirect assay formats may be used, with quantitation of the target analyte in unknown sample achieved by interpolation of binding response on a calibration curve acquired with authentic standards. Unlike physicochemical separation techniques, SPR-based immunoassay provides an estimate of the biologically active analyte content, in contrast to total concentration, a feature that is particularly significant when structurally labile proteins are of interest.

While there are now several commercial vendors of pre-configured *closed-box* SPR-based instruments, e.g. Biacore, Affinity Sensors, IBIS Technologies, and Texas Instruments, that includes the growing diversification into imaging technologies, Biacore® is globally dominant for the conventional SPR applications described above. Since the first commercial SPR-based system released in 1990, there has been a significant growth in publications (mostly in life science and drug discovery applications) with a total of ca. 4,500 articles to the end of 2004. Excellent reviews of affinity biosensors and SPR are available.¹⁻³

What's Happening in New Zealand?

There are currently eight Biacore instruments here, of which five are designed for the development and routine use of concentration immunoassays in foods and other biological materials, and three are configured for higher resolution kinetics and affinity applications. In comparison, Australia has 45-50 instruments with major applications to life science in academia, and to biotechnology that focuses on antibody therapeutics, drug discovery, membrane interactions, DNA interactions, and receptor-ligand and protein-protein interactions.

Analytes relevant to the food industry can generally be assigned among three categories when targeted for concentration analysis. The first includes low molecular weight nutrients or contaminants that are usually determined by chromatographic methods. The second group includes various proteins or other immunogenic macromolecules for which conventional immunoassay techniques are used, while the last group includes intact microorganisms, generally assayed by microbiological methods. Biosensor techniques based on SPR-based concentration immuno-

assay of food components can be configured for each of these analyte categories and there are now ca. 100 peer-reviewed publications describing specific applications to vitamins, pathogenic microorganisms, β -lactam antibiotics, steroid hormones, proteins, food adulteration, allergens, drug residues, marine biotoxins, coumarins, and GMOs. In fact, publications related to food analysis are one of the fastest growing applications of SPR-based systems.

In general, the sensitivity, specificity, and quantification range of bio-specific methods are determined by ligand-analyte affinity. Therefore, an optimized SPR-immunoassay relies predominantly on appropriate ligand selection and immobilisation chemistry, as well as buffer conditions, contact time, and the regeneration protocol.

SPR and Food Analysis

Vitamins

Within Fonterra, the principal usage of SPR instrumentation has been in the development and application of immunoassays for routine compliance testing of specific B-group vitamins in supplemented cow milk-based paediatric formulae, and other milk-based foods.

B-group vitamins are commonly consumed as dietary supplements to the extent that ca. 60% of respondents in a survey reported their use, although they are now being challenged by new botanical ingredients. Nevertheless, vitamins are produced commercially to more than 100,000 tons per annum, representing an almost \$7 billion industry in the US alone. The water-soluble vitamins folic acid, biotin, riboflavin, pantothenic acid, and vitamin B₁₂ are added as supplements to many foodstuffs and animal feeds. For infant formulae designed to substitute for breast milk, their inclusion is legally required. Thus, reliable and accurate concentration estimates of these vitamins are mandatory for compliance during food processing to ensure that labelling needs are met and that vitamin dosage is controlled during the production of fortified products. Furthermore, the demands of the modern processing environment and the sensitivity of vitamins to environmental factors demand a rapid analytical procedure.

Traditionally, the concentration of B-group vitamins is measured using microbiological assays that require a high level of skill, and suffer from relatively poor precision. HPLC-based methodologies are also available but reliable results from complex food matrices such as milk are difficult to reproduce and are not yet routine for biotin, folate and vitamin B₁₂. These assays are especially challenging because of the very low levels present and the high lability of the vitamins during multiple sample extraction steps. SPR-immunoassays that yield vitamin concentrations utilising Biacore instrumentation are configured with an inhibition format, and have been demonstrated to be accurate, rapid, sensitive, and highly suited to a routine high-throughput compliance program. As with immunoassays in general, the biological specificity of the detecting molecule results in the need for minimal sample preparation. With a single instrument and a range of vitamin-specific kits, a laboratory is equipped to fulfil the requirements of food and dietary supplement manufacturers, international

regulatory bodies, and consumers.⁴⁻⁷

AgriQuality Laboratory Services (Auckland) uses a Biacore Q for a range of compliance concentration assays for folic acid, biotin, and vitamin B₁₂ in fortified dairy products and foods. They are also evaluating the technique for the routine detection of antibiotic residues. The assays are kit-based with standards, antibody/antigen, sensor chip, and running buffers included. In general, vitamin supplements in foods present no particular difficulties except when starch is present, *e.g.* in cereal foods. For such cases, and when endogenous vitamins are required for analysis, more sophisticated sample preparation is necessary for analyte release prior to the SPR-based immunoassay. Thus, sample preparation protocols that are recommended with the kits have been modified to allow several food matrices to be tested to verify fortification levels. Current work is proceeding to optimise such strategies, incorporating various enzyme treatments, protein precipitation, and acid or alkaline hydrolysis for more reliable estimates of food folate.⁸

Milk Proteins

Milk contains numerous minor proteins with physiological properties targeted at providing immunoprotective, growth, and antimicrobial factors to the neonate. These are distinct from the nutritionally more significant major proteins. Many of these minor bioactive proteins are found in the whey fraction of mammalian milks, and are generally present at elevated levels in colostrum, reflecting their importance to early neonatal health. The increasing commercial interest in exploiting their therapeutic value has stimulated the need for reliable concentration assays for their determination at naturally occurring levels in milk and colostrum, at supplemental levels in infant formulas, and at pharmaceutical levels in milk protein isolates and nutraceuticals. Both liquid chromatographic (reversed-phase, ion-exchange and affinity) and conventional immunological methods (immunodiffusion, nephelometry and ELISA - *Enzyme-Linked Immunosorbent Assay*) exist for these proteins. Despite this, Fonterra has successfully developed and applied SPR immunoassay techniques for immunoglobulin G (IgG), folate binding protein (FBP), lactoferrin (Lf), and lactoperoxidase (LPO) in bovine milk and colostrum.⁹

Sensor surfaces were prepared with affinity-purified goat anti-bovine IgG, folic acid derivative, goat anti-bovine Lf, or rabbit anti-LPO on a carboxymethyl-dextran-coated gold sensor chip (CM5) via amine coupling under instrument control. Samples were prepared for analysis by dilution to between 1:1,000 and 1:50,000 in an Hepes buffer, depending on analyte and level. Calibration curves were established by serial dilutions of authentic standards in buffer. Calibration standards and sample extracts were dispensed into 96-well microtitre plates and injected for 3 min. at 20 $\mu\text{L}/\text{min}$ (IgG), 8 min. at 20 $\mu\text{L}/\text{min}$ (FBP) or 5 min. at 10 $\mu\text{L}/\text{min}$. (Lf and LPO). Binding responses acquired 30 sec. after the end of the injection were measured relative to the initial baseline and used for generation of the calibration curve and interpolation of unknown samples. The surface was regenerated by injection of 25 mM

phosphoric acid (IgG), 75 mM sodium hydroxide (FBP), 10 mM glycine-HCl, pH 1.75 (Lf), or 10 mM glycine-HCl, pH 1.50 (LPO).

The *on-farm* extraction of Lf from milk during milking has been achieved at Dexcel. This was the culmination of work undertaken over 18 months by a team involving dairy farmers, Dexcel, Waikato University, and Sorsortec. The automated on-line fractionation unit, named *Bruce*, extracted Lf via a single-stage stirred tank with cation exchangers SP Sepharose Big Beads™ while the cow was being milked in Dexcel's robotic milking unit.¹⁰ Lf was measured using SPR technology with a Biacore 3000 and this allowed for the rapid measurements of yields from different sample matrices such as raw whole milk (feed), processed milk, and eluates.

The project was designed to prove that minor, high-value milk components could be extracted from whole milk with minimal disruption to the milking routine or to the bulk milk composition during milking.¹¹ In the initial run, *Bruce* continually extracted Lf from milk during the normal operation of the robotic milking process in which the cow presents herself for milking. The on-farm system proved effective and yielded 15% more Lf than is achieved in conventional factory processing systems. Similar work at Waikato University has targeted the optimisation of a rotating bed annular chromatographic system for the continuous separation of milk proteins including BSA and Lf.

Progesterone and Estrogen Steroids

HortResearch in Hamilton have utilised SPR technology in developing a number of high sensitivity immunoassays for progesterone in milk, in view of the value of this steroid hormone as an indicator of bovine oestrous.^{12,13} They utilised Biacore instrumentation, either as a final assay technique or for evaluation of antigen:antibody binding characteristics as a means to screen optimal binding partners for ELISA assay. Inhibition assay formats utilising monoclonal antibodies to progesterone have been exploited, with the progesterone immobilised directly via various length linkers, or via a protein conjugate. Strategies have included novel surface attachment and gold-tagged enhancement labels for binding antibody that have increased sensitivity and reduced detection limits by orders of magnitude. The surface chemistry enables >1000 cycles/chip with excellent precision, and the surface linkers facilitate projection of antigen into the fluid stream.

In addition to assay design and enhancement, SPR has been used to study the effects of conjugation chemistry on the ability of antibodies to recognize targets, which is very important for both biosensor construction and the design of small molecule-drug conjugates. Such studies include assessments of the effects of changing conjugation position on antibody binding for immobilised steroids such as estrogen, and developing new synthetic routes for producing derivatives with maximal antibody recognition properties.¹⁴

Sorsortec, in conjunction with the Waikato University, is currently involved in using SPR technology to measure

and/or confirm binding between progesterone and a conjugated enzyme-antibody for use in an alternative ELISA immunoassay system. The aim is to commercially exploit analysis of progesterone for improved on-farm monitoring of herd fertility.¹⁵

SPR and Biotechnology

PEGylated Proteins

The *in vivo* stability of proteins used for clinical and therapeutic use is vital. The Bioseparations and Biomolecular Engineering group at Waikato University (now located at Canterbury) has explored the interaction of PEGylated proteins with various surfaces using SPR. PEGylation is the covalent attachment of polyethylene glycol groups to the target drug and is a technique that has been reported to prolong the half-life of the therapeutic protein. Such surface interactions of biomaterials are fundamental to issues such as host response and biocompatibility, and SPR offers a valuable alternative to other techniques, such as quartz crystal microbalance, for their study.¹⁶

Antibody Characterisation

HortResearch (Palmerston North) implemented SPR in 1997 and was the first NZ laboratory to do so. It has had much success since then, through use of a manual Biacore X instrument, in the development of antibody-based protein arrays. Host systems designed for multiple protein expression have been established for the production of monoclonal antibodies. The instrument is used for epitope mapping of the produced antibodies, to determine the affinity constants (K_D) of the antibodies for their antigen, and for studying protein-protein interactions.

