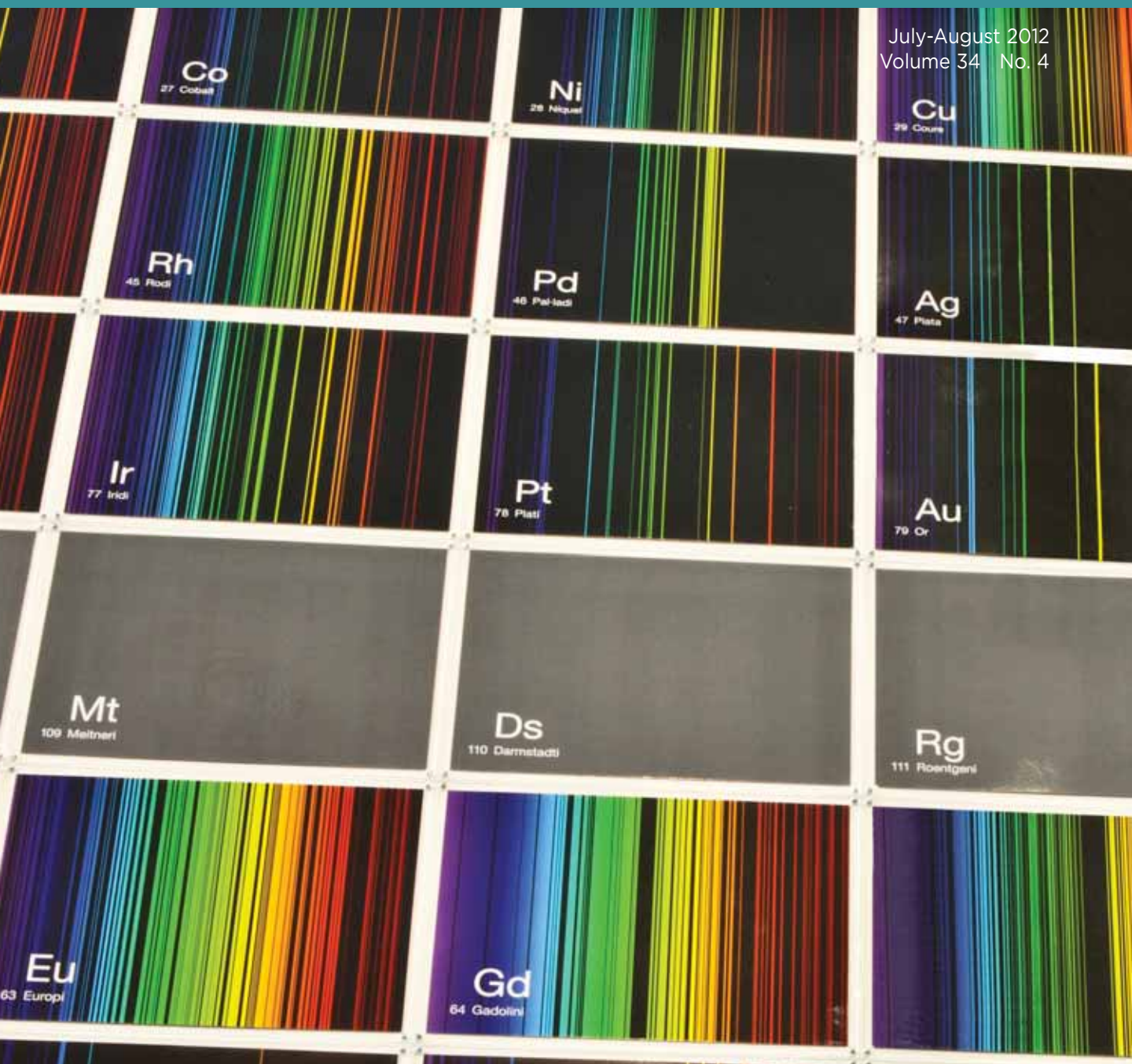


CHEMISTRY

International

The News Magazine of IUPAC

July-August 2012
Volume 34 No. 4



INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

Science for Haiti ►

Nanoparticle Toxicity Challenges ►



From the Editor

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For chemists and aficionados of chemistry of all ages, there is no equal to the iconic periodic table of chemical elements. The table is a symbol recognized universally, yet our understanding of its contents and underlying organization is still evolving. In this issue of *CI*, several aspects of this icon are put forth.

As we celebrated IYC2011, several projects focused on the table and its elements to instruct and intrigue. There were exhibits, essay competitions, and several drawing and video competitions around the world that resulted in unique tables. One such dazzling table was



scaled up and mounted as a mural in the Earth Science Museum at the University of Waterloo, Ontario, Canada. Read about the project and the unveiling event on April 2012 in the Wire section, page 20. Another IYC-inspired rendering of the table graces the cover of this issue: *Hommage to the Elements* by Eugènia Balcells, on display in the Atrium of the Chemistry Library at the University of

Barcelona, features each element's unique emission spectrum. Like all periodic tables, it displays order and yet, solicits questions. By its order, one can see in the table how the elements compare to each other and how in consequence they might react with one another. The table also raises questions, as the elements, and the chemistry they enable, are keys to future discoveries and solutions to today's numerous challenges.

As it just so happens, the family of recognized elements has grown a bit larger. In July 2011, the claims of discovery for element 114 and 116 were elucidated. Following that, the naming process was initiated and in December 2011 names were proposed. Now, the process is over and IUPAC has officially introduced flerovium, or Fl, as element 114 and livermorium, or Lv, as element 116. Read more on page 19.

While some scientists keep working at filling the gaps in the table, others are debating how the elements already in the table should be arranged. Group 3 seems to cause ambiguity and Eric Scerri is asking IUPAC to take a stand and clarify the issue. Read more page on page 28.

With contributions from artists of all ages and scientists of all disciplines, the table continues to spark interest and generate enthusiasm; all good signs for the creative future of chemistry?!

Fabienne Meyers

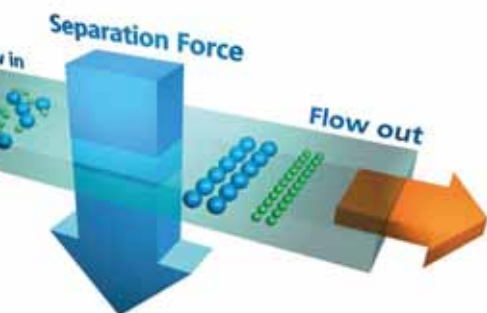
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Cover: A close-up of Hommage to the Elements, a permanent display in the atrium of the Physics and Chemistry Library at the University of Barcelona, Spain. "The work of multimedia artist Eugènia Balcells, is an invocation of the foundations of the universe and of life: matter and energy, light, and the chemical elements," writes Santiago Alvarez (see page 5).

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Back cover tear-off page: IUPAC Periodic Table of the Elements, version 1 June 2012

A System Comes of Age

by Kip Powell



Some 10 years after the initiation of the IUPAC Project System it is appropriate to restate its objectives and to reflect on what has been achieved. The core activity of IUPAC is to provide critical evaluations of methods and data and to make recommendations for nomenclature, terminology, metrology, and measurement standards. This outcome is achieved through its projects (the Project System).

The Project System encourages experts worldwide to contribute to this process, regardless of whether or not they are members of IUPAC's division (subject area) committees or standing committees. It makes this possible by funding meetings of task groups to plan and coordinate the contributions of team members working on an approved project.

IUPAC does not support original research, but the outcomes from projects provide the scientific community with authoritative articles based on the critical evaluation of peer-reviewed published literature. In this way, IUPAC is able to serve identified needs of industry, academia, teachers, and research chemists. In addition, several IUPAC projects are focused on enhancing the public's perception of the contribution of chemistry to their daily lives.

Are you at that stage in your career where you are able to contribute?

How Large is this Enterprise?

IUPAC generates a sizeable output through its projects. For example:

- Each year, an average of 40 new projects is initiated.
- Currently, there are over 900 chemists from 59 countries contributing to over 190 IUPAC-funded projects.

Most evaluations produce a Technical Report or an IUPAC Recommendation (if terminology or nomenclature is being defined) that is published in *Pure and Applied Chemistry*; some lead to databases that are made available via the web. Many also lead to dis-

semination of results in conference presentations or workshops. This output is consistent with a medium-sized multinational organization, but the projects, each of which is focused on a stakeholder group, have considerable added value.

Criteria for IUPAC Projects

A key requirement for a project proposal is that the task group has wide international (or continental) representation and has the necessary expertise. Key tests of the suitability of a project proposal are that the outcome has a well-defined group of stakeholders and that there is a well-established need for the evaluation, the report, or recommendations. The project proposal must emphasize how the outcomes will be communicated to the stakeholders (e.g., via publications, conference presentations, or workshops). Successful proposals must demonstrate the project's relevance to readily identified scientific communities and adequate methods of dissemination.

Scope of Current Projects

The scope of topics covered by IUPAC projects is illustrated by current projects from each of the 8 Divisions (subject areas):

- Recommended Reference Materials for Phase Equilibrium Studies
- Evaluated Published Isotope Ratio Data
- Rules for Abbreviation of Protecting Groups
- Critically Evaluated Rate Coefficients Associated with Initiation of Radical Polymerization
- Requirements for Proficiency Testing on Environmental Sampling
- Appropriate Consideration of Bioavailability of Metals/Metal Compounds in the Aquatic Environment
- Human Drug Metabolism Database
- Recommendations on Nomenclature of Flavonoids

Projects recently completed by Standing Committees—Committee on Chemistry Education (CCE), Chemical Research Applied to World Needs (CHEMRAWN) and Chemistry and Industry (COCI)—include:

- Enhancing the Capacity to Provide Quality Chemistry Education at Secondary and Tertiary Levels in Ethiopia
- CHEMRAWN XIX—A Renewable and Sustainable Energy from Biological Resources
- IUPAC-UNESCO-UNIDO Safety Training Program Workshop, San Juan, Puerto Rico

How Does the Project System Work?

The Project System is the *modus operandi* for IUPAC. A project proposal can be submitted at any time by any task group that is internationally diverse and has the appropriate expertise. After submission of a proposal to the Secretariat, it is reviewed by internal (division and/or standing committee) and external reviewers. If found to be appropriate to IUPAC's goals,¹ it can be funded by an IUPAC division or standing committee.

The system works by providing task groups with the funding to proceed with the working plan presented in their original proposal, to draft and discuss interim working documents, and prepare final documents for publication. Most work is usually achieved by electronic communications, which may precede or follow a meeting of the task group. After a rigorous review process (including by the Interdivisional Committee on Nomenclature, Terminology and Symbols, ICTNS) the output is published, most frequently in *Pure and Applied Chemistry*, although, with approval, some Technical Reports appear as publications in journals that more directly serve the stakeholder group. The process involves the appropriate division or standing committee, which will also maintain contact with the task group, monitor progress, and contribute to the refereeing of the final document(s).

IUPAC requires wide international participation in task groups and this is borne out by the 31 countries represented in the technical reports and recommendations published in *Pure and Applied Chemistry* in the last two years and by the 59 countries represented in the current list of project task group members.

IUPAC also seeks to engage chemists from "outside" its division and standing committees. Currently, 52 percent of task group members have no current or previous association with IUPAC committees. However, only 14 percent of task group chairs are in this category, so there is still scope for some improvement in capturing interest and contributions from outside of the IUPAC committee structure.

To find out more about the Project System, see the Guidelines and Application Forms on the IUPAC website.²

Support for Conferences

Conferences that seek "endorsement" by IUPAC (sponsorship or funding) are also managed as part of the Project System. As with projects that produce publications, conferences must also meet appropriate criteria: sound planning, scientific content, inter-

national participation within the advisory board and plenary lecturers, and accessibility to the international community and young scientists.

IUPAC Sponsored Conferences

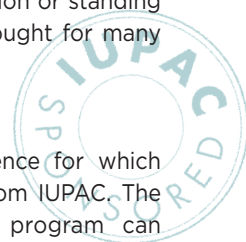
The majority of conferences that are "endorsed" by IUPAC are not funded by IUPAC, but are designated IUPAC-sponsored conferences. IUPAC sponsorship implies an IUPAC "seal of quality," an endorsement of the international calibre of the organization, key participants, and the program of the conference. Although IUPAC sponsorship does not imply any financial assistance, IUPAC will assist in the promotion of the conference through its publications. Applications are made through the Secretariat using the appropriate form³ and are reviewed by the relevant division or standing committee. This seal of approval is sought for many international conferences.

IUPAC Funded Conferences

There are two categories of conference for which modest funding may be requested from IUPAC. The Financial Support for Conferences program can provide assistance for conferences in "scientifically emerging regions" (FSC-SER) or for conferences in which a symposium or workshop is dedicated to "new directions in chemistry" (FSC-NDC). In both cases, the proposal must be endorsed and submitted by an IUPAC division or standing committee, thus ensuring that there is close communication between the conference organizers and IUPAC. Applications are made through the Secretariat using the appropriate forms.⁴ The first step is often an enquiry from conference organizers, but divisions and standing committees are also encouraged to take the initiative and identify conferences that could benefit from IUPAC participation and support.

For the FSC-SER program, the host country does not have to be a member of IUPAC. The thrust of this program is to facilitate conference attendance for young scientists and advanced students from the host country and surrounding emerging scientific communities.

The success of this program is illustrated by the fact that during the last two years, it has helped over 200 students/young researchers from Ethiopia, Nepal, Thailand, Romania, India, Croatia, Southern and Central African states, and Sri Lanka to attend conferences and benefit from presentations on contemporary topics by internationally recognized plenary lecturers.



Project Committee Chair's Column


The FSC-SER program also makes it possible for an "IUPAC lecturer" to attend; typically this person, in addition to promoting the aims of IUPAC, provides a plenary lecture at the conference and also visits other institutions in the host country or city.

For the FSC-NDC program, funding is focused on supporting one or two keynote speakers around whom a conference symposium/workshop dedicated to a "new direction in chemistry" can be built. Symposium themes might encompass contributions of an emerging field to the core topic of the conference, or explore new "frontiers" or new interdisciplinary developments that benefit chemistry or are enhanced by chemical knowledge and methods. To receive FSC-NDC support, the host country must be a National Adhering Organization of IUPAC. The FSC-NDC program enables an IUPAC division or standing committee to make a strategic, leading-edge contribution to an international conference that will stimulate progressive and boundary-breaking research.

An Opportunity to Make a Difference

IUPAC sees itself as a catalyst for enabling those who have gained expertise in their fields to return a contribution to their profession by assisting in the critical evaluation of methods, data, standards, nomenclature, and terminology required by the practicing chemist.

- Are you at that stage in your career where you are able to contribute to the enhancement of the work of other chemists in your field of expertise?
- Are there issues in your field that require harmonization across countries or cultures?
- Does your industry or field of research have needs for critical evaluation of established methods, of interdisciplinary issues, or of emerging techniques?
- Would you consider contributing to the work of IUPAC through its Project System?

If yes is your answer, IUPAC provides you with an opportunity to make a difference. 

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Kip Powell <kip.powell@canterbury.ac.nz> has been chair of the Project Committee since 2008. Previously he was a member of the Analytical Chemistry Division Committee, serving as president for 2004–2005. He is a professor in the Chemistry Department at the University of Canterbury in Christchurch, New Zealand.

I U P A C



Advancing Worldwide
Chemistry



IUPAC Prize for Young Chemists

Supporting the future of chemistry

The encouragement of young research scientists is critical to the future of chemistry. With a prize of USD 1000 and paid travel to the next IUPAC Congress, the **IUPAC Prize for Young Chemists** encourages young chemical scientists at the beginning of their careers. The prize is based on graduate work and is given for the most outstanding Ph.D. thesis in the general area of the chemical sciences, as described in a 1000-word essay.

Call for Nominations: Deadline is 1 February 2013.

For more information, visit www.IUPAC.org.

or contact the Secretariat by e-mail at secretariat@iupac.org or by fax at +1 919 485 8706.

An Artist's Hommage to the Elements

by Santiago Alvarez

The School of Chemistry of the University of Barcelona culminated the celebration of the International Year of Chemistry (IYC) with the installation of *Hommage to the Elements* in the atrium of the Physics and Chemistry Library. It is placed right above the printed collection of *Chemical Abstracts*, a monumental compendium of twentieth-century chemistry, and under the large windows through which percolate the lively human activity of the campus. *Hommage to the Elements*, the work of multimedia artist Eugènia Balcells, is an invocation of the foundations of the universe and of life: matter and energy, light, and the chemical elements. It takes the shape of a periodic table in which each element is represented by a collection of lines from its emission spectra and combines two of the best known icons of science or, as some like to say, constitutes the bar code of Nature.

Hommage to the Elements was born as a counterpoint to the multimedia exhibition *Frequencies*, presented for the first time by Balcells in Barcelona in 2009. Through the collaboration of the artist's workshop with physicists and chemists from the University of Barcelona, and thanks to the sponsorship of chemical companies Solvay and BASF and the support of the Catalan Societies of Physics and Chemistry, 20 copies of the wall installation were produced to commemorate the IYC. A poster of the exhibit was also produced.

Born in Barcelona, Eugènia Balcells has developed a wide trajectory in the fields of conceptual art, experimental film-making, and multimedia installations in New York and Barcelona. Her work was recognized in


2010 with the Visual Arts prize of the Catalan government, and with the medal of Fine Arts by the Spanish government.

The wall installation of *Hommage to the Elements* offers both scientists and nonscientists the opportunity to reflect on historical and philosophical aspects of chemistry. One obvious question many people pose when faced with it is, why do elements 100 (fermium) to 112 (copernicium) appear as empty gray boxes? These are the artificial elements for which emission spectra are as yet unknown, because these "atoms are brief, a game of inventiveness that lasts just long enough to deserve a name and vanishes," in the words of

poet and physicist David Jou.

For chemists, this spectral periodic table invokes our ancestors, such as Bunsen, Kirchhoff, Seaborg, Mendeleev, Davy, Priestley, Lavoisier, Ramsay, Curie, and many others. Both chemists and nonchemists may recall the artists that taught us new ways of seeing color, such as Mark Rothko or Anish Kapoor, or those who theorized on light and color, such as Newton, Ostwald, Goethe, Delacroix, or Josef Albers. It may also make us think about writers such as Howard Phillips Lovecraft, who wrote about a mysterious substance: "when upon heating before the spectroscopy it displayed shining bands unlike any known colors of the normal spectrum. There was much breathless talk of new elements, bizarre optical properties, and other things which puzzled men of science are wont to say when faced by the unknown."

Institutions interested in installing *Hommage to the Elements* should contact the workshop of Eugènia Balcells. More information on *Frequencies* and *Hommage to the Elements* can be found in <http://araa-horanow.blogspot.com>. To learn more about Eugènia Balcells and her work, visit www.eugenialbalcells.com. Copies of the poster can be ordered through the virtual bookstore of the Institut d'Estudis Catalans: <http://publicacions.iec.cat>.

Balcells' *Hommage to the Elements* is featured on the cover of this issue of *Chemistry International*. 

