

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

# CHEMISTRY

## International

November-December 2006  
Volume 28 No. 6



### GEOTRACES

Chemistry Takes Center  
Stage in Marine Science

Would Einstein  
Have Approved?

Nanotechnology: Lessons  
from Mother Nature



# From the Editor

## CHEMISTRY International

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

[www.iupac.org/publications/ci](http://www.iupac.org/publications/ci)

**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

Metcalfe 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

### Printed by:

Cadmus Professional Communications,

Easton, MD, USA

### Subscriptions

Six issues of *Chemistry International* (ISSN 0193-6484) will be published bimonthly in 2006 (one volume per annum) in January, March, May, July, September, and November. The 2006 subscription rate is USD 99.00 for organizations and USD 45.00 for individuals. Subscription orders may be placed directly with the IUPAC Secretariat. Affiliate Members receive *CI* as part of their Membership subscription, and Members of IUPAC bodies receive *CI* free of charge.

### Reproduction of Articles

Unless there is a footnote to the contrary, reproduction or translation of articles in this issue is encouraged, provided that it is accompanied by a reference to the original in *Chemistry International*.

Periodicals postage paid at Durham, NC 27709-9990 and additional mailing offices. POSTMASTER: Send address changes to *Chemistry International*, IUPAC Secretariat, PO Box 13757, Research Triangle Park, NC 27709-3757, USA.

ISSN 0193-6484

Which IUPAC book has a nickname, color, author, and now URL that are the same? The answer is the Gold Book, i.e. the *Compendium of Chemical Terminology*.

The compendium, first published in 1987, had a gold colored cover, and the first author/compiler was Victor Gold. Gold deserves the credit for initiating this project and contributing to the compilation of terms and their definitions. Unfortunately, Victor Gold passed away in September 1985, just a few months before the first edition was finally completed. The



work was later completed by Kurt Loening, Alan McNaught, and Pamil Sehmi. The compendium was soon popularized as the Gold Book in recognition of Gold's initial work.

The book was a hit as soon as it was published and plans were made to expand the compendium by including new and revised defini-

tions recommended by various specialized groups within IUPAC. In 1998, when the second edition was published, the book cover was again gold, and Alan McNaught was again one of the compilers along with Andrew Wilkinson. At this stage, the compendium included nearly 7 000 terms.

A couple of years after the second edition was released, the book was made available online as a collection of PDF files. Everyone was now just a few keystroke away from the compendium and all its definitions. This was quite an achievement at the time, one that was possible thanks to the help of the Royal Society of Chemistry.

Today, following the continuous growth in web technologies, we can all look at the Gold Book in a whole new light ... an XML version was recently completed—a copy of which is provided to you on the enclosed CD.

Turn to page 28 for details about this brand new product. The contributions of Miloslav Nic, Jiri Jirat, and Bedrich Kosata in transforming the compendium into a contemporary tool are remarkable. This achievement is clearly deserving of great appreciation from IUPAC and the chemistry community.

One of the most valuable functions of the XML technology is the easy linkage between definitions and the multitude of indexes. XML allows for regrouping of entries according to structures, physical constants, symbols, acronyms, etc—all generated automatically.

As it so happened, the release of version 1.0.0 of the XML Gold Book was completed on 29 September 2006—the 21st anniversary of Victor Gold's death. In his lifetime Gold could not have dreamed of all the improvements now added to the compendium he initiated, but I suspect that today he would have approved!

Fabienne Meyers

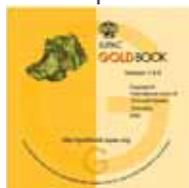
[fabienne@iupac.org](mailto:fabienne@iupac.org)

[www.iupac.org/publications/ci](http://www.iupac.org/publications/ci)

**Cover:** This SeaWiFS image of the global biosphere was taken in May 2002. In the oceans, the regions with increasing phytoplankton abundance and higher chlorophyll-a concentrations are shown in lighter blues, greens, yellows, and reds. Source: <http://oceancolor.gsfc.nasa.gov>.