The Biacore X has also been used to develop competitive immunoassays for small molecules such as organophosphate pesticides, antibiotics, and phytotoxins. For such work, the group has developed their own monoclonal antibodies and synthetic haptens.¹⁷

Microbial Pathogenesis

At Auckland University, the Molecular Bio-discovery team are investigating the mechanisms of microbial pathogenesis. A Biacore 2000 has been used to study the interaction between secreted pathogenicity factors from *Staphylococcus aureus* and *Streptococcus pyogenes* and components of the innate and adaptive immune response.¹⁸ Common studies include the rapid screening of toxin mutants to identify and map binding sites that can then be combined with protein crystallographic studies to provide a complete picture of the *modus operandi* of individual toxins. Analysis involves qualitative comparisons of mutant binding with wild-type toxins to their targets coupled to sensor chips, followed by quantitative analyses to determine association (k_a) and dissociation (k_d) rates and the calculation of K_D to provide information on affinity.

One example of past studies is the analysis of the binding of the potent super antigenic toxin SMEZ-2 to soluble recombinant forms of Major Histocompatibility Complex Class II and T Cell Receptor molecules. SPR was employed to demonstrate that mutants of SMEZ had reduced

affinity to the T Cell Receptor in comparison to the wild type toxin. These results were used in conjunction with other immunoassays to confirm the exact location of the TcR binding site, and the effects of individual mutations in the binding site on the toxicity of SMEZ-2. The studies were essential in the construction of a modified toxoid version of SMEZ-2 that forms the basis of a commercial vaccine conjugate to enhance the immunogenicity of proteins, peptides and carbohydrate antigens.

This group has also studied the interaction between the human epithelial Na^+ channel (hENaC) and domains of human ubiquitin-protein ligase hNedd4, where SPR was utilised to characterise the interaction affinities of synthetic binding domains of proteins.¹⁹ Other studies have reported nanomolar estimates of K_D for the interaction between staphylococcal superantigen-like protein SSL-7 and IgA by both kinetic and equilibrium affinity experiments.²⁰

SPR-Mass Spectrometry

The ability to use SPR to both confirm the presence of a binding partner and extract its interaction kinetics and affinity is enhanced by the opportunity to identify structure via coupled mass spectrometry. A group at AgResearch have utilised the capability of the Biacore 3000 to assist identification of a binding partner to a newly identified protein associated with muscle atrophy and plan to utilise SPR-MS to structurally characterise the binding protein.

Problems Inherent to SPR

Most of the difficulties with SPR measurements originate with the sample rather than the optics, which are relatively problem-free. Although ligand immobilisation is always required for an SPR experiment, there are a number of strategies that cover most instances. Non-specific interactions and bulk refractive index differences are probably the most difficult issues to deal with. It has been stated²¹ that *the good news is that everything has an SPR signal and the bad news is that everything has an SPR signal* and hence, overcoming potential non-specific interactions represents the major challenge for both kinetic and concentration applications of SPR detection.

Conclusions

In food compliance alone, the global food diagnostics market currently stands at *ca.* \$US 1.4 billion, and the application of biosensors is currently under-exploited, perhaps because of both an inherent conservatism and an occasionally inflexible regulatory system within this industry. The basic SPR instrument is not expected to change dramatically in the future, although there is potential for low-cost and field-type alternatives. Although acceptance of SPR technology has been relatively slow in NZ, recent installations have dramatically increased the visibility of this tool and it is likely that its attributes will become more apparent across analytical chemistry.

Acknowledgements

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John Mitchell, Yinqiu Wu, and Jing Yuan (HortResearch), Rob Orchard (Sensortec), John Fraser and Fiona Clow (Auckland University), Pathik Vyas (AgriQuality,) and Rick Filonzi (Biacore-Australia).

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NZIC Salary Survey update.

The first stage of the Salary Survey has been completed. 224 forms have been received and entered into a database. The usefulness of the survey is completely dependent on the information obtained so thanks to the members that took the time to correctly fill out and return their forms. Helpful notes and suggestions for future surveys were also valued. Appreciation is due to Biolab and MEP Instruments Ltd, who helped support this survey by providing prizes for those that returned their forms on time. The following people were the lucky ones to be drawn at random and receive prize packs.

Nicola Scholes
Al Shakarchi
Norrie Pearce
John Skipper
Graeme Gainsford
Robert Rankin

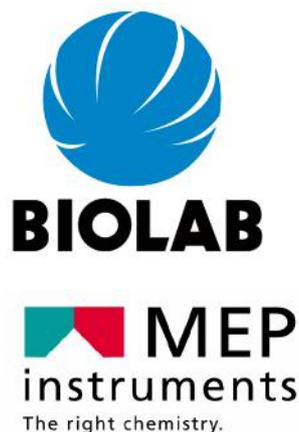
An answer that made for interesting reading was one given to the "What other benefits do you receive?" question by a self employed person. They had listed the benefit of "freedom".

One person wrote a note asking how the prizes would be awarded when the survey was anonymous. It would appear this person then read the paragraph detailing how this would be done directly under the paragraph about the draw and crossed out their note. Their ethnic background was listed as Australian.

While not everyone listed their gender 184 surveys were received from males and 39 from females. There was an \$80,000 difference between the highest male and the highest female base salary. The highest female salary came in 45th overall so if some higher paid females did not fill in their surveys the data will be skewed on gender.

Now the collection phase is complete, the data is going to be statistically analysed and a summary of the results will be written up in a forthcoming issue of *Chemistry in New Zealand*. This data will also be compared with the results of the last salary survey undertaken by the NZIC in 2000.

The NZIC thanks our sponsors



Nanotechnology - Does It Have a Sporting Chance?*

Dr. Alan Smith

Associate Director, Micro Nano Technology Network, UK

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It's been hard to miss the hype that's surrounded nanotechnology the past few years. On one side, industrialists and academics hype nanotechnology's wide-ranging potential applications, hoping to garner government funding. On the other side, advocacy groups agitate about the potential dangers of exposure to nanoparticles, working to stir up public awareness—and gain membership fees, to boot. As usual, the truth about nanotechnology lies somewhere in-between the two sides' positions, but it is important that the debate does not go the same way as the dispute over genetically modified foods.

Nanotechnology is debated as though it was a new technology, but it's not. Our own bones are composed of self-assembling nanostructures; car tires have included carbon black nanoparticles for decades; the red and yellow colours in sunsets are caused by nanoparticulate pollution (both volcanic and from chimneys); and many food products are nanoemulsions or particulates. Scanning tunnelling microscopy enabled us to observe objects at the nano-scale, revealing that at that level, thermal, optical, mechanical, electronic, magnetic, and surface properties change. This realization has driven the search for new products, and the sporting goods industry has led the way.

From Bowling Balls to Tennis Balls

For example, bowling balls are usually covered in scratches; hardly surprising when they hit the pins at the end of the alley with such force. One enterprising company used nanoparticulate coatings to give the balls a scratch-resistant surface, enabling them to look pristine for months. A similar technology is being used for the final lacquer coating on a number of Mercedes vehicles, and the results have been impressive.

Wilson Sporting Goods recently introduced a nanocomposite tennis racquet, currently used by Switzerland's Roger Federer. Use of the racquet has enabled Federer to consistently hit the ball harder. Wilson also offers a new *Double Core* tennis ball that keeps its pressure longer, even when Federer and others hit it in excess of 150 mph. The new balls have a butyl rubber nanocomposite coating inside that acts as a barrier, preventing air from getting out. This same technology is also being used for footballs and for food packing, helping slow degradation by preventing flavor from getting out of the packaging and oxygen and ultraviolet light from getting in.

Golf Clubs, Fly Rods, and Racing Bikes

Nanocomposite materials are also being used in fly-fishing rods from Redington; the rods' nano-titanium resin layer gives them a lighter weight and stronger frame

than has previously been possible. Nanocomposite golf balls are on the market, and Wilson is leading the way with Nanotech golf clubs. These new drivers and fairway woods have a nanocomposite material that reduces the weight of the crown of the club, lowering the center of gravity and giving longer and straighter drives. These clubs also have carbon nanotubes in the tip section of the shaft to improve stability and add to the length of the shot. Pdraig Harrington, Ireland's leading golfer, attributes his recent success to the new clubs. His caddy is grateful for nanotechnology as well; Harrington's golf bag is made from a new nanofabric that has reduced the weight of the bag by 52%.



Nanotechnology has also made inroads in the textile industry. Stain-resistant clothing has been available for the past few years, and a new fabric has been designed specifically to repel grass stains and help *whites stay whiter* — an advance sure to be welcomed by cricketers around the world. Socks are available that are based on the antimicrobial properties that silver nanoparticles impart. And many sunscreens now on the market contain nanoparticulate titanium dioxide, which blocks so-called “bad” ultraviolet rays while letting tan-giving rays through. Surfers and other athletes who cover their lips and noses with sunscreen will appreciate the distinction.

BMC, the leading Swiss bicycle brand, has developed a revolutionary bike for the number-one Pro Tour Team Phonak for the latest Tour de France. The company's enhanced resin system contains carbon nanotubes and exploits the fact that nanotubes have a strength-to-weight ratio a hundred times better than that of aluminium, and far

better than that of normal carbon fibers. The combination of good riders and excellent bikes has put Team Phonak at the top of the worldwide UCI ProTour ranking.

In the Cold and In the Shower

Winter sports are also benefiting from nanotechnology, with nanofibers being used to windproof and waterproof ski jackets. And skis and snowboards themselves are being coated with a high-performance nanowax that produces a hard, fast gliding surface.

Micro-electromechanical systems (MEMS) — small, integrated devices that combine electrical and mechanical components — are commonplace nowadays, and top range cars often contain 50 to 100 sensors. As the trend from micro to nano continues, the sports industry will see increasing use of sensors in sports goods. Suunto markets a wide range of sensor-packed, wrist-top computers. One of their golf models has GPS incorporated into it and can indicate which club to use to reach the pin and avoid water and bunkers. Who needs a caddy — especially because the golf bags are so lightweight?



The author in action.

The use of nanotechnology in Formula One motor racing has not been widely discussed, but lighter-weight materials and nanosensors offer an advantage that will likely be seized upon. To the extent that the race depends heavily on the type of tires used, there is a good chance that manufacturers such as Bridgestone and Michelin are investigating replacing their carbon black nanoparticle tires with better-wearing and lighter nanocomposite products.

Even the changing rooms at the gym will be using more and more nanotechnology, as easy-to-clean and antimicrobial products become more prevalent. Nanocoated glass surfaces are already available for showers that prevent water droplets from sticking to the glass, keeping the surfaces cleaner longer. Samsung is using this technology to keep refrigerators fresher, and black mold in showers will become a thing of the past as tile and sealant manufacturers adopt this development.

A Trillion-Dollar Market

Markets of between one-half to one trillion dollars for nanotechnology are being forecast in 10 years time, so even a 1% share of the market will add more than \$5 billion to a country's economy. MEMS sensors and nanomaterials are predicted to reach \$100 million in 2009 for the sporting goods market. High-tech sporting goods are leading the way for nanotechnology, but other industry sectors are quickly jumping on board. If concerns about exposure to nanoparticles continue to be addressed successfully at an international level, all industries utilizing nanotechnology will have a sporting chance of success.