Santiago Alvarez <santiago.alvarez@qi.ub.es> is a professor in the Department of Inorganic Chemistry at the University of Barcelona in Spain. This September, he co-chairs the 40th International Conference on Coordination Chemistry in València, 9–13 September 2012.



Measurement Helps Solve Nanoparticle Toxicity Challenges

by Louise Dean

Lord Kelvin was famously quoted as saying “... when you can measure what you are speaking about, and express it in numbers, you know something about it; but when you cannot express it in numbers, your knowledge is of a meagre and unsatisfactory kind”

In case you missed it, World Metrology Day¹ was observed on 20 May 2012, celebrating the signing of the Metre Convention by representatives of 17 nations 137 years ago. The Metre Convention created the International Bureau of Weights and Measures and set the framework for global collaboration in the science of measurement and its application in industry, innovation, and society. The worldwide uniformity of measurement remains as important today as it was in 1875.

World Metrology Day has become an established annual event during which more than 80 states celebrate the impact of measurement on our daily

lives—an important, though not always immediately apparent, aspect of modern society. This year, the theme was “Metrology for Safety,” a topic that concerns us all in a variety of commonplace ways. One such concern has emerged from the field of nanomaterials: Measurement procedures must be developed for establishing the potential toxicity of nanoparticles in consumer products and their effect on humans and the environment.

Nanoparticles are already incorporated in over 1300 commercial products,² from food and consumer products to electronics, automotive parts, and medical products. With the 2012 Olympic Games fast approaching, news of sports clothing containing nanoparticles has hit the headlines. Such materials offer the ability to produce lighter, stronger, or more streamlined athletic clothing (e.g., swimsuits with low levels of drag, running spikes with carbon nanotube reinforced plates, and sunglasses with a protective and anti-reflective polymer “nanofilm”). Our athletes are now kitted out in sportswear that not only looks great but also performs in a different league.

While the applications for nanomaterials in clothes are far ranging, the wider field of nanotechnology offers the potential to provide solutions to our biggest global challenges. For example, nanotechnology may provide a sustainable energy solution in terms of energy conversion, storage, and conservation. Nanotechnology may also offer better, more cost-effective medical treatment through improved drug delivery.

The increased use of nanotechnologies is driven by the unique mechanical, thermal, and catalytic properties that materials develop when structured at the nanoscale. However, it is these unique properties, while beneficial for technological innovation, which could also make nanomaterials toxic to biological tissues, raising concerns that they pose a risk to the environment and human health. The potential benefits of nanotechnology can only be fully realized if nanomaterials, particularly those for use in nanomedicine applications and consumer products, are shown to be non-toxic. Limitations in our knowledge of potential toxicity are partly due to the lack of methodology for the detection and characterization of nanoparticles in complex matrices. Therefore, in order to address this issue, the development of robust methods to provide adequate toxicity data, comparable between laboratories, is required.



Nanoparticle Tracking Analysis (NTA) in combination with FFF-ICP-MS characterized particles for size and elemental composition. Image courtesy of Andrew Brookes, www.andrewbrookes.co.uk.

The Challenge

As the name suggests, nanoparticles are very small—less than 100 nm, which means they could overcome some of the body's defense mechanisms, such as the cellular barriers, which protect against foreign objects. In order to take full advantage of the technological benefits of nanotechnology and to sustain competitive economic growth, it is becoming increasingly necessary to ensure that nanoproducts are safe at all stages of their life-cycle and that the public and the environment is adequately protected from any adverse effects.

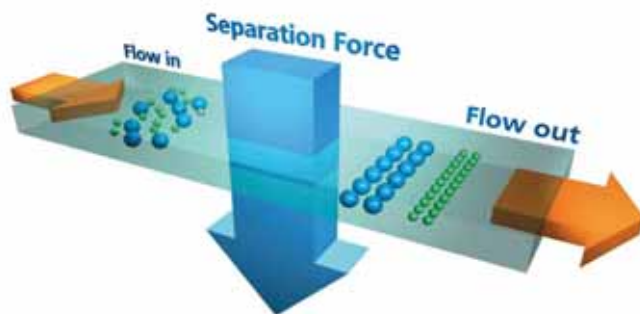
Current methods for understanding the potential harmful or toxic effects of nanoparticles rely on the well-developed in vitro and in vivo testing processes developed for assessing chemical, pharmaceutical, and consumer products. While comparisons can be drawn from these testing regimes, the unique properties of nanoparticles make measuring their potential toxic effects more problematic. As a consequence, it is difficult to predict the effects of nanomaterials on human health based on known risks for macrosized particles with the same chemical composition.

In addition, measuring the potential toxicity of nanoparticle-containing consumer products is often complicated by the complex matrix of the food or product. There is currently a lack of meth-

odology for the reliable characterization of inorganic nanoparticles added to food, and a lack of knowledge about the stability of such materials. Therefore, analytical methods are needed that will enable accurate element quantitation and rapid size characterization of nanoparticles in consumer products.

Method Development for Nanoparticle Extraction

Titanium dioxide is used predominantly as a white pigment in a variety of products, including coffee creamers, toothpastes, and sunscreens. In sunscreens, its high refractive index protects the skin from UV radiation from sunlight. Initially, titanium dioxide was considered to be an inert mineral, non-toxic to humans



The principle of FFF (field-flow fractionation).

Image courtesy of Postnova Analytics, www.postnova.com

and the environment. However, following its broad application, concerns have arisen that its toxicological risk has not been investigated sufficiently.

The accurate detection and identification of nanoparticles in food and consumer products requires an efficient sample preparation and extraction process to separate nanoparticles from the complex matrix of the product. Of the family of separation methods, field flow fractionation (FFF) is one of the most used and appropriate techniques for separation of nano-objects in complex matrices. FFF provides separation prior to detection and characterization of nanoparticles. The

separation process is similar to chromatography except there is no stationary phase and separation is based on physical forces as opposed to chemical interactions.

Separation occurs in a thin flow channel where the particles are forced downwards by the cross flow. Smaller particles will diffuse back into the channel flow more quickly, and will elute faster than larger particles (see figure above). By developing methods involving the coupling of FFF to inductively coupled plasma mass spectrometry (ICP-MS) and multi-angle light scattering (MALS), the technique has the potential to provide size-resolved data on the elemental composition of nanoparticles, which is critical to environmental and toxicological investigations of nanomaterials.

Using these techniques, LGC, the UK's designated National Measurement Institute for chemical and bio-analytical measurement, has developed a new method for the characterization of titanium dioxide particles in sunscreens which involves the development of an

... the unique properties of nanoparticles make measuring their potential toxic effects more problematic.

Size Matters

improved extraction method for nanoparticle isolation.³ This research forms the first systematic comparison and optimization of extraction methods for titanium dioxide nanoparticles in sunscreen samples. Sunscreens were selected for this research due to their wide use, high fat content, and highly complex matrix.

Previous published research has demonstrated the applicability of coupling FFF to ICP-MS in order to characterize nanoparticles.⁴⁻⁵ LGC is building upon this research by using a labelled titanium dioxide reference material as a spiking material for quality control and comparability. The novel approach of sample spiking with aluminium-labelled reference particles of known

the development of extraction methods able to preserve the size and composition of nanomaterials in the original sample. This method has been developed further and its feasibility investigated for determining size-based elemental speciation analysis in food.

While robust method development such as this is imperative for characterizing nanoparticle-containing products, the development of standards and reference materials are also essential. They enable standardization and comparability of toxicity tests, and support quality control of existing products.

Reference Materials for Standardization and Comparability

The National Measurement Institutes that reside throughout the world produce and distribute high-level measurement standards and measurement procedures, and provide metrological traceability to testing laboratories via their analytical and calibration facilities. LGC, in its designated National Measurement Institute role, is investigating the possibility of developing a standardized panel of reference nanomaterials to enable the development of traceable methods for improved in vitro toxicity measurement for safety assessment.

In vitro screens, which mimic the physiological environment of the human body, offer one of the fastest methods to measure the toxicity of nanoparticles. However, there is poor comparability between laboratories, due, in part, to the fact that when nanomaterials interact with biological systems, their physical and chemical properties can change significantly, affecting their functionality and behavior. For example, nanoparticles tend to become coated with proteins and form agglomerates in biological systems, changing their size and functional properties and altering their behavior under assay conditions. In addition, a lack of standardization in sample preparation methodology and the limited applicability of traditional sizing techniques for heterogeneous nanoparticles in complex matrices further complicate measurements. These issues make prediction of the potential toxicity of nanoparticles difficult. A number of reports⁶⁻⁷ have highlighted the critical need for a bank of nanomaterial reference materials to enable standardized measurement across laboratories.

Currently, there are a limited number of such reference materials available (e.g., 60 nm mono-dispersed gold-citrate [NIST RM-8013]). This inert reference material, although widely used for calibration of equip-



FFF-ICP-MS is used to determine the size distribution and elemental composition of nanoparticles in food and consumer products. Image courtesy of Andrew Brookes <www.andrewbrookes.co.uk>.

size enables the effect of extraction and separation conditions on particle size distribution to be studied. The sunscreens were analyzed and compared for titanium extraction efficiency, particle size distribution, and titanium dioxide recovery from the FFF channel. Using FFF-ICP-MS, the simultaneous detection of aluminium and titanium was proven, for the first time, to be very useful for tracking the spiked titanium oxide particles due to their much higher aluminium content when compared to native titanium dioxide particles in the sunscreen.

This research goes some way to addressing the emerging need for new validated methodology capable of reliably determining size and size-based elemental composition of nanoparticles, and in particular,


Measurement Helps Solve Nanoparticle Toxicity Challenges

ment, is not best suited for in vitro nanotoxicology due to its lack of toxicity. Recently, under ISO Guide 34 for the production of reference materials, the EU-Joint Research Centre produced a series of nanomaterials in powder-form, characterized for their physical characteristics. These materials are now being used by LGC to form the basis of a standardized panel of prototype reference materials that are stable, biologically active, have reproducible toxicity profiles, and are characterized under biologically relevant conditions.

In order to produce stable reference materials and prevent agglomeration, the behavior of the nanomaterials needs to be controlled by modifying the surface of the particles. These modified particles can then be characterized in biological solutions using instrumentation such as Nanoparticle Tracking Analysis (NTA), which offers a unique method for visualizing and analyzing particle size and size distribution by relating the rate of Brownian motion to particle size. In order to obtain reproducible toxicity profiles, a label-free, real-time, cell-electronic sensing system was used to measure changes in cell number following nanoparticle exposure. This technique enables continual analysis of cells exposed to nanoparticles using electrical impedance measurements and provides quantitative information about the rates and mechanisms of toxicity, which can be missed when using traditional assays. The system is not susceptible to measurement interference by the nanoparticles, thereby allowing the relationship between dose dependant toxic response in the cells and nanoparticle composition to be measured reproducibly. By combining this technique with NTA, nanoparticles in complex suspensions can be characterized in terms of size, distribution, and toxicity.

Once completed, it is anticipated that this research will produce a prototype panel of reference materials characterized for their properties (size, agglomeration state, elemental composition, and toxicity) in physiologically relevant systems so they can be applied as calibration standards in routine testing procedures. The research should support public acceptance of nanomaterial safety by providing reference materials that can be incorporated into testing regimes for regulatory processes.

The research should support public acceptance of nanomaterial safety . . .

The development of both methods to measure the size distribution and elemental composition of nanoparticles of relevance to food and consumer products, and the development of characterized reference materials is timely and important for supporting technological and societal challenges associated with sustainable development, competitiveness, food, health, safety, and environmental issues. 

Acknowledgement

The work described in this paper is funded by the UK National Measurement System.

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A Call for a Response from the International Chemistry Community

by Jorge Colón



A year ago, the American Association for the Advancement of Science (AAAS) published *Science for Haiti: A Report on Advancing Haitian Science and Science Education Capacity*. I was one of the coauthors of the report, along with

Gary Machlis and Jean McKendrey. This is a story of how that report came about. In addition, I summarize the report to the readership of *Chemistry International* and offer some recommendations on the current state of affairs in Haiti regarding the advancement of science and science education capacity and how the international chemistry community can respond to Haiti's current needs in these areas.

The *Science for Haiti* report was a response to the devastating earthquake of 12 January 2010 near Port-au-Prince, Haiti, that killed over 300 000 people, injured more than 300 000, and left over 1.3 million persons homeless and living in over 1300 camps and settlement sites. Much of the infrastructure, social institutions, economy, and environmental resources of Port-au-Prince and the surrounding areas were destroyed by the earthquake. Haitian education and research institutions, as well as the nation's science and science education capacity, were also badly damaged.

The earthquake devastated chemistry resources in Haiti. According to a study by the Inter-University Institute for Research and Development (INURED) from March 2010, around 90 percent of the physical infrastructure of the Université d'Etat d'Haiti (UEH), including laboratory space and classrooms, was destroyed. In addition, 380 students and 50 faculty and administrative personnel died in the earthquake. The four chemistry-teaching laboratories at the UEH were destroyed, although some of the materials and equipment were recovered. The earthquake killed 20 percent of Haiti's skilled professionals.

In February 2010, a month after the earthquake, during the AAAS Annual Meeting in San Diego, Gary Machlis of the College of Natural Resources of the University of Idaho and Science Advisor to the

Director of the National Park Service, suggested to the Committee on Opportunities in Science (COOS) for Minorities, Women, and Persons with Disabilities that the AAAS convene within 90 days of Haiti's earthquake a small meeting (20–30 people) in Puerto Rico to develop recommendations on how to help Haiti build capacity in science and science education for the long run. The COOS committee agreed, and the next day I was able to present this recommendation to the AAAS Board Meeting as part of my Caribbean Division Annual Report presentation as president of the division. Immediately thereafter, Gary and I started to organize the initiative with the help of Vaughan Turekian, chief international officer for AAAS.

We immediately agreed that science is an essential foundation for Haiti's future, but Haitian science must be Haitian-led and directed. We felt that one way in which the international scientific community could provide valuable assistance was to develop a set of well-founded strategies, policy recommendations, and proposed actions that could help guide the development of Haitian science capacity, prioritize a national program, and target international assistance. We were worried that many reports and plans being discussed by international organizations failed to mention science as an integral part of Haiti's future sustainable development and reconstruction efforts. Finally, we decided to hold in the summer a two-day workshop in San Juan, Puerto Rico, and then go to Port-au-Prince, Haiti, for two more days of workshops with Haitian stakeholders. Dr. Jean McKendrey, of the Association of American Geographers, joined Gary and me in organizing the workshops, with much needed logistical help from Dr. Fritz Deshommes, vice rector for research of the UEH.

Finally, on 10–12 July 2010, in a collaboration among the AAAS Caribbean Division and the AAAS International Office, the University of Idaho, the Association of American Geographers, and the University of Puerto Rico, the two-and-a-half-day workshop was held in San Juan, with the participation of 9 Haitian scientists and 11 other scientists from the Haitian diaspora, United States, Canada, Rwanda, and Puerto Rico. Then, from 15–17 July 2010, Gary, Jean, and I visited Haiti and met with about 60 Haitian scientists, school principals, and representatives of the Haitian government commissions on education and on information technology.

The objectives of the workshops were to 1) gather Haitian and international scientists, educators, and policy experts from diverse fields of science; 2)



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engage participants in dialogue on advancing capacity for Haitian science and science education; 3) draft strategic goals and recommendations to advance Haitian science and science education capacity; 4) prepare a formal report that could serve as a “road map” for advancing science for Haiti; and 5) present the report to Haitian officials and scientists, international scientific organizations, aid organizations, and the donor community.

The workshops were very successful and we obtained strong support from Haitian participants for initial and future collaborations. We established a network of contacts within the Haitian higher education and scientific communities. The main outcomes of the workshops were that a draft of the report was developed and that our Haitian colleagues committed to establishing a scientific society in 2010–2011.

The draft report was prepared by Gary, Jean, and me and sent to all workshop participants for review and comment. Then, the final version of the report was reviewed and approved by AAAS and published in June 2011. For the first time ever for an AAAS report, the executive summary was written in Creole, English, French, and Spanish. The report includes a one-page message from the AAAS CEO, Alan I. Leshner, encouraging “the governments of Haiti, the United States, and other nations, along with relevant scientific, development and aid organizations throughout the world, to recognize the skill and commitment of the Haitian science community and give the closest consideration” to the recommendations of the report.

The Science for Haiti report includes seven strategic goals for advancing science and science education capacity in Haiti:

1. **Advance** Haiti’s scientific capacity to link Haitian scientific expertise to Haiti’s development objectives.
2. **Invest** in science education, research, and technological innovation to generate sustainable development and prosperity for Haiti.
3. **Develop** Haitian scientific capacity and expertise to promote scientific management and

sustainability of Haiti’s natural resources.

4. **Support** existing scientific and educational organizations and institutions, and if needed, establish new ones to promote the role of science in Haitian society.
5. **Promote** the integration of Haitian science and scientists into the global scientific community, for the benefit of not only Haiti but the rest of the world.
6. **Increase** the connection of science to broader Haitian society through formal and informal education, so that all Haitian citizens have knowledge and understanding of science and its uses.
7. **Educate** Haiti’s leaders in government, business, religion, and culture, so that they better understand and value the role of science in Haiti’s economic and cultural development.

To support the achievement of the seven strategic goals, the workshop participants identified specific recommendations, policies, and actions to advance science in Haiti, each one linked to one or more of the strategic goals. The report includes 17 recommendations for advancing science capacity, such as establishing a national science and technology policy, conducting specific human capital studies, establishing internationally funded research programs that enable Haitian scientists and international colleagues to conduct collaborative research in Haiti, creating career opportunities for Haitian scientists, supporting Haitian graduate students, and developing creative approaches to promoting science within Haitian society.

The report also includes 15 recommendations to advance science education capacity, emphasizing that science education, both formal and informal, is essential at all levels of Haitian society. Among these recommendations are constructing regional “learning laboratories” and community gathering places and training more teachers and faculty to provide quality science instruction. In addition, the report recommends creating opportunities for students who excel in science to enhance their education, including internships with universities, the private sector, and government.

The report concludes with 11 recommendations to advance science governance in Haiti. One of the primary suggestions was to establish clear and constructive science, technology, and innovation policies (and where necessary, rules and procedures). To do this, the report recommends the establishment

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of an independent Haitian Academy of Science, which would inform and advise on such policy, and establish a system of accreditation that could be used to improve the quality of schools, and enforce established and new quality control standards. In addition, the report calls for the creation of effective governing bodies, well-supported institutions of higher education and research, and organizations to provide Haitian scientists with research opportunities, scientific interchange, and recognition. Participants stressed the need for the Haitian government to increase its level of support for science and science education, and urged the international scientific community to provide encouragement and assistance in developing “good governance” institutions for science.