# Contents

CHEMISTRY International November-December 2006 Volume 28 No. 6



<b>President's Column</b>	2
<b>Features</b>	
<b>GEOTRACES—Chemistry Takes Center Stage in Marine Science</b> <i>by David Turner</i>	4
<b>Would Einstein Have Approved?—A Discussion About the International Year of Physics</b> <i>Minella Alarcon's Interview with Judy Franz, Martial Ducloy, Francis Allotey, and Masno Ginting</i>	6
<b>Nanotechnology: Lessons from Mother Nature</b> <i>by Alan Smith</i>	10
<b>Tools of the Trade</b>	
The IUPAC International Chemical Identifier: InChI—A New Standard for Molecular Informatics <i>by Alan McNaught</i>	12
Using InChI <i>by Jeremy G. Frey</i>	14
<b>Up for Discussion</b>	
<b>The Canadian National Committee for IUPAC's Travel Awards Program—A Success Story</b> <i>by Chris I. Ratcliffe</i>	16
<b>Emerging Issues in Developing Countries: Standardization of Analytical Approaches and Analytical Capacity-Building in Africa</b> <i>by Robert Maybury, Walter Benson, and David Moore</i>	17
<b>IUPAC Wire</b>	
Young Chemists to the 41st IUPAC World Chemistry Congress	20
The XML Gold Book Online	20
IUPAC Elections for the 2008-2009 Term	21
Industry and IUPAC Meeting Halfway	21
IUPAC President Attends the International Chemistry Olympiad	22
InChI 1.01	23
Dewen Zeng Receives the 2006 Franzosini Award	23
<b>The Project Place</b>	
<b>Biophysico-Chemical Processes Involving Natural Nonliving Organic Matter in Environmental Systems</b>	24
<b>Trace Elements Analysis: Role of Grain Size Distribution in Solid Reference Materials</b>	24
<b>The Chemistry Clearing House as a Way to Better Chemistry Teaching</b>	25
<b>Teaching High-Temperature Materials Chemistry at the University Level</b>	26
<b>Provisional Recommendations</b> <i>IUPAC Seeks Your Comment</i>	26
<b>Making an impACT</b>	
<b>Standards, Calibration, and Guidelines in Microcalorimetry</b>	27
<b>Internet Connection</b>	
<b>Chemical Terminology at Your Fingertips</b> <i>by Miloslav Nic, Jiri Jirat, Bedrich Kosata</i>	28
<b>Free Information Resources for Chemists—Part 3</b> <i>by Leslie Glasser</i>	30
<b>Conference Call</b>	
<b>Solubility Phenomena</b> <i>by Heinz Gamsjaeger and Wolfgang Voigt</i>	31
<b>Green Chemistry: A Tool for Socio-Economic Development and Environmental Protection</b> <i>by Pietro Tundo and Kenneth R. Seddon</i>	32
<b>Polymers and Organic Chemistry</b> <i>by Shinichi Itsuno</i>	33
<b>Where 2B &amp; Y</b>	34
<b>Mark Your Calendar</b>	36
<b>Index for 2006</b>	38

## IUPAC Within and Without



by Bryan Henry

**I**n this brief column I want to touch on a number of issues and events that I believe are important or of interest to the IUPAC community.

A recurring concern of IUPAC officers and member organizations is how to allow everyone to get their issues "on the table." To address this problem, the

Executive Committee approved a proposal at its April 2006 meeting to hold a series of round table discussions at the next General Assembly (GA) in Torino, Italy, in August 2007. These discussions are intended to allow small groups of Council delegates to discuss subjects of mutual interest in a setting conducive to the easy exchange of ideas. National Adhering Organizations and Bureau members were invited to propose topics, and during the most recent Bureau meeting in Madrid on 7 October 2006, the following topics were identified:

- How can we attract more students to chemistry? Do we need to modify the curriculum? Can IUPAC play a role?
- How can we help regions and small countries to have a more effective voice within IUPAC?
- How can we interact more effectively with governments and other decision makers? How can we improve our interactions with industry, other unions, ICSU, UNESCO, etc.?
- How can we increase the global visibility of chemistry, enhance public understanding of chemistry, and improve its public image? How can we improve the visibility and image of IUPAC?

In each case, a couple of members of the Bureau will mediate the discussions. These discussions shall interest varied groups, including smaller countries within IUPAC who have needs and legitimate concerns that might be difficult to articulate and convey to the wider IUPAC community. For practical reasons, each round table will be limited to 40 participants. When registering for the Council, delegates will be asked to prioritize their interest in the discussion topics. Assignments to the various round tables will be based as much as possible on these priority interests. Hopefully, attendance

will be good and lively discussions will ensue at Torino. The results of these forums will be considered at future meetings of the Bureau and Executive.

