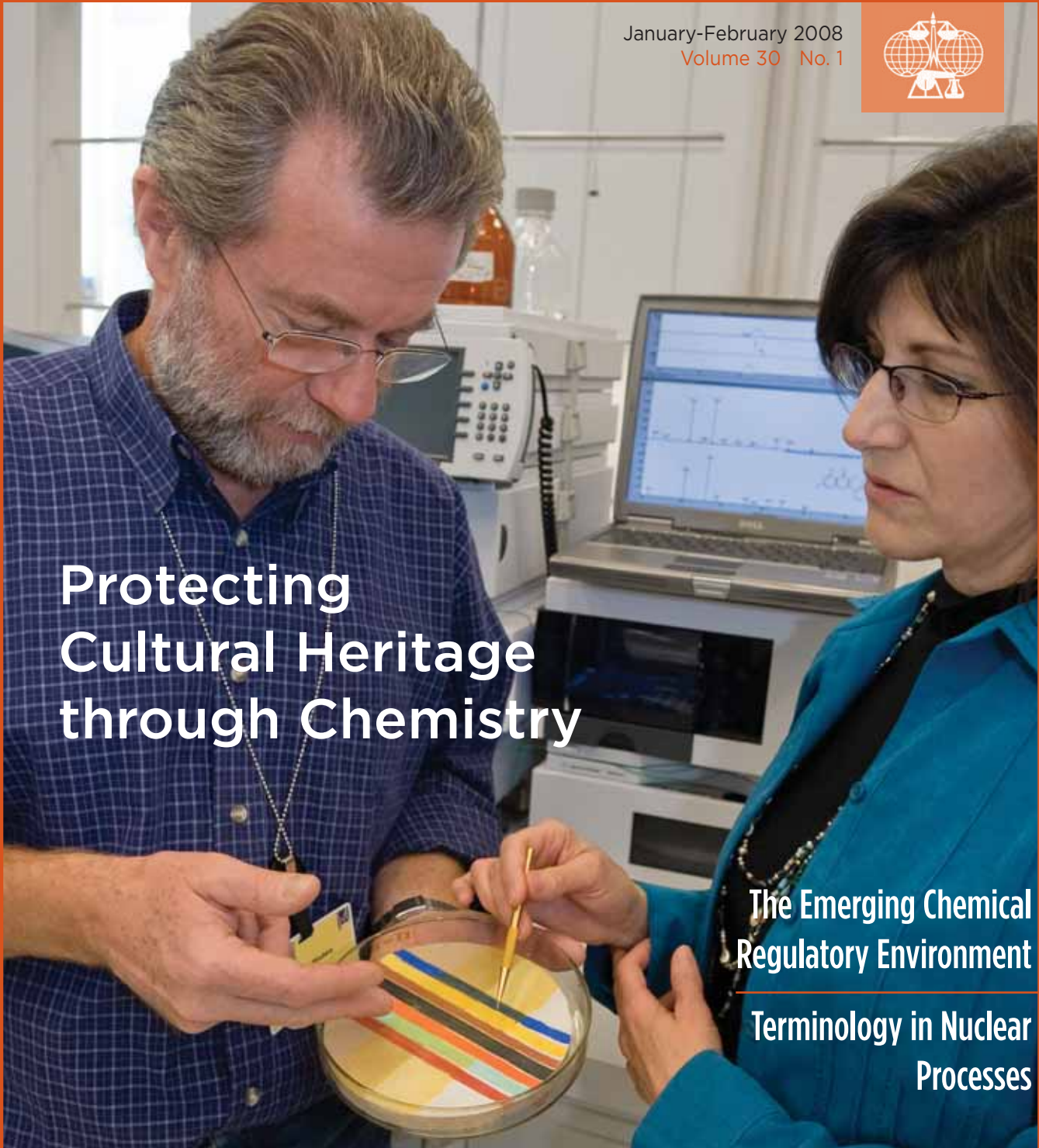


The News Magazine of the  
International Union of Pure and  
Applied Chemistry (IUPAC)

# CHEMISTRY

## International

January-February 2008  
Volume 30 No. 1



**Protecting  
Cultural Heritage  
through Chemistry**

**The Emerging Chemical  
Regulatory Environment**

**Terminology in Nuclear  
Processes**



# From the Editor

## CHEMISTRY International

The News Magazine of the  
International Union of Pure and  
Applied Chemistry (IUPAC)

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**Managing Editor:** Fabienne Meyers

**Production Editor:** Chris Brouwer

**Design:** CB Communications

### All correspondence to be addressed to:

Fabienne Meyers  
IUPAC, c/o Department of Chemistry  
Boston University  
Metcalf Center for Science and Engineering  
590 Commonwealth Ave.  
Boston, MA 02215, USA

E-mail: [edit.ci@iupac.org](mailto:edit.ci@iupac.org)

Phone: +1 617 358 0410

Fax: +1 617 353 6466

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In 2008, IUPAC will publish the 80th volume of its scientific journal *Pure and Applied Chemistry (PAC)* and the 30th volume of its news magazine *Chemistry International (CI)*.

By serendipity, the anniversary of *PAC* coincides with the recent unveiling of a new online interface that makes the journal contents more easily available and searchable. Online *PAC* provides access to slightly more than 30 years of IUPAC reports, recommendations, and selected lectures from IUPAC-sponsored conferences.

Thirty years is also the approximate age of *CI*. Year after year, *CI* has fulfilled its mission of providing news and views about IUPAC activities



and other areas of interest to its diverse international readership. *CI* has proved to be a valuable resource for members most involved in IUPAC activities who want to present their work in different ways and to various audiences. Nowadays, the newsmagazine also benefits from the availability of the internet as a reference and

supplement. While it is still a blend of news and reports emanating from within the Union, *CI* makes frequent links to online reports or supplementary information.

The content of *CI* has evolved and will continue to do so; that is only natural considering that IUPAC itself evolves, as does the media. Today's challenge is still to retain a diversity of articles that reflects the full spectrum of IUPAC activities.

In celebration of the *PAC* and *CI* anniversaries, I would like to express my thanks and gratitude to everyone who has contributed one way or another to these publications, including former editors and officers of the Union, and all who recognize the need to publish.

See YOU in *CI*, and have a 2008 pure and happy chemistry year!

Fabienne Meyers

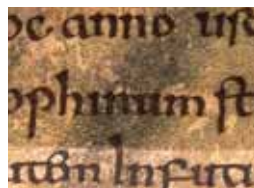
[fabienne@iupac.org](mailto:fabienne@iupac.org)

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*Cover: Jan Wouters (Head of Laboratory at the Royal Institute for Cultural Heritage, Brussels), a visiting scientist at the Getty Conservation Institute (Los Angeles), and Cecily Grzywacz, a Getty Conservation Institute scientist, discuss the construction, sampling, and analysis of a mock-up of ancient Chinese wall painting materials containing both inorganic pigment paints and an organic pigment glaze. Research on historical reconstructions can lead to better diagnosis of sources of materials and lower levels of destructiveness when studying historical objects. Read more regarding the Asian Organic Colorants project of the Getty Conservation Institute at <[www.getty.edu/conservation/science/asian/](http://www.getty.edu/conservation/science/asian/)>. Read more about Protecting Cultural Heritage on page 4. Photo by Emile Askey. © The J. Paul Getty Trust.*

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## Toward Global Leadership in Knowledge Sharing

—A Goal of Celebrating IUPAC's Centennial with 100 Member Countries

by Jung-Il Jin

**A**fter attending the IUPAC General Assembly and Congress in Torino, Italy, I felt, once again, that the number of attendees from so-called economically disadvantaged countries or emerging regions was far less than I had hoped to see. Every time I experience this disappointment at our GAs, I wonder what IUPAC should do to improve the situation.

At this point, I would like to remind readers what I mentioned in my candidate statement\* for the recent presidential election held in Torino. In particular, I noted that "more opportunity and support for increased participation of the representatives of the economically disadvantaged countries should be

---

\*To read Jung-Il Jin's full candidate statement, see <[www.iupac.org/news/archives/2007/44th\\_council/bios\\_070718.pdf](http://www.iupac.org/news/archives/2007/44th_council/bios_070718.pdf)>, page 26.

sought, and many different methods for achieving this goal will be explored."

In about 10 years, IUPAC is going to celebrate its centennial. Wouldn't it be great if 100 National Adhering Organizations (NAOs) and Associate National Adhering Organizations (ANAOs) could join together in the celebration of IUPAC's centennial? I propose that NAOs of "advanced" countries, together with IUPAC leaders, launch a new drive to dramatically increase the number of member countries. We now have only about 50 NAOs and 20 ANAOs, which amounts to slightly more than 35 percent of world nations. In order for IUPAC to truly be called an international union, there should be at least 100 NAOs and ANAOs. This drive to increase membership will also result in better and broader knowledge-sharing and partnership-building in the world chemistry community.

There have been many discussions about how to help more nations, scientists, and students participate in various IUPAC activities. Various IUPAC bodies have seriously discussed supporting the annual subscriptions of economically disadvantaged countries. In spite of IUPAC's strong desire to attract more participation among scientists from these countries, no practical action has been taken in this direction.

Knowledge sharing and partnership building are becoming ever more important in the knowledge-based society of the 21st century. IUPAC, without any doubt or prejudice, should try to become the global leader in fulfilling this international duty and responsibility. Improvements in the dissemination of chemical knowledge, something IUPAC has been working hard at lately, relies mostly on developing better electronic communications, mainly through the internet. There is no doubt that the internet is a powerful tool in knowledge sharing and partnership building, but one has to remember that presently only 18 percent of the world's population has access to this communication mode. More widespread e-communication will require significant investments in modern communication technology. This situation demands that we also utilize the classical, analog mode of communications, to a significant extent, when building global knowledge-sharing partnerships.

IUPAC has realized for some time that providing opportunities for chemists from economically disadvantaged countries,




*IUPAC leadership for 2008-2009 (from left): Secretary General David StC. Black, Past President Bryan Henry, Vice President Nicole Moreau, President Jung-Il Jin, and Treasurer John Corish.*

especially younger chemists, to participate in various IUPAC activities provides a long-lasting influence in their scientific careers and helps the Union build partnerships. One may wonder why IUPAC has not been doing more along this line. In fact, IUPAC has been trying hard to do more to help NAOs and ANAOs from economically emerging countries, but only to a limited extent due to budget limitations. The same has been the case in attracting new NAOs and ANAOs. Many chemical societies or associations are so financially fragile that they are unable to pay their annual subscriptions. Moreover, providing support for their scientists to travel to the IUPAC GA is almost unthinkable. I believe that we have a strong will to drastically improve the situation, but we have to find a way to achieve this goal. Not surprisingly, financing has been the most critical obstacle.

IUPAC has decided to formally request that the United Nations proclaim the year 2011 as the International Year of Chemistry. The year 2011 marks the one-hundredth anniversary of the Nobel Prize in Chemistry that was awarded to Marie S. Curie. IUPAC's role in proclaiming the Year of Chemistry and its participation in activities throughout the year will increase its visibility in the chemistry community and in the world. The event should provide us with a golden opportunity to convey our will to become the true global leader in knowledge sharing and partnership building.

Among the many possible approaches to broadening our membership, I propose that we start two feasible campaigns this year: a drive to raise a Special Fund and a partnership-building movement between the NAOs of so-called advanced countries and economically disadvantaged nations' chemical societies or associations. Let's try to enter IUPAC's second century by pursuing these worthy projects. Won't you all join me in this drive?

Last but not least, I would like to take this opportunity to express my heartfelt thanks to Bryan Henry and Leiv Sydnes, and also to earlier presidents, for their dedication and contributions to the prosperity of this Union. I wish you all the best. 

Jung-II Jin <jijin@korea.ac.kr> starts his IUPAC presidency this January 2008. Previously in IUPAC, he served as president of the Polymer Division. Jin is a professor at the Korea University, in Seoul, Korea.

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# Protecting Cultural Heritage

## Reflections on the Position of Science in Multidisciplinary Approaches

by Jan Wouters

Over the past 40 years, scientific research activities in support of the conservation and restoration of objects and monuments belonging to the world's cultural heritage, have grown in number and quality. Many institutes specifically dedicated to the study and conservation of cultural heritage have emerged. Small dedicated laboratories have been installed in museums, libraries, and archives, and, more recently, university laboratories are showing increased interest in this field.

However, no definition has been formulated to identify the specific tasks, responsibilities, and skills of a conservation scientist or of conservation science. This is contradictory to the availability of a clear *Definition of the Profession of a Conservator-Restorer*, published by the Conservation Committee of the International Council of Museums in 1984.<sup>1</sup> Conservation-restoration is also described as an academic discipline in the *Clarification of Conservation-Restoration Education at University Level or Equivalent*, published in the Clarification Document of the European Network for Conservation-Restoration Education (ENCoRE) in 2000.<sup>2</sup> At present, definitions on conservation and restoration, but not on conservation science, are under discussion in workgroup 1 of the Technical Committee 346 of the European Committee for Standardisation.

Hopefully, multidisciplinary research consortiums (e.g., executing research projects within European framework programs) will promote the synergy between the cultural heritage field and the natural sciences, and will generate elements for defining

conservation science. Important players in this field, which readily address interactivity and networking, are the recently started Episcon project in the European Community's Marie Curie program<sup>3</sup> and the five-year-old EU-Artech project.<sup>4</sup> The goal of Episcon is to develop the first generation of actively formed conservation scientists at the Ph.D.-level in Europe. EU-Artech provides access, research, and technology for the conservation of European cultural heritage, including networking among 13 European infrastructures operating in the field of artwork conservation.

The present absence of a recognized, knowledge-based identity for conservation science or conservation scientists may lead to philosophical and even linguistic misunderstandings within multidisciplinary consortiums created to execute conservation projects. This paper discusses sources of misunderstandings, a suggestion for more transparent language when dealing with the scientific term *analysis*, elements to help define conservation science, and the benefits for conservation scientists of becoming connected to worldwide professional networks.

## Disputable Terminology around "Analysis"

Modern analytical protocols involve ever-increasing sophistication of sample preparation procedures, instrumentation, and post-run data treatment. This, together with the frequent absence of explanatory terms around "analysis," may create an alienating effect on those professionals who are not familiar with the inherent terminology and evaluation processes, yet are closely involved in the multi- or interdisciplinary approach that must lead to the preservation of cultural heritage. There is no doubt that this may generate reservations when analysis of art is under discussion, even when such analysis is considered essential to reveal an object's conservation condition or to establish a conservation treatment. Among the most notable of such explanatory terms are destructiveness, invasiveness, representativeness, and resolution. Such terms tend to create a polarization between non-invasive/non-destructive interventions and destructive analytical approaches.

Inevitably, the withdrawal of a sample from an object of art or culture implies some kind of mutilation, even when executed in an inconspicuous area or when dealing with minute samples. Such handling is therefore called destructive to the object. On the other hand, there are analytical techniques available that may be applied directly to the object, without



*Dyes in Precolumbian Peruvian textiles: A combination of medium destructiveness and high resolving power allowed for the identification of biological sources used for dyeing, and revealed changes in use as a function of cultural periods (Jan Wouters and Noemi Rosario-Chirinos: "Dyestuff Analysis of Precolumbian Peruvian Textiles by High Performance Liquid*

*Chromatography and Diode-Array Detection."* Journal of the American Institute for Conservation 31,2(1992)237-255).

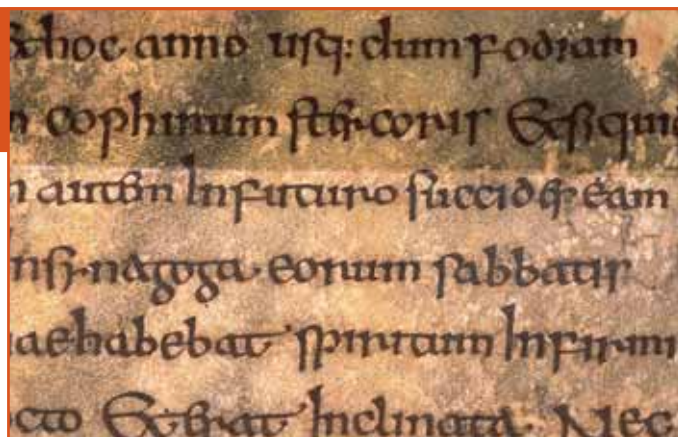
the removal of a sample. These techniques are often referred to as non-destructive and they are mostly applied to inorganic materials in art.<sup>5</sup> However, from a scientific point of view, any interaction between a material and an energy-bearing analytical vehicle, is unlikely to leave that material, or an accompanying-one, totally unaltered after the interaction.

The key issue in this discussion is the way in which one interprets damage. Obviously, the least critical evaluation of damage is performed by the naked eye: There is no damage if it cannot be “seen.” The most critical evaluation is from data generated at the molecular level by relevant spectroscopic techniques: There is no damage if the molecular compositional array at the spot of measurement has not changed beyond experimental deviations or beyond a preset level of tolerance. Sometimes, techniques applied directly to the object are called non-invasive. Although the term is correct since it is a non-sampling technique, the qualification may be misleading in terms of destructiveness for the reasons outlined above.

The complexity of the composition of artifacts such as paintings is expressed by their multilayer architecture, by the high level of heterogeneity of each individual layer, and by the further contribution to that heterogeneity by natural ageing processes and human interventions. Having to reveal production technology or damage patterns of an object by observing analytical data produced from a microsample or a microspot may come into conflict with the low representativeness of such a sample or spot. Obviously, the only ways to increase representativeness are through multiple sampling or increased spot size.

Multiple sampling increases damage to the object, but highly detailed results may be obtained by launching high-resolution mapping and imaging techniques to a set of microsamples.<sup>6</sup> Alternatively, non-invasive approaches may be applied, often with larger beam diameters than those used in high-resolution mapping and imaging. Those larger diameters are advantageous in terms of averaging and, hence, increased representativeness. But, due to the inherent lack of analytical resolution—both in the plane and in the depth of the artifact—they may miss phenomena vital to explaining technology and/or damage that would require conservation measures.

It may be clear from this discussion that invasiveness/destructiveness alone is not a good criterion to select an approach for analyzing artwork. One or more other parameters should be considered for evaluating the level and detail of information obtained.



*High-level destructiveness analysis of synthetic membranes without touching the 8th century parchment of the Codex Eycckensis revealed a polyvinylchloride polymer with 30 % (w/w) monomeric plasticizer; after the removal of the membranes, the Codex could be conserved by the application of an innovative parchment leafcasting technique (Jan Wouters, An Peckstadt, and Lieve Watteuw: “Leafcasting with Dermal Tissue Preparations: A New Method for Repairing Fragile Parchment, and Its Application to the Codex Eycckensis.” The Paper Conservator 19(1995)5-22.)*

## Toward New Terminologies<sup>7</sup>

So, should we stop using the often confusing terms that accompany “analysis” when discussing the ageing, damage, and manufacturing technology of artifacts? The answer extends beyond the suspected “yes”!