The report was not made public until 19 September 2011 when it was first delivered and presented to the Haitian scientific community by two of the authors. We were happy to learn in September that the Haitian scientific community had established the Haitian Association for the Advancement of Science and Technology (HAAST), with Fritz Deshommes as its first president, making this the first strategic goal to be implemented. The return visit to Haiti allowed the report authors to celebrate the establishment of the HAAST, meet with the Haitian scientific community, higher education leaders, business community, and secondary school principals and science teachers, and share and discuss the report with representatives of the U.S. Embassy and a counselor to Haitian President Martelly.

The news of the report's release and our visit to Haiti were well received internationally. The AAAS press release of 19 September 2011 generated over 100 stories in mainstream newspapers, magazines, television, radio, and online news sites throughout the world. A month after visiting Haiti, Gary, Jean and I presented the report's recommendations at the AAAS Headquarters in Washington, D.C. to representatives of government, universities, and NGOs, urging them to support Haitian-led efforts to build the nation's science capacity. Scientific and aid organizations from the United States and abroad expressed their support and are already sharing with us, and with the Haitian scientific community, possible avenues of collaboration and monetary support to begin implementing some of the ideas suggested in the report. The report is available online at www.aaas.org/go/haiti2011.



The initial workshop was held in July 2010 in San Juan, Puerto Rico. Photo by Edward W. Lempinen/AAAS.

The HAAST has already decided that one of their first efforts will be to enhance the image and understanding of science among the Haitian general population. To help achieve this goal, a two-day workshop on science reporting is planned for this year. To be held in Haiti, the workshop will feature science reporter Lisa Friedman of ClimateWire and winner of the 2009 AAAS Kavil Science Journalism Award for Online Reporting.

In addition, we have learned from a close counselor to Haitian President Martelly that they have already decided to implement another of the recommendations of the report and plan to establish the equivalent of a National Medal of Science and award it to a Haitian scientist, a Haitian science teacher, and a Haitian science student to increase recognition of science within Haitian society.

The international chemistry community can help in these efforts to advance science and science education in Haiti. One of the most rewarding ways to help is by volunteering to serve for a short period as a professor in Haiti. A good example of how this can be accomplished is the Volunteer Lecturer Program (VLP, see <http://vlpnas.ning.com>) established by the Commission on Development and Exchanges of the International Mathematical Union and supported by the Board on International Scientific Organizations of the U.S. National Academies of Science. The VLP program allows a professor to visit a developing country for a month and give an intense mathematics course. This program has allowed some countries to teach a whole Masters of Science program utilizing professors from this volunteer program. Once the students in the program receive their degrees, they have now the capacity to offer those courses and continue building homegrown capacity in that science. Encouraging international chemistry organizations to establish a similar program for volunteer chemistry professors would allow for our science to develop in Haiti by building Haitian capacity.

Some universities abroad have given fellowships to Haitian chemistry students to continue or begin

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M.S. studies at their universities. For example, the Río Piedras campus of the University of Puerto Rico gave scholarships to 13 students, including 3 chemistry students, to pursue graduate studies towards a master's degree starting in August 2011. An important lesson of the first year of the UPR program is that a one-year adjustment period should be provided to incoming Haitian students in which they can adapt to the culture, learn the language, and take advanced undergraduate courses, and become comfortable with their laboratories to prepare them for a competitive graduate program. This requires an integrated approach with all faculties and campus organizations engaged in the Haitian students' education.

However, as much as this and similar efforts throughout the world can be applauded, nothing can impact as much as teaching formally and informally to the Haitian students and population in Haiti. Doing so promotes the advancement of their country and reduces the possibility of brain drain. Understanding that science, especially chemistry, is an essential element of development in Haiti, a group of Haitian chemistry professors established the Groupe de Recherches et de Developpement de la Chimie en Haiti (GRDCH, <http://sites.google.com/site/haitichimie/grdch>). During the 2011 International Year of Chemistry (IYC), the project manager of GRDCH was approved as the local IYC representative and they had plans to conduct projects such as the Global Water Experiment. Some Haitian schools received the Global Water Experiment's kits through the national commission of UNESCO in Haiti and some conferences for students were held, but, unfortunately, due to a lack of financial support, the GRDCH was unable to organize IYC projects as planned and they are still waiting for funding.

GRDCH lists on its website some of the impediments to developing chemistry in Haiti: (1) lack of awareness of the importance of chemistry from national leaders and the population; (2) lack of higher education institutions offering a major in chemistry; (3) lack of interest in careers in chemistry among high school students; and (4) lack of qualified teachers and resources such as laboratories in the schools. GRDCH plans to prepare an annual report about issues surrounding chemistry in Haiti that we should read and to which we should properly respond.


On the other hand, there are some good indicators about the future of chemistry in Haiti. The undergraduate program in chemistry at the School of Science of UEH was launched in 2003 (this program had been closed since the 1980s), several students are currently enrolled in advanced studies in chemistry outside the

country (including staff of the GRDCH), and nowadays Haiti is globally more open to technology and science. GRDCH is committed to chemistry and its key role in the development process of Haiti. Its motto is "La chimie au service du developpement"—Chemistry in service of development.

There is reason to be optimistic for such development, with the planned construction of new science infrastructure. A new USD 150 million UEH main campus in 60 hectares of land is planned to be built in Damien, a district of Port-au-Prince 15 km from downtown, with buildings for classrooms, libraries, laboratories, dormitories, and restaurants to house 15000 students and 1000 professors, although funds for this project have not yet been approved. However, already a new university campus was inaugurated on 12 January 2012 at Lemonade in the north of Haiti, with USD 50 million from the government of the Dominican Republic, Haiti's neighboring country. Both campuses plan to have a strong science component.

Scientific capacity is required to advance technological innovation and economic opportunities in Haiti, improve medicine and health care, create access to drinking water, improve disaster preparedness and mitigation, develop sustainable agriculture and reduce hunger, manage natural resources, educate citizens, and promote human rights. The role of science in reconstruction, recovery, and development of Haiti will depend on the development of scientific capacity integrated into the full range of local, regional, and national efforts to rebuild the nation.

I urge the readership of *Chemistry International* to engage in collaborative efforts among Haitian and international scientists through the *Science for Haiti* report, which provides an initial "road map" for advancing science and science education in Haiti.

Access to the benefits of scientific progress is a human right as important as any other. Scientists should be committed to helping communities by sharing their knowledge and information and working jointly to allow them to solve their problems. We hope you will share this commitment with us and accompany us on this mission, since "Caminante no hay camino, se hace camino al andar." We as chemists can do our part. Join us in these efforts. 

Jorge Colón is a professor of chemistry at the Río Piedras Campus of the University of Puerto Rico, the immediate past president of the AAAS Caribbean Division, and one of the authors of the AAAS Report *Science for Haiti*. He can be reached at <jorge.colon10@upr.edu> to help establish contacts with the Haitian science and chemistry community.

Icons of Boron Chemistry

by Narayan S. Hosmane

This article is an effort to salute and revive the memory of 20 of the most-iconic figures in the field of boron chemistry. It is almost impossible to put a biographical sketch of each person in a paragraph or two. Therefore, by avoiding the detailed descriptions, the key features of their work are highlighted here, while maintaining a chronological order in accordance with their date of birth.



Anton Burg (1904–2003)

Anton Burg was the first American-born, American-educated boron chemist. He is our link to the distinguished past, to Herman I. Schlesinger, and through him to Alfred Stock, the pioneer of research on the boron hydrides. He is considered to be one of the pioneers of boron chemistry and is also credited as being the

“father of chemistry at the University of Southern California.” He joined USC as an assistant professor in 1939 and within a year became the chairman of the department. It was his relentless effort that helped the department of chemistry to succeed in acquiring major research grants and flourish within a few years. Burg was a major architect of many boron compounds that eventually became building blocks for more complex molecules. He was an athlete by nature and nationally ranked high jumper during his undergraduate studies. A bicyclist, who never drove a car, he passed away on 18 November 2003.

Boris M. Mikhailov (1906–1984)

Born in a village in Siberia in 1906, Boris Mikhailov received his Doctor of Science in Chemistry in 1948. He started as a head of laboratory at Zelinsky Institute of Organic Chemistry of the Russian Academy of Sciences in 1954 and remained there until his death.

He was considered to be a pioneer of modern organoboron chemistry along with Herbert C. Brown of the USA and Roland Köster of Germany. His group studied the bonding properties of various three- and four-coordinated compounds and it made several discoveries, including allylboratoin, rearrangements involving 1,3-boron shift, reduction of aromatic aldehydes with trialkylboranes, and allylboron-alkyne- and allylboron-allene condensation.

William Sweet (1910–2001)

William Sweet graduated from the Harvard Medical School in 1936. After finishing his residency in neurosurgery/neurology at Billings Hospital, Chicago, he returned to Harvard and the Massachusetts General Hospital, where his career spanned almost 60 years. During this time, Sweet made major contributions to the field of academic neurosurgery. Although he was able to concentrate on both basic and clinical research, his primary interests were focused on boron neutron capture theory, treatment syndromes of facial pain, treatment of persistent pain in general, diagnosis and treatment craniopharyngiomas, and diagnosis and treatment of optic gliomas. The founder of one of the first brain scan research laboratories, he performed one of the first successful carotid bifurcation reconstructions.



Herbert C. Brown (1912–2004)

Herbert C. Brown was born in London in 1912, received his doctoral degree in 1938 under the supervision of Herman I. Schlesinger from the University of Chicago, and worked briefly as a post-doctoral researcher under M.S. Kharasch in

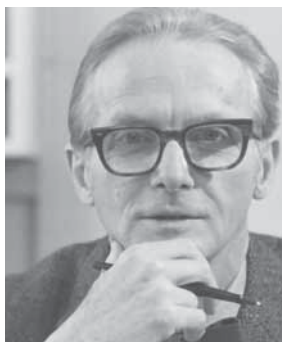
Chicago. He wrote in his autobiography that his failure to secure an industrial job led him to choose a career path that turned out to be the most beneficial for him, but also to the scientific community. After a short stay in Chicago as an instructor and at Wayne University as an assistant/associate professor, he joined Purdue University as a professor. He retired as a professor in 1978, but he was an active researcher until his death in 2004. The 1979 Nobel laureate won so many awards in his lifetime that to list them would require a whole article. Brown's tremendous scientific achievements included his earlier work involving synthesis of diboranes and sodium borohydride to the more recent development of quantitative methods to determine steric strains and the examination of the chemical effects of steric strains.

Robert W. Parry (1917–2006)

Born in Ogden, Utah, on 10 October 1917, Robert Parry graduated from the University of Illinois in 1946. After working for 23 years at the University of Michigan he moved to the University of Utah, Salt Lake City, and served there through the rest of his life. Along with his research distinctions, he was an accomplished educator with a life-long devotion to the profession of chemistry. He co-authored high school chemistry text books and won numerous awards, including the Priestly Medal in 1993, the highest honor from the American Chemical Society. He was the founding editor of the ACS journal *Inorganic Chemistry* and served as the president of the American Chemical Society.

William N. Lipscomb Jr. (1919–2011)

Nobel Prize winner of 1976 in Chemistry, William Lipscomb Jr. began graduate school as a physics major. He changed his major under the influence of Linus Pauling and graduated in 1945 from the California Institute of Technology. He began his academic career at the University of Minnesota and then moved to Harvard University in 1959 where he remained until retirement in 1990. But Lipscomb, also popularly known as “the Colonel,” never retired from Chemistry. His major involvement in boron chemistry was with the nature of the chemical bonds in boranes and carboranes. Later on, he focused on the structures of proteins and the reactivity of enzymes. A scientific genius with a great sense of humor, Lipscomb was an excellent mentor to many. Two of his graduate students and another one who spent some time in his laboratory went on to win Nobel Prizes.



Leonid I. Zakharkin (1923–2001)

Leonid I. Zakharkin was an outstanding scientist in many fields of organic and organometallic chemistry. He began his career at the Institute of Organoelement Compounds of the Academy of Sciences of USSR in 1954,



the year it was founded. His initial research was on the chemistry of flavor substances and the telomerization of dienes. Later, Zakharkin took a leading role in the field of organoaluminium compounds in the USSR and became one of the pioneers of the chemistry of carborane. He received several awards recognizing his talent, including the USSR State Prize in Science and Technology in 1986, followed by the Russian Federation State Prize for “Chemistry of Carboranes and Polyhedral Boranes” in 1996. He was also a successful supervisor of many boron chemists including Vladimir Bregadze, Igor Chizhevsky, Valeriy Kalinin, and others who are prominent in their respective fields.

F. Gordon A. Stone (1925–2011)

Francis Gordon Albert Stone was born in Exeter, England, on 19 May 1925. After receiving his Ph.D. from Cambridge University in 1951 he worked with Anton Burg as a post-doctoral researcher at the University of Southern California. He later joined Harvard University as an instructor and became an assistant professor in 1957. In 1963 he took a position as professor and chair of inorganic chemistry at Bristol University and remained there until his mandatory retirement in 1990. He then became the Welch Professor at Baylor University in Texas until his retirement in 2010, just a year prior to his death. Besides being an accomplished scientist, Stone was also inaugural co-editor of the series titled *Advances in Organometallic Chemistry* with Robert West. He was also a co-editor of *Comprehensive Organometallic Chemistry*, an encyclopedia of organometallic chemistry. In 1990, he was honored with the Civilian of the British Empire title by Her Majesty the Queen of Great Britain.



Earl Muettertief (1927–1984)

Earl Muettertief was born in Elgin, Illinois, on 23 June 1927. After graduation from Harvard University in 1952, he joined the Central Research Department at DuPont. He served as associate director until 1967 when he decided to explore the academic field and became part of the adjunct faculty, first at Princeton University and then at the University of Pennsylvania. In 1973 he took the opportunity to become a full professor at

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Cornell and stayed there until 1978. He finally moved to UC-Berkeley and ended his career there. During his stay at DuPont he worked with boron hydrides and extended the chemistry of polyhedral borane anions such as $B_{12}H_{12}^{2-}$ that was discovered earlier by Hawthorne at Redstone Arsenal in Huntsville, Alabama. He was a unique individual who undoubtedly made a significant contribution to modern inorganic chemistry.

Jaromir Plešek (1927–2010)



Born in Hostašovice, Moravia, on 21 September 1927, Jaromir Plešek graduated in 1952 with a Masters degree from Prague Technical University. He worked in the same institute as an assistant professor of Organic Chemistry until 1958 and then joined a company named Polymers for Human Medicine as a research chemist. In 1961 he started working as a scientist in the Laboratory for Special Inorganic

Chemistry in Řež. In 1965, he received his Ph.D. from Technical University, Pardubice, and became part of the Institute of Inorganic Chemistry at the Czech Academy of Sciences, where he remained for the rest of his career. He was an active researcher in the syntheses of boranes and heteroboranes, including their practical applications. He was also a co-founder of the IMEBORON conferences and the chairman of the organizing committee of the first meeting in 1971.

Robert Brotherton (1928–2001)

Born in Ypsilanti, Michigan, in 1928, Robert Brotherton received his Ph.D. in 1954 from Washington State University. After a few years of research at the University of Minnesota (as a DuPont Fellow from 1954–1955) and at Union Oil California (as a research chemist from 1955–1957) he joined U.S. Borax. He retired in 1993 from U.S. Borax as the vice president for research. Brotherton was the co-founder of Boron in the USA along with Narayan Hosmane. His expertise was high-energy boron fuels as part of Project ZIP. He pioneered diboron compounds and was the first to make tetra(hydroxy)diboron, tetra(amino)diboron, and tetra(dimethylamino)diboron, which are now important synthetic reagents.

Stanislav Heřmánek (1929–1999)

Stanislav Heřmánek, a close friend of Jaromir Plešek, was born in Tábor, Bohemia, on 13 June 1929. He graduated from Prague Technical University in 1952 with a master's degree and later in 1966 he received his Ph.D. degree from Technical University, Pardubice. He was a faculty member at The Institute of Chemical Technology from 1961 to 1974. Later, he joined Charles University as a professor and continued his service there until his death. Heřmánek was one of the founders of IMEBORON who was actively involved in the development of more sophisticated multinuclear NMR methods to identify new substances. A key early breakthrough was his recognition that the kinetics of the thermal gas-phase conversion of diborane into higher boranes, and ultimately, decaborane. The value of his contributions was recognized in 1968 by a Czechoslovak Academy of Sciences Award, and most recently by the award of the highly prestigious Heyrovsky Medal of the Academy of Sciences of the Czech Republic, a belated tribute to his lifelong achievements in boron science.

Hiroshi Hatanaka (1932–1994)

Hiroshi Hatanaka earned his medical degree from Tokyo University in 1957 and then came to the USA as a Fulbright Scholar, working under William Sweet at the Massachusetts General Hospital. He went back to Japan in 1968 and joined Teikyo University in Tokyo as a professor and neurosurgeon and served there until his death. Hatanaka successfully applied the concept of BNCT in Japan, where he began clinical trials in 1968. Hatanaka used improved boron compounds, such as sodium borocaptate, and applied radiation directly to surgically exposed tumors, rather than attempting to radiate the tumor through the patient's skin and skull. He was internationally recognized for advancing the brain tumor treatment through BNCT.

Ralph Fairchild (1935–1990)

Ralph Fairchild had a diverse educational background. Born in Trenton, New York, in 1935, he earned a master's degree in nuclear engineering in 1959 from St. Lawrence University and a Ph.D. in physics from Adelphi University in 1961. He started his career at Brookhaven Medical Department and continued there until his death in 1990. He was also a research associate professor at the Stony

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Brook School of Medicine of the State University of New York from 1979 to 1990. Fairchild was internationally recognized as a leading American investigator in BNCT. He was actively involved in the development of a new type of neutron beam at Brookhaven's Medical Research Reactor facility.

Lee J. Todd (1936–2011)

Born in Indiana in 1936, Lee Todd received his Ph.D. under Riley Schaeffer in 1963 from Indiana University. After a brief post-doctoral research at MIT, Todd joined University of Illinois in 1964 as an assistant professor. He moved to Indiana University-Bloomington in 1969 and remained there as a professor of chemistry until his death in 2011. Todd had an extreme passion for boron chemistry with unusual borane and carborane cages incorporating main group elements, forming the corresponding heteroborate anions as the ligands for converting them to metallaphospha- and azacarboranes. His tin chemistry was novel. He was active in using boron compounds to attempt to sequester and precipitate radioactive cesium from nuclear reactor wastes, to immobilize them so that they would be rendered "fixed" for long-term nuclear-waste disposal. Todd was also interested, later in his career, in making compounds for BNCT research.

John H. Morris (1937–2005)

John Morris was born in Cardiff, Wales, in 1937. He received his doctoral degree in 1961 from the University of Nottingham. In 1985, he received a D.Sc. from the same university. He worked in different universities, including the University of Newcastle as a senior research associate, Kingston College of Technology as a senior lecturer, and the University of Strathclyde in Glasgow as a senior lecturer where he was promoted to reader in 1969 and remained there until his death in 2005. His major research interests were in chemical and electrochemical studies of boranes, metalboranes, and boron heterocycles. He also became interested in the use of boron compounds in BNCT. To obtain access to neutron sources, he made many trips to Eastern Europe and, in particular, to Russia. He was an excellent preparative chemist with a lifelong fascination with the chemistry of boron.