Previous Council debates were concerned with the operational structure of IUPAC. After the last debate in Beijing, it was decided not to change the current structure, and instead to develop measures to streamline IUPAC operations and to make them more efficient. For this reason I have created a committee to examine such a possibility. The members of the Committee on Streamlining IUPAC Operations (CSIO) are Michael Jaffe (USA), Anders Kallner, (Sweden), Venceslav Kaucic (Slovenia), Kook Joe Shin (Korea), Fabienne Meyers (IUPAC Secretariat), and myself as chair. A second committee chaired by Secretary General David StC. Black will examine any changes needed in our statutes and bylaws to accomplish the recommendations of the CSIO, and make revisions that inevitably are needed periodically in such documents.

In order for the committee to have as wide a perspective as possible, we need input from all segments of the IUPAC community. Thus, we are requesting that you send us your suggestions. We consider this a matter of very high priority. The CSIO cannot possibly come up with a plan that reflects IUPAC's diverse community without your help.

One criticism of IUPAC that is germane to the streamlining initiative is that often IUPAC does not respond quickly enough to fast moving events. Perhaps this is not surprising for an organization that is so diverse in both membership and activities. Moreover, it is probably not reasonable to expect the same kind of response times in a volunteer organization—which needs to keep its members informed and motivated—as one would find in an organization with a hierarchical, top-down management structure and strict financial motivations. There is a price to be paid for democracy and universal involvement! Nevertheless, it is of interest that recently IUPAC had to respond to the unfortunate resignation of our vice president and president elect. The executive group responded to the situation in a timely and effective fashion. Of course, given that we are IUPAC, the decisions were taken to the Bureau meeting in Madrid for ratification.

One of our highest priorities within IUPAC is to involve young people in the excitement of chemistry. In that regard, I am pleased to announce that plans are now in place that will allow young chemists to participate in the 41st IUPAC Congress in Torino in August

2006 (see page 20). In addition, IUPAC renewed its commitment to invite a few young chemists to also participate in the debates of the GA, which are held concurrently. It is likewise rewarding to see that some National Adhering Organizations, such as those from the USA and the UK, continue their programs that offer grant support to young chemists to attend the GA.

A different way to expose young chemists to the international scene is presented in this issue of *CI* (see page 16). The Travel Awards Program of the Canadian National

Committee for IUPAC allows awardees to attend IUPAC-sponsored scientific conferences and present their research. Over its 25 years of existence, this nationwide competition has gained prestigious status within the Canadian scientific community. Small or large, all these programs are important to ensure the future of IUPAC. Might I invite all member countries to consider developing their own programs.

In that regard, it is regrettable that IUPAC has never been directly involved in the International Chemistry Olympiad. This is a competition with all the excitement and camaraderie that characterizes the Olympics. In July 2006, thanks to a gracious invitation from the organizing committee, I had the great privilege of participating in this event, which included speaking about IUPAC at the closing ceremonies, and, most importantly, presenting IUPAC Gold Books to the 28 gold medalists in a competition that involved more than 70 countries (read more on page 22).

The International Council for Science (ICSU) recently opened regional offices for Africa, Asia and the Pacific, and Latin America and the Caribbean. IUPAC participated in the opening conferences at all three sites: Pretoria (Piet Steyn), Kuala Lumpur (David StC. Black), and Panama (Bryan Henry). Chemistry has played an important role in ICSU from its founding in 1931, with IUPAC being one of its original members. Our hope is to use the contacts within these regional offices to help IUPAC become more involved with emerging countries and to extend our programs more effectively to these regions.

ICSU is attempting to revise and rationalize its dues structure for the more than 100 National Members and

approximately 30 Union members. They have invited our Executive Director John Jost to the first meeting of this Dues Committee to present a solution based on the IUPAC dues system.