Destructiveness could be replaced by “**degree of intervention**,” which might be described at three levels: molecular (low change), microscopic (medium change), or visual (high change). This would imply, for instance, that the withdrawal of a microsample or the generation of a permanently discolored microspot (as a consequence of prolonged remote radiation) reflect exactly the same degree of intervention. Using the older terms, microsampling would be called invasive and the radiation non-invasive, but apparently destructive. However, the degree of intervention and its discussion should be time-related. Indeed, discoloration caused by radiation in a focused beam may be either permanent or limited in time, which means that the degree of intervention could be further classified as medium or low intervention, respectively.

However, the degree of intervention does not explain at all why the analysis is proposed, requested, or executed, and by what party. More information is needed about the expectations of the requestor in terms of how analytical results will be used. It is suggested here that the terms “**usefulness**” and “**innovation**” can provide such information.

The assessment of the “usefulness” of the intervention should consider whether the intervention can establish what production technology was used, provide a damage assessment, and determine the

## Protecting Cultural Heritage

best conservation practice to use. "Innovation" may be formulated in terms of progress beyond the state of the art. Eventually, innovation could be assessed according to the degree of intervention<sup>8</sup> or usefulness<sup>9</sup> of analysis executed according to the newly developed approach. Hopefully, a high level of innovation would create data, insights, and experience which, in turn, would improve usefulness and probably even lower the degree of intervention in the long term.

The terms intervention, usefulness, and innovation may be rightfully used and combined to estimate the balance between the degree or level of intervention and the analytical outcome. And it is exactly this balance that must be discussed by all parties involved when selecting the most appropriate analytical approach. Transparency will be increased by specifying the degree of intervention, usefulness, and innovation when discussing scientific analysis in a multidisciplinary environment. Use of these terms also may improve the source's credibility, the receiver's attention, and the quality of the decision.<sup>10</sup>

### Towards a Definition of Conservation Science

The linguistic and philosophical issues discussed in the two preceding paragraphs illustrate how a natural scientist (chemist, physicist, biologist) working in the field of cultural heritage, must critically define pathways for proposing, executing, interpreting, and explaining analyses of art within a multidisciplinary and responsibility-sharing environment. To this must be added more specific research-related issues, including old manufacturing technologies, ageing phenomena, and the social, cultural, and political pressures to preserve the past for the future. All of these elements constitute criteria for improving the understanding of the specific requirements of conservation science.

The major objectives of conservation science should be to study all aspects (chemical, biological, physical) of the manufacture, decay, and preservation of objects of art and culture. Such studies require the following:

- reading and understanding data in historic literature (revealing the choice of sources, the preparation of products, and the combination of those products in the manufacturing technology of the final object), and the extrapolation of this data into a present-day scientific framework (to prepare mock-ups or to develop an analytical strategy)
- recognition of phenomena, at any level of observation (visual, microscopic, molecular), related to

manufacture and decay

- creation of reference collections and databases of analytical results of references and standards
- development of analytical approaches to enhance the ratio of information to destructiveness and taking into account levels of usefulness and innovation
- understanding of usefulness
- consideration and understanding of historical, geographical, and archaeological aspects of collections
- appropriate applications of statistics
- dedicated fundamental research and high-level interactivity with professionals from other disciplines

### A Multidisciplinary Research Forum in Cultural Heritage

Obviously, conservation scientists should have a strong interest in seeking and promoting interactions with others in their field. Such interactions will become more established within the framework of relevant professional organizations. A prominent player in this field is the Conservation Committee of the International Council of Museums (ICOM-CC).<sup>11</sup> This committee is the largest of 30 international committees of ICOM and is composed of 23 multidisciplinary working groups, covering all aspects of the investigation and conservation of museum collections. In this way, ICOM-CC helps to achieve ICOM's objectives, which are to exchange scientific information at an international level, develop professional standards, and adopt rules and recommendations. ICOM-CC membership, which is spread over 79 countries and has grown by 50 percent over the last seven years, is now more than 1500.

ICOM-CC organizes triennial conferences, where all working groups meet in dedicated sessions and where plenary sessions are organized on topics of general interest. At these conferences, working group members elect a coordinator and discuss a working program for the next three years.

### Conclusion

Multi- and interdisciplinary consortiums established to preserve cultural heritage will benefit from a better integration of conservation science. This may be achieved through establishing a definition of conservation science and through the formulation of end-terms—formed at the master level at



least—for conservation scientists. The terminology used nowadays to describe the potential damage to objects caused by analysis should be refined beyond the destructiveness/non-invasiveness polarization. A terminology should include at least “degree of intervention (low, medium, high),” “usefulness,” and “innovation.” The further development and integration of conservation scientists will improve with their participation in international networks that encourage multidisciplinary approaches. 🏛️

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Jan Wouters <[jan.wouters@kikirpa.be](mailto:jan.wouters@kikirpa.be)> is at the Royal Institute for Cultural Heritage, Brussels, Belgium.

See also [www.iupac.org/publications/ci/indexes/stamps.html](http://www.iupac.org/publications/ci/indexes/stamps.html)

## Stamps International

### A Hydrocarbon to Be Proud of

The stamp from Czechoslovakia illustrated in this note was issued on 4 July 1966 to celebrate the centennial of the Czech Chemical Society, which is one of the oldest chemical societies in the world and is still engaged today in all aspects of the chemical enterprise in the Czech Republic and elsewhere. Prominently featured on the stamp is a molecular diagram of adamantane, the well-known saturated hydrocarbon with a diamond-like structure and a smell reminiscent of camphor. It is a remarkably stable organic compound due to its conformational rigidity and, although it has relatively few applications,

some of its derivatives (e.g., amantadine, rimantadine) are important antiviral drugs against influenza.

Why is adamantane such an iconic molecule in Czechoslovakia, anyway? It turns out that this robust

cage hydrocarbon was first isolated in 1933 from a sample of Moravian crude oil analyzed by S. Landa and V. Macháček at the Czech Technical University (CTU) in Prague. Interestingly, there is another Czech connection to adamantane: It was first synthesized in 1941 by the famous Vladimir Prelog, co-recipient of the 1975 Nobel Prize in Chemistry. Although Prelog was born in Sarajevo (part of the Austro-Hungarian Empire at the time), he earned his Ph.D. from CTU in 1929 and worked in Prague until 1935. The 100th anniversary of Prelog's birth was remembered by Bosnia and Herzegovina with a stamp issued on 25 October 2006.

Written by Daniel Rabinovich <[drabinov@uncc.edu](mailto:drabinov@uncc.edu)>.

A brief history of chemistry in the Czech Republic was published in *Chemistry International* (1998, Vol. 20, pp. 77-80).



## Part II: Terminology in Nuclear Processes—Misconceptions and Inaccuracies\*

by Mauro L. Bonardi and David S. Moore

**T**here are few subjects that evoke a stronger response from most people than those associated with nuclear processes. The “power” of nuclear processes is not only  $E=mc^2$ , but also rhetoric, saber rattling, threats, fear, anguish, and horror. We wonder how much of the vehemence of such a response could be attributed to misunderstandings based on inaccurate and misleading terminology.

For example, using the terminology *atomic* energy to describe the energy produced by *nuclear* processes like fission is misleading, even if, unfortunately, it continues to belong to common language (e.g., peaceful uses of atomic energy, atomic bomb, atomic explosion, atomic reactor, Euratom, International “Atomic” Energy Agency, and so on). The IUPAC Gold Book, as well as Chapter 16 of the Orange Book, makes this distinction very clear. Terms that have to do with nuclear processes do not include the word “atomic” and vice versa. Similar misunderstandings accompany the use of the terminology “radiopharmaceutical” to designate labelled species for biomedical purposes (radio-diagnostic and metabolic radiotherapy), because no pharmacological effects are expected due to the negligible amounts of substance administered. Indeed, to be used in humans, a labelled compound must undergo a series of analytical and radioanalytical GLP and GMP investigations that are well described in the relevant literature (*National and International Pharmacopeia*).

This article seeks to describe the current situation and provide an understanding of preferred terms.

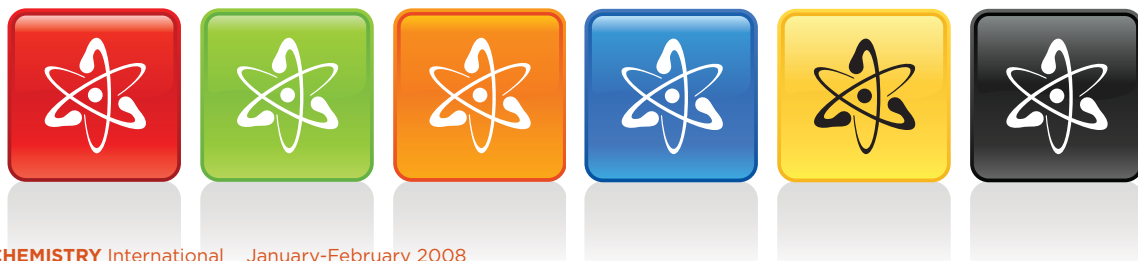
\*Part I focused on the role of radionuclides and radiochemistry in society (Nov-Dec 2007 *CI*).

## Radioanalytical and Nuclear Analytical Techniques vs. Atomic Techniques: How to Avoid Ambiguity?

At the time of their discovery, it was not clear to scientists that the atomic origin of Röntgen’s rays (subsequent to *atomic* electron rearrangement) was completely different from that of Becquerel and Curie’s rays (subsequent to a *nuclear* decay). As is explained below, today we can formulate an unambiguous distinction among them.

In order to proceed further, some definitions and statements are required. We can classify the field of analytical investigations on the basis of the *chemical-physical origin* of the process in question, rather than in terms of associated energy or time scale. This means roughly dividing the phenomena into *sub-nuclear, nuclear, atomic, molecular, or supra-molecular*. Hence, it is possible to classify the different branches of analytical chemistry and related analytical techniques as *radioanalytical and nuclear* (sometimes called nuclear analytical techniques or NATs) on one side and *atomic/molecular* on the other. However, no sub-nuclear processes are presently used on a routine basis for radioanalytical purposes. Therefore, the nuclear processes that are applied in nuclear and radiochemistry (N&R), and through related radioanalytical techniques, only involve the excitation or de-excitation of *nuclear* levels and not *atomic* or *molecular* levels, which are *subsequent* to spontaneous (radioactive decay) or induced nuclear reactions (either manmade or natural). Often, these nuclear processes are *followed* at different time scales by significant atomic and molecular modifications, fruitfully adopted as probes for analytical and structural investigations.<sup>1-5</sup>

In most cases, the processes concerning nuclear transition or transmutation involve much larger amounts of energy (several keV to many MeV or more, [i.e.,  $1 \text{ eV} = 1.60218 \cdot 10^{-19} \text{ J}$  or  $96 \cdot 485 \text{ J}\cdot\text{mol}^{-1}$ ]) than atomic and molecular processes (less than a few eV) and the *radiation* (both electromagnetic and corpuscular) associated with these processes is, as a rule, classified as “directly ionizing radiation,” like X-rays



or fast electron/charged-particle/heavy ion beams accelerated in high-energy acceleration devices (betatrons, Van de Graff, cyclotrons, synchrotrons, LINAC). These types of radiation must be distinguished from radiation that does not have sufficient energy for the *direct* ionization or excitation of the irradiated material or entity. As a useful figure, 30 eV is the average energy that is necessary to induce formation of an ionization/excitation entity in a material, compared to the first ionization energy of He (25 eV), the energy of Group 1 and 2 elements (4–9 eV), and the energy gap of TiO<sub>2</sub> photocatalyst (3.2 eV for anatase). This means that radiations from processes less energetic than UV light (less than a few eV) are not able to induce directly these phenomena and consequently are usually classified as “non-ionizing” radiation or simply by a term or abbreviation implying their energy range (NIR, UV, visible, IR, microwaves, radiowaves, cosmic background, etc.).

We believe the more correct approach to classifying the processes involved is not to describe the associated energy or the time scale, but the physical origin of the process itself. In fact, gamma rays originate from the decay (de-excitation) of nuclear levels in spite of the energy involved, while X rays originate from electronic rearrangements at the atomic levels. From the time-scale viewpoint, plenty of metastable nuclear levels are known and profitably used (radioisomers), with half-lives from fractions of seconds to many years.<sup>6,7</sup> On the basis of this simple classification it is possible to distinguish without any ambiguity between nuclear and atomic/molecular processes, even in the cases in which nuclear and atomic phenomena affect each other and cause significant chemical-physical effects on the chemical environment.

Surprisingly, the half-life of a radionuclide can be influenced by the atomic-electronic environment, especially if decay modes like electron capture or internal conversion on the innermost atomic shells are involved, because the decay probability of a radionuclide depends on the overlap between the nuclear and atomic wave functions. Unexpectedly, the half-life of metastable levels of nuclides is also affected by the chemical surroundings of the nuclides. The *hyperfine interaction* between nuclear levels and the *chemical microenvironment* (*chemical isomer shift*) is the basis of *Mössbauer spectroscopy* (MÖSSPEC, MOSPEC), a powerful radioanalytical tool for structural and analytical purposes. The interaction of decay emitted positrons, and the *positronium* quasi-atomic species Ps formed by binding with atomic electrons,

is affected by the chemical environment as well, giving rise to *positron annihilation spectroscopy* (PAS) and related radioanalytical techniques. On the other hand, other exotic quasi-atomic species like *muonium* and *antiatoms* have resulted to date in negligible analytical potentialities. These electronic effects following nuclear decay or nuclear reactions are, of course, not of direct nuclear origin and are normally called *extranuclear* or *atomic effects of nuclear transformations*. Among such effects are the emission of X-rays and Auger (and Coster-Kronig) monoenergetic electronic cascades after the rearrangement of electronic shells that occurs before most nuclear decay processes that are able to create electronic vacancies in the innermost atomic shells. Even *Bremsstrahlung* radiation (external and internal) generated by the deceleration/centripetal acceleration of fast particles through matter and Cherenkov shockwave visible radiation are not precisely of nuclear origin, but must be classified as atomic effects subsequent to a nuclear process.

In this framework, X rays and the X-ray based analytical techniques for chemical analysis in the energy range from some keV to some hundreds of keV have proved incapable of inducing nuclear processes. Let's remember that the binding energy of an alpha particle at rest is 28.3 MeV (or 7 MeV.nucleon<sup>-1</sup>), and the binding energy per nucleon of the 2 850 nuclides presently known varies from 2.2 MeV for the less stable, like <sup>2</sup>H, to 8.8 MeV for the more stable: Fe, Co, and Ni. Hence, analytical techniques based on the use of fast ion or electron beams with energy insufficient to induce nuclear reactions are normally called Ion Beam Analytical (IBA) techniques and are not nuclear techniques at all. Among them are PIXE, RBS, and a range of techniques based on the use of synchrotron radiation, even in the X-ray energy range (SRXRF, EXAFS, XANES).<sup>1</sup> Thus, elemental analysis techniques based on X-ray fluorescence, like XRF, TXRF, or ED-XRF, are not of nuclear origin, even if they are based on the use of radiogenic equipment or radioactive sources as excitation devices, which are incidentally installed at nuclear centers. Conversely, nuclear activation methods, like delayed and prompt neutron and charged particle *activation analysis*—in both instrumental or radiochemical versions, are properly classified as nuclear analytical techniques, because, in spite of the occasional low-energy projectile involved, they lead to a nuclear reaction on target nuclei, with delayed or prompt emission of de-excitation gamma rays or

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*Continued on page 25*



# The Emerging Chemical Regulatory Environment



## Proceedings of the World Chemistry Leadership Meeting

by Colin Humphris and Mark Cesa

**S**eventy-five delegates attended the World Chemistry Leadership Meeting (WCLM) on 10 August 2007 in Torino, Italy. The WCLM focused on the promising, yet challenging, global effort to meet the commitment that by 2020 chemicals are used and produced in ways that minimize significant adverse effects on human health and the environment. The 2020 commitment was made at the 2002 World Summit on Sustainable Development\* in Johannesburg and has led to new policy frameworks such as SAICM (UNEP/WHO) and regulations such as REACH (EU Commission).

The WCLM, held during the 44th General Assembly of IUPAC, attracted high-level representatives from industry, academia, and the UN. Speakers and panelists at the event included the following experts:

- Rainer Koch (International Council of Chemical Associations, ICCA)
- Carol Henry (American Chemistry Council, ACC)
- Richard Phillips (ExxonMobil)
- John Duffus (The Edinburgh Centre for Toxicology, Chair of the IUPAC Subcommittee on Toxicology and Risk Assessment)
- Elsa Reichmanis (Alcatel-Lucent)
- Alan Boobis (Imperial College School of Medicine)
- Matthew Gubb (UNEP)

WCLM attendees and speakers discussed the health and environmental safety of chemical products, emerging issues of societal concern, and the resulting regulatory trends, with the objective of identifying specific

contributions IUPAC could make through projects or through working with others. Participants recognized environmental health as an important aspect of applied chemistry for IUPAC and agreed that there is a need for an ongoing dialogue with key stakeholders, the industry, and UN on these matters. A consensus was also reached on the following important issues:

- The bulk of the environmental health concerns arising from the industrial application of chemistry lie in the developing world. IUPAC has a key role to play in education and capacity building to bring product stewardship toward the levels practiced in the developed world. IUPAC should seek to collaborate with industry and the initiatives it is undertaking, and with the SAICM process and its Quick Start Programme.
- Underlying many public concerns about the use of chemicals is a lack of understanding and appreciation of chemistry. This is a concern to both IUPAC and industry. The proposed UN/UNESCO International Year of Chemistry 2011 provides a strategic opportunity to celebrate both the contribution of chemistry to human development and the safe, responsible use of chemical products. IUPAC should invite industry to engage fully in the International Year of Chemistry.
- There is a need to strengthen the contribution of science to chemicals policy to ensure that future policy is soundly based. IUPAC is invited to provide chemical science input to the forthcoming SAICM implementation conferences and should consider the most appropriate processes to do this. Value is seen in working more closely with both UNEP and WHO and seeking formal recognition with both as an NGO.
- New health concerns are emerging from innovation (e.g., nanotechnologies) and our broader understanding of biochemistry and genetics, which cross the boundaries of chemistry, biology, toxicology, and medicine. It is important for IUPAC to remain alert to these concerns to ensure that it can contribute to questions of nomenclature, classification, and characterization and the development of appropriate methodologies (e.g., biomonitoring) to assess their toxicological, health, and environmental impacts.

\*The World Summit on Sustainable Development, WSSD or Earth Summit 2002, took place in Johannesburg, South Africa, from 26 August to 4 September 2002. It was convened by the United Nations to discuss sustainable development. WSSD gathered a number of leaders from business and non-governmental organizations, 10 years after the first Earth Summit in Rio de Janeiro <[www.worldsummit2002.org](http://www.worldsummit2002.org)>.