Dr. Alan Smith is an Associate Director of the UK government's Micro Nano Technology Network, which is coordinating activities in nanotechnology throughout the UK. He was re-elected as a member of the IUPAC Bureau at the Beijing IUPAC Congress.

Chemical Processes in New Zealand - now online

The second edition (1998) of our publication *Chemical Processes in New Zealand* is now out of print, but is still the most comprehensive account of the practice of chemistry in New Zealand. In addition to being bought and used by secondary schools, tertiary education institutions and public libraries, it was a source of information for, and used by, many businesses and organizations associated with chemistry in some way. Although many of the articles are no longer fully up to date, having it available in electronic form on the web allows access for all and gives us the opportunity to update it and develop it further.

The book contains 17 sections with self-explanatory headings, and various numbers of articles, (101 in all) under each heading. Individual articles can be easily downloaded.

The Institute would welcome offers of help and suggestions for the further development of this resource. See:

www.nzic.org.nz

The MacDiarmid Institute for Advanced Materials and Nanotechnology



Founded in 2002 and named after the 2000 NZ Nobel Laureate Alan MacDiarmid, the MacDiarmid Institute for Advanced Materials and Nanotechnology was one of NZ's first (now seven) Centres of Research Excellence. It is based in the School of Chemical & Physical Sciences of Victoria University, although its operations include Canterbury, Massey and Otago Universities, and the CRIs, IRL and IGNS in Wellington as partner institutions. Its director, Professor Paul Callaghan, PCNZM (Physics-VUW), arguably the most well recognised member of the NZ scientific community, has steered the MacDiarmid Institute from infancy to what is now a major player in the chemical and physical research arena not simply in this country but internationally. The aim of the Institute is to enhance NZ's capability in nanoscience and nanotechnology and to benefit the country both through graduate student training and technology spin-off. As Paul says



'We see ourselves as the premier NZ centre for innovation and knowledge creation in fundamental and applied materials science and technology'. In its four-year existence four spin-off companies (Anzode, magritek, Nanocluster Devices, and BioImprint/Bio-Chip) have been generated through use of targeted goals attained through *five* thematic areas each with its own *Theme Leader*. These are outlined below.



Theme I, Nanoengineered Material and Devices is led by Dr. Roger Reeves (Physics and Astronomy-Canterbury). In this area the nanofabrication of the ever decreasing sizes of integrated circuits (and the development of totally new devices) is critically explored, and an important thrust in the research is directed towards the discovery and development

of new materials that lend themselves to device fabrication. Within this area are research objectives covering the design and characterisation of new materials systems at the nano-scale, and the fabrication of devices from these or other materials that encompass optical and optoelectronic materials and devices, with targeted outcomes such as better UV-sensitive materials (for monitoring exposure to UV radiation), improved polarising filters (for TV displays or optical imaging systems), and ultra-sensitive op-

tical biomolecule detection devices.

Electronic and magnetic materials and devices are being examined with a view to better understanding of the way magnetic atoms interact in a non-magnetic host material. The fabrication of new types of magnetic sensors (for reading computer hard drives) using atomic clusters, and the development of new types of electronic device that rely on electron field emission, *e.g.* for improved flat-panel TV displays, form another area. Chemically and biologically active materials that could lead to devices with carbon-based surface self-assembly techniques (for creating selective arrays of bio-sensors), and the establishment of new techniques for manipulating cells and cell membranes (for miniaturized cellular diagnostics) and improved bio-sensors are also under investigation.

In many cases these objectives will assist in gaining a better understanding of materials and devices at the nano-scale, but new technologies will emerge for incorporation into products and processes that we all use every day. The diversity of research stems from the interests of the Principal Investigators who do not have to align their interests artificially to a small common set of objectives, but are given the freedom to explore, with the only requirements being those of excellence, ethical integrity, and an alignment to the overall objectives of the Institute.



Theme II encompasses novel electronic, optic-electronic and superconducting materials and its leader is Dr. Andy Edgar (Physics-VUW). The current frontiers in this challenging field are found in novel materials, in nano-scale architecture within new materials or composites, and in novel ways of understanding old materi-

als that remain elusive to theoretical description. The work is arranged under four objectives. The first is focused on determining the crystal structure and properties of previously unexplored metal nitrides since, with the exception of the wide band gap semiconductor GaN, others are unexplored. The second objective concerns a broad class of materials in which the interaction between electrons forces their motion and quantum states to be strongly correlated and is one of the most challenging problems in modern physics. The materials include the high temperature superconductors for which the IRL group (in particular Jeff Tallon and Grant Williams) is especially well-known. Objective 3 is concerned with composites that consist of glasses with nano-crystalline inclusions as such materials undergo a change in refractive index on

irradiation thereby forming the basis of a range of applications including Bragg gratings for optical fibre filters and optical memory devices. Some of the materials under investigation are close to commercialization as X-ray storage phosphors. The final area is one that provides theoretical support for the other objectives not simply of this area but also for those in the first, third and fifth themes. Moreover, a new initiative has been aimed at providing high-pressure capability for a number of programmes that range across several of the Institute themes. For example, pressure dependent effects provide a fundamentally important route to establishing the nature of electronic interactions, and high temperature spectroscopy represents a relatively unmapped frontier in the science of high-Tc superconductors.



The 3rd theme examines conducting polymers and is led by current NZIC President, Assoc. Prof. Keith Gordon (Chemistry-Otago). Here existing NZ expertise is used to create new materials based on conducting polymers, carbon nanotubes, nanofibres, and quantum dots. In turn, these materials are targeted for the fabrication of devices and thin

films used as light-emitting diodes, all-plastic solar cells, molecular sensors, and switchable surfaces. These materials are electro-active in the sense that they respond to or generate electrical energy. As the materials are crafted on a nanometer scale they are termed *nanostructured electromaterials*. The work is underpinned by computational modeling of the materials both at a molecular level (to understand properties such as mode of polymerisation and polaron structure) and in a bulk sense to gain insight into conduction mechanisms. Thus synthetic strategies provide monomer units with in-built electronic functionality such as donor-acceptor units, and fluorescence and phosphorescence capabilities, with the incorporation of additional functionality, e.g. alkoxy groups, to aid solubility and processability. These materials then form the feedstock for the generation of films, fibres, and nanoparticles that can subsequently be employed in the various devices.



Assoc. Prof. Kate McGrath (Chemistry-VUW) leads **Theme IV Soft Materials**. Soft materials and complex fluids represent one of the most challenging areas of interdisciplinary research as they possess both solid and liquid-like properties. These include polymer melts and solutions, lyotropic and thermotropic liquid crystals,

micellar surfactant phases, colloidal suspensions, and

emulsions. Complex fluid systems also include the class of materials known as *porous media*. The subject of flow, dispersion, and diffusion in porous media has major interdisciplinary significance and underpins chromatographic separation technology, biological perfusion, and wood treatment technologies to name but a few examples.

The molecular basis of soft material rheology, studied by use of NMR and optical methods, allows the links between nanostructure and rheology to be probed. Molecular assemblies at the basis of living organisms are the ultimate nanotechnology. Here structural organization is important at the molecular (a few nanometres), mesoscopic (many nanometres), microscopic (micrometres) and macroscopic (millimetres) scales. In comparison, motions range from very fast (tumbling water molecules) to comparatively slow (cell division). Adjustment of the macroscopic properties of complex fluids by control of the underlying nanostructure is aimed at giving, for example, better delivery systems and enhanced emulsion stability. Manipulation of the interfacial domain in emulsions is to be assessed by achieving controlled coalescence and the diffusion of a tagged macromolecule across the membrane interface.

Soft materials based upon biopolymeric networks are everywhere in nature and the technological arena. An elucidation of structure-function relationships in such biomaterials promises to reveal the design rules of nature and facilitate the use of biopolymers as engineering materials. The self-assembly of semi-flexible polymers in solution, in melts, and in blends is being examined experimentally and theoretically to gain better understanding of how important known polymers such as DNA have significant internal stiffness. Surface Enhanced Raman Scatterings (SERS) and plasmon resonance enhancement of fluorescence are new experimental tools. These are now being used to probe, at the molecular level, the physical and dynamic basis by which the mechanisms of biological processes take place – single biomolecule physics. The importance of plasmonics in current nanotechnology research is vast and researchers in this area use 3D assemblies of nanoparticles for surface enhanced Raman scattering. Here it is hoped to produce an entirely new type of materials for application in tracing molecules via Raman spectroscopy.



The 5th theme deals with advanced inorganic and hybrid nanostructured materials and is led by Assoc. Prof. Ken MacKenzie (Chemistry-VUW and IRL). It is concerned with the development of such innovative materials, inorganic polymers, composite and hybrid materials - including those utilizing conducting polymers with specific structures and surface properties. It

draws thematically on the idea of extending function and performance of conventional inorganic materials by in-

roducing novel surfaces and interfaces. These interfaces may be with organics in composite and hybrid materials, they may be nanostructured to provide steric selectivity and high surface area, or they may be internal interfaces in the form of topological defects associated with ultra-high strain. The associated science is complex and its elucidation is dependent upon a various spectroscopic techniques. However, the scope for structural, compositional, and functional variation within these materials is huge. The associated impact encompasses technologies for energy conversion and storage, environmental sustainability, sensors, electronics, and biotechnologies.

The research of this theme covers new materials design, synthesis, and characterization that will allow new approaches to energy conversion and storage, and to controlling surface functionality. Moreover, an understanding and control of the nano- and micro-structures of these

materials, of the reaction mechanisms, phase transformations, rates and processes involved, is vital to further development.

Integral to the theme is the world-class competence of its investigators and the need for instrumental methodologies that include Solid State NMR, X-ray Powder Diffraction, Electron Microscopy, Ion Beam Analysis, and SQUID magnetometry. For success in this area access to international centres of neutron diffraction, muon spin relaxation, and synchrotron X-ray science for the researchers is essential and has been arranged.

Compiled by the Scientific Editor from material supplied by Margaret Brown (Manager, MacDiarmid Institute for Advanced Materials and Nanotechnology); further articles describing the chemical work of the MacDiarmid Institute are to be provided by the chemically-based theme leaders and should appear in April 2007.

Conference Calendar

1st European Chemistry Congress, Budapest, Hungary, 27-31 August 2006

This Congress aims to be a showcase for chemical sciences in Europe and will bring together chemical and molecular scientists from industry, academia and government institutions across Europe and from around the world. Plenary lectures will be given by six Nobel Laureates.

For more information see
<http://www.euchems-budapest2006.hu/>

Green Chemistry Principles and Practice, Basel, Switzerland, 17-18 October 2006

A two day course given by Dr Peter Spargo aiming to provide chemists, engineers and managers in industry with the tools and information to meet and support their corporate environment goals.