Bernard F. Spielvogel (1937–2011)

Bernard Spielvogel graduated with a doctoral degree from the University of Michigan in 1963. His area of expertise was in synthetic boron chemistry and he was employed in different academic, government, and business positions. He worked in several universities, including the University of North Carolina at Chapel Hill, Duke University, North Carolina State University at Raleigh, Northern Illinois University, and Mt. Allison University in Sackville, New Brunswick, Canada. He was the program officer for the U.S. Army Research Office for decades and later became an entrepreneur. He was either founder or co-founder of five high-tech companies. The principal inventor on many patents in the field of boron analogs of amino acids, peptides, and nucleic acids, Spielvogel died on 10 May 2011 in Mount Airy, North Carolina.



Ralph Rudolph (1940–1981)

Ralph Rudolph, born in Erie, Pennsylvania, on 14 July 1940 died at age 41. He joined the University of Michigan faculty in the position vacated by his Ph.D. mentor R.W. Parry in 1969. At the University of Michigan, Rudolph continued his phosphine chemistry (which he learned from his Ph.D. work), particularly the chemistry of compounds having phosphorus-phosphorus bonds. However, he quickly proceeded to develop an active program in polyboranes and carboranes. From 1970 to 1977, his efforts not only resulted in further metallocarboranes with "naked metals," but also produced the synthesis of thiaborane in which a sulphur atom was incorporated into a boron cage structure. This compound proved to have a rich and interesting chemistry. Although still in the early stages of his career, he managed to publish over 60 research papers in peer-reviewed journals.

Clinton F. Lane (1944–2007)

A protégé of H.C. Brown, Clinton Lane joined the Aldrich Chemical Company after his graduation from Purdue in 1972. He worked there for more than 30 years during which time he was promoted to executive vice president in 1991. He chose to join academia in 2003 and became a research professor at North Arizona University, where he continued his research in organoborane chemistry until his death at 63.

Morris Srebnik (1947–2011)

Morris Srebnik received his Ph.D. from the Hebrew University in Jerusalem under Professor Raphael Mechoulam in 1984. He joined Professor H.C. Brown's group at Purdue University and studied the applications of organoboranes in organic synthesis until 1986. After doing research at Sigma-Aldrich Corporation, he returned to Brown's group. In 1990, he accepted a position at the University of Toledo, USA. In 1996, he returned to Hebrew University to become a professor at the School of Pharmacy. His research areas of interest included developing organometallic methodologies in synthesis of boron and zirconium compounds

and titanium. He had also investigated the potential uses of organoboranes in medicine and in isolating new sunscreen agents from natural sources such as cyanobacteria.

All of these extraordinary scientists made their major contributions in the field of boron chemistry. With their spectacular strides in science and lifelong devotion toward chemistry, they not only showed us the path of success, but also inspired us to achieve it.

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Stamps International

See also www.iupac.org/publications/ci/indexes/stamps.html

To Sneeze or Not To Sneeze

Allergies, among the most common ailments in the world, are abnormal reactions of the immune system that take place in response to otherwise harmless substances. Mild allergies often arise from exposure to widespread environmental allergens such as dust and pollen, which cause the red eyes, itchiness, and runny nose characteristic of hay fever. However, more severe allergic reactions may occur in some individuals, for example, upon ingestion of certain foods (e.g., peanuts), administration of penicillin or other antibiotics, or direct contact with the venom of stinging insects such as wasps and bees. Whether inhaled, ingested, or absorbed into the bloodstream, the offending substances trigger the release of copious amounts of histamine, an organic nitrogen compound derived from the amino acid histidine. Histamine is a potent vasodilator that increases the permeability of capillaries and leads to swelling of the affected tissues, redness, nasal congestion, sneezing, and other classic symptoms associated with allergic reactions. Most antihistamine drugs used in the treatment of allergies work by blocking the attachment of histamine to its cel-

lular receptors and thus suppressing the ensuing inflammatory response. Interestingly, other histamine antagonists operate instead by inhibiting the activity of histidine decarboxylase, the enzyme that catalyzes the biosynthesis of histamine.

The stamp illustrated in this note, issued in 2008, shows the structural formula of histamine and honors Daniel Bovet (1907–1992), the Swiss-born Italian pharmacologist who discovered the first antihistamine in 1937 while working at the Pasteur Institute in Paris. His seminal studies on the pharmacology of a vast range of substances that affect the function of the central nervous system, including acetylcholine, adrenaline, and curare,



a generic name used to describe various paralyzing South American arrow poisons, were recognized with the Nobel Prize in Physiology or Medicine in 1957. He published more than 300 papers, became a member of multiple learned societies, and is universally regarded as one of the forefathers of modern pharmacodynamics and mechanistic pharmacology.

Written by Daniel Rabinovich <drabinov@uncc.edu>.

Flerovium and Livermorium Join the Periodic Table

On 30 May 2012, IUPAC officially approved the name flerovium, with symbol Fl, for the element of atomic number 114 and the name livermorium, with symbol Lv, for the element of atomic number 116. The names and symbols were proposed by the collaborating team of the Joint Institute for Nuclear Research (Dubna, Russia) and the Lawrence Livermore National Laboratory (Livermore, California, USA) to whom the priority for the discovery of these elements was assigned last year. The IUPAC recommendations presenting these names is to appear in the July 2012 issue of *Pure and Applied Chemistry*.

The name flerovium, with symbol Fl, lies within tradition and honors the Flerov Laboratory of Nuclear Reactions in Dubna, Russia, where the element of atomic number 114 was synthesized. Georgiy N. Flerov (1913-1990) was a renowned physicist, an author of the discovery of the spontaneous fission of uranium in 1940 (with Konstantin A. Petrzhak), a pioneer in heavy-ion physics, and founder in 1957 of the Laboratory of Nuclear Reactions, part of the Joint Institute for Nuclear Research.

The name livermorium, with the symbol Lv, for the element with atomic number 116 is again in line with tradition and honors the Lawrence Livermore National Laboratory. A group of researchers at this laboratory took part in the work carried out in Dubna on the synthesis of superheavy elements, including element 116.

"These names honor not only the individual contributions of scientists from these laboratories to the fields of nuclear science, heavy element research, and superheavy element research, but also the phenomenal cooperation and collaboration that has occurred between scientists in these two countries," said Bill Goldstein, associate director of LLNL's Physical and Life Sciences Directorate.

Priority of claims to the discovery of the elements of atomic numbers 114 and 116 was determined by a Joint Working Party of independent experts drawn from IUPAC and the International Union of Pure and Applied Physics. The group's report was published in *Pure and Applied Chemistry* in July 2011. A newly appointed Joint Working Party has now begun work to assign priority for the discovery of elements 113, 115, 117, 118, and heavier elements.

 www.iupac.org

Future Earth: Research for Global Sustainability

The International Council for Science (ICSU), of which IUPAC is a member, announced a new 10-year initiative named Future Earth to unify and scale up ICSU-sponsored global environmental-change research.

Operational in 2013, this new ICSU initiative will provide a cutting-edge platform to coordinate scientific research to respond to the most critical social and environmental challenges of the 21st century at global and regional levels. "This initiative will link global environmental change and fundamental human development questions," said Diana Liverman, co-director of the Institute of the Environment at the University of Arizona and co-chair of the team that is designing Future Earth.

"Global environmental change affects our ability to access food, water, and energy. It increases our vulnerability to hazardous events, and erodes our ability to eradicate poverty," said Liverman. "Only by actively engaging natural sciences, social sciences, and humanities and by working with the full range of users and producers of knowledge, can we provide a full understanding of global change and its impact on societies and ecosystems."

Future Earth will have a new global governance body and secretariat, building on the strengths of existing core global environmental change programs, which are co-sponsored by ICSU. The program was officially launched in June at the United Nations "Rio+20" conference.

"We are very proud of the enormous scientific achievements of the ICSU-sponsored Global Environmental Change Programs over the last decades," said Yuan T. Lee, winner of the 1986 Nobel Prize in Chemistry and ICSU president. Lee stressed that "unifying the different efforts through this new broad partnership will provide the step-change needed in international research coordination to face the challenges posed by global environmental change." He added, "the enthusiasm and engagement of the whole community will be essential to the success of this endeavor."



 www.icsu.org/future-earth

Lois Rossi to Receive the IUPAC International Award for Advances in Crop Protection Chemistry

On 26 March 2012, the IUPAC Division on Chemistry and the Environment announced that the 2012 IUPAC International Award for Advances in Harmonized Approaches to Crop Protection Chemistry will be presented to Lois A. Rossi of the Office of Pesticide Programs at the U.S. Environmental Protection Agency.

The award recognizes individuals in government, intergovernmental organizations, industry, and academia who have exercised personal leadership for outstanding contributions to international harmonization for the regulation of crop protection chemistry. Awardees receive a USD 3000 honorarium plus travel

and per diem reimbursement to attend the award presentation ceremony. Corporate sponsorship for the award is provided by Dow AgroSciences.

Rossi joined EPA in 1978, and was active in leading pesticide reevaluation efforts during the 1990s, including implementation efforts for the Food Quality Protection Act of 1996. Since 2003, she has served as Director of the EPA Pesticide Registration Division, which evaluates and

approves new pesticide active ingredients and new uses. Rossi has been involved for more than 20 years with international regulatory harmonization efforts.

Rossi has been a tireless advocate for adoption of joint regulatory evaluations of new pesticide active ingredients, whereby the efforts of regulatory authorities in multiple countries are pooled and coordinated for harmonized data reviews. As part of her international regulatory harmonization efforts, Rossi has been involved in number of bilateral initiatives aimed at joint advancement of international approaches, and particularly active cooperation has occurred with such countries as China, Brazil, Japan, Taiwan and South Korea. Rossi has also been a frequent lecturer at IUPAC-sponsored and other international scientific conferences, and has become one of the most influential and respected advocates for regulatory harmonization.

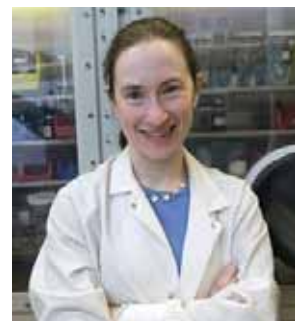


Lois Rossi.

 www.iupac.org

2012 Thieme–IUPAC Prize Awarded to Melanie S. Sanford

On 27 March 2012, Thieme Publishers, IUPAC, and the editors of *SYNTHESIS*, *SYNLETT*, *SYNFACTS*, and *Science of Synthesis* announced that the 2012 Thieme–IUPAC Prize in Synthetic Organic Chemistry was awarded to Melanie S. Sanford of the University of Michigan.



Melanie S. Sanford.

Professor Sanford becomes the 11th recipient of the prize, and joins a select group of scientists under the age of 40 years whose research has had a major impact on the field of synthetic organic chemistry. The prize, which is presented every two years and includes an award of Euros 5000, will be given to Melanie Sanford on July 3, 2012 at the ICOS-19 conference in Melbourne, Australia, after her Thieme–IUPAC lecture.

Professor Sanford has a particular interest in catalysis involving high oxidation state palladium complexes. She has shown that palladium(IV) complexes, which were earlier considered to be inaccessible under ambient conditions, can, with careful design of supporting ligands, be synthesized and studied in detail. More generally, her research program at the University of Michigan is at the leading edge of the use of transition metals to catalyze a variety of important reactions in organic synthesis and in the development of a fundamental mechanistic understanding of these organometallic reactions. She is internationally recognized as one of the foremost investigators in the development of catalytic processes for the site-selective functionalization of C–H bonds, an exceptionally challenging area of chemical research. Her research focus has included the development of new strategies for achieving this ambitious goal, providing the mechanistic understanding of how the reactions work, and clarifying the underlying mechanistic principles in a way that will allow their application in many further classes of reactions.

We heartily congratulate Melanie Sanford and look forward to hearing the latest exciting developments from her laboratories, an Account of which will be published in *Synlett*, at her award lecture in Melbourne, Australia.

 www.thieme-chemistry.com/our-service/thieme-iupac-prize.html

“G-Science” Statements Call for Action on Global Challenges

In May 2012, national science academies of 15 countries issued joint statements calling on world leaders who were about to meet at the G8 Summit and other international gatherings during the year, to give greater consideration to the vital role science and technology could play in addressing some of the planet’s most pressing challenges.

The “G-Science” statements recommend that governments engage the international research community in developing systematic, innovative solutions to three global dilemmas: how to simultaneously meet water and energy needs, how to build resilience to natural and technological disasters, and how to more accu-

rately gauge countries’ greenhouse gas emissions to verify progress toward national goals or international commitments.

The “G-Science” statements were signed by the leaders of national science academies from countries beyond the so-called G8+5. Many of these national science academies have expertise in the areas addressed in the statements, and academies around the world also collaborate and inform policymaking via their participation in groups such as the Global Network of Science Academies, the InterAcademy Council, the Academy of Sciences for the Developing World, and the International Council for Science.

 www8.nationalacademies.org/onpinews/newsitem.aspx?RecordID=05102012

An IYC Periodic Table Project Unveiled

To celebrate IYC 2011, Chem 13 News together with the University of Waterloo Chemistry Department and the Faculty of Science, Waterloo, Ontario, Canada, encouraged chemistry educators and enthusiasts worldwide to adopt an element and artistically interpret that element. The project created a Periodic Table as a mosaic of science and art.

The final product is an amazing table of artwork for each elemental tile designed by chemistry students from all Canadian provinces and territories, 20 U.S. states, and 14 countries. It can be viewed online and is available as a printed poster.

The Periodic Table Project is also displayed as a mural in the foyer of the Earth Science Museum at the University of Waterloo. The official installation of the 25-by-18-foot wall mural (about 8 by 6 meters) was on 10 April 2012. Over 140 people came out for the ceremony, including several of the student-artists who designed elemental tiles. Project sponsors, 3M Canada and the Chemical Institute of Canada, also were on hand to witness the event. 3M Canada manufactured the large wall mural with 3M™ Scotchcal™ Graphic Film for Textured Surfaces, a thin-layer polymer with high resolution and vibrant colors. 3M Canada also designed the electronic applications for the Periodic Table Project including apps for the iPad and Playbook. The celebration was an opportunity for participants,

organizers, and sponsors to gather together, some for the first time, to celebrate the collaborative effort of this International Year of Chemistry project.

 chemistry.uwaterloo.ca/iyc/periodic-table-project
www.chemistry2011.org/participate/activities/show?id=42



Some of the participants who were able to attend the mural installation ceremony held for project participants, organizers, and sponsors on 10 April 2012.

Rules for Abbreviation of Protecting Group

With the goal of presenting information in the scientific literature clearly and unambiguously, a set of rules for the abbreviation of protecting groups will be developed. It will be based on principles designed to be as descriptive and systematic as possible, but also being sufficiently pragmatic and flexible so as to accommodate the most important current abbreviations.

The Task Group's plan is to have an initial draft of the proposed set of rules available for discussion with interested parties at the IUPAC Division III Subcommittee on Organic Synthesis meeting that is to be held during the IUPAC-ICOS meeting in Melbourne in July 2012 (www.icos19.com).

For more information contact the Task Group Chair Margaret Brimble <m.brimble@auckland.ac.nz>.

 www.iupac.org/project/2011-044-1-300

Maintaining and Ensuring the Pesticides Properties Database

The Chemistry and the Environment Division has approved a project to create an international committee of scientists and a funding mechanism to provide continuing maintenance, enhancement, and quality assurance for the PPDB database, currently the best source of chemical and environmental information on pesticides publicly available. The database is currently being operated pro bono by staff at the University of Hertfordshire.

The PPDB is a database built principally from pesticide property data submitted by pesticide manufacturers in support of registration for crop protection chemicals and other uses. It is currently hosted on a server at the University of Hertfordshire, where it was developed. The PPDB is a major development in crop protection science—it is the most authoritative and complete source of chemical, environmental, ecotoxicological, and toxicological information on pesticide active ingredients ever assembled and contains data on 1700 substances. It is widely used free of charge by government, academic, and industry scientists. The development of this database has global significance for chemical science because of the quality and transparency of the information.

Although it is not immediately threatened, its future is not assured; the database is not currently funded

and is kept going in any spare time by the team responsible for it at the University of Hertfordshire, led by Kathy Lewis.

For more information contact the Task Group Chair Donald Wauchope <don_wauchope@citcom.net>.

 www.iupac.org/project/2010-060-1-600

Terminology of Nanomaterials and Nanotechnology in Polymer Science

With the advent of the application of polymers in high-resolution microlithography in the 1970s and thereafter the development of the all-embracing nanotechnology of the late 1980s, terms that are unfamiliar to polymer and materials chemists find ubiquitous use. Nevertheless, it is polymer science and material science that lead progress in these fields and by now scientists need a ready reference to the exact definitions of the unfamiliar terms that they will come across. Typically, microlithographers commonly use terms such as sensitivity, contrast, resolution, and dry etch resistance, and refer to techniques such as solvent development, aqueous-base development, and oxygen reactive ion etching. However, the explosion in so-called nanomaterials has added even less-familiar terminology. What, for example, is the correct definition of a nanostructure, a nanotube, a nanocomposite, a polymer nanofiber, a nanospintronic device, or nanoencapsulation? What is iontophoresis, superparamagnetism, or plasma-enhanced chemical vapor deposition? These and many other terms are now commonplace but precise definitions have never been compiled in one place for the benefit of polymer scientists and materials chemists.

The objective of this new project is to identify and define the terminology that is idiosyncratic to all aspects of the application of polymers in nanotechnology and in particular to high-resolution sub-micron lithography. This follows an earlier project "Analysis of the usage of nanoscience and technology in chemistry" (2007-040-2-200), the scope of which was confined to the mapping and critical evaluation the use of the prefix nano in various fields of chemistry. (See project report online; excerpts to be published in the Sep-Oct 2012 *CI*.)

Most materials of relevance are either polymers or other materials (usually inorganic) in a polymer environment, and the relevant technology invariably involves the manipulation of polymeric mate-

rials. Hence, this project will be led from within the Subcommittee on Polymer Terminology. The Interdivisional Subcommittee on Materials Chemistry will be closely involved to ensure that there will be no development of definitions that might conflict with those arising from future activities in its arena.