## Summaries of WCLM Lectures

### Rainer Koch (International Council of Chemical Associations, ICCA)

Koch began his lecture by describing the history of SAICM, which originated with the Johannesburg declarations in 2002:

“... aiming to achieve by 2020 that chemicals are used and produced in ways that lead to the minimization of significant adverse effects on human health and the environment using transparent science-based risk assessment procedures as well as science-based risk management procedures.”

As Koch explained, this declaration has led to a high-level political commitment from governments and stakeholders (including industry) and a policy strategy that lays out the key elements and principles to be adopted. From this, a Global Plan of Action was adopted as part of the Dubai Declaration (International Conference on Chemicals Management, ICCM 2006) to provide guidance and tools to enable governments to set priorities for chemicals management and regulation. REACH is a European example of this; a new regulation for chemicals management encompassing all stages of the value chain from primary manufacture to eventual consumer use. It will require the eventual preparation of some 80 000 registration dossiers.

Koch discussed the question “What does minimization of significant adverse effects actually mean?” Then he talked about how the Johannesburg declaration has made the following necessary:

- science-based risk assessment and management
- extensive data on chemical hazards and exposures
- education and capacity building in chemicals use

Koch recommended a number of ways in which IUPAC could help with this process:

1. improve knowledge/information on chemicals and chemical processes
2. develop sound risk assessment methodologies (targeted and comparative assessments)
3. contribute to the SAICM Quick Start Programme by proposing capacity building in developing countries

4. establish a scientifically sound interpretation or definition of the meaning of “minimization of significant adverse effects on human health and the environment,” the goal of the Johannesburg declaration
5. perform outreach to developing countries of science-based approaches to chemicals management: capacity building, education, and training
6. act as an active stakeholder in the SAICM implementation process, particularly in the upcoming international conferences
7. organize scientific sessions on key topics of SAICM in conjunction with IUPAC conferences
8. promote/support industry voluntary initiatives related to emerging science issues (e.g., ICCA Long-range Research Initiative [LRI] program)

### Carol Henry (American Chemistry Council)

Henry began her talk by describing the realities for the chemical industry today. She noted that “Discourse and debate about chemical products and their usage is too often fuelled by misinformation and lack of relevant facts and scientific research—fact versus fear.”

Henry described how the new global charter for Responsible Care, an industry initiative announced at the ICCM in Dubai (where SAICM was launched) will counter the tendency toward fear with more balanced information. The goal of Responsible

Care, she said, is to set a new vision for improved performance and strengthened engagement. It is designed to ensure consistency of approach across the world, with an increased focus on product stewardship (the Global Product Strategy [GPS]), and the management systems needed for its implementation. GPS sets out to improve the stewardship of chemicals from source to consumer through partnership, training, and dialogue and includes a commitment to participate in the necessary scientific enquiry to address health and environmental risk concerns through the industry’s LRI.

Henry appealed to IUPAC to engage with ICCA to develop a new paradigm of constructive engagement across the world of chemistry to replace “fact versus fear.” This would enhance discourse and partnership, promote engagement in the implementation of Responsible Care and GPS, encourage science and innovation (better products for a more sustainable future), and further chemistry education and capacity building.



# The Emerging Chemical Regulatory Environment

## Richard Phillips (ExxonMobil)

Phillips outlined why emerging science is so important to industry and policy makers when it is combined with societal change, encapsulated in the “right to know.” As he explained, when new questions emerge about the influence of people’s environments on their health, the debate rapidly moves to the need for action, which is often based on over-precaution and fear rather than thorough knowledge-based assessments. He noted that the European Union has set up an expert scientific committee to advise it on emerging risks.

Phillips provided examples of emerging science that will be helpful in assessing risks:

- nanotechnology to provide arrays for assessing the effects of chemical stimuli on cells (lab on a chip)
- biomonitoring as part of the assessment of an individual’s susceptibility to environmental chemicals and the need for new monitoring science for the environment, for the body intake, and for the assessment of pre-clinical responses (e.g., Gene-Environment Initiative, U.S. National Institutes of Health)
- epi-genetics, which is the science of the factors that effect gene expression and provides evidence of inheritable changes in response to environmental factors (exposures that may affect future generations)

He outlined a number of ways to maintain focus and support for incorporating new, improved technology in our risk assessments. Following are some of his suggestions:

- tools to link chemistry and biology in the new toxicology paradigms to be able to address the often subtle and more complex effects of real environments on health
- systems to manage, interpret, and apply the explosion of data that will follow from the application of new technologies
- education of the public to avoid policies that address “apparent problems,” but which could create greater adverse consequences
- improved science support to policy through
  - a renewed commitment to follow the scientific method
  - testing hypotheses and validating methods
  - confirming data and results clearly
  - communicating data and results clearly
  - considering alternative, biologically plausible and reasonable explanations for observations

## John Duffus (The Edinburgh Centre for Toxicology, chair of the IUPAC Subcommittee on Toxicology and Risk Assessment)

Duffus emphasized the importance of an authoritative and informed chemistry basis for policy and regulation. He cited a number of examples where the science basis for policy is questionable or ambiguous:

- the concept of no threshold for mutagenic activity
- the extrapolation of high-dose effects in mice and rats to humans
- the absence of real exposure data in epidemiological studies on which policy decisions have been based
- the absence of consideration of chemical speciation for all elements except carbon
- the need for new toxicological thinking when applied to nano-particles together with considerations of bio-availability for insoluble particles

Duffus concluded that “the assumptions inherent in regulatory toxicology should be reviewed regularly to bring them in line with current scientific thinking; this implies continuing revision of rodent (and other) test guidelines to ensure that the tests provide relevant data and that the data are correctly interpreted.” IUPAC should play its part in this work, he said.

## Panel and Discussion

### Moderated by Elsa Reichmanis (Alcatel-Lucent)

Alan Boobis reflected that there needs to be a chemical basis for concerns relating to chemicals and health. In some of the NGO activity that we see, this is missing; the focus is more on concerns of the unknown. Aside from well-known environmental toxicants and examples of environmental mismanagement, there is little evidence of human susceptibility to chemicals at the background environmental levels encountered in the developed world. Here, he said, current regulations are already precautionary and have served us well, providing adequate protection.

Boobis pointed out that policy makers do have a tough job however and many science gaps remain. Following are some of his ideas for how the scientific community and governments can fill these gaps:

- develop mechanistic insights to show that thresholds of activity exist
- ensure biomarker data is acceptable to regulators
- confirm that current multigenerational studies can identify multigenerational effects
- develop tiered approaches to risk assessment to enable a focus on priorities

## Proceedings of the World Chemistry Leadership Meeting

- understand the modes of action for different categories of chemicals

He agreed these were areas where chemistry needs to work with biology and medical science.

Speaking for UNEP, Matthew Gubb picked up on the theme that there is a need to strengthen the scientific base. This is a key component of SAICM, which he emphasised is a multistakeholder activity. As he explained, it is important to recognize that governments need to respond to societal concern and that authoritative science is needed to bridge that gap, improve understanding, and influence perceptions. He encouraged IUPAC to play an active role in the future SAICM conferences outlined by Koch, which will review progress and identify emerging issues. The conference in 2009 will include reports from science bodies which will recommend areas for action to provide a pathway to future regulation. It will be important that this is well grounded and that issues not yet addressed are highlighted. He foresaw IUPAC acting as a focal point in this regard.

The discussion continued with a fundamental question: What is a chemical? As Duffus noted, for the public the term “chemicals” has tended to mean products produced by the chemicals industry. Boobis stated that a chemical is a substance, natural or synthetic, that may interact with a biological system. Care is needed, he said, with the definitions and classifications in common use as toxicology is indifferent to the source of a chemical, which may be natural or synthetic. The feeling was that this is understood by regulators, but there is an educational question for the public. As a question of nomenclature, this may be something for IUPAC to consider, said Carol Henry.

The panellists and audience exchanged questions on a variety of topics. Are scientists part of the problem? Do they make it difficult to appreciate and objectively debate “chemicals” and “chemical issues” in public? What will be regarded as safe in 15 years and how can we continue to improve public health? Is the focus on chemicals fully justified, considering that many of the environmental problems come from human and mammalian waste? Don't most of the problems exist in the developing world, how can the developing world cope with capacity building, and are sufficient funds and resources available?

One way IUPAC can play an important role is in providing objective and authoritative science to the policy debate on complex chemistry issues. Such

authoritative “white books” have been prepared in the past and in response to the issues related to chlorine and endocrine disruption. Mapping emerging scientific issues of importance to industrial members would also be valuable, balancing the perspectives of the science, those of society, and those where IUPAC can have influence.

The relationship between regulation and public perceptions of chemistry was also raised. IUPAC is already seeking to address these public perceptions and felt this relationship could be addressed in the proposed UN/UNESCO International Year of Chemistry in 2011 which could serve to highlight both the benefits of chemistry and the effective management of hazards.

IUPAC President Bryan Henry concluded by summarizing points he had noted from the four presentations and the plenary discussion:

1. Rainer Koch's description of the industry response to the new regulatory environment and his recommendations for IUPAC to engage in SAICM
2. Carol Henry's description of the experience of Responsible Care, which highlighted the importance of public perceptions of both the industry and the application of chemistry
3. Richard Phillips' focus on key emerging issues such as nanotechnology, biomonitoring, and transgenerational effects in which chemistry needs to consider its contribution
4. John Duffus' identification of the ambiguity in the chemistry applied in many areas of regulation today

Henry noted that underlying many of the science and policy questions that were raised in the discussion was a lack of public understanding and appreciation of chemistry. The balance of science funding for cutting-edge and for applied research was important given the needs to develop practical public health methodologies such as biomonitoring. He said it was clear that many issues were raised where IUPAC can help and the dialogue (with industry and the UN agencies) should continue.

Colin Humphris <[cjhumphris@btinternet.com](mailto:cjhumphris@btinternet.com)> is a titular member on the IUPAC Committee on Chemistry and Industry (COCI). Until last year, he was executive director of research and science at CEFIC (The Chemical Industry Association in Europe). Mark Cesa <[Mark.Cesa@innovene.com](mailto:Mark.Cesa@innovene.com)> is chair of COCI; he is a process chemistry consultant for INEOS Nitriles in Naperville, Illinois, USA.

 [www.iupac.org/symposia/conferences/ga07/wclm07.html](http://www.iupac.org/symposia/conferences/ga07/wclm07.html)

# IUPAC in Torino, Italy—Part II

The 41st IUPAC World Chemistry Congress, which had the theme of “Chemistry Protecting Health, Natural Environment, and Cultural Heritage,” was held at the Lingotto Conference Center in Torino, Italy, 5–11 August 2007. The Congress, which was co-organized by the Italian Chemical Society, the National Research Council of Italy, the University of Turin, and the Polytechnic of Turin, is an international scientific conference that meets concurrently with the General Assembly, the meetings of the governing bodies and committees of IUPAC.

The Congress <[www.iupac2007.org](http://www.iupac2007.org)> attracted approximately 2 000 attendees from around the world. Plenary lectures were given by the following eminent chemists:

- Roald Hoffmann (Nobel laureate, Cornell University, USA), “Science and Ethics: A Marriage



Plenary lecturer Kurt Wüthrich (left) and Francesco De Angelis, co-chair of the Congress International Advisory Board and president of the Italian Chemical Society.

of Necessity and Choice for this Millennium”

- Kurt Wüthrich (Nobel laureate, ETH, Switzerland), “Protein Structure Biology Using NMR—At the Interface of Chemistry and Biology”
- Jan Wouters (Royal Institute for Cultural Heritage, Belgium), “Reflections on the Position

## “Chemistry is Beautiful”—A Report on the Opening Plenary Lecture by Roald Hoffmann

by Neil Gussman

“Chemistry has so much to be proud of,” said chemist, poet, playwright, and polymath Roald Hoffmann in his opening plenary lecture at the IUPAC Congress in Torino. Hoffmann’s talk, which began with chemistry then gave a glimpse of his views on philosophy and human nature, preceded a staging of his latest play, *Should’ve*.

Hoffmann, the 1981 Nobel laureate in chemistry, credits the chemical sciences with providing spiritual as well as material progress to humanity. “Knowledge of genetics, of the cosmos, of the color of cornflowers” is just part of an “incredible gain in knowledge” through chemistry, Hoffmann said. He noted that the knowledge that chemistry gave the world supplied “improvements for some, but not for all.”

Hoffmann then turned from chem-

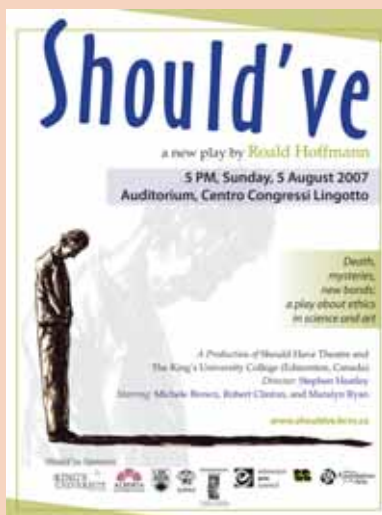
istry to its effect on society. “People are not happier,” Hoffmann said, referring to people in cultures that have the benefits of modern science, “and many do not praise technology” because “people are not happy by nature.” That comment started a small buzz in the audience. Hoffmann went on to say that the divide between those in the sciences and the wider population exists because “people are not machines. They are wonderful, vexing beings.

Science cannot understand people.”

Speaking of how little the general public understands chemistry, he said, “Half of the nitrogen atoms in me are from a chemical reactor through the Haber-Bosch process.” It was clear from the buzz and nods that this fact was news to many—even in an audience more familiar with chemistry than just about any similar-sized group on the planet. Since it went into use in Germany at the beginning of World War I, the Haber-Bosch process has been the source of an ever-larger fraction of the nitrogen available for biological processes.

Hoffmann then addressed the perception of chemistry among the wider public. “In the past 50 years, pollution has changed from normal entropy to a sin,” he asserted. The public perception of chemistry descended from a mid-20th-century source of innovation and products to make life better to a source of pollution and a threat to health. He then proposed a three-point plan to reconnect chemistry with the world at large. Chemistry leaders should:

1. accept human nature







of Chemistry in Multidisciplinary Approaches, Aiming at Protecting Cultural Heritage” (See related feature on page 4.)

- Robert Huber (Nobel laureate, Max-Planck-Institut für Biochemie, Germany), “Proteins and their Structures for Basic Science and Application in Medicine”
- Akira Fujishima (Kanagawa Academy of Science and Technology, Japan), “The Increasing Contribution of Photocatalysis to Comfort and Safety in the Urban Environment”
- Vincenzo Balzani (University of Bologna, Italy), “Molecular Devices and Machines”

A follow-up to Hoffmann’s lecture was the premiere performance of his new play *Should’ve* during the opening session of the Congress. The fully staged production of the play, which explores ethics through

the intersecting worlds of science and art, was presented by the Should Have Theatre, an independent professional theater company hosted by The King’s University College of Edmonton, Alberta, Canada. The play featured Michele Brown as Katie Wertheim, Maralyn Ryan as Julia Hollander, and Robert Clinton as Stefan Cardenas. Peter Mahaffy (The King’s University College), chair of the Committee on Chemistry Education, served as the liaison between IUPAC and the production team, which included his son Reuben, who was videographer and projection designer.

In another significant event, the City of Torino and IUPAC held an evening meeting at the Gallery of Modern Art in memory of Primo Levi, Turinese writer, chemist, and Jew, on the occasion of the twentieth anniversary of his death. Recollections of Levi were expressed by people who knew him and had worked with him, and through a film. Roald Hoffmann, himself

2. introduce ethical and ecological concerns in all chemical training
3. reawaken the primary motive of science, to meliorate the human condition

Hoffmann turned 70 in 2007. Born in 1937, his early life was marked by one of the worst crimes in human history. “The feeling of being dealt with unfairly causes real pain,” he said, yet he added, “I remain an optimist despite or because of surviving the Holocaust.”

Next he turned to the effect the free market can have on ethics, saying, “Market conditions alone do not provide motivation for ethical production decisions.” He cited the choice between producing malaria drugs and Viagra as an instance of where the free market can lead.

As he brought his talk to an end Hoffmann connected creativity and responsibility to describe the tension central to his latest play. He takes creativity as a given of human life: “As we create—we cannot help creating—we have a responsibility to ask about final use.”

He then took a seat with the




*On stage in Torino, Michele Brown as Katie Wertheim and Robert Clinton as Stefan Cardenas in the first production of Should’ve.*

*For more about Roald Hoffmann’s Should’ve, see May-June 2007 CI, pp. 4–7.*

audience and watched the premiere of his third play, which follows the family of a scientist who committed suicide as they deal with the consequences and the meaning of his death and the choices they made because of him.

Hoffmann remained in Torino for much of the week that followed, participating in discussions and public events during the biennial congress. He is very well known for saying


“Chemistry is beautiful.” Through plays and poetry, he brings his own perception of beauty to audiences who might otherwise never be able to see what he sees in chemistry. 

Neil Gussman <NeilG@chemheritage.org> works at the Chemical Heritage Foundation (CHF) [www.chemheritage.org](http://www.chemheritage.org). In Torino, he represented CHF and attended the meeting of the IUPAC Committee on Chemistry Education (see p. 16). CHF shares common goals with, and is an Associated Organization of, IUPAC.

## IUPAC in Torino, Italy—Part II

a Holocaust survivor, offered a very moving tribute to the works of Levi, who survived internment at Auschwitz, and the impact they had on his own teaching and writing.

Invited and contributed oral and poster presentations at the Congress were made within 10 topical groups: environment, health, cultural heritage, materials and nanotechnology, theoretical and computer chemistry, inorganic chemistry, analytical chemistry, organic and polymer chemistry, biological and biophysical chemistry, and chemical education.

The next IUPAC Congress and General Assembly will be held 1–9 August 2009, in Glasgow, Scotland. If you wish to look further ahead, Puerto Rico will be the venue of the Congress and General Assembly from 30 July–7 August 2011. 



[www.iupac2009.org](http://www.iupac2009.org)

[www.iupac2011.org](http://www.iupac2011.org)

## Division Roundups— Part II

Part 1 of the Division Roundups from the 2007 General Assembly in Torino, Italy, appeared in the Nov-Dec 2007 *CI* (page 7). That article covered Division IV: Polymer, Division V: Analytical Chemistry, Division VI: Chemistry and the Environment, and CHEMRAWN. Prior to the GA, all divisions and standing committees provided a written report that is part of the *Council Agenda* book available online <[www.iupac.org/symposia/conferences/ga07/council\\_agenda.html](http://www.iupac.org/symposia/conferences/ga07/council_agenda.html)>.

### Committee on Chemistry Education (CCE)

#### *Morton Z. Hoffman, U.S. National Representative*

The meeting of CCE, which was chaired by Peter Mahaffy, began with approval of the minutes of its previous meeting at the 19th International Conference on Chemical Education (ICCE) in Seoul, Korea, in August 2006, and a report of the executive strategy meeting that took place in Paris in March 2007.

Among the priority areas of concern of CCE are the ethical education of young chemists, the social responsibilities of scientists, the multiple uses of chemicals for peace and weapons, the relationship of chemistry and sustainable development, and the shift from teacher-centered to user-directed chemical education.