For more information see
http://scientificupdate.co.uk/training/green_chemistry/index.php

NZIC Conference Royal Lakeside Novotel, Rotorua, December 2-6 2006

Back to the Basics: From Small Molecules to Materials and Surfaces See full page advertisement elsewhere in this journal. Also a special symposium titled "Showcase, Industrial Chemistry in New Zealand"

For more information see www.massey.ac.nz/%7Eenzic/

4th International Conference on Advanced Materials and Processing, Waikato, Hamilton, 10 - 13 December 2006

Presentation topics include advanced polymers and composites, novel materials processing technologies and advanced metallic materials.

For more information see
<http://mape.waikato.ac.nz/icamp/>

Australian Colloid and Interface Symposium 2007, Sydney, Australia, 4-8 February 2007

ACIS 2007 is the international meeting of the RACI colloid and surface science division.

Themes:

- Spectroscopy and scattering in surface and colloid science (organisers: Jim McQuillan, NZIC & David Beattie)
- Pharmaceutical applications (organisers: Ben Boyd & Ian Larson)
- Hierarchical materials (organisers: Calum Drummond & Matt Trau)
- Surface forces, nanotribology and biological interactions (organisers: Roger Horn & Michelle Gee)
- Inorganic oxide surfaces (organisers: George Franks, Yang Gan & Jonas Addai-Mensah)
- Drops and Bubbles (organisers: Ray Dagastine & Clive Prestidge)
- Frontiers of Colloid and Interface Science (organisers: Greg Warr, Rob Atkin & Shannon Notley)

Further details available at the conference website: <http://www.colloid-oz.org.au/> or by email acis@pco.com.au Dr Erica Wanless, RACI Colloid and Surface Science Division

AMN-3 Third International Conference on Advanced Materials and Nanotechnology, 11-16 February 2007, Wellington, New Zealand

For more information see:
www.macdiarmid.ac.nz/AMN3



The International Union of Pure and Applied Chemistry: New Zealand Contributions

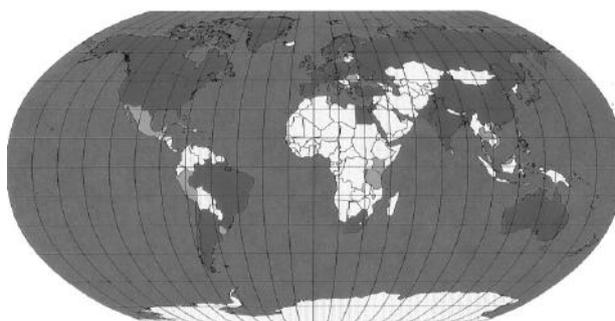
As a worldwide organization IUPAC has an impressive track record in enabling the language of chemistry to be understood globally. Its *mission* is to advance the global aspects of the chemical sciences and to contribute to the application of chemistry in the service of mankind. It promotes the norms, values, and ethics of science, it advocates free exchange of scientific information and access of scientists, and it addresses worldwide issues as a non-governmental, objective, international scientific body.

IUPAC acts as an independent authoritative agency to provide standards and outreach programmes for chemistry through:

- standardization of chemistry methods
- critical evaluation of physicochemical data, *e.g.* atomic weights
- the language of chemistry - nomenclature, symbols, terminology
- data exchange standards for computers and instruments
- chemistry education
- industrial safety and environmental programmes
- CHEMRAWN, its conference series that addresses Chemistry and Societal Impact
- sponsorship of major international conferences and symposia

It is nurtured, monitored, and organised by its elected management – the **Bureau** (President 2006-07: Prof. Bryan R. Henry), its **Secretariat** - an appointed administration at Research Triangle, NC, and its eight **Divisions** - each comprised of an elected membership – namely, I - Physical & Biophysical Chemistry; II - Inorganic Chemistry; III - Organic & Biomolecular Chemistry; - IV – Polymers; V - Analytical Chemistry; VI - Chemistry & the Environment; VII - Chemistry & Human Health; VIII - Chemical Nomenclature & Structure Representation. The regular business is handled by the five **Standing and Operational Committees** (each with Division representatives: Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS), Committee on Chemistry and Industry (COCI), Committee on Chemistry Education (CCE), the CHEMRAWN Committee, and finally the Committee on Printed and Electronic Publications (CPEP).

IPAC Member Countries



There are 45 National Adhering Organisations (NAOs; dark) and 21 Associate NAOs (gray) whose subscriptions financially sustain IUPAC; the level is proportional to the size of the country's chemical industry. New Zealand has membership through RSNZ and participates above its weight in IUPAC activities. Currently NZ has eight members of task groups for the *ca.* 150 current IUPAC projects, a number greater than for most other small nations. Recent and current NZ elected titular members of Divisional and Standing committees are:

A/Prof. Jim McQuillan (Otago)
Division I & CCE

Prof. Kip Powell (Canterbury)
Division V, President 2004-05

Dr. Patrick Holland (Cawthron) Institute
Div. VI, Secretary 1998-2005

Prof. Laurie Melton (Auckland)
Division VI

A/Prof. Richard Hartshorn (Canterbury)
Division VIII & CCE

While the following are the known project task group members (we apologise if we have inadvertently omitted some members from the list because our records are incomplete; please advise the editor accordingly):

A/Prof. Henrik Kjaergaard (Otago) Division I project, *Categorizing hydrogen bonding and other intermolecular interactions.*

Prof. Ken Marsh (Canterbury) Division I project, *Ionic liquids database.*

Dr. Gregory Russell (Canterbury) Division IV project, *Terminology for radical polymerizations with minimal termination.*

Ross Sneddon (Cawthron) Division VI project, *Remediation technologies for removing arsenic from water.*

Dr. Wayne Temple (Otago) Division VII project, *Training of school children on pesticides and health*.

Publications are an important part of IUPAC's outreach. The IUPAC journal *Pure and Applied Chemistry* publishes peer reviewed proceedings and plenary lectures from sponsored conferences, special topic articles and reviews, and IUPAC reports and recommendations. *Chemistry International* is the bimonthly news magazine that all Affiliates receive and there is an impressive book series that includes *Compendia of Nomenclature and Terminology*, *International Thermodynamic Tables of the Fluid State*, *Solubility Data Series*, *Analytical and Physical Chemistry of Environmental Systems* and *Chemistry for the 21st Century*. There are also some excellent electronic resources that include Educational materials, Databases, Nomenclature and Terminology, and some miscellaneous materials; see: www.iupac.org/publications/epub/index.html. Web access is available to most IUPAC projects, reports and publications, and further information is available at: <http://www.iupac.org>. This is very utilitarian but has a surprisingly wide range of information through the sub-pages and links.

IUPAC has a number of awards with the annual **IUPAC Prize for Young Chemists** being of broad interest and awarded for the most outstanding PhD theses in the general area of chemical sciences. In addition to a cash prize it supports attendance of the recipients at the biennial IUPAC Congress.

Projects

IUPAC was formed in 1919 and, until 1999, its scientific work was organised through Commissions. A reformation reinvigorated the work of the Union with emphasis on more open projects. The scope of the project system is still not well appreciated by many, but it lies at the very heart of IUPAC activities. It involves the efforts of close to 1000 volunteer scientists worldwide addressing issues of significance to the global chemistry community. These include nomenclature, terminology, and symbols, the validation and compilation of data, standardization of methods and procedures, education and the public understanding of chemistry and, lastly, topics requiring consensus among chemists worldwide.

The range of topics covers the whole gamut of chemistry from critically evaluated databases and precise and reliable atomic weights, to chemical education and the more political arenas of chemical disarmament, sustainable development, meeting the needs of developing countries, the requirements of chemical industry and a plethora of other topic areas in between. Any group of experts with a good idea can submit a *project proposal*. The proposals are assessed and, when approved, managed by the relevant Division; small budgets are allocated to cover the expenses of the project task groups. Principally, the emphasis is on voluntary inputs of time and expertise by a multinational task group that takes a 2-4 year lifetime to complete its job. Typically, a *Technical Report* or a *Recommendation* (including necessary terminology or nomenclature) is provided. The more applied projects often include outreach programmes, such as a workshop.

New Zealand Contributions

New Zealand members have been associated with the following projects in recent times.

IUPAC Stability Constants Database

This database provides the principal source of literature data for the *Critical evaluations of stability constants* at the core of Division V activity - a project chaired by Kip Powell. This database has wide relevance encompassing inorganic, physical, and environmental chemistry. Data compilation involves literature search, evaluation, and then data entry using the program SCenter; quality control checks are made on all entered data. The data are then sent to *Academic Software* for conflation of master files and addition of ligand structures. Some 58 main stream journals are abstracted with coverage current to the end of 2004 for 15 journals, to 2003 for 5, and 2002 for 14 journals. The current aim is to bring the literature coverage in the database up-to-date this year. A current aim is to establish a team of experts to supervise data entry and oversee quality control, thus assuring a succession of experts to continue the work beyond the current project (see: www.iupac.org/publications/scdb/index.html)

The Atmospheric Chemistry Database

This major Division I project on the evaluation of kinetic and photochemical data for atmospheric chemistry concludes this year. The database is now available on two websites (Cambridge and North Carolina) and the Cambridge site has had 4000 visits. There are 11 publications from the project that have gained 2600 citations (see: <http://www.iupac-kinetic.ch.cam.ac.uk/>).

XML in Chemistry and Chemical Identifiers

This Division VIII project has produced a *Public Chemical Identifier* to uniquely identify compounds. The essential feature of the problem is that the researchers require more advanced tools for data mining rather than an ability to move chemical data from A to B. The IUPAC/NIST Chemical Identifier (INChI) is a protocol for converting any chemical structure (connection table) to a unique, predictable character string. Version 1.0 of the Identifier was released in April 2005 and expresses chemical structures in a standard ASCII machine-readable format, in terms of atomic connectivity, tautomeric state, isotopes, stereochemistry, and electronic charge. It deals with neutral and ionic well defined, covalently-bonded organic molecules, and also with inorganic, organometallic and coordination compounds. Software, documentation, key links, source code and licensing conditions are available from the IUPAC website at <http://www.iupac.org/inchi>.

Richard Hartshorn is on the Task Group to develop a unified method for descriptors for all (higher) coordination numbers 7-12. The established method for lower coordination numbers involves identifying the appropriate coordination polyhedron, e.g. octahedron, and then defining the positions of the different ligands. Attempts to extend this to higher coordination numbers have all foundered to-date as a result of the larger number of possible geometries differing in relatively small ways one from another and the distortions from ideal geometries. A new project

for the promotion and extension of INChI aims to have the identifier used throughout the chemical information community, and to extend its applicability by including polymeric structures. The need for other extensions (including the ability to handle Markush structures) and an ability to include information on other attributes, such as phases and excited states is being assessed.