In late August, the European Association for Chemical and Molecular Sciences organized the 1st European Chemical Congress. This historic meeting was a great success and IUPAC was invited to present a brief address at the opening ceremony. In this talk, I had an opportunity to inform the more than 2 000 conferees about the

*One of our highest priorities within IUPAC is to involve young people in the excitement of chemistry.*

breadth of IUPAC activities. Too often we are viewed as a body whose sole function is nomenclature-related issues and critically evaluated data. Of course, these core activities continue to be very valuable and important, but IUPAC is much more diverse and far reaching. While IUPAC has close cooperation with regional chemistry organizations, it is worth noting that one of IUPAC's priorities should be to nurture the relationships it has, in principle, with more than 30 Associated Organizations. There is room to improve and cultivate relations with these international organizations. As the IUPAC Statutes underline, these organizations' "aims and activities are in harmony with those of the Union."

This column began with a description of measures to improve both the involvement of the smaller countries within IUPAC and our internal operational activities. The following paragraphs described outreach activities to other organizations. If there is a conclusion it is that IUPAC continues to evolve and to search for new opportunities to make the world a better place through chemistry. 

**Bryan Henry <chmhenry@uoguelph.ca> has been IUPAC president since January 2006. He is a retired professor of chemistry in the Department of Chemistry and Biochemistry at the University of Guelph, Canada. He has been a member of the Canadian National Committee for IUPAC since 1995, and served as chair from 1998–2003.**

## Chemistry Takes Center Stage in Marine Science

by David Turner

The enormous breadth and range of applications of modern chemistry are reflected in the wide range of activities within IUPAC. As a result, individual chemists can often feel that their own (all-important!) specialization is under represented in IUPAC's work. As a marine chemist, I am not immune to those feelings, but can at the same time point to some significant IUPAC contributions to marine science from the Analytical Chemistry Division (V) and the Chemistry and the Environment Division (VI). Much of the work of Division V on critical evaluation of stability constants and on chemical speciation modeling has been relevant to seawater systems, and in some cases specifically directed at seawater. Division VI has also contributed to marine sciences through books published in the "IUPAC Series on Analytical and Physical Chemistry of Environmental Systems."

In the late 1990s, I was given the opportunity to develop a marine initiative in IUPAC. At that time I

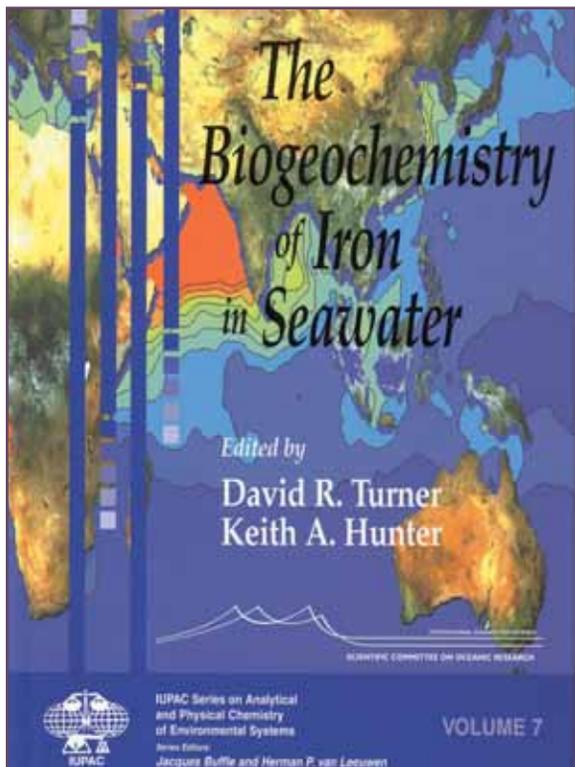
was the only chemist active in both IUPAC and in the International Council for Science's (ICSU's) Scientific Committee on Oceanic Research (SCOR). The leadership of the two organizations had agreed that collaborative projects would be a good idea, and I was given the task of turning this into reality. The result of this initiative was a joint project on iron in seawater, which resulted in the book *The Biogeochemistry of Iron in Seawater*, published in Division VI's book series in 2001 (John Wiley & Sons, 2001, ISBN 0-471-49068-7). Note the word "biogeochemistry," not just "chemistry" in the title: Chemical processes in the marine environment are intimately linked with both biology and geosciences, and it is those linkages which make marine biogeochemistry a key discipline in the science of global change.

The focus on iron in the IUPAC-SCOR collaborative project was no random choice of an interesting chemical element. It was during the 1990s that it became clear that iron is a key micronutrient in the oceans, whose bioavailability influences both the extent of primary production (photosynthesis), and also the plankton community structure. Indeed, the 1990s have been dubbed "The Iron Age of Oceanography."