Reports were presented from the subcommittee on the Public Understanding of Chemistry about

the procedures that would have to be followed in order for 2011 to be designated by the United Nations as the International Year of Chemistry (note was made that 2007 was the Year of Chemistry in Spain), and from the subcommittee on Chemistry Education for Development about the current Flying Chemists Program to revitalize tertiary education in the Philippines. This latter subcommittee also reported on the establishment of the Network for Inter-Asian Chemistry Educators, among Korea, Japan, Hong Kong, China, and Taiwan, which held a symposium in Taipei in July 2007.

Next on the agenda was a presentation by the Chemical Heritage Foundation (CHF). Edwin “Ted” Becker, long-time officer of both IUPAC and CHF, opened the session by describing the Philadelphia-based organization using its mission statement of treasuring the past, educating the present, and inspiring the future. Becker briefly described the collections, including thousands of rare books in the history of chemistry and early science, the world’s largest collection of art about alchemy, and many artifacts as varied as 18th century lab glassware and mid-20th century chemistry sets. Addressing CHF’s education outreach, he talked about the ways in which IUPAC and CHF could cooperate to extend the reach of both organizations, particularly through the web.

Becker was followed by Neil Gussman, who spoke about current programs at CHF and how he saw them fitting together with IUPAC efforts. Gussman is the communications manager for CHF and has more than 20 years experience in public relations for chemical clients. He was particularly impressed by the way the education committee considered real-world communications and the public image of chemistry in its efforts. Other organizations with the goal of increasing education outreach do not consider how the public will view such efforts, dooming them to failure.

Alistair Hay presented a brief report on IUPAC’s collaboration with the Organization for the Prohibition of Chemical Weapons (see Nov-Dec 2007 *CI*, pp. 23–25) that focused on producing educational materials. Hay discussed the newly developed web site <[www.iupac.org/multiple-uses-of-chemicals](http://www.iupac.org/multiple-uses-of-chemicals)>.

In more recent years, CCE has developed better communication with other IUPAC divisions. The chairman and Eva Åkesson, in her role of divisional liaison officer, visited all eight divisions during the General Assembly to present CCE. Some of the projects and priorities for the future were highlighted, such as the Young Ambassadors for Chemistry, International Year of Chemistry, 20th ICCE, and learner-centered edu-

## Division Roundups—Part II



**Morton Hoffman (left), U.S. national representative on the Committee on Chemistry Education, and Vincenzo Balzani, plenary lecturer at the IUPAC Congress.**

cation. Future collaboration and joint projects were discussed. A recurrent topic echoed from each group was the need to better plan for publication, including an educational component, and the need to assess carefully the accessibility level of that information.

Members of CCE presented reports about the chemical education issues that confront their countries, such as incorporating green chemistry into the curriculum, interesting students toward the study of chemistry, improving the abilities of chemistry students, and increasing the time spent by students on the study of chemistry at the primary and secondary levels. My report on the state of chemical education in the USA emphasized the important role of the ACS, its committees, technical divisions, and publications, in producing materials across the educational spectrum, reaching out to high school teachers, encouraging research in educational practices and teaching and learning, and working to reflect the changes that are taking place within chemistry and the other molecular sciences in curricular content and pedagogical approaches. Special mention was made of the proposed revision of the ACS Committee on Professional Training guidelines for the approval of departmental chemistry programs and the certification of their bachelor graduates by the ACS.

The 20th ICCE—Chemistry in the ICT Age will be held 3-8 August 2008 in Pointe Aux Piments, Mauritius <[www.uom.ac.mu/icce](http://www.uom.ac.mu/icce)>. Among the plenary lecturers will be Roald Hoffmann, Loretta Jones (University of Northern Colorado), Peter Mahaffy (The King's University College), Peter Atkins (Oxford University), Henry Schaefer (University of Georgia), Arthur Olson (Scripps Research Institute), and John

Bradley (University of the Witwatersrand, South Africa). The meeting will be preceded by an on-line conference on "Computational and Theoretical Chemistry Applications in Chemical Education," which will be part of the CONFICHEM Conferences on Chemistry of CHED <[www.ched-ccce.org/confchem](http://www.ched-ccce.org/confchem)>. A satellite conference at the University of Nairobi (Kenya) will follow the ICCE.

CCE voted to accept the bid of Taiwan to host the 21st ICCE in Taipei; the focus of the conference will be communication about the teaching of chemistry. Bids for the 22nd ICCE in 2012 are being accepted as well as expressions of interest for the 23rd ICCE in 2014; the plans for both future conferences will be discussed by CCE in Mauritius. For further information, please contact me as the CCE conference coordinator.

**Morton Z. Hoffman** <[hoffman@chem.bu.edu](mailto:hoffman@chem.bu.edu)> is a retired professor from Boston University; he is the U.S. national representative on CCE and the liaison with the ACS Division of Chemical Education.

### **Division VII. Chemistry and Human Health** **Mukund S. Chorghade, secretary**

Thanks to a proactive and rigorous effort by the nomination committee, Division VII's elections were a resounding success. Tom Perun, chair of the Nominating Committee, reported that the election process was smooth, the number of candidates of excellent caliber was high, and the electoral response was nearly 70 percent. We have a broad geographical representation and diversity on the Division Committee as well as significant new expertise. Doug Templeton was elected president-elect until January 2008. He will become president in January 2008 following the retirement of Paul W. Erhardt.

Erhardt presented the annual report that was submitted to the Bureau and mentioned the highlights/salient features. The division's report adhered to all prescribed guidelines and received favorable responses from other divisions. One of the highlights he mentioned was *Analogue-based Drug Discovery*, a book on medicinal chemistry that arose out of division projects and has received excellent reviews in professional journals and sold out its first print run of 800. Mention was also made of the successful IUPAC-Richter Prize venture. Erhardt also discussed the following important projects.

*Practical Studies for Medicinal Chemistry Students—An Integrating Approach for Developing Countries* by Antonio Monge (project 2004-028-1-700) was published as a web edition in January 2007. The book,

## Division Roundups—Part II

in Spanish or Portuguese and English, is available for free online.

Excellent progress has been realized on the following projects:

- concepts and structure for requests in clinical laboratories
- internationally agreed terminology for observations in scientific communication
- mapping of IFCC-IUPAC laboratory coding system to SNOMED CT
- securing and structural updating of information in the NPU coding system and its environment
- recent advances in Nomenclature, Properties, and Units: strategy for promoting SC-NPU achievements

The second edition of the glossary of terms used in toxicology was published in the September 2007 issue of *Pure and Applied Chemistry*. Philip Wexler, National Library of Medicine, Division of Specialized Information Services, will incorporate this into his book *Information Resources in Toxicology*.

Work has commenced on the “Explanatory Dictionary of Concepts in Toxicokinetics (part II)” and is expected to be completed within the stipulated time. Once complete and accepted for publication in *PAC*, parts II and I will be combined, revised, and reformatted into book form to be published by the Royal Society of Chemistry under the title *Concepts in Toxicology*.

The Division had four posters exhibited at the Congress in Torino. There was one general poster presenting the activities of the Chemistry and Human Health Division and one poster for each of the three subcommittees: SC on Nomenclature, Properties, and Units in Laboratory Medicine; SC on Medicinal Chemistry and Drug Development; and SC on Toxicology and Risk Assessment.

### Committee on Chemistry and Industry (COCI)

**Michael Booth, secretary**

The well-attended COCI annual meeting, held 6–7 August 2007, included 13 COCI members, four safety trainees, three divisional representatives, and the remainder either observers or invited participants. The meeting focused on the committee’s role and strategic priorities, organizational structure, and programs and accomplishments. COCI is currently considering joint projects with divisions and other standing committees with an emphasis on biomonitoring and aspects of human health. A number of members agreed to serve


on a fundraising committee to bolster the funds available to the committee over and above the operations and project budget.

The Safety Training Program, in which professional chemists and chemical engineers in developing countries are exposed to safety practices of the chemical industry in the developed world, continues. At the meeting, it was reported that two more trainees had undergone training at the Mitsui Corporation in Japan. There is no shortage of trainees wishing to participate in this program, which enjoys wide acknowledgement in IUPAC. A recurring problem, however, is the availability of host companies. An idea for a spin off of the program, initiated by one of the Uruguayan trainees, is to develop a safety training program in South America.

One of the new initiatives of the committee is to foster closer collaboration with trade associations, particularly with CEFIC (the European Trade Association) and the International Council of Chemical Associations. COCI organized the World Chemistry Leadership Meeting (WCLM) at the General Assembly as part of its process of collaboration. The proceedings of the WCLM will be reported on the IUPAC website (see feature on page 10).

COCI continued to promote the recruitment of new company associates and a new brochure expounding the merits of joining IUPAC is in the final stages of publication. The committee continues to work with the Committee on Chemistry Education on promoting the public appreciation of chemistry. A decision was also made at the meeting to forge closer interactions with National Adhering Organizations. As a pilot project, it was decided to run a workshop with NAOs in Europe as part of the annual meeting in Marl, Germany, in April 2008 (see IUPAC project 2006-030-1-022, <[www.iupac.org/projects/2006/2006-030-1-022.html](http://www.iupac.org/projects/2006/2006-030-1-022.html)>).

At the project meeting earlier in the year, new projects were proposed on biomonitoring, nanotechnology, and human health, and on biofuels. Presentations were made at the meeting to decide how project proposals should be advanced.

The possibility of introducing an award that recognizes and reinforces the ideals perpetuated by COCI was debated at the end of the meeting. Further recommendations will be advanced at the Marl meeting. 

**Michael D. Booth** <[caiainfo@iafrica.com](mailto:caiainfo@iafrica.com)> is from the Chemical & Allied Industries Association, in Auckland Park, South Africa. He has been a member of COCI since 1992 and secretary since 2006.

## Polymer International–IUPAC Award 2008: Call for Nominations

The executive editors of *Polymer International* and the IUPAC Polymer Division have established an award for creativity in applied polymer science or polymer technology. This new award, which celebrates the achievements of young researchers in the polymer community, will be presented at the IUPAC World Polymer Congress—MACRO 2008, to be held 29 June–4 July 2008 in Taipei, Taiwan.

The winner will be awarded USD 5 000 plus travel and hotel accommodation expenses to attend MACRO 2008, where he/she will present a plenary-type lecture. **All nominations are due by 15 March 2008** to Samantha Swann <[sswann@wiley.co.uk](mailto:sswann@wiley.co.uk)>. A Scientific Committee, representing *Polymer International* and the IUPAC Polymer Division, will select the winner on the basis of scientific merit from nominations received before this date.

Nominees must be under age 40 on 31 December 2008, and must be available to present a plenary-type lecture at MACRO 2008. Nominations must include the following information:

- name and address of person making the nomination
- full name and date of birth of nominee
- business address of nominee
- academic background and education (college or university, location, major field, degree, year awarded)
- academic honors
- employment history (position, organization, duties, dates)
- publications, patents, unpublished reports, papers presented at meetings (a list of those deemed pertinent)
- honors and awards
- scientific achievements for which the candidate is nominated for this award

 [www.iupac.org/news/archives/2007/PolymerInt-award.html](http://www.iupac.org/news/archives/2007/PolymerInt-award.html)

## IUPAC InChI/InChIKey Project Joins Microsoft BioIT Alliance

The continued development of new and powerful medications for treatment of disease relies more and more heavily on collaborative projects, involving organizations possessing a wide range of complementary skills. The discovery techniques developed over many years by the pharmaceutical industry can now be married with a new generation of genome-based technologies, enabling many quite different approaches to health



care. Information technology is an integral part of this enterprise. The vast collections of biomedical data now emerging require ultra-sophisticated methods of data-handling, and such methods are currently being developed and improved by teams of software engineers in a variety of IT organizations. The establishment of the BioIT Alliance in April 2006 by Microsoft and leading organizations in the life science industries was very much a reflection of this scenario. The Alliance has now been extended to include IUPAC.

The importance of IUPAC's contribution to the enterprise lies primarily in its responsibility for establishing standards for transmitting chemical information. IUPAC has long been well known for its internationally agreed recommendations for deriving names for chemical substances. With the number of known substances running into many tens of millions, including both those reported in the scientific literature and those synthesized in-house, this is no small achievement; however, conventional names are not best suited to the age of information technology, and IUPAC, in collaboration with the U.S. National Institute of Standards and Technology, has developed the machine-readable International Chemical Identifier (InChI), an open-source identifier algorithmically generated from a two-dimensional graphical structure <[www.iupac.org/inchi](http://www.iupac.org/inchi)>. This contains full structural information and can be converted back into the original structure.

On 5 September 2007, IUPAC launched the beta-version of software to generate a new fixed-length (25-character) identifier, derived algorithmically from InChI and known as InChIKey <[www.iupac.org/inchi/release102.html](http://www.iupac.org/inchi/release102.html)>. Although this version of the identifier does not itself contain information about chemical



structure, it will do the following:

- facilitate web searching
- allow development of a web-based InChI lookup service
- permit an InChI representation to be stored in fixed length fields
- make chemical structure database indexing easier
- allow verification of InChI character strings after network transmission

Stephen Heller (IUPAC Division of Chemical Nomenclature and Structure Representation) says: "The InChI/InChIKey is the first publicly available unique chemical identifier. Until IUPAC developed the InChI/InChIKey, it had not been possible to link and exchange information and data between the vast chemical world and the life sciences world that the Microsoft BioIT Alliance supports. The InChI/InChIKey is like a Digital Object Identifier for chemicals. The InChI/InChIKey is an agent of change and an agent of the future for linking the chemical, biochemical, and biomedical information and data on the web. The InChI/InChIKey provides the Microsoft BioIT Alliance with a unique, easy, accurate, universal, and free way to link the information they collect and use internally and provide externally to their customers. . . . I am very pleased that I am part of the team that has been able to put this one small, but vital link in place to support and enhance drug discovery and improve the health of all persons around the world."

According to Rudy Potenzzone, Microsoft's director of the BioIT Alliance and industry strategist for life sciences, "Microsoft is pleased to have IUPAC, the international chemistry standards organization, join the Microsoft BioIT Alliance. The IUPAC InChI/InChIKey is a critical link in making the goal of improving biomedical data interchange come to fruition in the near future. As more companies and organizations use the IUPAC InChI/InChIKey to connect information, the international scientific community will benefit. We hope their participation in the Alliance can help expand its usage."

### About the BioIT Alliance

Formed in 2006, the BioIT Alliance is a cross-industry group working to integrate science and technology in order to accelerate the pace of drug discovery and realize the potential of personalized medicine. Founding members include Accelrys Software, Inc.; Affymetrix, Inc.; Agilent Technologies, Inc.; Amylin Pharmaceuticals, Inc.; Applied Biosystems;

The BioTeam, Inc.; Digipede Technologies LLC; Discovery Biosciences Corporation; Geospiza, Inc.; Hewlett-Packard Development Company, L.P.; Illumina, Inc.; InterKnowlogy; Microsoft Corporation; Sun Microsystems, Inc.; The Scripps Research Institute; VizX Labs, LLC; and other companies in the pharmaceutical, biotech, hardware, and software industries. Additional information can be found on the BioIT Alliance website at <[www.bioitalliance.org](http://www.bioitalliance.org)>.

 [www.iupac.org/news/archives/2007/BioIT-alliance.html](http://www.iupac.org/news/archives/2007/BioIT-alliance.html)

## Chemical Heritage Foundation Names Thomas R. Tritton President

**T**homas R. Tritton, formerly president of Haverford College, will become president of the Chemical Heritage Foundation (CHF) effective 1 January 2008. He will be only the second president of CHF, succeeding Arnold Thackray, who founded the organization in Philadelphia 25 years ago and will continue with CHF in the new role of chancellor.

"I am enormously excited to be returning to my roots as a scientist," says Dr. Tritton. "My life has been devoted to education and the CHF position offers a new way to continue that calling in directions that are both original and challenging."

Tritton was selected following a worldwide search for someone with both scholarly and entrepreneurial talents, who combines a passion for the long sweep of chemistry and molecular sciences with the drive to build and sustain a successful enterprise.

"Scientist, scholar, inspiring leader, Tom Tritton is the right person at the right time for CHF," said Vincent Calarco, chairman of the CHF Board of Directors. "His passion for chemistry, his energy, his leadership will help CHF achieve its ambitious goals . . ."

"CHF's world-class scientific collections and holdings provide an outstanding resource for scholars and a natural linkage to both the humanities and to the social sciences," said Tritton. "Additionally, the work on science education, outreach, and public policy offers distinctive contributions to contemporary questions and societal needs."

 [www.chemheritage.org](http://www.chemheritage.org)



### Zafra Lerman Receives George Brown Award for International Scientific Collaboration

**T**he U.S. Civilian Research and Development Foundation (CRDF), based in Arlington, Virginia, USA, presented its George Brown Award for International Scientific Cooperation to an outstanding scientist 11 October 2007 at the U.S. Department of State. Zafra Lerman, head of the Institute for Science Education and Science Communication at Columbia College Chicago, was recognized for her use of international science collaboration to promote peace and prosperity.

Presented annually by CRDF, the George Brown Award honors the vision and legacy of the late Congressman George E. Brown Jr., a recognized advocate of science in the interest of peace. His vision and efforts helped to create the institutional framework for science and technology in the federal government, as well as several nongovernmental organizations, including CRDF. CRDF created the award three years ago to recognize individuals who continue Brown's scientific vision.

In her acceptance speech, Lerman described science as an international language and an invaluable way to build peace in such regions as the Middle East. Lerman has recently focused on connecting scientists from different countries within the Middle East to begin building the basis for serious cooperation and communication in the future—including an annual conference held in Malta that brings together scientists from Israel and other Middle Eastern nations. (See more about this IUPAC activity in the Mar-Apr 2006 *CI*, <[www.iupac.org/publications/ci/2006/2802/2\\_malin.html](http://www.iupac.org/publications/ci/2006/2802/2_malin.html)>.)

"Science is probably the only field that contributes to the longevity and quality of life, but it can also cut life short. We have learned from the past that scientists can contribute to solving global issues by communicating with each other." said Dr. Lerman. "In the Middle East, there is some light at the end of this dark tunnel. Like other Americans, I have a dream that researchers in the Middle East will achieve peace by working together. Supporting activities like the Malta conference will go a great way towards building peace in the Middle East."

This year's award ceremony drew a large number of ambassadors, government officials, public health officials, and business leaders—including U.S. Congresswoman Jan Schakowsky, who represents

the Ninth District of Illinois. Ambassador Reno Harnish, III, the principal deputy assistant secretary of state in the Bureau of Oceans and International Environmental and Scientific Affairs, served as the keynote speaker.

#### About CRDF

CRDF is a nonprofit organization authorized by the U.S. Congress and established in 1995 by the National Science Foundation. This unique public-private partnership promotes international scientific and technical collaboration through grants, technical resources, and training.