IUPAC Colour Books'

The publication of glossaries is a standard IUPAC activity. They are developed for particular topic areas to facilitate communication among researchers, government regulatory authorities and chemists in associated professional areas. The core glossary of chemical terms is IUPAC's **Gold Book**, *Compendium of Chemical Nomenclature* (3rd revision 2003). A key project for Division 1 has been the preparation of the third edition of the **Green Book**, *Quantities, Units and Symbols in Physical Chemistry* that is expected to be on the internet later this year; it contains more quantum mechanical and spectroscopic terminology than previous editions. Division VIII has recently revised the IUPAC **Red Book**, *Nomenclature of Inorganic Chemistry*. This project was long term, lasting some five years and the publication is edited by Connelly, Damhus, Hartshorn, and Hutton, (RSC, ISBN 0-85404-438-8. 2005, pp. 366). Other IUPAC **Colour Books** are featured at:

<http://www.iupac.org/publications/books/seriestitles/nomenclature.html>

Glossary of Terms Relating to Pesticides (2006)

This Division VI project is to revise the 1996 glossary (created under the leadership of Pat Holland) and currently searchable at:

<http://www.iupac.org/reports/1996/6805holland/index.html>

The revision contains definitions of more than 500 terms frequently used in relation to the chemistry, mode of action, regulation and use of pesticides for the wide range of disciplines involved in this field. Terms relate to pesticide residue analysis, sampling for analysis, good laboratory practice, metabolism, environmental fate, effects on ecosystems, computer simulation models, toxicology, and risk assessment. The number of terms has more than doubled since 1996, indicating the degree of integration with other scientific and regulatory disciplines over this time.

APAT/IUPAC International Workshop on Combining and Reporting Analytical Results

This workshop held in Rome in March this year typifies an IUPAC extension activity, in this case for Division V. Traceability and measurement uncertainty in comparisons of analytical data were explored as they represent a significant challenge for the analysts from the uncertainty in combining and reporting data, and the role of reference materials to improving the quality of data through interlaboratory comparisons.

IUPAC Conference Sponsorship

IUPAC sponsors about 30 major international conferences and symposia in the chemical sciences annually. It sel-

dom involves funding except for meetings in developing countries or those focused on new directions in chemistry. IUPAC members (or affiliates) are frequently involved on the programme committees ensuring that the meetings are of a high standard with open access; proceedings are normally published in *Pure & Applied Chemistry*. Upcoming conferences include the 19th *International Conference on Chemical Education* (Aug. 2006, Seoul), the 11th *IUPAC International Congress of Pesticide Chemistry* (Aug 2006, Kobe), the 12th *IUPAC International Symposium on Mycotoxins and Phycotoxins* (May, 2007, Istanbul), and the 41st *IUPAC Chemistry Congress - Chemistry Protecting Health, Natural Environment & Cultural Heritage* (Aug 2007, Turin).

Committee on Chemical Education - the Flying Chemists Program

In January 2005 a new initiative, the Flying Chemists Program (FCP) was inaugurated with its aim of supporting emerging countries in improving the teaching and learning of chemistry at primary, secondary, and tertiary levels. The FCP provides a country with necessary expertise to strengthen chemistry education and to assist it in its development. So far FCP project have been conducted India (2005) and Sri Lanka (2006).

Emerging Issues in Developing Countries

A recent contribution by NZ member Kip Powell was to organise a series of articles on this topic in *Chemistry International* over the past 12 months. By way of illustration one topic was *Ambiguous (chemical measurement) terminology as a barrier to fair trade*.

Tools of Trade

A series of articles for *Chemistry International* starting in September is to highlight the contributions of IUPAC Divisions to the goal "...to facilitate the advancement of research in the chemical sciences through the tools that it provides for international standardisation and scientific discussion". These articles, again initiated from an NZ initiative, will illustrate topics such as the many IUPAC electronic resources and databases; the *Colour* books; metrological traceability and laboratory proficiency documents; CHEM-RAWN publications, etc.

New Zealand Institute of Chemistry

supporting chemical sciences

July News



Executive

Error: In the April issue we inadvertently published the name of the second Vice-President as **Prof. Brian Nicholson** (Waikato). This is incorrect. The 2nd VP is **Prof. Bill Henderson**.



Prof. Bill Henderson

Bill was born in Darlington and grew up in Stockton-on-Tees in northeast England. He studied chemistry and geochemistry (University of Leicester), and gaining his PhD there in organometallic chemistry (supervised by Dr. Ray Kemmitt). Postdoctoral work at Northwestern University (Evanston, IL) with Professor Du Shriver then followed. Bill then returned to industry in England (Albright & Wilson Ltd.) where he carried out research and development in organophosphorus chemistry and surfactants. In 1992 he took up a lectureship at Waikato. He was promoted to Assoc. Prof. (2000) and then a full chair in 2005; he has been Chairperson of Chemistry since 2002.

Bill's research interests centre on the characterisation of inorganic compounds using mass spectrometry and span the chemistry of the platinum group metals and gold, and applications of organophosphorus chemistry to the synthesis of novel ligands and the immobilisation of enzymes. He

has published over 160 articles and three textbooks to date.

Chemistry in New Zealand

The *Journal* is now available on-line 6-monthly in arrears. Individual articles may be downloaded free of charge as PDF files.

BRANCH NEWS

AUCKLAND

The Branch has had two interesting speakers recently. In April we had a meeting aimed at new members with pizzas galore, followed by a presentation from **Rachel Bennett** (Total Laboratory Systems) on her studies of *Forensic Isotope Ratio Mass Spectrometry* while she was at ESR Ltd. We thank the Waikato Branch for alerting us to her interesting topic in a previous issue of *Chemistry in New Zealand*.

In May, members were treated to a stimulating talk by **Prof. David Williams** on sensors, ranging from their scientific conception through to commercial reality. David recently joined the Chemistry Department at Auckland University as Professor of Electrochemistry. He has been involved personally in the development and commercialisation of sensors for ozone through to pregnancy testing. The audience appreciated both his coverage of the topic and his enthusiastic presentation style – particularly his demonstrations of assorted sensors from the consumer market.

Chemistry Department UA

The Medicinal Chemistry programme at Auckland celebrated the graduation of the first 11 BSc (Hons.; Med. Chem.) students in May. Four of the students were awarded Bright Futures Top Achiever Awards for PhD study. At the Departmental graduation breakfast it was announced that **Drs. Sanjaya Senanayake** (supervisor **Hicham Idriss**) and **Roslina Halim** (supervisor **Margaret Brimble**) were

jointly awarded the L.H. Briggs Prize for best PhD thesis in Chemistry. Roslana was also awarded a University Best Doctoral Thesis prize.

Prof. Jonathan Sessler (University of Texas, Austin) has been visiting the University of Auckland having research interests in the medicinal chemistry, supramolecular chemistry, and macrocyclic synthesis. **Prof. Abhik Ghosh** (University of Tromsø, Norway) is also visiting and is hosted by **Penny Brothers** and **Peter Boyd**. Here for another six months, his research areas encompass bioinorganic chemistry, porphyrin chemistry and computational modelling.

Linus Parander joined the Light Metals group an honorary research fellow on 1 April 2006. Linus was, until February, at the Process Chemistry Centre at Åbo Akademi University and has been involved mainly with thermodynamics and high-temperature- and combustion chemistry.

CANTERBURY

March saw the **Annual Student BBQ**, and in May an evening talk from the Department's Erskine visitor **Prof. Greg Jackson**.

Chemistry Department UC

The Chemistry Department beat Physics in the *quasi-annual* Rutherford Shield Cricket. In June, **Dr. Emily Parker** started as Senior Lectureship in organic chemistry. Emily was an undergraduate and BSc (Hons.) student here before doing a PhD in the UK. **Prof. Don House** is here for the year to replace **Prof. Peter Steel** who is indulging in his James Cook Fellowship.

Prof. John Blunt is the 2006 recipient of the NPR Lecture Award 'in recognition of his international reputation and the huge importance of the marine metabolites review to the profile of Natural Products Review'. **Dr. Maya Mitova**, currently a postdoc-

toral in the Marine Chemistry group has received a prestigious Humbolt Fellowship; she was previously the holder of a Marie Curie Fellowship. **Daniel Packwood** has been awarded the University of Canterbury's 2006 Undergraduate Scholarship to attend the Australian Institute of Nuclear Science and Engineering Winter School in July.

Thomas Cain graduated as recipient of the inaugural Cuth. J. Wilkins Prize, which is awarded each year to the top MSc (Hons.) in Chemistry student in the 12 months prior to the award. The prize is in memory of **Prof. Cuth Wilkins**, who was a student, staff member, and Emeritus Professor in Chemistry for more than 70 years.

On May 14 our longest servicing member of our technician staff, **Russell Gillard**, completed 45 years service. Well done!

Mary Gower and **Andrew Muscroft-Taylor** have recently been awarded PhD degrees. Mary's thesis *Synthesis and Biological Evaluation of Inhibitors of the Shikimate Pathway Enzyme 3-Dehydroquinase Dehydratase* was supervised by **Prof. Andrew Abell**. She has just been awarded a NZ Science & Technology Postdoctoral Fellowship to work with **Prof. Jon Clardy** at Harvard Medical School. Andy's thesis **Investigations of the Type II Intramolecular Diels-Alder Reaction Directed Towards Natural Product Synthesis** was on work under the supervision of **Dr. Jonathan Morris**, who is now at the University of Adelaide.

Prof. Greg Jackson (Australian Defence Force Academy, University of New South Wales) is currently a visiting Erskine Fellow. **Dr. David Havlicek**, an inorganic chemist from Charles University, Prague, made a short return visit. **Philipp Kuegler** (University of Constance, Germany) is an undergraduate student spending the year with the Marine Group (**Blunt, Munro**).

The appointments of **Denis Hogan** and **Dr. Quentin McDonald** as Adjunct Senior Fellows in the Chemistry Department have been extended for three further years.

Three long-standing and valuable

members of the staff recently retired after great service to the Department. They are **Bruce Whitfield** (27 years in the Store), **Geoff Speer** (18 years in the workshop) and **Bruce Clark** (18 years as mass spectrometrist). **Axel Neffe** has completed his postdoctorate and returned home to Hamburg.

CPIT

The CPIT Year 12 Chemistry competition was held in mid-May, and involved more than 60 students from schools around Canterbury. The focus of the evening was organic chemistry with students spending a busy hour identifying unknown organic compounds using chemical tests and constructing models of stereoisomers. After a supper of pizza, prizes were awarded to the top schools as: 1st - Riccarton High School, 2nd - Burnside High School, and 3rd - Hillmorton High School. Competitions for Years 10 and 11 are planned for later in the year.

ESR

ESR Christchurch Science Centre has announced the retirement of long serving food chemist **Dr. John Love**, and the resignation of **Dr. Rosemary Whyte** who is to pursue a career growing mushrooms.