For more information contact the task group chairs Chris Ober <cko3@cornell.edu> and Richard G. Jones <kapitimana@googlemail.com>.

 www.iupac.org/project/2012-001-1-400

Metal-Binding Organic Ligands

The trace metals iron (Fe), copper (Cu), nickel (Ni), cobalt (Co), cadmium (Cd), and zinc (Zn) are essential micronutrients to marine phytoplankton, controlling primary productivity in up to half of the open ocean, from tropical to polar regions. Consequently, these metals exert a major influence on the global carbon cycle and play a key role in regulating climate. However, the availability of these metals to the biota is governed by speciation, whereby trace metals are bound by organic ligands that may reduce or enhance metal bioavailability, depending on the metal and the resulting metal-ligand complex. Organic ligands are defined as molecules that can bind to, and form a stable complex with, trace metals in the aquatic dissolved (typically <math><0.2 \mu\text{m}</math>) phase. Electrochemical techniques have shown that trace metals in seawater are overwhelming bound (up to 99.999%) by organic ligands, and that these ligands are ubiquitous in the ocean. More recently, organic geochemical techniques have shown that at least some Fe-binding ligands are produced by the biota. Over the past three decades, major advances in analytical techniques have led to a consensus on accuracy and precision for total dissolved trace metal analyses and dramatically improved our knowledge on the global and regional distributions of trace metals. In contrast, our understanding of trace metal-binding ligands and their pivotal biogeochemical functions remains at a comparatively early stage. To date, we know little about the composition, distributions, and provenance of metal-binding ligands, which is hindering further advances in the field of trace metal biogeochemistry.

By combining the expertise and analytical advances of trace metal biogeochemists, organic geochemists, and modelers, this community is poised to make a significant step towards assessing metal-binding ligands in the ocean and defining new research direc-

tions for metal speciation. This will enable trace metal speciation data to be better incorporated into global climate models to predict how organic complexation, and consequently trace metal cycles, will respond to projected changes in ocean acidification and oceanic oxygen minimum zones. To facilitate this effort, an ICSU Scientific Committee on Oceanic Research (SCOR) Working Group 139: Organic Ligands—A Key Control on Trace Metal Biogeochemistry was formed.

This SCOR Working Group met for the first time in February 2012 following the ASLO Ocean Sciences Meeting in Salt Lake City, Utah, to approve and commence on the Working Group's terms of reference. Members of Working Group 139, comprised of trace metal biogeochemists, organic geochemists, and biogeochemical modelers, have identified three overarching goals to be advanced over a four-year term:

1. promote improvements in quality, accessibility, and development of analytical methodologies for characterizing metal-binding ligands in seawater
2. characterize which components of the dissolved organic matter pool make a significant contribution to biogeochemistry of trace metals in the oceans
3. identify the role of ligands in microbial ecology and marine biogeochemical cycles

Following the first meeting, the Working Group has begun working towards building a database to link trace metal biogeochemistry and organic geochemistry data at established time-series stations, advancing the ligand intercalibration program initiated by GEOTRACES, and summarizing methodological approaches to assess metal-binding ligands in seawater. The next SCOR Working Group 139 meeting will be on 16 February 2013 preceding the ASLO Aquatic Sciences Meeting in New Orleans, Louisiana. We have proposed a scientific session for the Aquatic Science meeting to complement the SCOR Working Group 139 goals.

Anyone interested is welcome to join our e-mail list by contacting the co-chairs and to participate in the proposed scientific session. Information, progress, and updates on future meetings, database development, and upcoming intercalibration exercises may be found via the SCOR website.

 www.scor-int.org/Working_Groups/wg139.htm

For more information, contact Kristen N. Buck <kristen.buck@bios.edu>, Bermuda Institute of Ocean Sciences, Bermuda; Maeve C. Lohan <maeve.lohan@plymouth.ac.uk>, University of Plymouth, United Kingdom; or Sylvia G. Sander <sylvias@chemistry.otago.ac.nz>, University of Otago, New Zealand.

Chlorine-Free Synthesis for Green Chemistry

F. Arico, A. Vavasori, Z. Liu, and T. Jiang (eds.)
Special Topic Issue, *Pure and Applied Chemistry*,
2012, Vol. 84, No. 3, pp. 411-860

A special topic issue of *Pure and Applied Chemistry* published in March 2012 and titled "Chlorine-free synthesis for Green Chemistry" explores the restriction, or preferably prevention, of the use of halogenated compounds, whenever feasible, through the assembly and reporting of already identified information. Innovative synthetic pathways using clearly identified production drivers (e.g., environmental and health impact, energy consumption, economical feasibility, etc.) have been elucidated. In past decades, scientific knowledge and feasible technologies were unavailable, but now there is enough expertise to pursue discontinuation of hazardous and toxic reagents. This PAC Special Topic issue presents a collection of useful and industrially relevant examples for alternatives to chlorine in synthesis.

Overview

by *Pietro Tundo**

In the last 20 years, chemists have put enormous effort into designing chemicals with various applications ranging from medicines and cosmetics to materials and molecular machines. However, for the most part, their work demonstrated a quite surprising lack of interest in taking hazards into consideration in the design process. The goal was often to design substances that were robust and could last as long as possible. This philosophy has resulted in a legacy of persistent toxic and bio-accumulative substances and lingering toxic waste sites. Nowadays, it is known that it is more desirable to avoid substances that persist indefinitely in the environment or in a landfill, and to replace them with substances designed to degrade after use. Polymeric materials, for instance, should have no negative effect on the environment during their production, utilization, or disposal. Therefore, the

* Department of Environmental Sciences, Ca' Foscari University of Venice, Venice, Italy; E-mail: tundop@unive.it; reproduced in part from *PAC* 84(3), pp. 411-423, 2012; <http://dx.doi.org/10.1351/PAC-CON-12-02-02>.

design of safer chemicals cannot be limited to hazards associated with the manufacture and use of the chemical, but also to its disposal (i.e., its full life cycle).

Among halogens, chlorine is by far the most abundant chemical in nature and also the easiest to produce and use. This explains its predominant and seemingly irreplaceable role in the chemical industry (see figure). Five hundred companies at 650 sites around the world have the capacity to produce over 58×10^6 tonnes of chlorine and 62×10^6 tonnes of its co-product, caustic soda, per year.

For example, the European chloro-alkali industry had a production in 2009 of 9.1×10^6 tonnes at about 80 plants, mostly (about 95 percent) via electrolysis-based techniques (chlor-alkali industry); the sector directly employs about 40 000 people in 20 European Union countries. Germany is Europe's largest chlorine producer, accounting in 2009 for 43.5 percent of European production.¹ Owing to their peculiar characteristics, halogens are widely used by all sectors of the chemical industry to produce solvents, catalysts, building blocks, additives, and drugs. Chlorine is a major building block in today's chemistry. More than 90 percent of pharmaceuticals contain or are manufactured using chlorine, which is also used in the production of 86 percent of crop protection chemicals. Furthermore, halogens are contained in several commodities that we all use daily as plastics (e.g., chlorine is contained in polyvinyl chloride, PVC, one of the most widely used plastic materials), solvents for dry cleaning and metal degreasing, textiles, agrochemicals and pharmaceuticals, insecticides, dyestuffs, household cleaning products, and disinfectants. Chlorine is used extensively in organic and inorganic chemistry as an oxidizing agent (i.e., water disinfectant) and as a leaving group in substitution and elimination reactions.

Chlorine compounds find use as intermediates in the production of a number of important commercial products that do not contain chlorine. Foremost examples are polycarbonates, polyurethanes, silicones, polytetrafluoroethylene, carboxymethyl cellulose, and propylene oxide.

Through a chain of chemical derivatives and relatively easily made compounds and intermediates, such molecules have used the intrinsic energy available through the use of chlorine primarily produced via electrolysis.

Environmental and Health Concerns

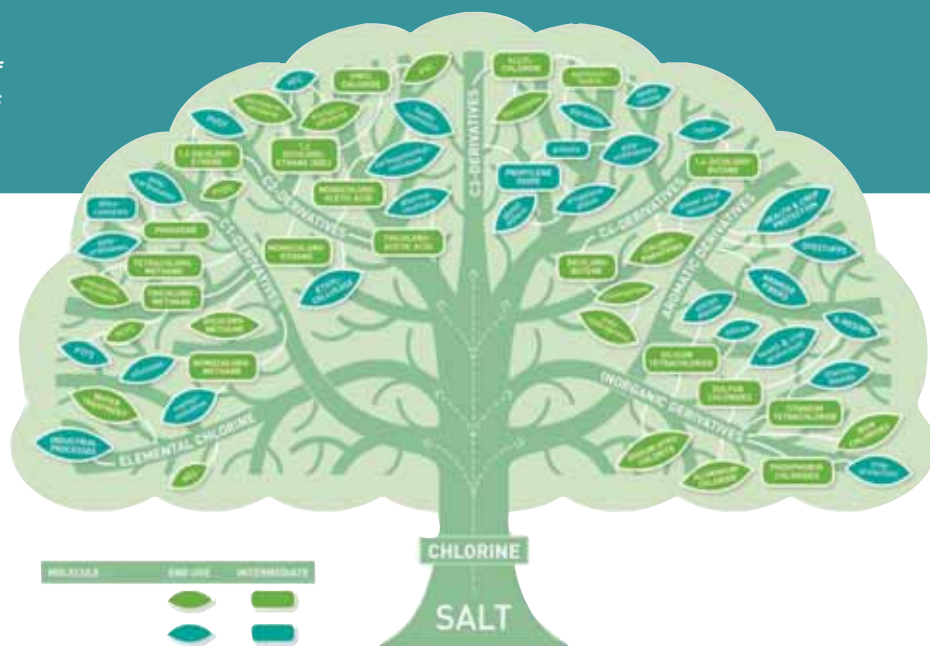
The widespread use of halocarbons was often driven by observations that most of them were more stable

than other substances. Their stability tended to encourage beliefs that they were mostly harmless, but starting from the mid-1920s it was discovered that they can cause chloracne or fatal liver diseases in workers in the chemical industries. By the 1950s, toxicity and health hazards related to halocarbons were widely reported. Concerns about the environmental and health impact of halocarbons were first raised early in the 1960s in studies about

DDT and other halocarbon pesticides. Today, they are widely recognized as persistent pollutants and doubts were recently (2006) raised even about very stable molecules such as perfluorooctanoic acid (PFOA) and Teflon, just to mention a few.

Today, European and international legislation for environmental protection is becoming stricter and recognizes that there is a growing need for replacement of halogenated compounds at a productive and end-user level. Besides EU directives, which tackle global environmental concerns (e.g., sustainable development) through prescription about chemical production in the frame of a multi-sector approach (political, scientific, economical, and social), some regulations are specific to ban or restrict the production of some chemical compounds or byproducts at an industrial level.

The EU has recently established REACH (Registration, Evaluation, Authorization and Restriction of Chemicals), a single integrated system for the registration, evaluation, and authorization of chemicals, together with the European Chemicals Agency (ECHA). REACH requires firms that manufacture and import chemicals to evaluate the risks resulting from the use of those chemicals and to take the necessary steps to manage any identified risk. Industry has the burden of proving that chemicals placed on the market are safe. By the end of 2008, ECHA received approximately 2.75 million requests for preliminary authorization concerning about 150 000 compounds collected in an ECHA online database. Among them, over 20 000 substances are chlorinated and more than 4 000 are brominated (this excludes those where "chlorine is used in the making", which would increase these numbers considerably). The process for authorization will be long (possibly ending in 2018), but a significant fraction of halogenated substances are at



risk of rejection, thus forcing their replacement at a productive level.

Furthermore, some international conventions ban or restrict production of specific chemicals. At least two need to be mentioned. The Stockholm Convention on Persistent Organic Pollutants (most of which contain chlorine; byproducts of both domestic and industrial activities) and the Montreal Protocol on Substances that Deplete the Ozone Layer which control the phase-out of ozone depleting substance (ODS) production and use. The application of both is managed by the United Nations Environmental Program, and all their prescriptions will come into force within 2020. Finally, we must cite the Kyoto Protocol about greenhouse gas (GHG) emissions, which was adopted almost worldwide and then mostly disregarded. International agreements about a follow-up to the Kyoto Protocol are currently in progress.

Today, the European and international legislation and EU directives for environmental protection are becoming stricter and recognize that there is a growing need for replacement of particular halogenated compounds at a productive and end-user level. In 2007, the Intergovernmental Panel on Climate Change stated that some halocarbons were a direct cause of global warming, owing to their nature as GHGs. Some of them are ODSs. Halogen-based materials may show an indirect toxicity or eco-toxicity, releasing halogen atoms/molecules and/or harmful compounds (e.g., in case of accidental fires, a case of particular interest for the electric distribution industry).

Energy

Since the industrial revolution, the halogen chlorine remains "an iconic molecule" for industrial chemical production. Even though its production by the electrolysis of sodium chloride is very energy-intensive,

it is still used because it allows the manufacture of chlorinated derivatives in a very easy way, owing to its high energy and reactivity; for example, easily obtained from chlorine are AlCl_3 , SnCl_4 , TiCl_4 , SiCl_4 , ZnCl_2 , PCl_3 , PCl_5 , POCl_3 , COCl_2 , etc., which in turn are pillar intermediates in the production of numerous everyday goods. This kind of chloride chemistry is widely utilized because the energy is transferred to these intermediates, making further syntheses easy; a good number of fundamental reactions of the industrial production are based on the synthesis of chloride compounds obtained by reaction with SOCl_2 , COCl_2 , or AlCl_3 as a catalyst.

Besides their (eco-) toxicity, a major concern with chlorine derivatives is the large amount of energy necessary for their production, and this is why chlorinated molecules have both a direct (as GHGs) and indirect (CO_2 production) impact on climate change at a global level.

Estimates of the global warming potential (GWP) resulting from chlorine use by the chlorine industry in Europe is 0.29 percent of the total GWP, while the estimate from the primary energy consumed is 0.45 percent of the total GWP.

The chlorine industry is extremely energy-intensive: its CO_2 emissions is comparable to that of the iron and steel industry and higher than for cement (1.5 kg CO_2 /kg for the chlorine industry vs. 1.7 for iron and steel and, 0.95 for cement) and that for a world production of the order of 40×10^6 tonnes (covering Europe and China in 2008) vs. 1.2×10^9 tonnes of iron and steel, and 2.3×10^9 tonnes of cement.²

Beyond Chlorine Chemistry

Can we pursue an intrinsically safer, cleaner, and more energy-efficient alternative to chlorine chemistry? Many of society's greatest challenges and fortunes depend on the development of the chloro-alkali industry; but is chlorine-based chemistry sustainable?

Chlorine-based chemistry very often does not obey the principles of atom economy and waste minimization introduced, respectively, by B. Trost³ and R. Sheldon⁴; in fact, halogen anions are byproducts of many organic reactions and represent a waste to be disposed of. The environmental and health constraints (toxicity and eco-toxicity, ozone layer depletion) and the growing need for energy (energy efficiency, climate change) force us to take advantage of available

knowledge to develop a new chemical strategy. By the motivation given, it seems appropriate to refer to chlorine-free chemistry as "beyond-chlorine chemistry."

The beyond-chlorine strategy has two approaches, bottom-up and top-down, as follows:

- The bottom-up approach involves investigating halogen-free reactions and processes on a lab scale in academies and then scaling them up for production by industry (the most appropriate term would be green chemistry).
- The top-down approach involves industry collaboration with academic partners to design halogen-free alternatives for industrial products and processes (the most appropriate term would be sustainable chemistry).

Beyond-chloro does not mean, of course, that we should avoid chloride anion, for example in foods or as disinfectant. The substitution of chlorine compounds and of compounds where "chlorine is used in the making" means that we avoid electrolysis as the primary energetic source; however, this makes chemistry "without chlorine" considerably more difficult and illustrates why it has not been adopted before.

The rationale behind this Special Topic issue is to seek useful and industrially relevant examples for alternatives to chlorine in synthesis, so as to facilitate the development of industrially relevant and implementable breakthrough technologies. The 29 papers included in the issue are partitioned into the following parts:

1. Chlorine-Free Reagents And Reaction Selectivity
2. Chlorine-Free Catalysts
3. Carbonate Chemistry
4. Chlorine-Free Solvents
5. Benign Chloro-Free Methodologies
6. Metrics On Chlorine-Free Syntheses

 www.iupac.org/publications/pac/84/3/

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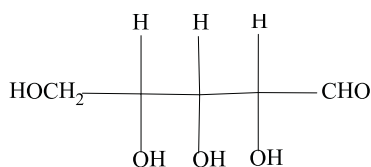
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Nomenclature Notes

Non-IUPAC Nomenclature Systems

by Jeffery Leigh

In the second “Nomenclature Notes” (May-June 2012 *CI*, p. 28) we alluded to various kinds of nomenclature that fall under the aegis of IUPAC. There are other nomenclatures in wide use, to some of which IUPAC contributes. For example, biochemical nomenclature is reviewed regularly by a committee which has joint membership from both IUPAC and IUBMB (International Union of Biochemistry and Molecular Biology). It is fair to say that biologists and biochemists are often not interested in systematic nomenclature in the way that chemists are. For them it may be sufficient that a given name is specific and defined so as to make the compound to which it refers unequivocally and universally recognized within the discipline. The IUPAC requirement that a name should convey the structure of a compound is not necessary or even desirable, as long as all practitioners accept it. For example, the compound



may receive a perfectly good IUPAC name, 2,3,4,5-tetrahydroxypentanal, but this might not be recognizable to biochemists unless the compound were named as a sugar, specifically an open-chain form of ribose. As this molecule also contains three chirality centers (asymmetric carbon atoms) to which are assigned the locants 2, 3, and 4, a more complete name would be (2*R**,3*R**,4*R**)-2,3,4,5-tetrahydroxypentanal. Biochemists would also prefer to know the absolute configuration at carbon atom 4, representing it by small capital letters, either *D* or *L*, and they would be very comfortable with a name such as *D*-ribose. When even more complex structures are considered, such as amino acids, steroids, and proteins, the use of defined but semisystematic names becomes necessary for ease of communication and comprehension in biochemical and biological contexts.

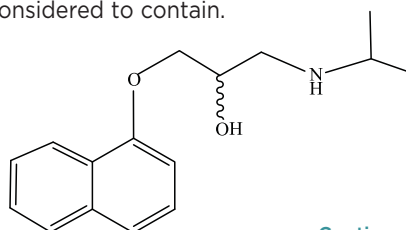
A system of nomenclature which is independent of IUPAC, but which is widely used by chemists, is due to the Chemical Abstracts Service (CAS) of the

American Chemical Society. This has been developed to produce names for CAS use in both running text and indexes. Although nomenclaturists of CAS have contributed substantially to IUPAC, they cannot afford the leisurely contemplation of data in which IUPAC indulges. They have to make decisions rapidly to meet publication deadlines, and CAS names are designed to be adaptable for use in indexes. Because an index compiler would wish to locate all derivatives of, say, the parent compound butane, at the same place in the alphabetical index, CAS names are sometimes termed “inverted,” because, in this specific case in an index the parent name butane would always be cited first. In its Index Guide, CAS explicitly states that, outside of a CAS index, a name should be used in its uninverted form. In contrast, IUPAC nomenclature presents a name written in a continuous and linear fashion from left to right, and which contains prefixes and suffixes in a specific, linear order. The consequence is that IUPAC names for derivatives of a given parent compound would appear at different places in an index using IUPAC names because the initial letters of the names depend upon the specific prefixes employed. Two examples follow:

IUPAC, 2-sulfanylethanol CAS, 2-mercaptoethanol CAS inverted, ethanol, 2-mercapto-

In a similar sequence, we have: 4-(methylsulfanyl)benzoic acid, 4-(methylthio)benzoic acid, and benzoic acid, 4-(methylthio)-

In addition to these nomenclatures, others are current in the literature. IUBMB categorizes and specifies and names of enzymes according to the types of reaction they catalyze. Considerations of enzyme chemical structure are secondary here. The World Health Organization produces a list of nonproprietary names for drugs which are shaped so as to allow easy conversion to languages other than English and which indicate the action of the drug. Hence, the names of beta-blockers all carry the ending -olol. An example is propranolol, the structure of which is hardly reminiscent of that of propane, though the name was apparently suggested in part by the propane residues it may be considered to contain.