 [www.crdp.org/georgebrown](http://www.crdp.org/georgebrown)



### In Memoriam: The Oldest Active Chemist Dies at the Age of Nearly One Hundred

**A**li Rıza Berkem, born in 1908 in Izmir, Turkey, died on 22 May 2007. He was the head of the Turkish Chemistry Association (Türkiye Kimya Derneği), one of the National Adhering Organizations of IUPAC.

Following high school, Berkem was one of the young Turks selected after an examination to continue their educations in a European university, mostly in Germany, France, or England. Berkem studied chemistry at Montpellier University (1928-1932), graduated as a laureate student, and received the Coulouma prize. This was the first time such an honor was given to a foreigner by the university. He returned from France to Izmir to teach chemistry at his old high school.

In 1933, the young Turkish Republic decided to reform the university system. To bring modern methods and teaching systems to Turkey, the time was ripe to invite uneasy Jewish-German professors to Turkey, pay them quite good salaries, and give them a free hand to bring a rather quick change in the university system. At the same time, young Turkish scientists were divided among various faculties according to the fields in which they were educated in Europe.

Prof. Valensi became the physical chemistry professor and Berkem was given to his lab as an assistant. After getting his doctorate degree in France in 1938, Berkem came back to the same institute, and this

## IUPAC Wire

time became head of the department. He formed the nucleus of the Physical Chemistry department in the Faculty of Sciences, publishing 30 scientific books and a large number of research papers. He could often be found in the lab with his graduate students.

After the war, new universities were founded in various cities. Berkem was always ready to work, advise, take part, and give lectures until these institutions had enough faculty members. Berkem was also a visiting scholar at European and American universities, including Oregon University and Oak Ridge Nuclear Center in 1956. In 1950, after becoming a full professor, he was elected as the Dean of the Faculty for two terms. After that he was elected to the University Senate as the representative of the Faculty of Sciences. He was honored many times by his colleagues and by various institutions. He was given the title "ombudsman" by the Turkish Chemical Society with the approval of every single member.

Anatolian University, now the biggest in Turkey gave him an honorary doctorate and in 2002 the Science

and Technology Institute of Turkey gave him an honorary membership. He also received honorary memberships from the Société de Chimie Industrielle of France and the Turkish Society of Chemical Industry.

Berkem married a biochemist who was his student once, and together they had three daughters.

In addition to his scientific books and articles Berkem had many semi-scientific articles in popular science journals and social articles in daily newspapers. He never retired, working enthusiastically until the very last few weeks when he died from kidney failure. He always had goals to be achieved, dreams to be realized, and expectations to make life more meaningful and memorable. He was kind, understanding, tolerant, optimistic, and a determined person. His heart was full of love not only for his family and his students, but also for mankind.

Submitted by Prof. Ayhan Ulubelen, faculty member at the University of Istanbul, Turkey, and titular member of Chemrawn.

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## Electrochemical DNA-Based Biosensors: Terms and Methodology

Biosensors based on deoxyribonucleic acid (DNA) are well recognized among the family of chemical sensors. With respect to the specific role of DNA in organisms, there are some remarkable specific features of DNA-based biosensors that are applied mainly to the investigation of DNA itself. These biosensors are used to determine the concentration, structure, and chemical reactivity of DNA in relation to drugs and chemicals, including pro- and antioxidants, and for the detection of specific genes or mutant genes associated with human genetic diseases and infectious agents. With electrochemical signal transducers, the main advantages of biosensors are their low cost, fast response, simple design, small dimensions, and low power requirements at their high-detection potentialities.

In 1999, the IUPAC technical report "Electrochemical Biosensors: Recommended Definitions and Classification" was published. This report did not deal extensively with DNA as the biological recognition element, but considered its use in the future. Since that time, significant progress has been achieved in the development and application of electrochemical sensors based on DNA and other nucleic acids (including aptamers and peptide nucleic acids). Yet, so far there have been no efforts at essential classification in this dynamically developing field. This project is intended to produce a critical evaluation of the terms and methodology related to DNA-based biosensors.

The project deals with the following:

- DNA-based biocomponents (natural, biomimetic), including their electrochemical responses
- type of interaction to be addressed (DNA hybridization, DNA-drug, interactions, aptamer-antigen interactions, etc.)
- detection principles (label-free, label-based, reagentless, indicator-based, etc.)
- construction of DNA biosensors and DNA chips
- their specific performance criteria

This project should be valuable to academic, biomedical, environmental, and food-testing researchers, as well as to drug-developing labs and sensor producers.

For more information and content, contact the Task Group Chair Jan Labuda <[jan.labuda@stuba.sk](mailto:jan.labuda@stuba.sk)>.

 [www.iupac.org/projects/2006-026-1-500.html](http://www.iupac.org/projects/2006-026-1-500.html)

## Recent Advances in Nomenclature, Properties and Units: Strategy for Promoting SC-NPU Achievements

In clinical laboratory sciences a nomenclature is required to facilitate electronic exchanges. SC-NPU provides a database that is set according to ISO and CEN standards, and IUPAC and IFCC recommendations. The objective of this project is to promote the database.

The SC-NPU database has been freely available in English, Danish, and Swedish for several years and is currently used in Denmark and Sweden. It is now being developed in Catalan, French, German, Portuguese, and Spanish versions. Notes, explanations, and links to other relevant websites will also be added to the database. Once these new versions of the SC-NPU database are available, it is important that they are promoted widely. Clinical laboratory professionals in the countries where these languages are spoken need to be informed about this database.

In order to do so, the SC-NPU project team intends to organize a worldwide information campaign aimed at the clinical laboratory sciences community. To start, this project will involve the publication of articles in various clinical laboratory sciences journals, presenting the database and demonstrating its advantages. To complete this communication campaign, the project team will present posters and organize workshops and roundtables at international and regional congresses, such as those organized by IUPAC and IFCC.

These communications will publicize the useful aspects of the SC-NPU database, including the fact that it has a multilanguage terminology set, which is constantly revised according to scientific advances, and that it is free online for any clinical laboratory professional. The syntax of the terms is simple and unique and based upon ISO and CEN standards and IFCC and IUPAC recommendations. The SC-NPU database includes descriptions of 15 000 properties covering all fields of clinical laboratory sciences, each with a specific and ready-to-use code.

The project team plans to disseminate its work through IUPAC and IFCC contacts. The help of National Adhering Organizations and Company Associates will be enlisted to promote the SC-NPU database.

For more information, contact the Task Group Chair Françoise Pontet <[francoise.pontet@free.fr](mailto:francoise.pontet@free.fr)>.

 [www.iupac.org/projects/2006/2006-048-2-700.html](http://www.iupac.org/projects/2006/2006-048-2-700.html)

## The Project Place

### A Multilingual Encyclopedia of Polymer Terminology

This project is aimed at preparing a web-based and user-friendly multilingual encyclopedia of polymer terms and definitions that initially will be based on the "Glossary of Basic Terms in Polymer Science" (IUPAC Recommendations 1996). Once available on the IUPAC website, the user will be able to look up any term and its definition, as well as its translation into languages other than English. In the first instance, translations into Czech, French, Polish, and Portuguese will be incorporated. At a later stage, the more complex task of including languages based on character sets of non-Latin origin will be addressed. Since all the content will come exclusively from IUPAC documents that have already been published, it is expected that this electronic encyclopedia will be flexible enough to accommodate updating and the addition of further terms in a straightforward fashion.

The task group is truly international and includes 12 members from 10 countries: Giuseppe Allegra (Italy), Maximo Baron (Argentina), Taihyun Chang (Korea), Alain Fradet (France), Jiasong He (China), Michael Hess (Germany), Jung-Il Jin (Korea), Tatsuki Kitayama (Japan), Przemyslaw Kubisa (Poland), David Tabak (Brazil), and Jiri Vohlidal (Czech Republic).

For more information, contact the Task Group Chair Cláudio dos-Santos (Brazil) <[claudio@iceb.ufop.br](mailto:claudio@iceb.ufop.br)>.

 [www.iupac.org/projects/2007/2007-008-1-400.html](http://www.iupac.org/projects/2007/2007-008-1-400.html)

### "Global Climate Change"— Monograph for Secondary Schools

The first goal of this project was to translate a booklet on global climate change produced by the Italian Consorzio Interuniversitario Nazionale (INCA) from Italian into English, Spanish, and Portuguese. The booklet, titled *La Chimica per L'Ambiente*, constitutes one of the early chapters of the senior secondary textbook *Introduction to Green Chemistry*, which will be produced by INCA as part of its Green Chemistry Series. The monograph is gaining considerable popularity in Italy and has been adopted by numerous science teachers for inclusion in their curriculum. The translations permit for a wider distribution, including to parts of Europe, UK, Australia, New Zealand, South Africa, and most countries in North and South America.



In the original version of the booklet, the "Perspectives" section was dedicated to the Kyoto protocol and issues closely tied to Europe and Italy. In the translations, this section was updated and customized to address issues facing each user country.

The English, Spanish, and Portuguese translations were published by INCA in July 2007 and are now available online at <[www.incaweb.org/publications/papers.php](http://www.incaweb.org/publications/papers.php)>.

More recently, as part of IUPAC project 2007-035-1-300, work on a translation into Romanian was initiated. This latest project is headed by Aurelia Pascariu from the Romanian Academy, Institute of Chemistry of Timisoara.

For more information, contact Pietro Tundo <[tundop@unive.it](mailto:tundop@unive.it)>.

 [www.iupac.org/projects/2005/2005-015-1-300.html](http://www.iupac.org/projects/2005/2005-015-1-300.html)  
[www.iupac.org/projects/2007/2007-035-1-300.html](http://www.iupac.org/projects/2007/2007-035-1-300.html)

### Recommendations for Codes of Conduct

What obligation does a scientist have to ensure that his/her work is used for the benefit of mankind? That serious question is being asked frequently these days, especially in the biochemical and microbiological communities, where pathogenic organisms can easily be created. Chemists also must consider the ethical implications of their work. Ultimately, each chemist must decide individually how to address such ethical issues, but IUPAC has embarked on a project to provide guiding principles for codes of conduct for chemistry that might be developed locally, nationally, and internationally.

The work of those engaged in science and technology using chemicals needs to be, and perceived to be, in compliance with international treaties, national laws, and regulations prohibiting chemical or biological weapons and illicit drugs. Among the most important of the laws and treaties governing banned and severely restricted chemicals are the Chemical Weapons Convention, the Biological and Toxin Weapon Convention, the Conventions on Narcotic Drugs and Psychotropic Substances, the

## The Project Place

Rotterdam Convention on the Prior Informed Consent Procedure, the Stockholm Convention on Persistent Organic Pollutants, the Montreal Protocol, and the Basel Convention on Hazardous Wastes.

Increased attention is being given to ethical principles and codes around the world, including initiatives such as those of the UNESCO Division of Ethics of Science and Technology. Furthermore, the new generation of chemists is keen to see ethical and other considerations, such as the environment, taken into account. Guiding principles for a code of conduct would strengthen international chemistry, and help to achieve high standards of excellence and relevance in academic, governmental, and industrial activities. Such a code would also promote the service of chemistry to society and to global issues.

Guiding principles for a code would recognize the extraordinary benefits to the quality of life, public health, and agriculture throughout the world made available by the knowledge, methods, and techniques involving chemicals. It would promote all aspects of chemistry, not just among members of the profession, but increasingly to the worldwide community. While chemistry is central to life and provides many valuable benefits for humankind, it can also raise important ethical issues. These issues can evolve as more

development and uses of chemistry occur and guiding principles for a code of conduct would provide a framework within which to consider such issues.

In developing the guiding principles, a process of widespread consultation involving different cultural perspectives from around the world will ensure that the recommended codes are informed by the experience of other professional bodies that have codes, such as the International Council of Chemical Associations, which developed the Responsible Care Global Charter. In addition, UNESCO and ICSU have worked extensively on education and codes.

In order to have an impact on practice, codes need to be dynamic rather than static, and need to be incorporated into a continuing process that is considered prior to each new piece of work. The project team will consider how to ensure that IUPAC can, in the future, engage in processes that help the recommended guiding principles for codes to be embodied in the practice of chemistry.


For more information and comments, contact the Task Group Chair Graham S. Pearson <[graham\\_pearson@compuserve.com](mailto:graham_pearson@compuserve.com)>.

 [www.iupac.org/projects/2007/2007-022-2-020.html](http://www.iupac.org/projects/2007/2007-022-2-020.html)

*Continued from page 9*

### Radionuclides and Radiochemistry: Part 2

fast particles of nuclear origin (nucleons or clusters of nucleons). Further, due to their nature as neutral particles, neutrons can induce nuclear reaction even at the most probable thermal energy of only 0.025 eV (i.e.,  $\langle E \rangle = 2 m_n v^2 = k.T$ ).

As a final comment, it is known that some nuclear levels have energies well below the typical energies of X rays of atomic origin: In this framework, the discovery of a nuclear level at 3.5 eV of the radioisomer  $^{229m}\text{Th}$  led to the invention of the term “nuclear light” to stress the evidence that the energy of this nuclear phenomenon is of the same order of magnitude of typical UV radiation. Later on, the nuclear metastable level at 14 keV of stable nuclide  $^{57}\text{Fe}$ , successfully used in MOSPEC for radioanalytical purposes, lies well below the atomic X-ray energy range of heavier elements, which are easily—even roughly—predictable by Moseley’s equation, confirming the conclusion that the classification of these phenomena on the energy scale is quite misleading. 

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Mauro L. Bonardi <[mauro.bonardi@mi.infn.it](mailto:mauro.bonardi@mi.infn.it)> is a professor at the Università degli Studi di Milano, Accelerators and Applied Superconductivity Laboratory, in Segrate, Italy. David S. Moore <[moored@lanl.gov](mailto:moored@lanl.gov)> is at the Los Alamos National Lab, in Los Alamos, New Mexico, USA.

## Provisional Recommendations

*Provisional Recommendations are drafts of IUPAC recommendations on terminology, nomenclature, and symbols made widely available to allow interested parties to comment before the recommendations are finally revised and published in Pure and Applied Chemistry.*

 [www.iupac.org/reports/provisional](http://www.iupac.org/reports/provisional)

### Metrological Traceability of Measurement Results in Chemistry

In commerce, society, and science, metrological comparability of measured quantity values and various published values is essential to determine their spatio-temporal differences, ratios, and drifts. Achieving metrological comparability of measurement results requires definition of calibration hierarchies providing metrological traceability chains which enable the establishment of metrological traceability of measured quantity values to a common metrological reference.

Experience has shown that the understanding of the concepts involved, their relation, role, definition, and use is insufficient and varied. Consequently, an attempt is made in this study to arrive at a set of consistent concept systems with associated terminology for measurement in chemistry. The systems build on definitions of concepts and associated terms from the new 3rd edition (2007) of the *International Vocabulary of Metrology—Basic and General Concepts and Associated Terms*, such as quantity, measurand, calibration, measurement procedure, measurement uncertainty, measurement standard, calibrator, and reference material. Additional concepts such as metrological equivalence of measurement results are also given.

Flow charts of generic calibration hierarchies are presented as well as a variety of examples.

The establishment, assessment, and reporting of metrological traceability are discussed, including the needed metrological institutional hierarchy and the role of interlaboratory comparisons.

Recommendations are made about the essential steps in planning and performing a measurement, and reporting a measurement result.

#### Comments by 29 February 2008

Prof. Paul De Bièvre  
TEL: +[32] 14 851 338  
FAX: +[32] 14 853 908  
E-MAIL: paul.de.bievre@skynet.be

 [www.iupac.org/reports/provisional/abstract07/fajgelj\\_290208.html](http://www.iupac.org/reports/provisional/abstract07/fajgelj_290208.html)

### Glossary of Terms Used in Pharmaceutics

This Glossary of Terms in Pharmaceutics is needed by practitioners in the field of pharmaceutics—a field that fulfills an important and crucial role, different from the roles of other scientific disciplines involved in the drug-making process. The glossary contains 156 definitions used in pharmaceutics. These are related to various aspects of this discipline such as 1) physicochemical characterization of pharmaceutical preparations and the active ingredients they contain; 2) unit operations used in the practice of pharmaceutics; 3) terms related to the various dosage forms; 4) terms related to the various modes and routes of drug delivery; and 5) terms used in pharmacokinetics and biopharmaceutics in general, and additional miscellaneous terms. Since the field of pharmaceutics is multidisciplinary, with practitioners from a variety of fields such as chemistry or various biological sciences, a glossary containing authoritative definitions would be useful to them. The terms used in pharmaceutics are rarely covered by existing glossaries, and in cases where they are, their definitions are often inappropriate for the field of pharmaceutics and require new or modified definitions to better fit the new context.

#### Comments by 30 April 2008

Prof. Eli Breuer  
Hebrew University of Jerusalem, Department of Medicinal Chemistry, P.O. Box 12065, IL-91120 Jerusalem, Israel  
TEL.: +[972] 2 675 8704  
FAX: +[972] 2 675-8934  
E-MAIL: breuer@cc.huji.ac.il

 [www.iupac.org/reports/provisional/abstract07/breuer\\_300408.html](http://www.iupac.org/reports/provisional/abstract07/breuer_300408.html)

## Representation of Configuration in Coordination Polyhedra and the Extension of Current Methodology to Coordination Numbers Greater than Six (IUPAC Technical Report)

Richard M. Hartshorn, Evamarie Hey-Hawkins, René Kalio, and G. Jeffery Leigh

*Pure and Applied Chemistry*

Vol. 79, No 10, pp. 1779–1799, 2007

doi:10.1351/pac200779101779

In this report, established IUPAC recommendations for the representation of configuration are reviewed briefly, and then methodologies are examined for dealing with regular polyhedra that are typically used when working with coordination numbers greater than 6. More than one method is available and can be used for many such geometries, but the deviations from regular polyhedral geometries that are typically found in such molecules can make it difficult to arrive reproducibly at the same description for a complex using purely objective criteria. Recommendations are made for some geometries of coordination numbers 7, 8, and 9, but not for higher coordination numbers.

 [www.iupac.org/publications/pac/79/10/1779](http://www.iupac.org/publications/pac/79/10/1779)

## Definitions of Terms Relating to the Structure and Processing of Sols, Gels, Networks, and Inorganic-Organic Hybrid Materials (IUPAC Recommendations 2007)

J. Alemán, A.V. Chadwick, J. He, M. Hess, K. Horie, R.G. Jones, P. Kratochvíl, I. Meisel, I. Mita, G. Moad, S. Penczek, and R.F.T. Stepto

*Pure and Applied Chemistry*

Vol. 79, No 10, pp. 1801–1829, 2007

doi:10.1351/pac200779101801

This document defines terms related to the structure and processing of inorganic, polymeric, and inorganic-organic hybrid materials from precursors, through gels to solid products. It is divided into four sections—precursors, gels, solids, and processes—and the terms have been restricted to those most commonly encountered. For the sake of completeness

and where they are already satisfactorily defined for the scope of this document, terms from other IUPAC publications have been used. Otherwise, the terms and their definitions have been assembled in consultation with experts in the relevant fields. The definitions are intended to assist the reader who is unfamiliar with sol-gel processing, ceramization, and related technologies and materials, and to serve as a guide to the use of standard terminology by those researching in these areas.