MANAWATU

The Manawatu Branch members have enjoyed several meetings and activities recently. Thus, at our annual student barbeque **Simon Hall** (Anzode) gave an entertaining account of how his group has taken basic research from the laboratory bench to a commercial venture; a select group made a visit to the Hawke's Bay wine regions including a tour through the Mission and Montana wineries – the scale of the Montana plant was especially impressive. **Barry Scott** (Merck) organised a chemistry quiz night, with **Trevor Kitson** as quizmaster and the phosphazene team (**Andrew Brodie, Eric Ainscough, Carl Otter**) were the clear winners; it must be noted that a certain team headed by a recent Past-President of the Institute managed to score *zero* in the *math* round, much to the dismay (delight?) of the physical chemists present.



My supervisor went to Penn State and all I got was this t-shirt – the look on Carl Otter's face says it all. Manawatu's Quiz Night Champions – The Atom Antz.



Captain Bob (obscured) and the NanoWarriors in action at Quiz Night.

Massey University

This year will see many IFS staff retiring or taking up reduced contracts, primarily because of the rapid expansion of the late 1960s and early 1970s. Amongst these are **Roger Reeves, Ken Jolley, Dean Halford** and **David Parry**. We also have **Carol Taylor, Emily Parker** and **David Officer** moving on and several others contemplating retirement. **Scott Walker, Aidan Harrison** and **Hemi Cumming** will be joining the crusade with Emily at Canterbury University.

A farewell was held for **Roger Reeves** in mid-February. A large turnout of friends and former colleagues was pleased to have the opportunity of wishing Roger well in his new venture in Melbourne. Roger has had a very long and distinguished career at Massey and his loss will be keenly felt by those in the Chemistry Discipline, the Institute, and the College of Sciences as a whole. The occasion was marked by an appropriate ditty composed by **Paul Buckley**. This was performed by the mass choirs of IFS and IMBS and as has become the tradition for the more senior staff members at the time of their retirement.

Massey welcomes back **Bin Yu Qin**, who completed his PhD with **Geoff**

Jameson in 1999, producing a couple of landmark papers on β -lactoglobulin. Since then he has been a postdoctoral researcher with **Kai Lin** (Massachusetts Medical Center). Bin has produced, generally as lead author, a series of beautiful papers on kinase signalling pathways and regulatory mechanisms and is in NZ for a one year post-doctoral position that **Jim Salvador** held, working on the proton transport pathway of manganese superoxide dismutase.

Mila Webb has joined the Technical General Staff working with the Chemistry group servicing the teaching laboratories. Mila has a background in science and will help ensure that the 100-level operation is back to full strength. **Geraldine Wood** has transferred from the College of Education to take the role of Chemical Services Technician assisting **Penny Abercrombie** in the Chemical Stores. Geraldine also has a science background and knowledge of the University and IT procedures.

During her four month work placement, **Veronique Durand** will try to develop a set of complexes, and test how they bind to certain anions. Veronique has joined **Paul Plieger's** group in between completing her MSc in analytical chemistry at Poitiers University (France). Massey University welcomed a number of students earlier in the year - **Angela Bennett** (with **Mark Waterland**), **Sara Wright** (**Shane Telfer**), **Lauren Ferguson**, **Sam Bruere** (**Paul Plieger**), **Rachel White** (**Dave Harding**), **Ross Davidson** (**Brodie/Ainscough**), **Adam Stephenson** and **Robert Bruekers** (**David Officer**) and **Helen Hsu** (**Geoff Jameson**) all commenced Honours or Masters studies this year.

This year the chemistry research symposium was held in late February. There was a very good turn-out with numerous industry representatives present. Twelve talks were given during the course of the day representing research from the Parker, Jameson, Waterland, Harding and Brodie/Ainscough groups as well as representation from the Nanomaterials Research Centre. Everyone did a fantastic job of keeping to time – possibly due to the ever vigilant Mr Blinky! (who is rapidly becoming the most hated member

of staff).

Innovators of Los Alamos National Laboratory gathered early this year to recognise and reward copyrights, patents and technological licenses garnered in 2005. **Simon Hall** was honoured with the patent award for his work in *Reversible Electro-optic Device Employing Aprotic Molten Salts and Method*. **Trevor Kitson** won the 2005 Vice Chancellor's Award for Excellence in First Year Teaching. This follows on from his success in gaining the NZIC Chemical Education Award in 2005.

Andrew Brodie spent 3 weeks in the US, mainly with **Harry Allcock's** group (Pennsylvania State University) where he held discussions with members of the group on enhancing collaboration on polyphosphazenes. He also gave talks at Drexel University (Philadelphia), SUNY at Binghamton, and Carnegie Mellon (Pittsburgh). PhD student, **Steve Kirk** from the Ainscough/Brodie group spent a month in the Allcock laboratory in June to learn more about polyphosphazenes.

OTAGO

The Otago branch has had several fun events with more planned for later in the year. In March the Branch visited the Otago Polytechnic Mellor Restaurant for dinner and talk by **Dr. Leo Schep** (National Poisons Centre) on *Alexander the Great's mysterious death. Was it poison?* - it does indeed look like foul play may have been responsible. A chemistry SuDoku evening was held in April defying the local flooding and proving to be a great success. On May 31 everyone went to the Emerson Brewery Tour to experience first hand *a quantum leap in the flavour of NZ beers*. During this period **Prof. Karl Wieghardt** (Max-Planck Institute for Bioinorganic Chemistry-Mulheim) visited the Chemistry Department and was hosted by **Prof. Sally Brooker**. Prof Wieghardt met with colleagues in the Chemistry and Biochemistry Departments and also came along to the Otago Branch dinner and talk in March; he also visited other Chemistry Departments in the country. In May **Dr. Brook Nunn** gave a seminar in the Biochemistry Department on differential proteomics focusing on phytoplankton which was

much appreciated by all those in attendance.

On the marine side of things, work by the chemists in Crop & Food Research - Plant Extracts Research Unit, (based in Otago's Chemistry Department) is illustrated by their part in a recently published international patent application *Anti-inflammatory compounds*. AN 2006:269600: PCT Application WO 2006031134 (2005) (Denny, W. A., Copp, B. R., Pearce, A. N., Berridge, M. V., Harper, J. L., Perry, N. B., Larsen, L. and Godfrey, C. A.) that covers the application of some new marine natural products and synthetic analogs as anti-inflammatory treatments. These have arisen from work in the TerraMarine Pharmaceuticals collaboration. At the more fundamental end of the research scale, **Assoc. Prof. Chi-Hwan Lim**, on sabbatical from Chungnam National University, Korea, is studying unusual diterpenes from New Zealand vegetable sheep. Working with **Rex Weavers** and **John van Klink**, Chi-Hwan is following up on the unique diterpenes identified in *Raoulia* species by Stephen Bloor (then IRL, now Biodiscovery).

WAIKATO

Waikato University

An evening was held for Hamilton secondary school Chemistry teachers at which **Brian Nicholson** gave a very interesting and informative talk entitled *Fluoridation of our water supply-protecting or poisoning the population?* This was especially topical considering the recent referendum that Hamilton had to determine whether to continue with fluoridation of the city water supply or not and probably assisted the audience in making their voting decision as it presented the facts not the hype!

Richard Coll recently attended two conferences in the USA. He presented work on use of analogies and models in chemistry teaching (based on his chapter in a recently released book), at the National Association for Research in Science Teaching annual conference. He also attended an editorial board meeting of the *Journal of Research in Science Teaching*, of which he is a member. The second conference, at the University of Cincin-

nati, celebrated the 100th anniversary of the birth of cooperative education (degrees and other programmes of study that integrate work experience with academic work). Richard's work here was on the perspectives of full fee-paying international student experiences in a work-integrated learning science and engineering programme. **Anne Hume** (EdD) and **Cathy Bunting** (PhD) have been working with Richard as supervisor and have now submitted their theses.

Kelly Kilpin has started a PhD with **Brian Nicholson** and **Bill Henderson** on Cyclometallated complexes. **Bevan Jarman** has started a PhD with these and **Merilyn Manley-Harris** on carbohydrate derived ligands.

NIWA

Dr. Michael Ellwood left NIWA at the end of May to take up a lectureship in Earth and Marine Sciences at the Australian National University. We were sorry to see Michael and Kitty (a former Branch Secretary), depart and wish them well. They were both active in Waikato Branch affairs. **Dr. Mike Stewart** has joined the NIWA Hamilton group as a natural products chemist and will be working on various *bioactives* studies. Mike comes to us from the University of Queensland and will be a welcome addition to the chemistry team. **Dr. Burns Macaskill** retired in March but has been contracted back to work on a number of commercial projects.

WELLINGTON

Recent meeting of the Branch have focused on nanomaterials with the March meeting addressed by **Prof. Kiyoshi Okada** (Metallurgy & Ceramics Science, Tokyo Institute of Technology) on *Highly functional porous ceramics for environmental protection produced by controlling their nanostructures*. With the importance of porous ceramics increasing as global environmental issues become more urgent, these materials can be used to protect and improve the environment and Prof. Okada described some of the developments made in this field. These included the preparation of zeolite and mesoporous silica from a kaolin clay that are derived from by heating kaolinite at 600-800°C fol-

lowed by selective acid leaching. Examples of composites containing TiO₂ with synergetic adsorption and photocatalytic properties including a film of porous TiO₂/hydroxyapatite and a TiO₂/montmorillonite material with a porous structure were described. The film composite synergetically enhances the decomposition of proteins, while the montmorillonite composite decomposes 1,4-dioxan thereby showing them to be extremely promising candidates for medical and environmental applications. In April **Dr. Andreas Markwitz** (Principal Scientist, GNS Science) discussed the *Growth of silicon nanostructures under high vacuum electron beam annealing (EBA)*. He focused on the potential of raster-scanned, computer controlled, electron beam annealing (EBA) for creating silicon-based nanostructures under high vacuum conditions. The system at GNS Science Lower Hutt utilises a 20 keV electron beam to heat samples under high vacuum conditions up to 1200°C for periods ranging from seconds to minutes. Wafer-silicon forces the silicon surface to form pyramidal nanostructures at 1000°C for 15 s. Silicon nanostructures, called *silicon nanowiskers*, are produced with an average height of 5 nm and they cover the entire surface with an average density of 20 μm⁻². The pillars are square-based and align to common axes which correspond to the [110] directions of the base Si substrate. The process is rapid and offers high throughput with formation of the disordered surface and subsequent self-assembly of the nanostructures requiring only a single fabrication step.

The May meeting consisted of a presentation and a site tour of the Naenae plant of Resene Paints Ltd., one of NZ's industrial chemistry successes. **Dr. Scott Dickie** (R&D Chemist) outlined the process of paint manufacture, and the research and development being carried out was described ahead of the plant visit. He was ably assisted by **Danusia Wypych**, (Technical Manager) and **Dr. Jeff Jurlina** (Industrial Coatings Manager). As one member stated – *It was the best site visit the Branch has had for years* – thanks Resene.

