

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

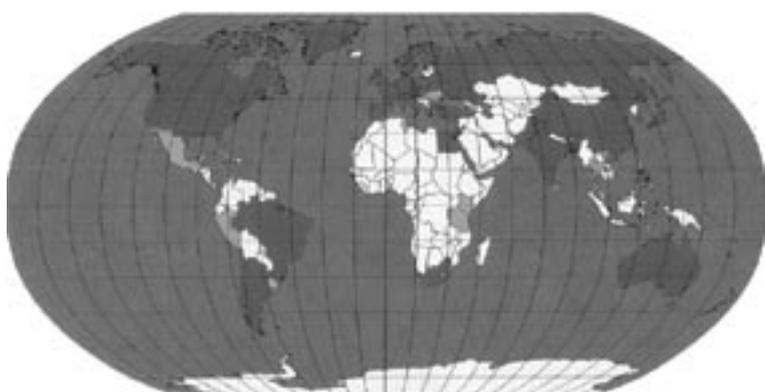
As a worldwide organization IUPAC has an impressive track record in enabling the language of chemistry to be understood globally. Its *mission* is to advance the global aspects of the chemical sciences and to contribute to the application of chemistry in the service of mankind. It promotes the norms, 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: Inter-divisional 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 scientific 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 is 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. 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 seldom 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 projects 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; CHEMRAWN publications, etc.

Compiled by Dr. Pat Holland (Cawthron Institute) from IUPAC and locally supplied materials.