 [www.iupac.org/publications/pac/79/10/1801](http://www.iupac.org/publications/pac/79/10/1801)

## Alcohols with Water

**IUPAC-NIST Solubility Data Series. 82**

*Journal of Physical and Chemical Reference Data*, 2007

In this five-part series published in 2007 in the *Journal of Physical and Chemical Reference Data* (volume 36), the mutual solubility and related liquid-liquid equilibria of C<sub>4</sub>, C<sub>5</sub>, C<sub>6</sub>, C<sub>7</sub>, and C<sub>8</sub>–C<sub>17</sub> alcohols with water are exhaustively and critically reviewed. Reports of experimental determination of solubility are compiled for the chemically distinct binary systems that appeared in the primary literature prior to end of 2004. For most of the systems, sufficient data are available to allow critical evaluation. All data are expressed as mass percent and mole fraction as well as the originally reported units. In addition to the standard evaluation criteria used throughout the Solubility Data Series, a number of new methods based on the evaluation of all experimental data were used.

 [www.iupac.org/publications/sds/2007/82\\_abstract.html](http://www.iupac.org/publications/sds/2007/82_abstract.html)

New IUPAC projects have recently been initiated that will evaluate solubility data useful to industrial processes. The projects will cover nitriles C+3: binary and multicomponent systems; mutual solubility of esters with water; solubility of higher alkynes in liquids; and solubility in systems with lithium and/or sodium nitrates.

 [www.iupac.org/divisions/V/502](http://www.iupac.org/divisions/V/502)

## Nomenclatura de Química Inorgánica (Recomendaciones de la IUPAC de 2005)

Spanish language version of  
*Nomenclature of Inorganic  
Chemistry*  
translated and adapted  
by Miguel A. Ciriano and  
Pascual Román Polo of the  
book by Neil G. Connelly,  
Ture Damhus, Richard M.  
Hartshorn, and Alan T.  
Hutton  
ISBN 978-84-7733-905-2  
Editorial Prensas  
Universitarias de Zaragoza,  
June 2007

This book contains the full translation and adaptation to Spanish of the IUPAC recommendations on nomenclature of inorganic and organometallic compounds published at the end of 2005. It is now available from Editorial Prensas Universitarias de Zaragoza, Spain.

The book was translated so that Spanish-speaking chemists can have a uniform and consistent understanding of chemical terms. In this context, the translators carefully reviewed the vocabulary of the Spanish version of *Nomenclature of Inorganic Chemistry (Recommendations 1990)* by L.F. Bertello and C. Pico Marín, which this new edition of the Red Book supersedes. The earlier Red Book proved to be a significant resource among Spanish-speaking chemists and was distributed widely.

 [www.iupac.org/publications/books/author/RedBook-spanish.html](http://www.iupac.org/publications/books/author/RedBook-spanish.html)



## “Photochemistry for A Better Life”

A special issue of *L'Actualité Chimique*, May/June 2007, edited by E. Amouyal and T.H. Tran-Thi

reviewed by Marie-Laure Viriot, Bernard Valeur,  
and Thu-Hoa Tran-Thi

“Photochemistry for a Better Life” was the theme of the June 2007 special issue of *L'Actualité Chimique*, the official journal of the French Chemical Society that is aimed at popularizing chemistry. For this issue, the journal editor offered the French Group of Photochemistry the opportunity to write about the multiple applications of photochemistry in everyday life. The result is an issue covering four main themes: Light and Life; Photons for Lighting, Detection, and Analysis; Light for the Protection of the Environment; and Solar Energy: Energy for the Future?

“How does light interact with living organisms?” is the question addressed by the authors of the Light and Life section. Five major topics are discussed, with the central idea that light is a tool with which to observe, analyze, and understand the chemical reactions in living organisms, but with the caveat that light can be harmful and beneficial at the same time.

UV radiation for instance provokes “DNA Photodamage.” Under this topic, the main DNA lesion

routes induced by UV radiation are described, in particular those involving the formation of pyrimidine dimers and guanine oxidation. The approaches used for the elucidation of the mechanisms involved in their formation include the synthesis and photochemical studies of model compounds, as well as experiments performed by time resolved spectroscopy. The role of UV radiation is also considered in the topic “Amino Acids and Proteins in Photochemistry,” which focuses on protein photo-fragmentation and protein photo-inactivation by ruthenium complexes. In the chapter on “Cellular Photoperception and Photoactive Proteins,” the authors show how real-time laser spectroscopy allows the characterization of the crucial photochemical steps in light-induced intracellular energy transduction. The proteins presented are involved in vision (bacteriorhodopsin), microorganism photomotility (yellow protein and oxyblepharismine), and plant phototropism (cryptochrome), and can also be used as a temporal probe (green fluorescent protein).

The beneficial role of light is pointed out in “Photodynamic Therapy,” which targets the destruction of carcinogenic tissues by combining the actions of a photoactive drug or photosensitizer with light and oxygen. Additional topics discussed include the search for new efficient and selective photoactive compounds, the photosensitization mechanism at the molecular level, and the main applications in therapy.

In “UV and Skin: Mechanism and Photoaging Treatment,” aspects of the skin aging process are

\* This review was first published in the June 2007 *Newsletter of the European Photochemistry Association* <[www.unibas.ch/epa](http://www.unibas.ch/epa)> and is reprinted with permission.



described, and different approaches for its prevention and treatment are discussed.

Sustainable energy production based upon renewable resources is achievable. This is the message conveyed by the authors of "Solar Energy: Energy for the Future?" A strategy for converting visible light into electrical current is described in "New Nanocrystalline Solar Cells," with examples of credible devices able to produce electricity from sunlight with an overall efficiency of 11.1%. Another strategy described in this section involves new methods for efficiently splitting water into H<sub>2</sub> and O<sub>2</sub> without using noble metals as catalysts. Many bio-inspired artificial systems elaborated for light harvesting, energy transfer, and charge separation, including a hybrid photobiofuel cell, are reviewed in the section "Bio-Inspired Constructs for Sustainable Energy Production and Use." In "Water Photolysis by Molecular Biomimetics," the authors describe recent progress and findings on the structure of the water oxidizing enzyme of natural photosynthesis.

"Light for the Protection of the Environment" covers four topics. A rapid survey of the treatment and disinfection of spring water with UV and V-UV, and also of air treatment using V-UV irradiation, is given in "Photons Can Directly Destroy Pathogens and Pollutants." In "Solar Light to Eliminate Pollutants," the focus is on the solar-induced transformation of organic pollutants present in the upper layer of water surfaces, and on the surfaces of soil or leaves, which can lead to stable and more or less toxic compounds. To illustrate the photo-transformation of the pollutants, three examples are given. In "Detecting the Pollutants in Air and in Water," the authors show the large panoply of tools and methods (LIDARs, chemiluminescence, fluorescence) developed for the analysis and detection of pollutants (particulates, nitrogen oxides, formaldehyde, heavy ions) in various environments. In section on "Photocatalysis for the Elimination of Pollutants," the main concepts of photocatalysis are described and the latest research developments in the field are reviewed. A special focus is on the strategies aimed at improving the efficiency of TiO<sub>2</sub>, such as the use of dopant, surface treatments, coupling of TiO<sub>2</sub> with dyes absorbing in the visible, and modifications of the structure and morphology of the photocatalyst. Also reviewed are the principal commercial and industrial applications for water and air depollution or disinfection.

Under the theme "Photons for Lighting, Detection, and Analysis," the main "Lighting Sources" are first described: incandescent lamps, discharge lamps, and

light emitting diodes (LED). Future prospects are presented with special attention to environmental concerns. Fluorescent lighting is of particular interest, and current efforts focus on "Phosphors for Fluorescent Lighting," with the aim of find-

ing more efficient materials in which "cascades of photons" occur. The second section deals with the use of light as a tool of detection in the field of security. For instance, "The Detection of Explosives" is of major importance in preventing terrorist attacks and facilitating mine clearance. Polymer-based fluorescent sensors show much promise in this respect. In the article "Light to Fight Counterfeiting," various marking techniques are discussed that concern not only bank notes and artwork, but also more common commercial products. "Light and Trace in Police Inquiry" are strongly associated: Fluorescence and chemiluminescence for are currently used at crime scenes.

The third theme concerns light and art. In the article "Optics for a Better Knowledge of Works of Art," various techniques and applications are presented: identification of pigments by diffuse reflectance, identification of varnishes by fluorescence under UV illumination, and distinction of different artistic techniques by goniophotometry and colorimetry. "Dating by Luminescence" is the subject of the last article. The energy accumulated by minerals with time, as a result of the natural radioactivity, can be released in the form of light with heating (thermoluminescence) or with light irradiation (optically stimulated luminescence), with the amount of light proportional to the elapsed time.

This issue can be ordered online through the website of *L'Actualité Chimique*. A second special issue on "Photochemistry to Transform Matter" is scheduled in 2008.

Marie-Laure Viriot <malou.viriot@free.fr>, Département de Chimie Physique des Réactions, France; Bernard Valeur <valeur@cnam.fr>, Laboratoire de Chimie Générale, CNAM, France; and Thu-Hoa Tran-Thi <thu-hoa.tran-thi@cea.fr>, Laboratoire Francis Perrin, CEA / CNRS, Saclay, France.

 [www.lactualitechimique.org](http://www.lactualitechimique.org)

## ChemSpider and Its Expanding Web

### Building a Structure-Centric Community for Chemists

by Antony Williams

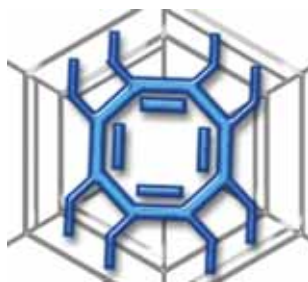
To declare that the worldwide web has changed our lives is really an understatement. The impact on commerce, information exchange, social networking, and provision of access to a myriad of other forms of interaction and data, while breathtaking, continues to expand at an astounding pace. In the domain of chemistry, scientists have long had access to text-based searching provided by any of the primary search engines such as Google, Yahoo, and so on. When those search efforts are facilitated by a provider such as Google and focused on patent searches<sup>1</sup> and literature articles<sup>2</sup> then chemists can directly probe those domains of information. In a similar way chemists today have access to tens of thousands of chemistry articles via searches on platforms including PubMed,<sup>3</sup> Google Scholar,<sup>4</sup> and ChemRefer.<sup>5</sup>

While the general nature of text-based searches provides a familiar environment for chemists to search and review their results, chemists' natural affinity for communicating via chemical structures demands the need to perform searches in a "natural language." Ask a chemist about his/her preferred manner for searching chemistry databases and he/she will generally state they prefer structure-based searching. There are certainly commercial solutions that provide chemical-structure-based searches of literature and patent data (CAS,<sup>6</sup> Infochem,<sup>7</sup> and Elsevier MDL<sup>8</sup> to name a few) as well as a myriad of solutions for managing in-house organizational data collections.

In a world changed forever by the dominance of web-based searching and the freedom that blogging now offers to scientists in terms of creativity, criticism, and connectivity, a focus on the management of only highly curated, peer-reviewed data is leaving untouched the information deposited and exchanged across the web on a daily basis. With daily updates of Open Access<sup>9</sup> articles, with online theses now exposing research,<sup>10</sup> and Open Notebook Science<sup>11</sup> starting to grab the attention of scientists, chemistry that was previously "lost"<sup>12</sup> might be available for all to review, if

only it could be found. The challenge is finding chemistry—specifically chemical *structures* across the web. Maybe ChemSpider can help?

ChemSpider<sup>13</sup> was initially developed as a hobby project by a small group of dedicated cheminformatics specialists. The intention was to aggregate and index available sources of chemical structures and their associated information into a single searchable repository that would be available to everybody, at no charge. The success of the PubChem project<sup>14</sup> had demonstrated both the value and attractiveness of an online structure



database for facilitating the connections between structures and associated data. While PubChem delivered on its mission to host and disseminate data associated with the Molecular Libraries Roadmap Initiative,<sup>15</sup> the plethora of possible extensions to such an approach to provide value to the chemistry community remained attractive to the ChemSpider team.

ChemSpider, unveiled to the public on 24 March 2007 in time for the Spring ACS meeting, delivered on one of the initial concepts. There are tens if not hundreds of chemical structure databases such as literature data, chemical vendor catalogs, molecular properties, environmental data, toxicity data, analytical data etc. and no single way to search across them. Many of these databases are for profit and there is no way to easily determine the availability of information within these commercial or open access databases. One of the initial concepts for ChemSpider was to aggregate into a single database all chemical structures available within open access and commercial databases and to provide the necessary pointers from the ChemSpider search engine to the information of interest. When the system first went online, only the PubChem data sources, around 10 million structures, were hosted as a proof of concept. As of this writing, the ChemSpider database has indexed over 8 million additional unique chemical compounds. The data hosted today comes from over 80 different data sources, including include chemical vendors, chemistry database vendors, online chemistry resources, aggregated data sets from the literature, virtual libraries, and user submissions.

Rather than provide here a detailed examination of the functions and capabilities associated with ChemSpider, the reader is pointed to the online overview<sup>13</sup> of the capabilities of the system. The capabilities include flexible text and structure-based searching of the database to facilitate structure iden-



tification, the text-based searching of over 50 000 open access chemistry articles, structure/substructure-based searching of U.S. and European patents, structure and spectra deposition to share data across the chemistry community, and the prediction of chemical properties using software provided by a series of collaborators.

ChemSpider continues to grow in its reach into the chemistry community with a number of specific missions:

- 1. Improving the quality of available information.** A number of blog postings<sup>16</sup> have pointed to the quality of information available in online databases. With millions of indexed compounds, ChemSpider has enabled a community-based curating process<sup>17</sup> to help improve the association between a chemical compound and a set of identifiers (systematic names, trade names, synonyms, registry numbers).
- 2. Increased access to chemistry-related information.** There are many types of data and information that can be associated with chemical compounds and made available to the benefit of the chemistry community. As an example, the association of analytical data<sup>18</sup> has been demonstrated, the integration to patent searches,<sup>19</sup> and, presently in progress, the integration to QSAR-based modeling.<sup>20</sup> These efforts will continue.
- 3. Provide access to online tools and services.** ChemSpider already serves up the online prediction of certain chemical properties for chemists to take advantage of and a number of software algorithms provided by collaborators will be added into the system. Web services such as the recently released InChI<sup>21</sup> and OpenBabel services will continue to be made available as a service to the community.<sup>22</sup>

ChemSpider is proving to be a success based on a number of measures. On average over 1 200 unique visitors frequent the site every day.<sup>23</sup> Tens of thousands of transactions are initiated monthly. The community continues to expand as more and more people register to become data depositors and curators. The real success comes from the acknowledgment that real-world problems are being solved and that information is being found in a facile manner, and at no charge to the user, to allow them to make decisions and move on.

The intention for ChemSpider remains true to its initial vision—to build a structure-centric community for chemists. The manner by which we get there is changing with experience and available tools, but hopefully we will be part of the overall team of passionate individuals working to make the worldwide web searchable by chemical structures, improving accessibility to scientific information, and speeding the process of discovery. ChemSpider will continue to demonstrate the potential of the semantic web.<sup>24</sup>

#### Acknowledgments

I would like to acknowledge the development team of ChemSpider. They continue to amaze me with their passion, energy level, and commitment to making a difference. We have used a number of Open Source tools on ChemSpider, but I would especially like to thank the OpenBabel team, the InChI team, and the JSpecView team. My acknowledgements to ACD/Labs, Igor Tetko, and ChemAxon for providing prediction algorithms for the system. My personal thanks to many of my fellow bloggers who keep the conversations entertaining, especially Joerg Wegner, Egon Willighagen, Jean-Claude Bradley, Peter Murray-Rust, and Rich Apodaca. My thanks to the advisory group of over 20 people from across the industry—you help make it all possible.

#### References

All of the references for this article are URLs, which are available online at <[www.iupac.org/publications/ci/2008/3001/ic\\_chemspider.html](http://www.iupac.org/publications/ci/2008/3001/ic_chemspider.html)>.

**Antony Williams is the host of ChemSpider. He has spent over a decade in the commercial scientific software business as chief science officer for Advanced Chemistry Development. He is an NMR spectroscopist by training with over 100 peer-reviewed publications. He has taken his passion for providing access to chemistry related information and software services to the masses and is now applying his time to hosting ChemSpider, working alongside the intellect and innovation making up its development team and immersing himself in the experience of blogging. He can be contacted at <[antony.williams@chemspider.com](mailto:antony.williams@chemspider.com)>.**

# Conference Call

## The Evolving Identity of Chemistry

by *D. Thorburn Burns and Brigitte Van Tiggelen*

A widely attended international conference of more than 110 participants from 26 countries gathered in Erasmushuis at the University of Leuven, Belgium, from 28 August-1 September 2007 for the **6th International Conference on the History of Chemistry (6ICHC)**, organized by the Working Party on History of Chemistry of the European Association for Chemical and Molecular Sciences (EuCheMS). A major aim of these conferences is to facilitate communication between chemists interested in history and historians of chemistry from all over Europe. The first such conference was organized in Hungary in 1991. Since then the working party has fostered the creation of what is now a well-connected community that meets every two years.

Previous conferences were held in Budapest in September 2003 and in Lisbon in September 2005. The 2007 theme "Neighbors and Territories: The Evolving Identity of Chemistry" focused on the disciplinary identity of chemistry and its changing relationships with other fields. The Program Committee was chaired by José R. Bertomeu-Sanchez (University of Valencia) and the Belgo-Dutch Local Committee was chaired by Brigitte Van Tiggelen (University of Leuven and Mémosciences).

So, why would members of EuCheMS, IUPAC, and, more generally, active practicing chemists be interested in this conference? First, it should be noted that many of the questions investigated by historians and philosophers are naturally rooted in their experiences, reflections, and views on the present state of chemis-

try. The severe attacks on chemistry's public image has led for several decades to various counter-strategies, many focused on costly advertising campaigns, others on popularizing the discipline and developing new teaching techniques. To historians, the problem is not just one of image; the recent emergence of new fields (material science or biotechnology to name but two) clearly raises the question of the identity of chemistry. Putting this question in historical perspective is a good reminder that chemistry actually never held a definite and unchanging identity. On the contrary, the science of matter (chemistry) and its transformations with time are very much controlled by reactivity to changes in the scientific and social environments.

Throughout its history, chemistry has been shifting ground between different identities. From its roots in artisan technologies, pharmaceutical workshops, and alchemistic philosophy, it has developed into an archetypical laboratory science of the eighteenth and nineteenth centuries, ultimately claiming full academic status. Chemists have invaded many new fields, from agriculture and industry, to medicine, public hygiene, and pharmacology. In the twentieth century, chemistry contributed to the major scientific developments in molecular biology, quantum mechanics, environmental science, and nanotechnology. Chemists also gained key positions in the oil, plastics, and pharmaceutical industries. This broad and continuous adaptation of the discipline to various fields of endeavour has brought chemistry in close contact with neighboring disciplines and to social pressures. Time and again, chemists have needed to carve out their own territory, to negotiate with other specialists, and to gain particular expertise in widely divergent fields. How chemists achieved this aim was a major thread in the meeting.