Victoria University

Recently gaining their research degrees **Rangituatahi Te Kanawa** submitted the first thesis in the recently created *Heritage Materials* area, namely *Consolidation of Degraded Iron-Tannate Dyed Phormium tenax fibres using Zinc Alginate* (MSc) from work with **Gerald Smith**. **Pascale Savigny**, a student from France working with **Kate McGrath**, successfully submitted *Cell membrane dynamics during exocytosis in anterior pituitary cells* for MSc. **Xianming Liu** completed his PhD under **John Spencer** and **Alan Kaiser** (*Synthesis of Multi-walled Carbon Nanotubes by Chemical Vapour Deposition and Post-Synthesis Treatment on Carbon Nanotubes by Dielectrophoresis*) while **Hannah Brackley**, working in Palmerston North under **Jim Johnston's** supervision gained her PhD for *Land to Ocean Transfer of Erosion-related Organic Carbon, Waipaoa Sedimentary System, East Coast, New Zealand*.

Dr. Kate McGrath is on research and study leave until the end on January next but is spending most of the time here (from September) in **Paul Callaghan's** group learning about different diffusion NMR techniques for investigating soft matter. Currently she is visiting Carole Perry's group (silica based biomineralisation and materials synthesis- Nottingham) and then the groups of Perdita Barran (MS of biological molecules and probing molecular self-assembly), Philip Camp (theoretical materials chemistry), and Wilson Poon and Mike Cates (emulsions) in Edinburgh. Kate has been Branch Secretary almost from her arrival in Wellington and her departure from the role will be sorely missed. Likewise our long-standing Branch Treasurer (and former administrator) has signified his intent to retire after some 10 years of providing the best sets of accounts the NZIC treasurer has seen from any Branch! We wish them both well in their future endeavours and encourage them and others to recycle themselves in the future.

Prof. Okada's visit to VUW (see Branch meeting above), hosted by **A/Prof Ken MacKenzie**, was to negotiate an arrangement between the Tokyo Institute of Technology and VUW for the exchange of research students and

staff working in materials science. The drafted agreement has now been signed by the Dean of Science in each institution. Ken also hosted a visit (to the SCPS and the MacDiarmid Institute) of a party of ten Korean scientists from Universities and major industries here to make contact with advanced materials and nanotechnology research groups. They had spent the preceding day at a workshop on advanced materials organised by FRST that had introduced them to some of the work being done in NZ in the area. In June Ken presented an invited paper at a conference in Vienna, and is presenting another at a materials engineering conference in Switzerland as this issue is in distribution.

IRL

Dr. Gary Evans attended the NZ

Society of Oncologists meeting in Hamilton in early May and met with representatives of Mundipharma NZ Ltd., the licensors of IRL's anticancer Drug Fodosine™. **The Carbohydrate Chemistry Team** has launched a new website associated with their Fine Chemicals web-based sales business that markets many valuable enzyme inhibitors internationally (see: www.finechem.co.nz).

The science within the Chemistry Operations Group at IRL was recently reviewed by **Prof. Andrew Holmes**, AM, ScD, FRS, FAA, formerly of Cambridge University and now Head of the Bio21 Institute at Melbourne University. He concluded that this platform is one of the jewels in the crown of the IRL and that it should be given an unfettered opportunity to develop and expand what has been de-

scribed as *the most valuable IP portfolio in the country*.

IRL's GlycoSyn business unit manufactured Mito-Q, the active pharmaceutical ingredient in the Antipodean Biotechnology Ltd. mitochondria-targeted anti-oxidant for the treatment of Parkinsons disease. We were thrilled to see its progression to Phase II trials here in NZ well reported in the national press.

The **Hon. Trevor Mallard**, Minister of Economic Development and local MP, visited the Gracefield Campus in late April to meet with members of the Carbohydrate Team and to tour the GlycoSyn cGMP manufacturing facilities. **Drs Evans, Furneaux & Tyler** of the group also attended the Wellington Gold Awards as finalists in the *Discovering Gold* category.

CHEMISTRY AUSTRALASIA

THE PREMIER SINGLE-VOLUME TEXT FOR FIRST YEAR NEW ZEALAND CHEMISTRY STUDENTS

Publishing August 2007

Allan Blackman (University of Otago), **Steve Bottle** (Queensland University of Technology), **Siegbert Schmid** (University of Sydney), **Mauro Mocerino** (Curtin University), **Uta Wille** (University of Melbourne)

Published by **John Wiley & Sons**

Traditionally, first-year chemistry students at New Zealand universities have had no choice but to study from textbooks that are written overseas and do not really cater for their needs. Apart from having no local content, they often require students to work in imperial units and contain insufficient organic chemistry coverage. As a consequence students have been required to purchase two text books to obtain the required reading content for the subject.

John Wiley & Sons is therefore delighted to announce Chemistry Australasia - a textbook written for local students by local authors.

ABOUT THE TEXT

Chemistry Australasia has been in development since late 2004. This single-volume text is a complete course in first-year chemistry that provides a thorough coverage of organic, inorganic and physical chemistry. It is not what is commonly known as an "adaptation" of an existing US text – this is a totally reworked publication which draws on the wealth of resources available from Wiley's long involvement in Chemistry Publishing. The author team's experience in first-year Chemistry educa-

tion is one of the text's greatest assets. In particular, the authors' experience in teaching students from diverse backgrounds, disciplines and skill levels has greatly informed the development and organisation of this text.

WILEY – THE WORLD'S LEADING CHEMISTRY PUBLISHER

Globally, Wiley are renowned for their leading Chemistry journals such as *Angewandte Chemie* (Wiley VCH) and the quality continues with our editorial team for Chemistry Australasia. Their direct experience in Chemistry puts Wiley in a unique position to offer quality and expertise throughout the whole development process. Our Senior Editor has a PhD in Chemical Engineering and the developmental Editor is a member of the Australian Science Communicators.

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The New Zealand Science Scene

Data immersion on a new scale.



The first three screen stereo projection theatre in New Zealand has opened at the University of Canterbury's Human Interface Technology Laboratory (HIT Lab).

VisionSpace offers groups another way to view and interact with three-dimensional data.

The theatre overcomes current limitations of viewing data on traditional computer monitors in two dimensions. It is especially useful for geospatial and biomedical data. HIT Lab NZ Director Dr Mark Billingham says "Being immersed in your data is a truly remarkable experience we want to share with others in New Zealand."

Complex data is rendered as 3D virtual imagery and since several users can view the same screen it is a powerful tool for collaboration.

The theatre has three large projection screens that can be moved to different configurations depending on the number of people needing to view the data. The users wear polarised glasses to experience the 3D effect and there is surround sound available.

There are also portable single screen versions available. These use an active stereo single lens video projector that interleaves a stream of left and right images. Shutter glasses are worn by the users, which are synchronized to the projector and block the appropriate images from the appropriate eye to create a stereo effect.

HITLab has also collaborated on another innovative venture using graphics to enhance understanding. Tobi Gefken, an intern with HITLab NZ, has developed interactive graphics to help doctors and medical students gain a deeper understanding of clinical pharmacology with the Department of Clinical Pharmacology at Christchurch Hospital. The graphics can be viewed via the internet or PDAs. By changing conditions on the pages, users can visualise the effects of their changes to understand concepts such as half life drug elimination and drugs in pregnancy. The project is continuing to grow with possible uses including helping patients gain a better understanding of their condition.

Money for bridge between business and science

Business and Academia links were strengthened in Christchurch in late March with an injection of \$2.4million from the Government.

The money is to set up a joint venture between Lincoln and Canterbury Universities.

The venture will bring private sector, biotechnology, science entrepreneurs into contact with students and researchers. This aims to enhance courses to prepare students for the commercial world and to help identify commercial potential in research projects.

Sue Suckling, a former Business-woman of the Year, was elected as the first chair of the project's joint industry advisory board. Other Industry representatives on the Advisory Board are; Dr Richard Garland, CEO, NZ Pharmaceuticals Ltd; Bruce Foulds, CEO, Keratec Ltd; Dr Mike Dumbier, foundation CEO of Crop and Food Research Ltd, a director of Dairy Insight Inc, and Chair of the Board of the National Centre for Advanced Bio-Protection Technologies; and Jim McLean of Genesis Research and Development Corporation Ltd. University representatives are Dr Chris Kirk, Deputy Vice-Chancellor of Lincoln University and Professor Ian Town, Deputy Vice-Chancellor of the University of Canterbury. Project Leaders are Dr Garth Carnaby at Lincoln University and Dr Bill Swallow at the University of Canterbury.

The advisory board will be specifically working in the area of biotechnology with Lincoln and Canterbury Universities.

Students showed the way and now Victoria University has followed.

Interface, the student computer science club, set up an experimental wireless network in June 2003. The university recently announced the completion of the WirelessVic Network on Kelburn, Karori, Pipitea and Te Aro campuses.

Students and staff with suitably capable laptops can now wirelessly access their email, files and the internet at 189 "hotspots" throughout the four campuses. This means collaboration over data can happen over coffee in one of the cafes and provides the opportunity to catch up on the latest scientific news or papers before a lecture.

Chmoogling along

Have you found your way to chmoogle yet? Chmoogle is a website that allows you to draw a chemical structure and perform a search for that structure and best of all, to do it for free.

It's mission is to discover, curate and index all public chemical information and make it available.

The site works across different computer platforms and internet browsers. It performs the searches very quickly. To

search for a particular structure, simply click on the draw structure button and a new window pops up. Click on a component you want for your structure and then click in the white box and you are away drawing your molecule. It is possible to search for substructures or exact molecules as well as common and trade names.

The site also provides code so users can embed it into their own websites for direct access to Chmoogle.

Chmoogle.com is the product of eMolecules Inc and was launched in November 2005. eMolecules Inc has headquarters in San Diego. Chmoogle is not affiliated with Yahoo, Google, or MSN.

Recognition received

The Hon. Margaret Austin received an honorary Doctor of Science degree at Lincoln University's Graduation Ceremony at the Christchurch Town Hall on April 28. She received the honorary doctorate in recognition of her lifetime dedication to education and commitment to science.

She is a former Head of Science at Christchurch Girl's High School and Assistant Principal at Riccarton High School. She is more well known for her 12 years in parliament including being the Minister of Research, Science and Technology and in 1995 helped found the United New Zealand Party. Margaret was Chancellor for Lincoln University from 2000 until 2004 and also served a total of ten years on the Lincoln University Council.

The New Zealand Order of Merit was awarded to Dr Ruth Bonita, Emeritus Professor at Faculty of Medical and Health Science at the University of Auckland, and Robert Beaglehole formerly a Professor of the University's School of Community Health.

The award was for their work in public health with the World Health Organisation in Geneva. The couple are looking to return to New Zealand next year.

The first New Zealander elected as a Fellow of the United Kingdom's Academy of Medical Sciences was admitted to the prestigious Academy in June. Professor Peter Gluckman is, Director of the Liggins Institute and his major field of research is the physiology of the time around birth.

Election to the Academy is considered recognition for achieving at the highest levels. Only twenty two of the 800 Fellows are based outside the United Kingdom.