Continued on page 31.

Mendeleev's Periodic Table Is Finally Completed and What To Do about Group 3?

by Eric Scerri

The ninth of April 2010 was a rather special date for the discovery of the elements. First of all, it was the day on which an article was published in a physics journal to announce the synthesis of element 117. Second, and perhaps more important, it represented the completion of the 7th row in the periodic table, which contains 32 elements. As of that day, the periodic table of Mendeleev was finally completed in a way that it never was before. This is because there are now absolutely no gaps in the periodic table, although there may well be some new elements to follow in a 8th row that will probably begin to form very soon. Such a situation has never existed before because in the past there were always gaps within the boundaries of the elements that had already been discovered.

To appreciate the full impact of this development, we need to briefly consider the history of the periodic table. It was discovered over a period of about nine

years from 1862 to 1871.¹ There were several different versions of the table published, but what they all had in common was this; if all the elements were arranged in a sequential fashion based on the weights of their atoms, the elements showed an approximate repetition after a particular sequence of elements. In these early periodic tables things appeared to be rather simple because the repeat distance, or length of each period, was the number eight throughout the table. Among these short-form tables, the one designed by the Russian chemist Dimitri Mendeleev is widely considered to be the most important, displaying Group I to VIII over 8 columns and 12 series (or periods) as shown in figure 1.

As the table shows, Mendeleev left a number of gaps in his table. He was more or less forced to do this in order to make the other elements fall into vertical columns to reflect their similar chemical and physical properties. The periodic table therefore began life with many gaps within it.

Mendeleev, unlike some of the other discoverers, made predictions about the properties of these missing elements. As is also well known, many of his predictions turned out to be remarkably accurate.

As time went by, it became increasingly clear that a better design for the periodic table could be obtained by relaxing the notion that all periods have the same number of elements. It was realized that period lengths show a variation and that the 4th and 5th periods show a length of 18 elements, as shown in the medium-long form (figure 2). Rather than lump-

ing together say lithium (Li), sodium (Na), potassium (K), copper (Cu), silver (Ag), and gold (Au) as Mendeleev had done, it is better to separate the first three from the last three of these elements to form two different groups. This change was also applied systematically to a number of other groups in Mendeleev's original table. As a further example, beryllium (Be), magnesium (Mg), and calcium (Ca) which Mendeleev initially placed in the same group as zinc (Zn), cadmium (Cd), and mercury (Hg) now gave rise to two new groups. The net result of these changes was to

Figure 1. Short-form or eight column periodic table as devised by Mendeleev in 1871.

MENDELÉEFF'S TABLE I.—1871.

Series.	GROUP I. R ₂ O.	GROUP II. RO.	GROUP III. R ₂ O ₃ .	GROUP IV. RH ₄ , RO ₂ .	GROUP V. RH ₃ , R ₂ O ₅ .	GROUP VI. RH ₂ , RO ₃ .	GROUP VII. RH, R ₂ O ₇ .	GROUP VIII. RO ₄ .
I	H=1							
2	Li=7	Be=9.4	B=11	C=12	N=14	O=16	F=19	
3	Na=23	Mg=24	Al=27.3	Si=28	P=31	S=32	Cl=35.5	
4	K=39	Ca=40	—=44	Ti=48	V=51	Cr=52	Mn=55	Fe=56, Ce=59 Ni=59, Cu=63
5	(Cu=63)	Zn=65	—=68	—=72	As=75	Se=78	Br=80	
6	Rb=85	Sr=87	? Y=88	Zr=90	Nb=94	Mo=96	—=100	Ru=104, Rh=104 Pd=106, Ag=108
7	(Ag=108)	Cd=112	In=113	Sn=118	Sb=122	Te=125	I=127	
8	Cs=133	Ba=137	? Di=138	? Ce=140
9
10	? Er=178	? La=180	Ta=182	W=184	Os=195, In=197 Pt=198, Au=199
11	(Au=199)	Hg=200	Tl=204	Pb=207	Bi=208	
12	Th=231	U=240

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo		Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La		Ta	W		Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po		Rn
	Ra	Ac	Th		U												

Ce	Pr	Nd		Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
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Figure 2. Medium-long form periodic table as it looked circa 1915 with seven missing elements between the old boundaries from hydrogen to uranium.

period of 32 elements was discovered by the American chemist Glen Seaborg while he was in the process of attempting to synthesize more new elements. Seaborg realized that the elements actinium (Ac), thorium (Th), protactinium (Pa), and uranium (U) did not belong in the places shown in figure 2, but that they formed part of a new 14 element series which became known as the actinides. Now, the case for arranging the elements in a long-form table became more compelling. Seaborg and others began to

produce what is termed the medium-long form periodic table as shown in figures 2 and 3.

Notice that there are several gaps in this periodic table. In 1914, Moseley discovered that it was better to order the elements according to atomic number rather than atomic weight. This change resolved a number of “pair reversals” such as the one involving the elements tellurium (Te) and iodine (I) which were incorrectly ordered according to the atomic weight criterion.

But the use of atomic numbers did not result in any profound changes to the form of the periodic table although it did eventually reveal that there were precisely seven gaps to be filled within the limits of the old periodic table, consisting of the elements ranging between atomic numbers 1 (hydrogen) and 92 (uranium).

Meanwhile, a separate development was taking shape. As far back as the earliest periodic tables it had been evident that some elements could not easily fit into the system at all. This became such a difficult problem for Mendeleev that he handed the task to a Czech colleague, the chemist Boruslav Brauner who had some partial success. The elements in question included cerium (Ce), praseodymium (Pr), and neodymium (Nd) that are so similar that they appear to belong in the same place in the periodic table. But this would be going against a basic principle of the periodic table, namely one element, one place.

Another solution was to place these so called rare earth elements into a separate row at the foot of the main body of the table as seen in figures 2 and 3. Some chemists realized that this move necessitated an even longer period consisting of 32 elements, but this did not have any serious influence on those who designed periodic tables who stuck with the medium-long format and its 18 columns.

Starting in the 1940s, new elements began to be synthesized, thus extending the periodic table beyond the original 92 elements. Soon afterwards, a second

publish long-form tables such as in figure 4.

Curiously though, such long-form designs are still not the most commonly encountered format of the periodic table in textbooks and wall charts. This is likely because it is not very convenient to represent the periodic table in this more correct form. Such tables stretch a little too far horizontally and so tend to be avoided by designers of periodic tables, even though everyone agrees that they are scientifically more correct. One clear advantage that the long-form table has is that it lists all the elements in sequential order of increasing atomic number whereas the medium-long form displays a couple of anomalous jumps which occur between barium (Ba) and lanthanum (La) and another between radium (Ra) and actinium (Ac).

In any case, whether the medium-long or long-form table was used, there were still several gaps that

Figure 3. Medium-long form periodic table (reproduced from reference 1).

H																	He	
Li	Be											B	C	N	O	F	Ne	
Na	Mg											Al	Si	P	S	Cl	Ar	
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
Rb	Sr	Y	Zr	Nb	Mo		Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
Cs	Ba	La		Ta	W		Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra																	

La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No

Editors note: The latest release of the Periodic Table of the Elements, dated 1 June 2012, is reprinted on the back cover pull-out of this issue. It includes, for each element, its symbol, name, atomic number, and standard atomic weight.

Up for Discussion

1	2												3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18			
H																													He		
Li	Be																	B	C	N	O	F	Ne								
Na	Mg																	Al	Si	P	S	Cl	Ar								
K	Ca															Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr															Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn						

H																													He		
Li	Be																	B	C	N	O	F	Ne								
Na	Mg																	Al	Si	P	S	Cl	Ar								
K	Ca															Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr															Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn						

H																													He			
Li	Be																	B	C	N	O	F	Ne									
Na	Mg																	Al	Si	P	S	Cl	Ar									
K	Ca	Sc																Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y																Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
Fr	Ra	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn							

Figures 4–6 (top to bottom): Three different long-form, or 32-column, periodic tables with differences highlighted.

Figure 4 (top): Version with group 3 consisting of Sc, Y, Lu, and Lr.

Figure 5 (middle): Version with group 3 consisting of Sc, Y, La, Ac. The sequence of increasing atomic number is anomalous with this

assignment of elements to group 3, e.g., Lu (71), La (57), Hf (72).

Figure 6 (bottom): Third option for incorporating the f-block elements into a long-form table. This version adheres to increasing order of atomic number from left to right in all periods, while grouping together Sc, Y, La and Ac but at the expense of breaking up the d-block into two highly uneven portions.

remained to be filled in the seventh row of the table. As more and more elements were synthesized these gaps were reduced until the last piece in the jig-saw puzzle was filled on 9 April 2010 with the announcement of the discovery of the elusive element 117.

The Group 3 Question

In an article in the Jan-Feb 2009 issue of *Chemistry International*, page 5, Jeffrey Leigh correctly pointed out that IUPAC does not take a position on what should be regarded as the correct periodic table.² There is no such thing as an IUPAC-approved table, contrary to the label “IUPAC periodic table” that one might see in some books or on certain websites.

Leigh was responding more specifically to the debate that had been conducted, mostly in the chemical education literature, concerning the membership of

group 3 of the periodic table.³ In this article, I propose that IUPAC *should* in fact take a stance on the membership of particular groups even if this has not been the practice up to this point. This would not of course amount to taking an official position on an optimal periodic table since it would concern the placement of elements into groups rather than any other aspect of the periodic table such as what shape or form it should take or whether it should be two or three dimensional.

Some years ago, following some work by physicists, it was pointed out that the elements lutetium (Lu) and lawrencium (Lr) show greater similarities with scandium (Sc) and yttrium (Y) than do lanthanum (La) and actinium (Ac).⁴ As a result, many textbooks and websites, but by no means all of them, have adopted this new version of group 3 (as depicted in figure 3). This has led to a situation in which chemistry students and professionals alike are often confused as to which

Up for Discussion

version is more “correct” if any. Quite apart from arguments based on electronic configurations, chemical and physical properties, which are not completely categorical, I will present an argument here that I believe renders the newer grouping of Sc, Y, Lu, and Lr rather compelling.⁵

In addition to arranging all the elements in a more correct sequence of increasing atomic numbers, the decision to move to a long-form or 32-column table forces the periodic table designer towards just one possible option regarding the question of which elements to place in group 3. The natural choice, turns out to be the placement of Lu and Lr into group 3, as seen in figure 4, because the other option fails to maintain an orderly increasing sequence.

I suggest that any reluctance to accept this grouping as opposed to the more frequently seen grouping of Sc, Y, La, and Ac (as shown in figure 5) stems entirely from a reluctance to display the periodic table in its 32-column format. If this obstacle is removed and the rare earths are taken up into the main body of the table the choice of how to do so is almost entirely in favor of a group 3 consisting by Sc, Y, Lu, and Lr.

I say “almost entirely” because there does exist a third option, although this can be dismissed on the grounds that it represents a very asymmetrical possibility. As seen in figure 6, the third option requires that the d-block elements should be broken into two very uneven portions consisting of one group, followed by the insertion of the f-block elements and continuing with a block of nine groups that make up the remainder of the d-block elements. Indeed, this form of the periodic table is also sometimes encountered in textbooks and articles, although this fact does not render it any more legitimate.

Of course, there may still be a preference for an 18-column table among many authors, in which case

one can easily revert to the form in figure 3, but with the knowledge that the group 3 issue is now resolved. At the risk of repeating myself, it is this question which I believe is in need of resolution and not the issue of the best shape for the periodic table, or indeed, whether it should be presented in a medium-long or long form. I am not, therefore, suggesting a change of IUPAC policy regarding a commitment to an “optimal format” for the periodic table. The latter must remain as a choice for textbook authors and individual periodic table designers.

Finally, given that the periodic table is now complete for the first time, and probably not for long, would it not be an occasion for IUPAC to turn its attention to the central icon and framework of chemistry in order to resolve a remaining issue that continues to confuse seasoned practitioners and novices alike? And who knows what discoveries might lie ahead if a more precise grouping of elements in group 3 were to be established after all the available evidence has been suitably weighed by the relevant IUPAC committees.

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 <http://ericscerri.com>

continued from page 27, *Nomenclature Notes*

The International Organization for Standardization lists names for pesticides, which bear a fleeting similarity to IUPAC names; for example, “trimesium” stands for “trimethylammonium.” There is also list of recommended names for cosmetic ingredients, the International Nomenclature of Cosmetic Ingredients. What characterizes these latter names is that they serve as specific identifiers for commercial and industrial materials which must be quickly recognizable by users who are nonchemists, but they are usually

inadequate for use by chemists. All these non-IUPAC nomenclatures are briefly described in the new edition of *Principles*, together with references allowing the reader to obtain more detailed information should it be required.

Jeffery Leigh is the editor and contributing author of *Principles of Chemical Nomenclature—A Guide to IUPAC Recommendations, 2011 Edition* (RSC 2011, ISBN 978-1-84973-007-5). Leigh is emeritus professor at the University of Sussex and has been active in IUPAC nomenclature since 1973.

 www.iupac.org/web/ins/2006-029-1-800

Next in this series will be a review of systematic and trivial nomenclatures.

Delivering Data in Science

by John R. Helliwell and Brian McMahon

Nowadays, there are many high-level activities focusing on the management of research data sets, their archiving and their re-use—in effect, their publication. On 5 March 2012 ICSTI, the International Council for Scientific and Technical Information, convened a one-day workshop, held at ICSU headquarters in Paris, on “Delivering Data in Science” to survey some of the most pressing issues.

The session on Data and the Policy Makers opened with an account by Ray Harris of the SCCID, the ICSU Strategic Coordinating Committee on Information and Data that he chaired between 2009 and 2011. As ICSU is an interdisciplinary and international body, the importance of these recommendations lies in their representing the priorities for science worldwide. The committee’s six main recommendations related to scientific data were as follows:

1. ICSU National and Union Members should adopt a guide to best practice (presented in the SCCID report) covering aspects of data policy, governance, planning and organization, standards and tools, management and stewardship, and data access. This should help to foster a common view of the significance of these issues across all domains.
2. ICSU Members should explore and agree on the terms used under the umbrella of “Open Access” to clarify a very muddled terminology and in consequence help to distinguish and prioritise factors leading to universal and equitable access to publications (guided by ICSTI and INASP) and data (CODATA).
3. ICSU Members should improve the whole process of creating data as a publication, with increased academic recognition, appropriate behavior modification, and a possible role for legal deposit libraries in providing infrastructure or services.
4. ICSU should use its affiliated organizations, CODATA and the World Data Service, more actively in managing large-scale data activities.
5. Practical help needs to be given to less economically developed countries, again using the existing networks of ICSU and its affiliated bodies.
6. There should be greater interaction with the private sector to use commercial expertise and resources for mutual benefit.

One potential weakness of SCCID’s analysis of data management is that it does not consider separate strategies for “raw” versus “processed” data. In part, this is a philosophical decision—many of the technical challenges of handling electronic information do not depend on the nature of that information within the scientific experiment/publication life cycle. Nevertheless, several later presentations did demonstrate how different strategies needed to be applied in different scientific fields to data that had undergone various stages of processing. In crystallography, IUCr Journals and Commissions have long promoted the exemplary position of requiring coordinates and structure factor amplitudes (our “processed data”) to be deposited. The IUCr’s Diffraction Data Deposition Working Group is now wrestling with the possible next step of archiving the “raw data.”

Four succeeding presentations at the workshop gave a survey of policy and funding support available from national and regional funding organizations, which will have a key role to play in realizing the vision laid out by ICSU.

Stefan Winkler-Nees discussed the recommendations on data of the Alliance of German Science Organizations. Research funding in Germany has a division of responsibilities between the federal government and the regional Lander, and in part by German research institutions’ traditionally strong relationships with private industry. Nevertheless, common principles for archiving and free access to publicly-funded research data have emerged that are similar to those of other countries, and there is a significant investment in funding to assist German science organizations to realize these principles. The speaker referred to a frequent perception among some authors that suitable data archiving was to “stuff a CD or DVD in a desk drawer”—clearly not easily accessible to a wide readership and subject to the author remaining alive during the lifetime of the publication. The working group learned that universities, at least in the UK, are beginning to wake up to the need to provide their staff with centralized archives not only as good practice but also to avoid inadvertent research malpractice.

Carlos Morais-Pires of the European Commission described the preparations for the next European framework program for research development and innovation (Horizon 2020) and emphasized the positive commitment to research and development, mirrored by a likely increase in funding of 40–45 percent over the coming seven-year period. Much of the commission’s emphasis will be towards Open Science, in the belief that open content, open infrastructures, and

an open culture will work together to create optimal sharing of research results and tools. The impetus for data management strategy in this program comes from the influential *Riding the Wave* report of October 2010.

Rob Pennington of the U.S. National Science Foundation described the cyberinfrastructure for the 21st Century program (CIF21), which will make some USD 200 million available for data infrastructure investment. NSF has been very keen to assess how best to distribute funding within the new and still poorly understood paradigm of data-driven science. Pennington described the detailed consultation and review processes that have informed CIF21. It is built around several grand challenges, but is seeking to provide multidisciplinary and multiscale integration to draw real and useful science out of the sea of data. While NSF feels that it has been “behind the curve” in this area, it is moving forward with a very strong and focused commitment. Already funded projects are required to provide a data archiving plan in grant proposals and account for themselves in their annual reports to the NSF and at the end of their grant awards. This “policin” of its own policy is an important step in itself.

Runda Liu, a replacement for Peng Jie of the Institute of Scientific and Technical Information of China (ISTIC), described the Chinese Scientific Data Sharing Project of which ISTIC is an active participant. China wishes to follow the western model of data sharing and reuse across research institutes and end users, and has been building up a national distributed network that now includes 10 data centers and over 100 branches and nodes, covering over 3000 databases. China is an active participant in CODATA activities and is enthusiastic about participation in the World Data System. ISTIC works with the Wangfang Data Agency to provide digital object identifier (DOI) registration for scientific data sets in China, and there is significant investment in the development of scientific data classification and navigation systems, and building an Internet platform for scientific data resource information.

A session on “Data in Practice” brought some ground-level perspectives to these high-minded policy objectives. Todd Vision described DRYAD, a system within the life sciences that allows authors to deposit their supporting data sets at the same time as they submit a research article for publication. Currently there are 25 journals with deposition/submission integration in this field; each deposited data set has a unique DataCite-supplied DOI. The philosophy behind

the system has been to make it easy and low-cost for authors to deposit their data, and this strategy is broadly working. The down side, however, is that the deposited data sets are described by limited meta-data. There is some encouraging evidence of re-use of deposited data sets by other researchers; but there is also some concern that providing too easy a route for deposition might hurt existing curated data centers by diverting material away from them.