Although this was a meeting on the history of chemistry, many speakers brought the discussions



*Participants at the 6th International Conference on the History of Chemistry.*

up to date. The opening plenary lecture discussed the current popular polarization of chemistry into separate areas, namely bio- and nanotechnologies. For Bernadette Bensaude-Vincent (Université Paris X), "The New Identity of Chemistry as Biomimetic and Nanoscience" does not erase the need for broad chemical expertise which is, and will be, needed more than ever to advance these new fields.

The conference was attended by more than 110 participants. Europe was of course well represented, but what was more striking was the growing presence of overseas historians of chemistry or historically-minded chemists: Some came from the fringes of Europe, Israël, or Russia, others from much further away, including Canada, USA, Mexico, Brazil, Taiwan, and Japan.

Fifty-nine oral presentations were given in 18 sessions; posters were available to view throughout the conference. The wide range of material covered is indicated by the session topics: alchemy and early chemistry to early modern chemistry; identity and boundaries in the seventeenth, nineteenth and twentieth centuries; boundaries between physics and chemistry, chemistry, medicine and pharmacy, organic chemistry, biochemistry and molecular biology; the development of macromolecular chemistry; and teaching and knowledge in transit.

The plenary lectures reflected the many facets of the main theme. Ana Simoes (University of Lisbon) investigated the emergence and identity of quantum chemistry in her talk "Dangerous Liaisons or Unavoidable Associations: Quantum Chemistry at the Crossroads of Chemistry, Physics, and Mathematics." Lawrence Principe (The Johns Hopkins University) showed through his lecture, "Transmuting Chymistry into Chemistry: Eighteenth-Century loss of Chrysopoeia and its Repudiation," how the disappearance of alchemical pursuits at the Paris Academy of Science was triggered by the local French context with the suspicions of poisoning at the court and not so much by a shift in the aims of exact sciences. With his presentation "Close Neighbours, but Different Chemistries: Chemistry in the Low Countries 1600-1900," Ernst Homburg (University of Maastricht) demonstrated clearly the influence of local political, social, or economical context by contrasting the development of the discipline in two very different settings.

This conference lived up to expectations, based upon experiences of earlier ICHC, in content, ambience, mix of participant's backgrounds, warmth of welcome, and in the ensuing social program and

interactions. As usual, the conference outings were private visits to museums of interest, this time in Ghent. The first visit, which deserves a special mention, was to the Museum for the History of Sciences at the University of Ghent. The museum has an excellent collection of instruments used in teaching and research since its foundation in 1817. The director, Kristel Wautier expertly introduced the main collections and the temporary exhibition she had prepared about Leo Hendrik Baekeland (1863-1944), the inventor of Bakelite, who studied chemistry in Ghent under Théodore Swarts (1839-1911). On show was the Bakelite volumetric apparatus, resistant to hydrofluoric acid, which Baekeland made for his step-brother, Frédéric Jean Edmond Swarts (1866-1940). This was a most significant and useful gift to Swarts, a pioneer in the organic chemistry of fluorine. The museum collection also includes memorabilia of August Kekulé (1829-1896); Kekulé was professor of the University of Ghent from 1858 to 1867. The contemplation of such chemical heritage was at least as significant and meaningful to those who devote themselves to the current practice or to the history of chemistry.

Duncan Thorburn Burns <profburns@chemistry.fsbusiness.co.uk> is professor emeritus of Analytical Chemistry at The Queen's University of Belfast. He was first elected to IUPAC in 1979 to the Commission on General Aspects of Analytical Chemistry, serving as chairman from 1987-1989 and then as National Representative for Ireland. Brigitte Van Tiggelen <vantiggelen@memosciences.be> is at the University of Leuven and Mémosciences <www.memosciences.be>; she co-chaired the program committee of 61CHC.

Further details of the recent and ongoing activities of the Working Party for the History of Chemistry can be found on the EuCheMS web-site <www.euchems.org>.

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## Heterocyclic Chemistry

*by Roger Read*

Australia was pleased to host the biennial **International Congress for Heterocyclic Chemistry (ICHC21)**, 15-20 July 2007, for the first time in the history of the Congress. It attracted well over 400 delegates from more than 40 countries. As always, the standard of the conference was high, due to the quality of the plenary, award, and keynote lectures, and the many stimulating contributed papers that were presented in oral and poster form across the full range of topics in heterocyclic chemistry.

## Conference Call

### The Venue

The venue, at the University of New South Wales (UNSW), close to the center of Sydney, provided an attractive, modern academic backdrop to the conference. The university provided convenient access to coastal beach scenery and lively attractions in and around Sydney Harbor and Darling Harbor. The Congress was organized under the auspices of the International Society for Heterocyclic Chemistry and a local committee headed by David Black. The program, ably coordinated by Kate Jolliffe (University of Sydney), was designed to bring together heterocyclic chemists from industry and government research laboratories, as well as academia, and care was taken to engage and showcase local industry.

### The Opening

Delegates and guests were welcomed by Margaret Brimble (University of Auckland), president of the ISHC. The Congress was officially opened by the New South Wales Governor, Her Excellency Professor Marie Bashir, who spoke of the importance of heterocycles as drug candidates, bioactive materials, and chemicals that had played major roles in agriculture and the pharmaceutical industry. She also praised the many important advances in fundamental science and applied technology



*Professor Margaret Brimble, president of the ISHC, speaking at the opening ceremony.*

that had resulted from the study of heterocyclic compounds and their chemistry.

### The Program

With his lecture on cycloaddition reactions of 2-azoniaheterodienes, professor Scott Denmark (University of Illinois) then set the scene for what was to be a week-long feast of formal scientific presentations, including two poster sessions, a trade exhibition, and informal networking.

New cycloaddition and annulation strategies were revisited later in the conference through lectures by Rick Danheiser (Massachusetts Institute of Technology), Shengming Ma (Shanghai Institute of Organic Chemistry) and Andrew Holmes (University

of Melbourne), who adopted them for synthesis of a range of heterocycles of biological interest. Ferenc Fülöp (University of Szeged) also gave an overview of his contributions toward understanding the ring chain equilibrium of 1,3-(*X-N*)-heterocycles.

There followed expositions of new synthetic methods to unusual classes of heterocycles, such as silole heterocycles, by Masahiro Murakami (Kyoto University), and a fascinating study by Alan Rowan (University of Nijmegen) of polymer threading mechanisms that have found importance in the development of processive rotaxane catalysts. The topic of catalysis and the design of new catalysts and catalytic processes was picked up later in the conference, particularly around the lecture on chiral phenyl-bis(oxazoline) derivatives in asymmetric catalysis by Hisao Nishayama (Nagoya University).

The relevance of new technologies, such as microwave acceleration, in heterocyclic chemistry was summarized in a series of presentations by pioneers of the field, Rajendar Varma (U.S. Environmental Protection Agency) and Nicholas Leadbeater (University of Connecticut), and put into practical context by Keller Barnhardt (CEM Corporation). The power of programmed self-assembly in providing new heterocycle-based materials for molecular electronic and optoelectronic applications and opportunities in functional nanomaterials was beautifully presented by Takuzo Aida (University of Tokyo) and Thomas Carell (University of Munich).

Others, including Toshiaki Mase (Banyu Pharmaceutical Company), David Tschaen (Merck USA), and Naresh Kumar (UNSW), provided updates on the establishment of commercially viable synthetic chemistry in support of the use of biologically active heterocyclic molecules for drug development. Presenters on these topics described the discovery and adoption of natural products and natural product analogues in the development process, and efforts to harness supramolecular chemistry of heterocyclic derivatives, including those of Troger's base and novel macrocyclic systems, to develop functional and diagnostic materials. Efforts to understand and mimic natural heterocyclic systems provided another theme of enquiry in *de novo* and biological control studies, and this topic was developed by Cynthia Burrows (University of Utah) in her lecture on guanine oxidation in genomic and mitochondrial DNA. Such oxidative damage leads to hydantoin products by previously unrecognized pathways.

Total synthesis and improvements in existing synthetic methods were featured in much of the work

## Conference Call



*Presentation of congress plaque by Professor Girolamo Cirrincione, chair of ICHC20, to Professors David Black and Roger Read, co-chairs of ICHC21.*

described, but plenary lectures in this area included the work of Mikiko Sodeoka (RIKEN Institute of Physical and Chemical Research) on enantioselective synthesis of heterocycles based on palladium enolate chemistry, the underlying methods developed by Thorsten Bach (Technical University Munich) for the total synthesis of heterocyclic natural products, and the design and synthesis of heterocyclic cleft-shaped receptors for molecular recognition and transport (Phillip Gale, University of Southampton).

### Awards for Heterocyclic Chemistry

Other scientific highlights of the program included the presentations of the ISHC Senior Prize in Heterocyclic Chemistry (sponsored by Pfizer) to Professor K.C. Nicolaou (Scripps Research Institute), and the ISHC Katritzky Junior Award in Heterocyclic Chemistry to Professor David MacMillan (Princeton University), respectively. Each gave marvelous award lectures that illustrated the power and elegance of their discrete areas of heterocyclic chemistry and reinforced the outstanding contributions that they have made to modern heterocyclic chemistry, especially in the areas of targeted synthesis and generally applicable synthetic methods.

The organizers were thankful to have the support of the Australian heterocyclic chemistry community and local sponsors and exhibitors, including the New South Wales Department of State and Regional Development, who ensured the viability of the meeting. But no conference can be a success without the delegates, some of whom had come from the far side

of the globe, and with some hardship. We recommend attendance at the next ICHC, which will be held in St John's, Newfoundland, August 2009.

 [www.chem.unsw.edu.au](http://www.chem.unsw.edu.au)

## Greenhouse Gases: Mitigation and Utilization

*by John M. Malin*

While there are citizens who still deny it, the scientific community has largely accepted the premise that anthropogenic emissions of carbon dioxide and other greenhouse gases (GHG's) are raising GHG concentrations in the atmosphere and the resulting "greenhouse effect" is driving global warming. Governments, industry, scientists, and private citizens are grappling with the problems posed. The phenomenon has profound economic implications as industry seeks to reduce emissions, but lacks appropriate technologies and clear direction from government. Policymakers and politicians struggle to balance environmental responsibility against immediate economic goals and the needs of the developing world, while the scientific community is engaged with understanding the nature, causes, and solutions of the GHG problem.

To explore these important issues, CHEMRAWN, together with the International Conferences on Carbon Dioxide Utilization (ICCDU), co-sponsored the **CHEMRAWN XVII** and **ICCDU IX** conference on Greenhouse Gases: Mitigation and Utilization. The meeting, attended by 200 people from 30 countries, took place 8-12 July 2007 at Queens University, Ontario, Canada. It was organized around three main themes: (1) policy issues and strategies, (2) sequestration of GHGs, and (3) their mitigation and utilization. Many of the presentations are posted on the conference website <[www.chem.queensu.ca/Conferences/abstract.asp](http://www.chem.queensu.ca/Conferences/abstract.asp)>.

Because of the worldwide economic significance of greenhouse gas sequestration and mitigation, international policy issues are of key importance. In his keynote lecture, Dimitri Zhengelidze from Her Majesty's Treasury (UK), who is also a member of the Stern Review on the Economics of Climate Change, discussed how the Stern Review employs a combination of economics and ethics to assess in broad terms the costs of anthropogenic climate change and of stabilizing emissions. Increasing atmospheric CO<sub>2</sub> levels, they say, will produce severe economic consequences.



Environmental degradation due to climate change and the accompanying rises in sea levels will, they forecast, disrupt food supplies, limit access to potable and irrigation water, pose serious medical risks to human health, and ultimately create a refugee problem that will threaten the world's stable societies. If emissions are not limited, the current concentration of CO<sub>2</sub> in the atmosphere, some 425 ppm, is projected to rise to 550 ppm by 2050 and to 650 ppm by 2100. These changes correlate with at least a 50 percent probability of increases in average global temperature of 3 and 5 degrees Celsius, respectively. Zhengelis pointed out that the average temperature rise since the most recent ice age has been 5 degrees.

The Stern Review urges that steps to curb carbon dioxide emissions should begin immediately. The costs of inactivity, Zhengelis noted, are far greater than those of action and they are likely to increase. If nothing is done, the poorest countries will suffer disproportionately—even though they have made the smallest contributions to GHG emissions.

Economic models for a “business as usual” scenario predict the overall risks and losses due to climate change amount to at least a 5 percent decrease in gross domestic product (GDP) per year. On the other hand, said Zhengelis, meeting the challenge by reducing emissions of greenhouse gases may cost no more than 1 percent of GDP annually. Global emissions of CO<sub>2</sub> in the year 2000 were near 42 Gigatons per year, with power generation accounting for 24 percent of the CO<sub>2</sub> produced, transport and industry each producing 14 percent, buildings at 8 percent, and miscellaneous sources at 5 percent. Non energy-related sources included 18 percent from nonagricultural land use and 14 percent from agriculture.

Important components to an international strategy to combat global temperature rise include (1) *Emissions trading*, through which funds from larger countries could help pay for the transition to low-carbon development trajectories in economically disadvantaged countries; (2) *Technology cooperation*, through product standards and shared R&D targeted at raising energy efficiency; (3) *Action to reduce deforestation*, which both contributes carbon to the ecosphere and eliminates a “CO<sub>2</sub> sink”; and (4) *Adaptation*, by sharing regional information on effects of climate change and developing crop varieties that are resistant to both flood and drought.

In his plenary lecture, Henry Hengeveld of Environment Canada further explored the question of how human activities are causing climate change. Quoting the latest report by the Intergovernmental

Panel on Climate Change, published in February 2007, Hengeveld pointed out that 25 percent of the greenhouse effect is caused by CO<sub>2</sub>, 65 percent by water vapor (whose atmospheric concentration increases when the temperature rises), and 10 percent from other gases, including methane. Greenhouse gas concentrations, he said, are now at levels unprecedented in the past 650 000 years and recent paleoclimatic studies indicate that the past 50-year period has been unusually warm. Global temperatures, he said, have risen by 0.74 °C in the last century while snow cover is decreasing and many glaciers are shrinking. Sea levels will rise due to thermal expansion of the oceans and the melting of land ice.

Extreme precipitation events, said Hengeveld, are likely to become more frequent in some areas while droughts will occur more often in others. Yet, temperate regions such as North America may derive benefits from a warmer environment. These would include lower snow removal costs, less ice cover on the Great Lakes and along Canada's east coast, longer, warmer growing seasons, and lower costs for space heating. These advantages would be offset in tropical regions by loss of habitable land due to floods and sea level rise, crop loss due to droughts, and threats to health caused by poor air quality and extreme weather. Hengeveld described the scientific community's best estimates on the level of effort that will be needed to stabilize the level of CO<sub>2</sub> at 550 ppm, which may bring risks to an acceptable level. In particular, emissions must be reduced by at least 50 percent.

Pieter P. Tans of the U.S. National Oceanic and Atmospheric Administration's Earth Systems Research Laboratory noted that the pre-industrial levels of CO<sub>2</sub> were close to 280 ppm. Tans cited a striking correlation over the past 650 000 years between the levels of atmospheric CO<sub>2</sub> and changes in the global temperature. The pre-industrial atmosphere contained 600 Gtons of carbon as CO<sub>2</sub>. Since then, humans have contributed 330 Gtons of carbon as CO<sub>2</sub>, of which 210 Gtons have persisted in the atmosphere with the remainder being absorbed by the ocean. The potential for future anthropogenic increases is very real since current coal resources are assessed at 4000-8000 Gtons of carbon, while oil and gas resources are some 500-1000 Gtons.

Like Hengeveld, Tans emphasized that the least expensive option is to begin immediately in applying a portfolio of techniques. “If we want to avoid massive, and accelerating climate change,” said Tans, “we have to greatly reduce CO<sub>2</sub> emissions, eventually to zero.” “Science cannot,” he continued, “provide at this time

## Conference Call

with confidence a 'safe' atmospheric CO<sub>2</sub> level that we should try not to exceed. The risks of dramatic climate change will increase with increasing emissions."

John Grefford of CRO Engineering, Ltd., provided an overview of carbon-neutral energy sources and options for the future. Grefford emphasized both mitigation and adaptation to environmental warming scenarios. Hermann Ott of the Wuppertal Institute, Berlin, described the mission of the developed countries. He outlined the challenges in building political support, emissions trading, choosing effective policy instruments, and fostering technological innovation. Ott noted that the choices made by policy makers will be crucial.

Truman Semans, director of the Business Environment Leadership Council of the Pew Center for Climate Change, described international efforts to strengthen global cooperation. Following positive discussions at the recent G-8 summit at Heiligendamm, the Pew Center convened a meeting of 25 governmental leaders from 15 countries to develop a framework for global climate policy. Semans urged that the USA and other developed countries must implement CO<sub>2</sub> mitigation measures, and he discussed how these measures should include the issues of international competitiveness and participation by developing countries.

John Drexhage, director of Climate Change and Energy for the International Institute for Sustainable Development, discussed the history of federal climate change policy in Canada. He noted that Canada signed the Kyoto Protocol in 1998 but, like many countries, has encountered bumps in the road toward compliance. Canadian projections of CO<sub>2</sub> emissions total some 809 Mtons for 2010, while the Kyoto target for Canada is 571 Mtons, 6 percent below the 1990 level. The USA has not signed the Kyoto Protocol.

James Meadowcroft of Carleton University contrasted Canada's climate change strategy with that of the European Union. Between 1990 and 2005, said Meadowcroft, Europe's CO<sub>2</sub> emissions did not increase while Canada's emissions rose by some 25 percent. The EU, he noted, evolved a suite of policies, including a burden sharing agreement and an emissions trading system. The UK, for example, initiated the Stern Report, established a carbon change levy and a carbon budget, provided incentives for renewable energy programs, and encouraged conservation through "zero carbon" homes. Germany has implemented conservation measures and an extensive wind

power program and Sweden employs nuclear energy extensively. The EU, he said, is "delivering on Kyoto," even though national attainment is uneven across the Union. Canada, in contrast, has yet to develop and deliver an effective strategy. Meadowcroft noted that political leadership is needed in this field. Canadian policymakers, he urged, must realize that emissions control, rather than being ruinous, is highly possible.

Of course, for any mitigation efforts to take effect, the public must "buy in" to the proposed measures. "If we want to facilitate effective communication between policy experts and the public, it would be useful to understand how the public understands climate policy while designing the communication programs," said Stephen Hill of Trent University. Employing interviews and focus groups, Hill carried out a revealing study of the public understanding of economic instruments for climate change policy. "The public has been led to believe that climate policies will require little or no inconvenience to their lifestyles," he said. "People do not grasp the deep cuts in carbon emissions (e.g., 60 percent to eliminate a 2-3 °C temperature rise) required within a few decades." Hill added that the policy debate has been clouded by "unhelpful controversies" at the expense of discussion about what we actually can do to reduce GHG's and to prepare for climate change.