### Why GEOTRACES Now?

SCOR has recently launched a major new global program, GEOTRACES, in which marine biogeochemistry takes center stage. There is a clear focus on trace elements, not just because they are fascinating (which they are!), but for what they can tell us about the functioning of the ocean and its role in global change. This is the first large-scale coordinated program in this area since GEOSECS (Geochemical Ocean Sections Study) in the 1970s. So, with three decades elapsed between programs, what makes GEOTRACES timely just now? The answer to this question lies partly in developments in sampling and measurement techniques, and partly in our ability to interpret and model data on a global scale.

It was during the 1970s that much of the methodology of "trace metal clean handling" was developed and put into practice. In plain English, this means ensuring that the trace metals measured came from the sample, not from the analyst, sampling vessels, reagents, or laboratory atmosphere. Earlier studies of trace metal chemistry in seawater were bedeviled by contamination, giving rise to misleading and uninterpretable results. For example, it was recognized in the 1920s and 1930s that iron concentrations in seawater



could be so low as to limit primary production, but it was not until the advent of clean handling techniques that this could be confirmed by experiment. Even now, the accuracy of measurement of subnanomolar iron concentrations in seawater is a matter for concern (and iron concentrations are subnanomolar for the most part). Significant progress has been made through an intercalibration project within the framework of the IUPAC-SCOR project on iron (see Bowie et al., 2005. *Marine Chemistry*, 98, 81-99. doi:10.1016/j.marchem.2005.07.002).

The global oceanography programs of recent decades such as the World Ocean Circulation Experiment and the Joint Global Ocean Flux Study (JGOFS) have shown how field measurements, coordinated on a global scale, can be combined with satellite observations and modelling to develop a new understanding of the oceans' role in the Earth System. These programs have included an increasing amount of trace elements chemistry, most particularly in JGOFS during the "Iron Age of Oceanography." This has in turn stimulated the development of methods for high-density sampling and analysis, yet another methodological advance that will be important to GEOTRACES.

## The GEOTRACES Program

GEOTRACES has formulated a guiding mission: "To identify processes and quantify fluxes that control the distributions of key trace elements and isotopes in the ocean, and to establish the sensitivity of these distributions to changing environmental conditions." Within this guiding mission, GEOTRACES has identified three overriding goals, focusing on the past, present, and future.

**Past:** "To understand the processes that control the

concentrations of geochemical species used for proxies of the past environment, both in the water column and in the substrates that reflect the water column."

**Present:** "To determine global ocean distributions of selected trace elements and isotopes, including their concentration, chemical speciation, and physical form, and to evaluate the sources, sinks, and internal cycling of these species to characterize more completely the physical, chemical, and biological processes regulating their distributions."

**Future:** "To understand the processes involved in oceanic trace-element cycles sufficiently well that the response of these cycles to global change can be predicted, and their impact on the carbon cycle and climate understood."

I will not in this short article try to provide further details of the background and approach to these goals, but refer the interested reader to GEOTRACES's ambitious Science Plan, which can be found at its website <[www.geotraces.org](http://www.geotraces.org)>. Individuals interested in becoming involved in GEOTRACES can do so by either contacting their national GEOTRACES committee or by sending an e-mail to <[geotraces@ideo.columbia.edu](mailto:geotraces@ideo.columbia.edu)>.