Business award for pharmaceutical supplier

The winner of this year's University Business Link award is a company that started out in Massey's Old Dairy Building.

A shortage of ingredients for pharmaceutical products in the 1970s saw New Zealand Pharmaceuticals Ltd step forward as an international supplier of bio-chemicals.

The recipient of the University's 2006 Business Link Award, NZ Pharmaceuticals was founded in 1971 between the freezing industry and Tasman Vaccine Laboratories. Its first contract with a French pharmaceutical company was to process concentrated animal bile into deoxycholic acid – a component of steroid drugs.

The business outgrew its rented laboratories in the University's Old Dairy Building, but remained in the Manawatu to become a high-tech enterprise with a \$25 million turnover under the management of Dr Richard Garland. It employs more than 90, ranks in the nation's top 500 companies and, in November, will complete a new factory purpose-built to produce its latest product – complex sugars developed from simple sugars found in prawn shells.

Dr Garland received the Business Link award from Deputy Vice-Chancellor Professor Ian Warrington at a graduation function co-hosted by the University and Vision Manawatu. A variety of local businesses enjoyed the opportunity to network during one of Palmerston North's busiest weeks.



Dr Richard Garland

2007 ROYAL SOCIETY OF CHEMISTRY AUSTRALASIAN LECTURESHIP

Applications are called for the 2007 Royal Society of Chemistry Australasian Lectureship.

This lectureship, financed by an annual grant from the RSC to Australia and New Zealand, is held by a New Zealand resident every fourth year. The 2003 lecturer was Professor Geoffrey Jameson (Massey University). The 2004-2005 lecturers were Professors Bob Gilbert (University of Sydney) and Allan Canty (University of Tasmania).

The lectureship involves lecture tours in Australia and New Zealand, coordinated by the respective RSC Local Representatives: Prof. Graham Bowmaker (University of Auckland) and Prof. Alan Bond (Monash University).

The selection panel for the 2007 Lectureship will be Prof. Graham Bowmaker (Auckland), Prof. John Spencer (Wellington), Prof. Leon Phillips (Christchurch) and A/Prof. Keith Gordon (President of the NZIC).

Applications should include a CV, and an account of the work to be covered in the lectures. The major part of the work should have been carried out in New Zealand.

Applications should be sent to:

Prof. G.A. Bowmaker
Department of Chemistry
University of Auckland
Private Bag 92019
Auckland
Email: ga.bowmaker@auckland.ac.nz

by the closing date of 31 August 2006.

Can You Patent an Old Dog Doing New Tricks?

By Blair Hesp

This issue marks the 10 year anniversary of the *Patent Proze* column being published in Chemistry in New Zealand. Accordingly, at this time it may be appropriate to ask a question that may interest a lot of chemists: "Can I patent an old dog doing new tricks?" Potentially you can. The most well known New Zealand example being the discovery, patenting and subsequent court battle over the antibiotic amoxicillin.

SELECTION INVENTIONS

Amoxicillin was developed in the seventies and patented by Beecham Group in the face of strong opposition from Bristol-Myers Company on the basis that amoxicillin was broadly claimed in an earlier patent, and its likely antibiotic activity was known (*Beecham Group Ltd v. Bristol-Myers Company* [1980] 1 NZLR 192). Following numerous court battles around the world on the subject, subsequent patent applications by Beecham for the preparation of a composition for oral administration containing amoxicillin were generally accepted as patentable a "selection invention". This goes against conventional wisdom, in that most people would presume that once a group of compounds is claimed by one inventor, another inventor cannot then claim the same compound.

There were two key issues at stake in this case. First of all, despite Bristol-Myers claiming amoxicillin under a patent for ampicillin-derivatives, amoxicillin (6[(-)-oc-amino-p-hydroxyphenylacetamido]penicillanic acid) had not previously been isolated or specifically synthesised, from the racemic mixture containing both the (-)- and (+)-epimers of 6(oc-amino-p-hydroxyphenylacetamido)penicillanic acid. Subsequently, Beecham purified amoxicillin and discovered the compound's surprisingly good oral absorption when compared to the other ampicillin-derivatives claimed by Bristol-Myers. Because Beecham was the first to purify amoxicillin and identify its significantly better oral absorption properties the patent applications for amoxicillin succeeded because the compound amoxicillin, which had been 'selected' out of all the compounds claimed by Bristol-Myers, exhibited a "special and unexpected advantage" over any of the other claimed compounds. The term 'selection invention' is used to describe a subsequent invention borne out of an earlier, and usually more generically defined invention. All of the compounds which are the subject of a selection invention must exhibit some unexpected

properties, or overcome a disadvantage, of the earlier class of compounds. Therefore, selection inventions tend to be directed to a narrow class of compounds.

COLLOCATION OF KNOWN AGENTS

A further example of a patentable invention is the combination of two or more previously known agents which together exhibit a working interrelationship to produce a benefit or to overcome a disadvantage. An example of this could well be a process which normally occurs at a very slow rate, but which is sped up by an otherwise inactive catalyst, or a combination of drugs exhibiting synergistic activity. For example, amoxicillin is an effective antibiotic to which bacteria quickly became resistant. Clavulanic acid is a beta-lactamase inhibitor with no bacteriocidal activity in itself, but when co-administered with amoxicillin, potentiates the antibiotic effect of amoxicillin. Subsequently, this combination was patented because the effectiveness of the combination was superior to what could be expected by simply adding the two compounds together.

SECOND MEDICAL USES OF DRUGS

While a new use for an old invention is generally not patentable, there is an exception when it comes to second medical uses for previously known drugs. In other words, if it is found that a well known drug is effective against condition A, but is later found to also be effective against condition B, it is possible to patent the drug for use in preparations designed to treat condition B. A potential example where a second medical use could have been claimed is the anti-inflammatory drug aspirin, which was subsequently found to be useful when administered in low doses for the prevention of potentially deadly blood clots.

Therefore, if you do find that it is possible 'to teach an old dog new tricks' then it may be possible to secure patent rights over any 'new trick' which is developed.

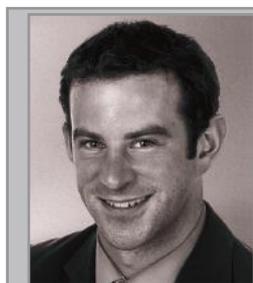
A reminder: if you have any queries regarding patents, or indeed any form of intellectual property, please direct them to:

Patent Proze

Baldwins

PO Box 852, Wellington.

Email: email@baldwins.com



Blair Hesp of Baldwins specialises in chemistry and biotechnology patents. Blair joined Baldwins in 2006. He has a PhD in pharmacology from the University of Otago as well as a NZDipBus with a management focus. Blair is currently studying towards a law degree and registration as a patent attorney.

NZIC Education Specialist Group

Suzanne Boniface, Chairperson NZIC Specialist Education Group



Suzanne Boniface with pupils at Queen Margaret College

Last November a meeting was held in Wellington to consider ways in which the Institute could better support Chemistry Education. While *Chemical Education* is a specialist group (see the website) it has not been active for some time. The meeting was called by Council with a view to reactivating this group. Each NZIC Branch was asked to send a delegate and some had more than one attending. The initial discussion indicated that every Branch was actively involved in some form of chemical education initiative, often in conjunction with the local Universities. The level of support these initiatives receive varies widely as does their geographical coverage. Considerable discussion took place about the needs of chemistry educators – particularly in the secondary sector – and how best a voluntary organisation such as NZIC could respond to these needs. Some Branches were discouraged in that their meetings or professional development opportunities they set up were poorly attended, and that too few teachers are members of NZIC.

So what does the Institute offer the education sector and what more can be done? National initiatives that NZIC is currently supporting include the publication of ChemNZ, the production of Level 2, Level 3 and Scholarship mock examinations, and the ChemEd conference series. Local Branches run professional development days for teachers, chemistry competitions for students, and they support local science initiatives such as science fairs. Reinvigorating the NZIC Education Specialist Group and giving it a definite presence was seen as a further opportunity to ensure on-going support for all of these things and to encourage the search for new initiatives to support chemistry education in NZ.

It was agreed to provide professional support for people involved in chemistry education at the primary, secondary and tertiary levels by:

- Co-ordinating and distributing information about current education initiatives/events,
- Setting up opportunities to promote Chemistry, particularly in the secondary sector,
- Providing a forum for discussing curriculum needs and initiatives,

- Providing access to up-to-date resources about:
 - the latest developments in chemistry,
 - new ideas for teaching chemistry,
 - chemistry developments/processes that are taking place in the country,
- Supporting the professional development of teachers, particularly in the area of pedagogical content knowledge.

Plans are underway to set up an *Education* page on the NZIC website so as to provide easy access to all the Chemistry Education happenings and resources in NZ. It is hoped that some of the RSC Secondary Schools publications can be offered to NZ schools at a reduced rate and distributed through NZIC. In the future we would like to be able to run a nationwide *Chemistry Quiz* which would involve local Branch competitions in the middle of the year with the winning teams coming to Wellington for a playoff in the October holidays. Of course, this will be dependent on securing sponsorship for the event and it could even become part of a bigger initiative of having a nationwide *Chemistry Week* that promotes Chemical Science in our communities.



A 2005 Schools Quiz Night

In the longer term this group would like to see *Chemical Processes in NZ* turned into an interactive resource and find ways of promoting seminars on *Careers in Chemistry* for secondary school students. The Specialist Group will also provide ongoing support for ChemEd conferences and other national events that promote chemistry.

These are small beginnings but we have to start somewhere. The future direction of the group will depend on the enthusiasm and energy of those involved, and the support they get from their local Branch and its Chemistry Educators. The availability of funds and sponsorship to support some of these activities could also be an issue.

Feedback about current programmes and suggestions for further initiatives would be much appreciated and can be sent to: Suzanne Boniface [Suzanne.Boniface@qmc.school.nz].



NZIC Conference 2006

Back to the Basics: From Small Molecules to Materials and Surfaces

December 2 - 6, 2006
Novotel/Convention Centre, Rotorua

Plenary Speakers: Mark Barteau (Delaware),
Harry Gray (Caltech), **David MacMillan** (Caltech),
Warren Roper (Auckland), **Richard Zare** (Stanford)

Organizing Committee: Peter Schwerdtfeger (Chair), Matthias Lein,
Jim Metson, Alastair J. Nielson, Gordon W. Rewcastle, Tilo Söhnel
Secretary: Vesna Davidovic-Alexander

Session Chairs:

John Spencer, Victoria (Inorganic and Organometallic Chemistry)
Margaret Brimble, Auckland (Organic and Medicinal Chemistry)
Hicham Idriss, Auckland (Materials and Surface Chemistry)
Henrik Kjaergaard, Otago (Physical and Theoretical Chemistry)
Geoff Jameson, Massey (Biochemistry and Molecular Biology)

Special Symposium: Showcase Industrial Chemistry in New Zealand
Chair: Jim Metson (Auckland)

<http://www.massey.ac.nz/~nzic/>