Hill's study found that the public does not understand the "cap and trade" system by which emissions permits are auctioned. Most people view emissions trading as "copping out" (i.e., selling a problem that we should be solving ourselves). The idea of a carbon tax, which on the other hand was well-understood, tended to be disfavored because people thought it would "just add to the cost of doing business." However, some believed the idea would be supportable if the tax revenues were used for purposes of reducing GHG emissions, such as improving home insulation. It seems clear that these policy instruments will need to be explained more effectively to the public. Eric Lachapelle of the University of Toronto noted that, while only six OECD countries have a carbon tax, all OECD countries tax motor fuels, with the lowest rates being those in the USA and the highest in Sweden.

John M. Malin <jmalin023@comcast.net> was the chair of the CHEMRAWN Committee in 2007; he has been involved with the committee since 1998.

Part II of this report will cover sequestration and mitigation strategies —see March-April 2008 CI.

# Where 2B & Y

## Emulsion Polymers

2-6 June 2008, Bethlehem, Pennsylvania  
USA

This one-week short course on **Advances in Emulsion Polymerization and Latex Technology** will be offered by the Emulsion Polymers Institute at Lehigh University in Bethlehem, Pennsylvania, USA, from 2-6 June 2008. The course is an in-depth study of the synthesis, char-

acterization, and properties of high polymer latexes. The subject matter includes a balance between theory and application as well as a balance between chemical and physical problems. Lectures will be given by leading academics and industrialists. Lectures will begin with introductory material and reviews, and will progress through recent research results.

 [http://fp2.cc.lehigh.edu/inemuls/epi/lehigh\\_sc.htm](http://fp2.cc.lehigh.edu/inemuls/epi/lehigh_sc.htm)

## Applied Thermodynamics

29 May-1 June 2008, Cannes, France

The 23rd **European Symposium on Applied Thermodynamics** (ESAT2008) will be held on the French Riviera from 29 May-1 June 2008. The goal of the event is to bring together engineers and scientists (from universities, industry, and research institutes) to discuss applications of chemical engineering thermodynamics.

Theoretical and experimental aspects will be covered, and researchers are encouraged to report new results and theories. Speakers will consider future applications based on today's results, offer solutions for current problems, and discuss the present state of the art.

Major topics covered will be as follows:

- Phase equilibria
- Petroleum fluids
- Supercritical fluids

- Molecular simulation
- Product and process design
- Sustainable development (resources, energy, environment, storage and capture of greenhouse gases)
- Ionic liquids
- Polymers
- Biochemical systems
- Colloidal and interfacial systems
- Electrolytes
- Experimental techniques and data

During the conference, the "ESAT2008 Best Poster Award" will honor a young researcher who has presented a poster of exceptional merit dealing with a subject related to thermodynamics. All young researchers are encouraged to participate in this competition.

 [www.esat2008.com](http://www.esat2008.com)

## Polar Research

8-11 July 2008, St. Petersburg, Russia

The Scientific Committee on Antarctic Research (SCAR) and its Arctic counterpart IASC (International Arctic Science Committee) have organized a conference on **Polar Research—Arctic and Antarctic Perspectives in the International Polar Year** that will take place in St. Petersburg, Russia, 8-11 July 2008. Natural and social scientists are invited to present abstracts under a series of session headings that address the themes of the International Polar Year.

In addition, the Association of Polar Early Career Scientists (APECS) and the U.K. Polar network (the British branch of APECS) wants to help young scien-

tists form connections through an international network of early career polar and cryosphere scientists and researchers. These groups are organizing a one-day professional-development workshop for 7 July 2008, the day before the SCAR/IASC open science conference. The meeting will include invited keynote speakers, panel sessions, and discussion groups. For more information, contact Liz Thomas <liz.thomas@polarnetwork.org> or go to <www.arcticportal.org/apecswww.arcticportal.org/apecs>. The application deadline is 29 February 2008.

 [www.scar.org](http://www.scar.org)  
[www.scar-iasc-ipy2008.org](http://www.scar-iasc-ipy2008.org)



## Solid State Chemistry

6–11 July 2008, Bratislava, Slovakia

The scope of the **8th Conference on Solid State Chemistry** is solid state chemistry in the broadest sense, including results of various experimental and theoretical methods applied in investigation of solid state substances.

This conference is a continuation of the previous conferences on solid state chemistry, held biannually in the Czech and Slovak republics. It is endorsed by the three organizing institutions and by the Slovak Chemical Society, Slovak Clay Group, and Slovak

Silicate Society. The scientific program of SSC 2008 will comprise the following sections: Synthesis and Characterization of Materials; Crystal, Electronic, and Magnetic Structure; Electrochemistry and Molten Salts; Chemistry of Glasses; Novel Inorganic Materials and Nanomaterials; Layered Compounds, Clathrates and Intercalates; and Deposited Films and Surface Chemistry.

See **Mark Your Calendar** on page 40 for contact information.

 [www.ssc2008.sav.sk](http://www.ssc2008.sav.sk)

## Stable Isotope

31 August–5 September 2008, Presqu'île de Giens, Var, France

The second Joint European Stable Isotope Users group Meeting (JESIUM) is being organized by the French Society of Stable Isotopes under the coordination of Jaleh Ghashghaie. It will take place in southern France from 31 August–5 September 2008.

The specific objectives of JESIUM 2008 are as follows:

- discuss the role of isotopic measurements for a better understanding of
  - processes of life
  - ecology
  - mechanisms in terms of physical chemistry, biology, circulation, evolution

- interactions within and between ecosystems and environmental compartments
- terrestrial and extra-terrestrial geologies
- human activities and practices
- impact and resolution of problems generated by human activities and practices
- diagnostic and decision tools for society
- stimulate discussion and reflection on the importance of quality in measurements
- stimulate exchanges in Europe between nonprofit scientific societies and organizations promoting the use of isotopic measurements
- create a formal European Federation of Associations of Stable Isotope Users

 <http://sfis.snv.jussieu.fr/jesium2008/>

## Polymer Processing

15–19 June 2008, Salerno, Italy

The **2008 Annual Meeting of the Polymer Processing Society** (PPS-24) will take place in Salerno, Italy, 15–19 June 2008. Scientists and engineers working in polymer processing and related fields are invited. See program online.

The Polymer Processing Society was founded in March 1985 at the University of Akron, Ohio, USA, with the intent of providing a mechanism and format for interaction and presentation of research results in the international polymer processing community. The

goals of the group are to foster scientific understanding and technical innovation in polymer processing by providing a discussion forum for the worldwide community of engineers and scientists in the field. The thematic range encompasses all formulation, conversion, and shaping operations applied to polymeric systems in the transformation from their monomeric forms to commercial products. Membership in PPS is open to all researchers in the field, and to all persons who feel the activities of the society advance their professional development.

 [www.pps-24.com](http://www.pps-24.com)

2008

 IUPAC poster prizes to be awarded

**8–11 January 2008 • Agrochemicals • New Delhi, India**

*International Conference on Agrochemicals Protecting Crop, Health and Natural Environment*,  
Dr. N.A. Shakil, Division of Agricultural Chemicals, IARI, New Delhi 110 012, India, Tel.: +91 009818196164,  
Fax: +91 11-25843272

**2–8 February 2008 • Photodynamics • Havana, Cuba**

*5th International Meeting on Photodynamics*  
Prof. Jesús Rubayo Soneira, Instituto Superior de Tecnologías y Ciencias Aplicadas, Ave. Salvador Allende y  
Luaces, A.P. 6163, Havana 10600, Cuba, Tel.: + 53 7-2041188, Fax: +53 7-2041188, E-mail: [jrs@instec.cu](mailto:jrs@instec.cu)

**17–21 February 2008 • Advanced Materials • Lucknow, India** 

*POLYCHAR-16—World Forum on Advanced Materials*  
Prof. Poonam Tandon, Department of Physics, University of Lucknow, Lucknow 226 007, India, Tel.: + 91 522 274,  
0840 | Fax: +91 522 274 0840, E-mail: [contact@polychar16.com](mailto:contact@polychar16.com)

**9–12 March 2008 • Heterocyclic Chemistry • Gainesville, Florida, USA**

*9th Florida Heterocyclic Conference*  
Prof. Alan R. Katritzky, University of Florida, Dept. of Chemistry, Gainesville, FL 32611-7200, USA,  
Tel.: +1 352 392 0554, Fax: +1 352 392 9199, E-mail: [katritzky@chem.ufl.edu](mailto:katritzky@chem.ufl.edu)

**2–6 June 2008 • Molecular Order and Mobility in Polymer Systems • Saint-Petersburg, Russia**

*6th International Symposium on Molecular Order and Mobility in Polymer Systems*,  
Prof. T.M. Birshtein, Institute of Macromolecular Compounds, Russian Academy of Sciences (IMC RAS), Bolshoi  
pr. 31, Saint-Petersburg, RU-199004 Russia, E-mail: [birshstein@imc.macro.ru](mailto:birshstein@imc.macro.ru)

**22–27 June 2008 • Organic Synthesis • Daejeon, Korea** 

*International Conference on Organic Synthesis (ICOS-17)*  
Prof. Sung Ho Kang, Department of Chemistry, KAIST, Daejeon 305-701, Korea, Tel.: +82-42-869-2825,  
Fax: +82-42-869-2810, E-mail: [shkang@kaist.ac.kr](mailto:shkang@kaist.ac.kr)

**29 June–4 July 2008 • Macro 2008 • Taipei, Taiwan** 

*Polymers at Frontiers of Science and Technology*  
Conference Secretariat, MACRO 2008, Department of Chemical Engineering, National Tsing-Hua University,  
101, Section 2, Kuang-Fu Road, Hsinchu, 30013 Taiwan, Tel.: (03) 5713131 ext. 33683, Fax: (03) 5715408,  
E-mail: [acsu@mx.nthu.edu.tw](mailto:acsu@mx.nthu.edu.tw)

**6–11 July 2008 • Solid State Chemistry • Bratislava, Slovakia**

*8th Conference on Solid State Chemistry*  
Dr. Milan Drabik, Ceramics Department, Institute of Inorganic Chemistry, Slovak Academy of Sciences, SK-84536  
Bratislava, Slovakia, Tel.: +421 (7) 5941-0474, Fax: +421 (7) 5941-0444, E-mail: [uachmdra@savba.sk](mailto:uachmdra@savba.sk)

**13–18 July 2008 • Biodiversity and Natural Products • Charlottetown, Prince Edward Island, Canada** 

*International Conference on Biodiversity and Natural Products (ICOB-6 & ISCNP-26)*  
Prof. Russell Kerr, Department of Chemistry, University of Prince Edward Island, 550 University Avenue  
Charlottetown, PEI C1A 4P3, Canada, Tel.: + 1 902 566 0565, Fax: +1 902 566 0632,  
E-mail: [rkerr@upei.ca](mailto:rkerr@upei.ca). Ann Worth, Conference Manager, E-mail: [info@iupac-icbnp2008.com](mailto:info@iupac-icbnp2008.com)

**13–18 July 2008 • Physical Organic Chemistry • Santiago de Compostela, Spain** 

*19th International Conference on Physical Organic Chemistry (ICPOC-19)*  
Prof. J. Ramón Leis, Faculty of Chemistry, Universidad de Santiago de Compostela, E-15782 Santiago de  
Compostela, Spain, Tel.: +34-98-156-3100, Fax: +34-98-159-5012, E-mail: [qfjrleis@usc.es](mailto:qfjrleis@usc.es)

**20–24 July 2008 • Polymer Colloids • Prague, Czech Republic**

*2008 Prague Meetings on Macromolecules—48th Microsymposium “Polymer Colloids: From Design to  
Biomedical and Industrial Applications”*  
Dr. Daniel Horák, Institute of Macromolecular Chemistry, Heyrovský Sq. 2, CZ-162 06 Prague 6, Czech Republic  
Tel.: + 42 029 680 9260, Fax: +42 029 680 9410, E-mail: [horak@imc.cas.cz](mailto:horak@imc.cas.cz)

**20–25 July 2008 • Coordination Chemistry • Jerusalem, Israel**

*38th International Conference on Coordination Chemistry*  
Prof. Dan Meyerstein, The College of Judea and Samaria, P.O. Box 3, Ariel 44837, Israel, Tel.: + 972 3 906 6153,  
Fax: +972 3 972 7555, E-mail: [danmeyer@bgumail.bgu.ac.il](mailto:danmeyer@bgumail.bgu.ac.il)

**27-31 July 2008 • Solubility Phenomena • Dublin, Ireland** 

*13th International Symposium on Solubility Phenomena Including Equilibrium Process (ISSP-13)*  
Prof. Earle W. Waghorne, Chairman, School of Chemistry & Chemical Biology, University College, Belfield, Dublin 4, Ireland, Tel.: +353 1 716 2132, Fax: +353 1 716 2127, E-mail: earle.waghorne@ucd.ie

**27 July-1 August 2008 • Carbohydrates • Oslo, Norway**

*24th International Carbohydrate Symposium (ICS 2008)*  
Prof. Berit Smestad Paulsen, School of Pharmacy, University of Oslo, P.O. Box 1068 Blindern, N-0316 Oslo, Norway, Tel.: +47 22 856 572, Fax: +47 22 854 402, E-mail: b.s.paulsen@farmasi.uio.no

**28 July-1 August 2008 • Photochemistry • Gothenburg, Sweden** 

*XXII IUPAC Symposium on Photochemistry*  
Prof. Devens Gust, Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ, USA, 85287-1604, USA, Tel.: +1 602 965 4547, Fax: +1 602 965 2747, E-mail: gust@asu.edu

**3-8 August 2008 • Chemical Education • Pointe aux Piments, Mauritius** 

*20th International Conference on Chemical Education: Chemistry in the Information & Communications Technologies Age, (20th ICCE)*  
Dr. Ponnadurai Ramasami, Department of Chemistry, University of Mauritius, Reduit, Mauritius, E-mail: p.ramasami@uom.ac.mu

**3-8 August 2008 • Chemical Thermodynamics • Warsaw, Poland** 

*20th International Conference on Chemical Thermodynamics*  
Questions should be addressed to E-mail: info@icct2008.org. Comments, concerns, proposals, etc., should be addressed to E-mail: secretariat@icct2008.org.

**14-20 September 2008 • Green Chemistry • Moscow, Russia** 

*2nd IUPAC Conference on Green Chemistry*  
Prof. Valery V. Lunin, Chairman Russia Chemistry Department, M.V. Lomonosov Moscow State University, Leninskiye Gory 1, build. 3, 119992 Moscow Russia, Tel.: +7-495-9394575, Fax +7-495-9394575, E-mail: vvlunin@kge.msu.ru

**14-20 September 2008 • Humic Substances • Moscow, Russia**

*14th Meeting of the International Humic Substances Society (IHSS-14)*  
Prof. Irina V. Perminova, Department of Chemistry, Moscow State University, 119992 Moscow, Russia, E-mail: iperm@org.chem.msu.ru, Tel: +7 495 939 5546, Fax: +7 495 932 8846

**12-17 October 2008 • Biotechnology • Dalian, China**

*13th International Biotechnology Symposium (ISB 2008): "Biotechnology for the Sustainability of Human Society"*  
Prof. Fengwu Bai, Dept. of Bioscience & Bioengineering, Dalian University of Technology, 2 Linggong road, Dalian 116023, China, Tel.:+86 411 84706329, Fax:+86 411 84708083, E-mail: fwbai@dlut.edu.cn

**26-30 November 2008 • Soil Science • Pucon, Chile**

*International Symposium of Interactions of Soil Minerals with Organic Components and Microorganisms*  
Dra. Maria de La Luz Mora, Universidad de La Frontera, Ciencias de Recursos Naturales, Temuco, Chile, Tel: +56 45 325479, Fax: +56 45 325053, E-mail: mariluz@ufro.cl

**Chemistry in a Changing World—New Perspectives Concerning the IUPAC Family**

**25 April 2008, Marl, Germany**

The IUPAC Committee on Chemistry and Industry (COCI) will organize a **Workshop on "Chemistry in a Changing World—New Perspectives Concerning the IUPAC Family"** to increase knowledge among the National Adhering Organizations (NAOs)/chemi-



cal societies in the European Union (plus Norway and Switzerland) about the role of COCI/IUPAC and to foster communication and discussion about the emerging role of IUPAC in a changing world. Representatives of NAOs/chemical societies in the EU, Norway, and Switzerland will be invited to participate and to develop a framework for future actions.

Anyone interested in participating should contact Michael J. Droescher at < michael.droescher@degussa.com > or any member of the task group or of COCI.

 [www.iupac.org/projects/2006/2006-030-1-022.html](http://www.iupac.org/projects/2006/2006-030-1-022.html)



# International Union of Pure and Applied Chemistry

Advancing the worldwide role of chemistry for the benefit of Mankind

**Mission Statement**—IUPAC is a non-governmental organization of member countries that encompass 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.

**President:** JUNG-IL JIN (Korea)

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## National Adhering Organizations

Australian Academy of Science (*Australia*)  
Österreichische Akademie der Wissenschaften  
(*Austria*)

Bangladesh Chemical Society (*Bangladesh*)

National Academy of Sciences of Belarus  
(*Belarus*)

The Royal Academies for the Sciences and  
Arts of Belgium (*Belgium*)

Brazilian Chemistry Committee for IUPAC  
(*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*)

Czech National Committee for Chemistry  
(*Czech Republic*)

Det Kongelige Danske Videnskabernes Selskab  
(*Denmark*)

National Committee for IUPAC (*Egypt*)

Chemical Society of Ethiopia (*Ethiopia*)

Suomen Kemian Seura—Kemiska Sällskapet i  
Finland (*Finland*)

Comité National Français de la Chimie (*France*)

Deutscher Zentralausschuss für Chemie  
(*Germany*)

Association of Greek Chemists (*Greece*)

Hungarian Academy of Sciences (*Hungary*)

Indian National Science Academy (*India*)

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Israel Academy of Sciences and Humanities  
(*Israel*)

Consiglio Nazionale delle Ricerche (*Italy*)

Caribbean Academy of Sciences—Jamaica  
Chapter (*Jamaica*)

Science Council of Japan (*Japan*)

Jordanian Chemical Society (*Jordan*)

Korean Federation of Science and Technology  
Societies (*Korea*)

Kuwait Chemical Society (*Kuwait*)

Koninklijke Nederlandse Chemische Vereniging  
(*Netherlands*)

Royal Society of New Zealand (*New Zealand*)

Norsk Kjemisk Selskap (*Norway*)

Chemical Society of Pakistan (*Pakistan*)

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Sociedade Portuguesa de Química (*Portugal*)

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Russian Academy of Sciences (*Russia*)

Union of Yugoslav Chemical Societies (*Serbia  
and Montenegro*)

Slovak Chemical Society (*Slovakia*)

Slovenian Chemical Society (*Slovenia*)

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