## A Role for IUPAC in GEOTRACES?

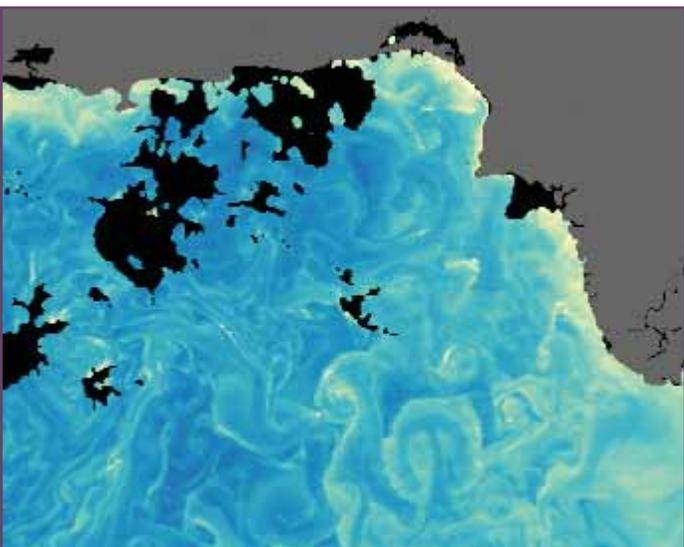
Chemistry is central to the GEOTRACES program, which can only benefit from a dialogue with the international chemistry community represented by IUPAC. This could, for example, take the form of new joint IUPAC-SCOR projects. An important first step towards further development of such collaboration would be to fill the currently vacant position of IUPAC representative to SCOR. I have now relinquished this position due to the pressure of other engagements. I would be very happy to see a successor appointed. 🤖

David Turner <[davidt@chem.gu.se](mailto:davidt@chem.gu.se)> is a professor in the Department of Chemistry at Göteborg University in Sweden. From 1998–2005 he acted as IUPAC representative on SCOR.

👉 [www.geotraces.org](http://www.geotraces.org)

*This clear view of chlorophyll concentrations in the northeastern Arabian Sea was collected by MODIS on the Aqua satellite on 22 February 2005.*

Source: <http://oceancolor.gsfc.nasa.gov>.



# Would Einstein Have Approved?

## A Discussion About the International Year of Physics\*

*Minella Alarcon's interview with Judy Franz, Martial Ducloy, Francis Allotey, and Masno Ginting*

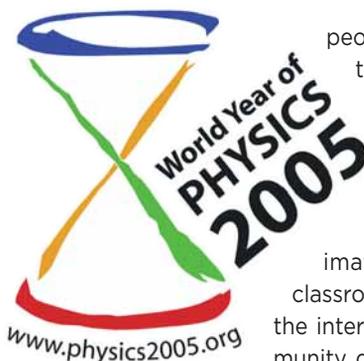
**H**ow successful was the International Year of Physics? In celebrating the 100th anniversary of Einstein's *annus mirabilis* in 1905, the Year was intended to serve as a rallying point for the public by recalling the important benefits physics has brought society over the past century.

Four leading physicists speak frankly about their individual experiences with the Year: Prof. Judy Franz from the USA is secretary general of the International Union of Pure and Applied Physics (IUPAP) and executive officer of the American Physical Society; Prof. Martial Ducloy from France chaired the International Steering Committee for the Year and is former president of the European Physical Society; Prof. Francis Allotey from Ghana is president of the Society of African Physicists and Mathematicians; and Prof. Masno Ginting from Indonesia is president of the Indonesian Physical Society.

**What did the physics community you represent hope to gain from the Year and how did it go about achieving this goal?**

**Judy Franz (J.F.)** We wanted to make nonscientists more excited about physics. We helped organize national events and many local ones and provided a website, which listed over 600 events, so that

\*This interview was first published in *A World of Science* 4(2), April-June 2006. Reprinted with permission. *A World of Science* is the UNESCO Natural Sciences Quarterly Newsletter; it is available online at <[www.unesco.org/science](http://www.unesco.org/science)>. French and Spanish versions are also available.

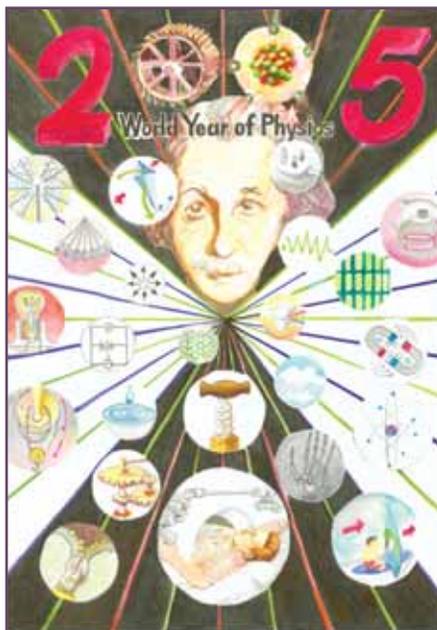


people across the country could see what was happening in their region. We also organized programs that were carried out in approximately 10 000 school classrooms. Overall, I think the international physics community did an excellent job of promoting the public understanding of physics. Of course, in some countries, physicists achieved much more than in others.