If DRYAD handles “long-tail” scientific data, the opposite extreme is faced at the particle physics facility CERN, as described by Tim Smith. In 2012, over 22 petabytes of data were recorded on the Large Hadron Collider (LHC), although this is only a fraction of the amount that can be generated by the experiments. CERN must invest heavily in data filtering procedures to trap only the small fraction of the experimental results that may be of interest to specific experiments. Even then, the large volume of data (most of which is reduced and analyzed in research institutions outside of CERN) requires very large data storage facilities distributed around the world, and dedicated high-bandwidth optical private networks to transport the data between nodes. An interesting feature of particle-physics “information” was that, as one moved along the data pyramid from large volumes of raw data through smaller volumes of processed data to the relatively small volume of published results, the proliferation of multiple copies of more highly processed information actually amplified the data management problem. It was estimated that the 22 petabytes of raw data collected in a year gave rise to a total of 70 petabytes of duplicated and derivative data that needed to be tracked, verified, and reconciled. One beneficial aspect of the data explosion was that for each generation, the archiving of previous generations’ output (including content migration to new-generation media) became progressively less burdensome. Another feature of the LHC’s data output is that the data is not really digestible by many other research workers; it is almost as if all those that could digest the data are already co-authors on the publication(s)!

Toby Green of OECD demonstrated the visualization and access gateways to data sets published by the Organisation for Economic Cooperation and Development. Where there is a significant holding of well-characterized and homogeneous data, it becomes cost-effective to develop tools to make it easier for end-users to access and visualize those data. For the OECD data sets, simple web-based applications allowed the extraction and combination of data sets in many ways. Very granular dataset DOIs facilitated

Conference Call

linking statistical tables to publications, and the potentially difficult issues of tracking time-variable data sets were being tackled initially by detailed versioning.

The after-lunch session on Global Initiatives began with a description by Michael Diepenbroek of the ICSU World Data System, the federation of data centers largely in the earth sciences. Much of the impetus behind this system is the establishment of common norms of quality and interoperability across a very diverse spread of activities, and early attention is focusing on organizational aspects, including the establishment in Japan of a coordinating International Program Office. Among the technical aspects of the new system are the orderly registration of DOIs and linking to associated publications in a way that will give due credit to those collecting and curating the data.

Jan Brase, Managing Agent of DataCite, and overall Chair of the Workshop, explained how DataCite acted to register data DOIs across the sciences.

Geoffrey Boulton previewed the forthcoming Royal Society policy report "Science as an open enterprise", which would discuss the major policy issues surrounding research data management, drawing on recent cases such as the "Climategate" affair and on the perception that the data deluge offers both challenges, in terms of handling vast quantities of data, and opportunities to involve a wider research community, and indeed the citizen scientist.

Françoise Genova closed this session with an account of the Astronomical Virtual Observatory, a good example of a discipline-wide and international approach to data handling and linking to publications.

In the final session, Publishers and Data, three academic publishers gave their perspectives on the integration of data management and archiving with the much longer-established business of learned journals.

Eefke Smit of the International Association of STM Publishers (representing over 100 publisher members) described some individual journal initiatives to enhance scientific articles through linking to associated data sets, and spoke also of the PARSE-Insight survey ("Permanent Access to the Records of Science in Europe") that had identified the current patchy distribution of scientific data archived in orderly and accessible ways. Fred Dylla of the American Institute of Physics (AIP) preferred to emphasise the traditional added value of the publishing enterprise and see integration with supporting data as a simple extension of the existing paradigm. Alicia Wise of Elsevier described some initiatives within the Elsevier stable of journals to enhance linking between articles and data sets.)

Overall, this workshop provided a helpful snapshot of the state of play in making research data available within the framework of the record of science. There are encouraging signs that public policy is well informed and is moving towards encouraging orderly curation of data across many disciplines. Within this framework, public funding is available for well-defined data management activities, and this may provide some resources for individual disciplines to address any needs they have that cannot be met by existing academic funding. There is, of course, huge disparity both in the types of data across different disciplines, and in the sophistication of different communities with the management of their data. This does provide a continuing challenge to publishers, especially large organisations publishing across many different scientific fields. As yet, the ability of publishers to take advantage of specific data handling opportunities seems rather limited. Initiatives such as DOI, which now provides persistent unique identifiers in both the publishing and data worlds, do of course facilitate linking and citation, which are important first steps. But there is still a great deal to do before there is routine validation, visualisation and reuse of data across the whole field of science. It is very beneficial that organisations such as CODATA and ICSTI are both aware of the problems, and well placed to work together with the many relevant stakeholders to bring this vision closer to reality. Full report and workshop presentations are available online.

 www.icsti.org/spip.php?rubrique42

Agrochemicals

by J.B. Unsworth, N.A. Shakil, J. Kumar, G.A. Kleter and J.B.H.J. Linders

The global population is predicted to grow from about 7 billion today to 9 billion in 2050, with a corresponding need to increase the food supply, which is one of the greatest challenges of our time. Today, there is an urgent need to review advances made in crop protection research and formulate future strategies to achieve a secure food supply and at the same time ensure that this is done in a sustainable way.

The **Second International Conference on Agrochemicals Protecting Crops, Health and Natural Environment—The Role of Chemistry for Sustainable Agriculture** was held on 15–18 February 2012 at the Indian Agricultural Research Institute (IARI), in New Delhi, India, the practical conference arrangements



The opening ceremony. From left: Dr. Pankaj, Dr. J.B. Unsworth, Dr. N.A. Shakil, Shri Harish Rawat, Prof. V.L. Chopra and Dr. J. Kumar.

and invitations were organised by Dr. N.A. Shakil and Dr. J. Kumar (senior scientists at IARI) and the National Organising Committee was chaired by Dr. H.S. Gupta (Director, IARI). The conference, which was sponsored by IUPAC, together with IARI, the Indian Council of Agricultural Research (ICAR) and the Society for the Promotion of Sustainable Agriculture (SPSA), attracted 415 delegates including a significant number of international delegates and it was pleasing to note the presence of a large number of young scientists. The scientific program was organised with 20 technical sessions consisting of 17 plenary lectures, 28 invited lectures, 82 oral presentations and 176 poster presentations, of which the three judged to be the most meritorious received awards.

The opening ceremony was chaired by Dr. V.L. Chopra (former President, National Academy of Agricultural Sciences) and, after a traditional welcome, the inaugural address was given by the Chief Guest Shri Harish Rawat (Union Minister of State for Agriculture, Food Processing Industries and Parliamentary Affairs). In his address he emphasised the need for an increase in food production and that the approach taken would include many of the issues to be addressed by the conference, particularly in the plenary lectures.

Plenary lectures given by Dr. C.D. Mayee (former chairman of the Agricultural Scientists Recruitment Board) and Dr. S. Singhal (PI Industries Ltd.) focused on pest management and food security in India. Today Indian agriculture needs major reforms which will allow increased productivity and at the same time contribute to the farmers' wealth; a "Second Green Revolution". Significant crop losses still occur but pesticides are not always used effectively to combat these losses. In addition, new pesticides can take a significant time to reach the market. Integrated Pest Management (IPM) strategies are being strongly promoted and have been developed for all major crops, but so far uptake has been limited as they need to be tailored to local conditions and require a high level of expertise. Interestingly IPM, when used appropriately with lower pesticide inputs, can also help in reducing the carbon footprint as was outlined by Dr. K.R. Chauhan (US Dept. of Agriculture), for example, by the use of pheromones to either attract beneficial insects for biocontrol or for mating disruption of insect pests.

The search for new crop protection products is an ongoing challenge as was explained by Dr. K.J. Divakar (Syngenta) and Dr. A. Klausener (Bayer CropScience). The number of new pesticides is decreasing and their development is becoming increasingly more expensive and time-intensive, with a higher risk of

failure. An example of a recently introduced insecticide, Cyazapyr™, with a novel mode of action was given by Dr. I. B. Annan (DuPont Crop Protection). Research into novel pesticides was described by Professor K. Matsuda (Kinki University, Nara, Japan) who concentrated on the neonicotinoid family of insecticides and the possibility of designing insecticides that are safe for mammals and beneficial insects. Another approach was given by Dr. R.J. Nachman (US Dept. of Agriculture) who discussed the role of insect neuropeptides and the use of biostable mimetics as a possible new strategy for pest control. Dr. M.J. Kennedy (Dept. of Employment, Economic Development and Innovation, Queensland, Australia) described a research program to extract bioactive compounds from the hardwood of the white cypress (*Calitris glaucophylla*) and the development of delivery systems based on nanoparticles.

Methods for risk assessment are essential to ensure that pesticides can be used safely. An example of environmental risk assessment was described by Dr. J.B.H.J. Linders (formerly RIVM, Bilthoven, the Netherlands). The aim of this IUPAC funded project is to harmonize approaches to risk assessment between nations. It was concluded that methods based on a tiered approach and adapted to the local region and growing conditions are preferred over a strictly hazard approach, as fewer pesticides would be discontinued. In ensuring the safe use of pesticides it is necessary to be able to quantify trace levels in various substrates. Dr. S.K. Raza (Institute of Pesticide Formulation Technology, Gurgaon, Haryana, India) described current chromatographic methods, coupled with mass-spectrometry, which are highly selective and have excellent sensitivity. Dr. D.B.G. Williams (University of Johannesburg, South Africa) explained a novel technique for the analysis of pesticide residues using bubble-in-drop single-drop micro-extraction (BID-SDME) for which sensitivity in the ng/L range was achieved for triazines in water.

Biotechnology is increasing in importance in agriculture and Dr. S.M.P. Khurana (Amity Institute of Biotechnology, Haryana, India) explained how traits introduced by genetic modification can help increase food production, whilst other types of modification can help fight malnutrition; a good example is Golden Rice engineered to biosynthesize beta-carotene, a precursor of pro-vitamin A. When crops have been modified to be resistant to a given pesticide it is important to verify that the residue definition, initially proposed for the non-GM crop, is still valid. This is the basis of an IUPAC funded project led by Dr. G.A.

Kleter (RIKILT-Institute of Food Safety, Wageningen University and Research Center, Wageningen, the Netherlands). The project team investigated data on residue levels for herbicides applied to GM herbicide-resistant crops. The outcome was that no generalized inferences could be made about the nature or level of the residues of either the herbicide active ingredients or their metabolites. Each case, therefore, must be examined separately.

Registration of pesticides is mandatory before pesticides can be commercialized. The Organization for Economic Cooperation and Development (OECD) plays a key role in harmonizing regulations. Dr. S. Poret (OECD, Paris, France) explained that the current aim is mutual acceptance of data and that by 2014 governments will routinely accept dossiers and monographs in OECD format. In addition, OECD is working on "best practices" for topics such as IPM, risk assessment, and reduction in animal testing.

There is a great deal of information available about pesticides online and Dr. J.B. Unsworth (Consultant, UK) described an IUPAC-funded project that was set up to highlight sites that are reliable and objective. A "Pesticide Portal" has been developed to give access to publicly available information on pesticides and provide links to relevant documents (see <http://pesticides.iupac.org>).

It is also important that stakeholders understand current thinking on pesticides and agricultural policy. This was the subject of the plenary lecture delivered by Prof. E. Capri (Research Centre on Sustainable Agriculture, Piacenza, Italy) who described how policy recommendations or detailed studies and suggestions for national implementation are developed. Current examples are the outcome of discussions on the EU common agriculture policy and work on the Directive on the Sustainable Use of Pesticides.

Based on the presentations the following recommendations were formally adopted during the closing ceremony:

Pesticides: chemical pesticides are extremely important for ensuring a secure food supply but in some areas there is a reluctance to use them, in these cases extension services should educate farmers in the safe use of appropriate pesticides in order to increase their crop yields. If crops are destined for export it is essential that the pesticides used are acceptable to the importing country.

Regulations: In order to ensure that new pesticides are registered with a minimum of delay increased

resources from government should be made available for this task. In addition, the safety assessment of pesticides should be based on actual risk under local conditions, rather than on the inherent hazard of the pesticide. Support should be given by government to the OECD initiative on the harmonisation of regulatory requirements.

Public awareness: The media give the impression that chemical pesticides are inherently unsafe. Industry, academia, and government, together with the help of international organizations, should increase the awareness of the public that chemical pesticides can be used safely and pose no problem to human health or the environment. In addition, in order to ensure public confidence, industry must ensure that products are clearly and accurately labelled and have instructions for use in an understandable manner.

Integrated pest management: The importance of integrated pest management should be stressed and training of farmers by qualified experts should be carried out to ensure that this technique is used appropriately and effectively in controlling target pests.

Biotechnology: New techniques are being enabled by biotechnology. These techniques should be built on to develop not only herbicide resistance or insecticidal properties but also, for example, new traits in crops such as adding health benefits (golden rice) or other benefits such as drought resistance and increased storage times (increased shelf life). Along these lines, a program should be initiated for identifying those naturally occurring metabolites responsible for repelling insect pests of plants, and crop plants should be engineered, through both molecular breeding and GM technology, to produce these biochemicals for plant defence.

Biopesticides: Although biopesticides derived from natural products have a role to play in crop protection, their sometimes suboptimal efficacy, and consequent lower crop yields, means that their use should be limited to crops where a higher price premium can be demanded (i.e. where there is a demand for organic produce). Organic farming on its own will not ensure a secure food supply.

N.A. Shakil (jamshakil@gmail.com) and J. Kumar are senior scientists at the Indian Agricultural Research Institute, New Delhi, India; J.B. Unsworth (current Chair), G.A. Kleter and J.B.H.J. Linders are members of the IUPAC Advisory Committee on Crop Protection Chemistry.

Where 2B & Y

Open Data and Information for a Changing Planet

28–31 October 2012
Taipei, China

Never before have scientific data and information played such a major role in addressing the problems and challenges facing our planet. The calls for freely available, publicly accessible data are gaining a stronger voice. The June 2011 editorial in *Nature* highlighted the value of open access to global nuclear-monitoring data, and the benefits of such data for a variety of applications, “in times of both calm and crisis.”

The theme of the **23rd International CODATA Conference “Open Data and Information for a Changing Planet”** encompasses some relevant issues in data-intensive scientific fields. Nurturing an open environment for data and information is crucial for disseminating research results to a wide audience and allowing thorough, collaborative analysis. Also, the theme distinguishes between data and information and by so doing highlights the role data-intensive science plays in transforming raw observations into applicable, intelligible results and discoveries. Furthermore, the theme emphasizes that our scientific endeavors, and the data that sustain them, are key to providing reasoned solutions to the problems we face with

climate change, population pressure, natural hazards, and other global issues. The theme supports not only the mission of CODATA, but that of ICSU, as it strives to strengthen international science for the benefit of society.

CODATA 23 will bring together stakeholders from industry, research, and academia who will highlight, debate, and address these issues over three days. It will provide an international forum where these stakeholders, in collaboration with the ICSU and CODATA international networks, and other networks can create a dialogue on legal, economic, and technological challenges; evaluate societal impacts; and put forward possible solutions that can in turn benefit the planet. Nurturing an open environment for data and information plays a pivotal role in this process. This will be the underpinning message of the conference.

CODATA 23 organizers recognize the importance of involving and working with early career scientists in discussing these issues. They are the scientists who will have to address these challenges tomorrow. CODATA 23 will thus build on strengthening interaction between young scientists and senior scientists on data. Special young scientist activities and social events will take place within the framework of the scientific program.

 www.codata2012.com

MacroMolecular Complexes

13–16 August 2013
Clemson & Greenville, South Carolina, USA

Following the basic scientific design and tradition of the previous MMC symposia, the **15th IUPAC International Symposium on MacroMolecular Complexes** (MMC-15:2013) will take place at Clemson University and Greenville, South Carolina, on 13–17 August 2013.

The themes for this year’s meeting are Energy Harvesting and Energy Industry, Sustainability and Green Chemistry, Biotechnology and Biomedicine, and Global Health. The symposium brings together leading researchers and commercial developers, scientists, and engineers to discuss the latest advances in macromolecule-metal complexes as they impact the foregoing themes.

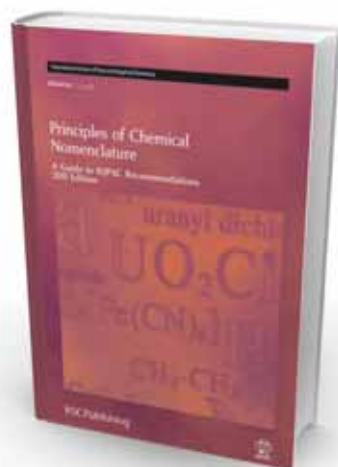
Macromolecular complexes play key roles in super capacitors (energy), separations (sustainability), drug

delivery and regenerative medicine (biomedicine), and in the development of low-cost diagnostics for resource-challenged regions of our planet (global health). Fundamental underpinnings are in polynuclear complexes, capped metal nanoparticles, organic-inorganic hybrids, supramolecular-nano complexes and self-assembled materials, and polyelectrolytes. Not only syntheses and characterization of those materials but also various properties and functions, such as conductive, photophysical, catalytic, electronic, optical, magnetic, and biological, as well as their application, are included for discussion.

MMC-15:2013 will feature 8 plenary addresses, 24 invited lectures, and contributed oral and poster presentations. This year will mark the introduction of MMC Awards, student travel awards, and expanded poster prizes.

MMC has previously been held in Beijing (1985), Tokyo (1987), New Jersey (1989), Siena (1991), Bremen (1993), Kuang-chou (1995), Leiden (1997), Tokyo

IUPAC and RSC Publishing



Principles of Chemical Nomenclature

A Guide to IUPAC Recommendations 2011 Edition

Written by leading world authorities, this book enables teachers and students to obtain a sound training in IUPAC nomenclature. It outlines IUPAC recommendations for application in the principal branches of chemistry: organic, inorganic, organometallic, and polymer. The book also includes some basic biochemical nomenclature, clearly explaining the fundamental principles of nomenclature methods.

The book is replete with examples for guidance and there are extensive tables to direct the reader to information quickly. This book will enable readers to apply the principles of nomenclature accurately and with confidence.

ISBN 9781849730075 | 2011 | £24.99

Other IUPAC References

Compendium of Polymer Terminology and Nomenclature

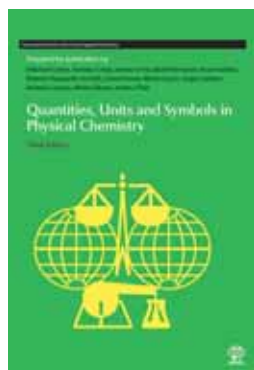
IUPAC Recommendations 2008



This new edition collects the most important position papers on the nomenclature and terminology of several types of polymers into one extensive volume.

ISBN 9780854044917 | 2009 | £139.99

Quantities, Units and Symbols in Physical Chemistry



This is the definitive guide for scientists and organizations working across a multitude of disciplines requiring internationally approved physical chemistry nomenclature.

ISBN 9780854044337 | 2007 | £39.95

Nomenclature of Inorganic Chemistry

IUPAC Recommendations 2005



The 'Red Book' is the definitive guide for scientists requiring internationally approved inorganic nomenclature in a legal or regulatory environment.

ISBN 9780854044382 | 2005 | £49.95

Where 2B & Y

(1999), New York (2001), Moscow (2003), Pisa (2005), Fukuoka (2007), Conception (2009) and Helsinki (2011).

English will be the working language of the conference. All participants should submit their one-page abstracts electronically and register by visiting www.macromolecularcomplexes.org. Under the guidance of

the International Advisory Board, reviewed abstracts accepted for presentation will be accompanied by the submission of a full paper for peer-reviewed publication in Wiley's *Macromolecular Symposia*.

 www.macromolecularcomplexes.org

IUPAC Poster Prizes

Since 2004, IUPAC Poster Prizes have been regularly awarded at IUPAC Congresses and Division-sponsored conferences to recognize outstanding poster presentations. Upon request from a National Adhering Organization, such prizes may also be awarded at a single chosen national conference each year. The conference organizers oversee the selection of the prizewinners and, typically, two or three prizes are awarded. The winners of the IUPAC Poster Prizes receive a certificate signed by the IUPAC president, a copy of an IUPAC book, and a year's subscription to *Chemistry International*.

Guidelines

- Prizes will be awarded at all IUPAC Congresses and Division sponsored meetings where poster sessions are held.
- Prizes will be awarded at national meetings if requested. Not more than one meeting per country a year will apply, and that meeting should be selected by the relevant NAO.

- In all cases except IUPAC Congresses, there will be normally two, but a maximum of three, prizes per conference.
- Selection of prizewinners is in the control of the conference organizers.
- Each prize will consist of (i) a certificate signed by the president (ii) a copy of an IUPAC book (iii), and one year's subscription to *Chemistry International*.

National Adhering Organizations are asked to inform their national chemical societies of this program and to inform the IUPAC Secretariat of any plans to award IUPAC Poster Prizes at a national meeting. Likewise, Division Committees are asked to inform the organizers of meetings sponsored by their Divisions of this opportunity.

Starting again with this issue of *CI*, each IUPAC-sponsored conference eligible to award poster prizes will be flagged in the Mark Your Calendar section. Over the most typical two- to three-year cycle, about two dozen events are usually eligible to award IUPAC poster prizes.

Visas

It is a condition of sponsorships that organizers of meetings under the auspices of IUPAC, in considering the locations of such meetings, should take all possible steps to ensure the freedom of all bona fide chemists from throughout the world to attend irrespective of race, religion, or political philosophy. IUPAC sponsorship implies that entry visas will be granted to all bona fide chemists provided application is made not less than three months in advance. If a visa is not granted one month before the meeting, the IUPAC Secretariat should be notified without delay by the applicant.

How to Apply for IUPAC Sponsorship

Conference organizers are invited to complete an Application for IUPAC Sponsorship (AIS) preferably 2 years and at least 12 months before the conference. Further information on granting sponsorship is included in the AIS and is available upon request from the IUPAC Secretariat or online.

 www.iupac.org

2012 (after 15 July)

 IUPAC poster prizes to be awarded

15–20 July 2012 • Photochemistry • Coimbra, Portugal 

XXIVth IUPAC Symposium on Photochemistry

Prof. Hugh D. Burrows, University of Coimbra, Dept. of Chemistry, P-3004 535 Coimbra, Portugal

Tel.: +351 239 854 482, Fax: +351 239 827 703, E-mail: burrows@ci.uc.pt

15–20 July 2012 • Change in Chemistry Education • Rome, Italy 

22nd International Conference on Chemical Education (ICCE) and 11th European Conference on Research In Chemical Education—Stimulating Reflection and Catalysing Change in Chemistry Education

Prof. Luigi Campanella, Conference Chair; Agency YES Meet, organizing secretariat

Tel: + 39 081 8770604, Fax: + 39 081 8770258, E-mail: info@iccecrice2012.org

22–27 July 2012 • Solubility Phenomenon • Xining, China 

15th International Symposium on Solubility Phenomena and Related Equilibrium Processes

Prof. Dewen Zeng, Qinghai Institute of Salt Lakes, Xining Road, # 18, Xining 810008, China

Tel.: +86 13 618 496 806, Fax: +86 971 630 6002, E-mail: dewen_zeng@hotmail.com

22–27 July 2012 • Carbohydrate • Madrid, Spain

XXVIth International Carbohydrate Symposium

Prof. Jesús Jiménez-Barbero, Centro de Investigaciones Biológicas, Consejo Superior de Investigaciones Ciencias, Ramiro de Maeztu 9, E-28040 Madrid, Spain

Tel.: +34 91 837 3112, Fax: +34 91 536 0432, E-mail: jjbarbero@cib.csic.es

5–10 August 2012 • Chemical Thermodynamics • Búzios, Brazil 

22nd International Conference on Chemical Thermodynamics and 67th Calorimetry Conference

Prof. Watson Loh, Universidade de Estadual de Campinas, Instituto de Química, Caixa Postal 6154, Campinas, São Paulo 13083-970, Brazil, Tel.: +55 193 521 3001, Fax: +55 193 521 3023, E-mail: wloh@iqm.unicamp.br

25–29 August 2012 • Biomolecular Chemistry • Beijing, China 

9th International Conference on Biomolecular Chemistry

Prof. Liangren Zhang, School of Pharmaceutical Sciences, Peking University Health Science Center, 38 Xueyuan Road, Beijing 100083, China, Tel.: +86 10 82 802 491, Fax: +86 10 82 802 638, E-mail: liangren@bjmu.edu.cn

25–29 August 2012 • Green Chemistry • Foz do Iguacu, Brazil 

4th International IUPAC Conference on Green Chemistry

Prof. Vania Gomes Zuin, Federal University of Sao Carlos, Department of Chemistry, Rodovia Washington Luis, Sao Carlos, 1365-905, Brazil, Tel.: +55 163 361 8096, Fax: +55 163 361 8350, E-mail: vaniaz@ufscar.br

9–13 September 2012 • Coordination Chemistry • Valencia, Spain

40th International Conference on Coordination Chemistry

Prof. Eugenio Coronado, University of Valencia, Institute of Molecular Sciences, C/ Catedrático José Beltrán 2 E-46980 Paterna, Valencia, Tel.: +34 963 544 4415, Fax: +34 963 543 273, E-mail: eugenio.coronado@uv.es

9–13 September 2012 • Physical Organic Chemistry • Durham, United Kingdom 

21st International Conference on Physical Organic Chemistry

Professor Ian H. Williams, Department of Chemistry, University of Bath, Claverton Down, Bath BA2 7AY, United Kingdom, Tel.: + 44 1225 386 625, Fax: + 44 1225 386 231, E-mail: i.h.williams@bath.ac.uk

11–14 September 2012 • Polymer-Solvent Complexes • Kiev, Ukraine

9th International Conference on Polymer-Solvent Complexes and Intercalates

Professor L. Bulavin, Kiev National Taras Shevchenko University, Department of Physics, Volodymyrska, 60, UA-01610 Kiev, Ukraine, Tel.: +380 044 526 45 37, Fax: +380 044 526 44 77, E-mail: bulavin221@gmail.com

15–20 September 2012 • Pesticide and Environmental Safety • Beijing, China 

4th International Symposium on Pesticide and Environmental Safety & 8th International Workshop on Crop Protection Chemistry and Regulatory Harmonization

Prof. Zhang Jing, China Agricultural University, Centre for Chemicals Applications Technology, Yuanmingyuan West Road, Beijing 100193, China, Tel.: +86 10 6273 1456, Fax: +86 10 6273 3688, E-mail: zj810515@163.com

15-20 September 2012 • Catalysis in Organic Synthesis • Moscow, Russia

International Conference on Catalysis in Organic Synthesis

Prof. Mikhail P. Egorov, Russian Academy of Sciences, Zelinsky Institute of Organic Chemistry, 47 Leninsky Prospekt, B-334, RF-119991 Moscow, Russia, Tel.: +7 095 135 5309, Fax: +7 095 135 5328, E-mail: mpe@ioc.ac.ru

16-21 September 2012 • Biotechnology • Daegu, Korea

15th International Biotechnology Symposium and Exhibition

IBS 2012 Secretariat, 6F, Sunghwa B/D, 1356-51 Manchon, 1-Dong, Suseong-Gu, Daegu 706-803, Korea
Tel.: +82 53 742 5557, Fax: +82 53 742 9007, E-mail: info@ibs2012.org

14-19 October 2012 • Novel Materials • Xian, China 

8th International Conference on Novel Materials and their Synthesis

Prof. Yuping Wu, Fudan University, Department of Chemistry, New Energy & Materials Laboratory, Shanghai, 200433, China, Tel.: +86 21 55 664 223, Fax: +86 21 55 664 223, E-mail: wuyup@fudan.edu.cn

23-26 October 2012 • Green Chemistry • Moscow, Russia

4th International Chemical Assembly on Green Chemistry

Prof. Ekaterina S. Lokteva, Moscow State University, Department of Chemistry, Leninsky Gory, 1, RF-119991 Moscow, Russia, Tel: +7 495 939 3337, Fax: +7 495 939 4575, E-mail: les@kge.msu.ru

5-9 November 2012 • Mycotoxin • Rotterdam, Netherlands 

7th World Mycotoxin Forum and XIIIth International IUPAC Symposium on Mycotoxins & Phycotoxins

Ms. Helena B. Bastiaanse (Program Coordinator), Bastiaanse Communication, P.O. Box 179, NL-3720 AD Bilthoven, Netherlands, Tel.: +31 302 294 247, Fax: +31 302 252 910, E-mail: helena@bastiaanse-communication.com

21-25 November 2012 • Supramolecular Architectures and Materials • Coimbatore, Tamil Nadu, India

6th International Conference on Macro- and Supramolecular Architectures & Materials (MAM-2012)

Dr. Venkatchalam Rajendran Director, Center for NanoScience & Technology, K.S. Rangasamy College of Technology, K.S.R. Kalvinagar, Tiruchengode, Namakkal, Tamil Nadu 637 215, India
Tel.: +91 428 827 4880, Fax: +91 428 827 4880, E-mail: veerajendran@gmail.com

2013



IUPAC poster prizes to be awarded

17-22 February 2013 • Scanning Electrochemical Microscopy • Ein Gedi, Israel

7th Workshop on Scanning Electrochemical Microscopy

Prof. Daniel Mandler, The Hebrew University of Jerusalem, Department of Inorganic and Analytical Chemistry, Safra Campus, IL-91904 Jerusalem, Israel,
Tel.: +972 2 658 5831, Fax: +972 2 658 5319, E-mail: mandler@vms.huji.ac.il

25-30 March 2013 • Polymer Characterization • Daegu, Korea 

21st International Conference on Polymer Characterization—World Forum on Advanced Materials (PolyChar-21)

Prof. Witold Brostow, University of North Texas, Department of Materials Science & Engineering, P.O. Box 305310, Denton, TX 76203-5310, USA, Tel.: +1 940 565-4358, Fax: +1 940 565-4824, E-mail: brostow@unt.edu

19-23 May 2013 • Clinical Chemistry & Laboratory Medicine • Milan, Italy

20th IFCC-EFLM European Congress on Clinical Chemistry & Laboratory Medicine; 45th Congress of the Italian Society of Clinical Biochemistry & Clinical Molecular Biology

Dr. Ferruccio Ceriotti, Istituto Scientifico Ospedale San Raffaele, Servizio di Medicina di Laboratorio, Via Olgettina 60, I-20132 Milano, Italy, Tel.: +39 10 226 432 282, E-mail: ceriotti.ferruccio@hsr.it

28 July-2 August 2013 • Novel Aromatic Compounds • Taipei, Taiwan

15th International Symposium on Novel Aromatic Compounds (ISNA-15)

Prof. Ken-Tsung Wong, Taiwan National University, Department of Chemistry No. 1, Sec. 4, Roosevelt Road, Taipei 10167 Taiwan, Tel.: +886 2 3366 1665, Fax: +886 2 3366 1667, E-mail: kenwong@ntu.edu.tw

11-16 August 2013 • IUPAC 44th Congress • Istanbul, Turkey 

44th IUPAC Congress—Clean Energy Through Chemistry

Prof. Mehmet Mahramanlioglu, Turkish Chemical Society, Istanbul University, Department of Chemistry, TR-34320 Avcilar, Istanbul, Turkey,
Tel.: +90 212 591 1996, Fax: +90 212 591 1997, E-mail: mehmah@istanbul.edu.tr, www.iupac2013.org

I U P A C

ADVANCING THE WORLDWIDE ROLE OF CHEMISTRY FOR THE BENEFIT OF MANKIND

MISSION

IUPAC is a non-governmental organization of member countries that encompasses more than 85% of the world's chemical sciences and industries. IUPAC addresses international issues in the chemical sciences utilizing expert volunteers from its member countries. IUPAC provides leadership, facilitation, and encouragement of chemistry and promotes the norms, values, standards, and ethics of science and the free exchange of scientific information. Scientists have unimpeded access to IUPAC activities and reports. In fulfilling this mission, IUPAC effectively contributes to the worldwide understanding and application of the chemical sciences, to the betterment of the human condition.

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Kazuyuki Tatsumi (Japan)

Vice President:
Mark C. Cesa (USA)

Past President:
Nicole J. Moreau (France)

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René Deplanque (Germany)

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NATIONAL ADHERING ORGANIZATIONS

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Österreichische Akademie der Wissenschaften (*Austria*)
Bangladesh Chemical Society (*Bangladesh*)
The Royal Academies for the Sciences and Arts of Belgium (*Belgium*)
Brazilian Chemical Society (*Brazil*)
Bulgarian Academy of Sciences (*Bulgaria*)
National Research Council of Canada (*Canada*)
Sociedad Chilena de Química (*Chile*)
Chinese Chemical Society (*China*)
Chemical Society located in Taipei (*China*)
Croatian Chemical Society (*Croatia*)
Sociedad Cubana de Química (*Cuba*)
Pancyprrian Union of Chemists (*Cyprus*)
Czech National Committee for Chemistry (*Czech Republic*)
Det Kongelige Danske Videnskaberne Selskab (*Denmark*)
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IUPAC Periodic Table of the Elements

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1	H hydrogen [1.007; 1.008]	2	He helium 4.003	3	Li lithium [6.938; 6.997]	4	Be beryllium 9.012	5	B boron [10.80; 10.83]	6	C carbon [12.00; 12.02]	7	N nitrogen [14.00; 14.01]	8	O oxygen [15.99; 16.00]	9	F fluorine 19.00	10	Ne neon 20.18	11	Na sodium [22.989; 22.99]	12	Mg magnesium 24.31	13	Al aluminium 26.98	14	Si silicon [28.085; 28.086]	15	P phosphorus 30.97	16	S sulfur [32.059; 32.061]	17	Cl chlorine [35.446; 35.453]	18	Ar argon 39.95	19	K potassium 39.10	20	Ca calcium 40.08	21	Sc scandium 44.96	22	Ti titanium 47.87	23	V vanadium 50.94	24	Cr chromium 52.00	25	Mn manganese 54.94	26	Fe iron 55.85	27	Co cobalt 58.93	28	Ni nickel 58.69	29	Cu copper 63.55	30	Zn zinc [65.38; 65.40]	31	Ga gallium 69.72	32	Ge germanium 72.63	33	As arsenic 74.92	34	Se selenium [78.96; 78.97]	35	Br bromine 79.90	36	Kr krypton 83.80	37	Rb rubidium 85.47	38	Sr strontium 87.62	39	Y yttrium 88.91	40	Zr zirconium 91.22	41	Nb niobium 92.91	42	Mo molybdenum [95.96; 95.97]	43	Tc technetium	44	Ru ruthenium 101.1	45	Rh rhodium 102.9	46	Pd palladium 106.4	47	Ag silver 107.9	48	Cd cadmium 112.4	49	In indium 114.8	50	Sn tin 118.7	51	Sb antimony 121.8	52	Te tellurium 127.6	53	I iodine 126.9	54	Xe xenon 131.3	55	Cs caesium 132.9	56	Ba barium 137.3	57-71	lanthanoids	72	Hf hafnium 178.5	73	Ta tantalum 180.9	74	W tungsten 183.8	75	Re rhenium 186.2	76	Os osmium 190.2	77	Ir iridium 192.2	78	Pt platinum 195.1	79	Au gold 197.0	80	Hg mercury [200.59; 200.61]	81	Tl thallium [204.38; 204.41]	82	Pb lead 207.2	83	Bi bismuth 209.0	84	Po polonium	85	At astatine	86	Rn radon	87	Fr francium	88	Ra radium	89-103	actinoids	104	Rf rutherfordium	105	Db dubnium	106	Sg seaborgium	107	Bh bohrium	108	Hs hassium	109	Mt meitnerium	110	Ds darmstadtium	111	Rg roentgenium	112	Cn copernicium	113	Nh nihonium	114	Fl flerovium	115	Mc moscovium	116	Lv livermorium	117	Ts tennessine	118	Og oganesson

57	La lanthanum 138.9	58	Ce cerium 140.1	59	Pr praseodymium 140.9	60	Nd neodymium 144.2	61	Pm promethium	62	Sm samarium 150.4	63	Eu europium 152.0	64	Gd gadolinium 157.3	65	Tb terbium 158.9	66	Dy dysprosium 162.5	67	Ho holmium 164.9	68	Er erbium 167.3	69	Tm thulium 168.9	70	Yb ytterbium 173.1	71	Lu lutetium 175.0
89	Ac actinium	90	Th thorium 232.0	91	Pa protactinium 231.0	92	U uranium 238.0	93	Np neptunium	94	Pu plutonium	95	Am americium	96	Cm curium	97	Bk berkelium	98	Cf californium	99	Es einsteinium	100	Fm fermium	101	Md mendelevium	102	No nobelium	103	Lr lawrencium

Notes

- IUPAC 2009 Standard atomic weights abridged to four significant digits (Table 4 published in *Pure Appl. Chem.* 83, 359-396 (2011); doi: 10.1351/PAC-REP-10-09-14). The uncertainty in the last digit of the standard atomic weight value is listed in parentheses following the value. In the absence of parentheses, the uncertainty is one in that last digit. An interval in square brackets provides the lower and upper bounds of the standard atomic weight for that element. No values are listed for elements which lack isotopes with a characteristic isotopic abundance in natural terrestrial samples. See PAC for more details.

- "Aluminium" and "caesium" are commonly used alternative spellings for "aluminum" and "caesium".

- Claims for the discovery of all the remaining elements in the last row of the Table, namely elements with atomic numbers 113, 115, 117 and 118, and for which no assignments have yet been made, are being considered by a IUPAC and IUPAP Joint Working Party.

For updates to this table, see iupac.org/reports/periodic_table/. This version is dated 1 June 2012.
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