**Martial Ducloy (M.D.)** The goal of the Year was to improve communication between the physics community and society at large, including young people, in order to narrow the gap and recall the importance of physics in solving the societal problems of the 21st century. There was a large mobilization of physicists worldwide.

**Francis Allotey (F.A.)** The aim was to motivate more young people, including girls, to study physics and choose physics as a career. We hoped to make decisionmakers, and the general public in our part of the world, more aware of the important role physics plays in our daily lives and in industrial development. We informed the Minister for Environment and Science and Minister for Education and Sports about the aims of the Year. A national planning committee with various stakeholders was formed. We received financial support for local activities

from the government and from industry. The media was invited to our activities. We organized a series of lectures and physics exhibitions for students, teachers, and the general public on science in general and physics in particular, including topics such as Physics and Health Care, Physics for Wealth Creation, and Physics for Development. A physics outreach program was started: A Physics Talent Search and Physics Quiz



*First prize poster in the age 13-16 category of Science Across the World's Year of Physics poster competition. The artist is Stephanie Dorothy Yu of Hong Kong.*



were organized for young people throughout Ghana. The hour-long award ceremony for the winner of the Physics Quiz was televised live nationwide. Ghanaian young scientists participated in the International Junior Science Olympiads in Indonesia in 2004 and 2005, the Year's launch conference in Paris, and in the Young Physics Ambassador Symposium in Taipei from 30 December 2005 to 4 January 2006.

**Masno Ginting (M.G.)** We introduced competitions like the National Olympiad in Physics for junior and senior secondary school pupils and the International Junior Science Olympiad, in which pupils and the general public were invited to participate. The Indonesian Physical Society, in cooperation with the Indonesian Institute of Sciences (LIPI), organized a two-day seminar to which Nobel Laureate for Physics Prof. Douglas Dean Osheroff was invited as the keynote speaker. LIPI invited young scientists from all over Indonesia who had received science awards for their work, either in Indonesia or abroad, to attend this event. All of them presented their work during the seminar.

**How important was it for UNESCO to lend its support to the Year?**

**J.F.** Very important. For instance, in many countries the local government would not have given any funding without the official declaration by the United Nations and UNESCO. In all countries, this United Nations support helped attract media attention.

**M.D.** The support of international organizations, and of the United Nations in particular, gave an official seal to the Year and was essential for mobilizing the physics community in many countries. One may regret the absence of financial support.

**F.A.** UNESCO's support was critical. It showed the Ghanaian public that the Year was an important world event. This enabled us to receive financial support and full participation from the Ministry of Education and the Ministry of Science. Donations were also received from some local private organizations.

**M.G.** In my opinion, the United Nations/UNESCO support for the Year was very important for scientists all over the world and especially for physicists. The declaration of 2005 as the International Year of Physics stressed the importance of young people studying physics.

UNESCO supported the proclamation of the International Year of Physics 2005 as requested by the 58th session of the UN General Assembly. UNESCO organized activities for the celebration in close collaboration with the International Union of Pure and Applied Physics, the European Physical Society, and other regional and national physics societies all over the world. Approximately 90 countries implemented various activities. The Year provided UNESCO with a significant opportunity for international collaboration and networking among physics communities around the world. Worldwide, the activities of the International Year of Physics have developed a great momentum for physicists to reach out to the public at large.

Through its Physics Programme, under the Division of Basic and Engineering Sciences of the Natural Sciences Sector, UNESCO provided technical and financial assistance to the preparatory conferences and was fully involved in organizing two of the major events of the Year. The first was the launching conference, Physics for Tomorrow, held from 13–15 January 2005 at UNESCO Headquarters. This launch event, attended by more than 1 000 participants, brought together young people, the public at large, and distinguished scientists and Nobel laureates. It provided a rare opportunity for discussion and sharing of ideas on the role of physics in society and its impact on everyday life, the influence of Einstein on the science of the 20th and 21st centuries, physics teaching, and its links with other disciplines. UNESCO was also involved in the World Conference on Physics and Sustainable Development, held in Durban, South Africa, from 31 October to 2 November 2005. The conference offered a unique opportunity for the international physics community to come together and focus on how physics can bring more benefits to the developing world.

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

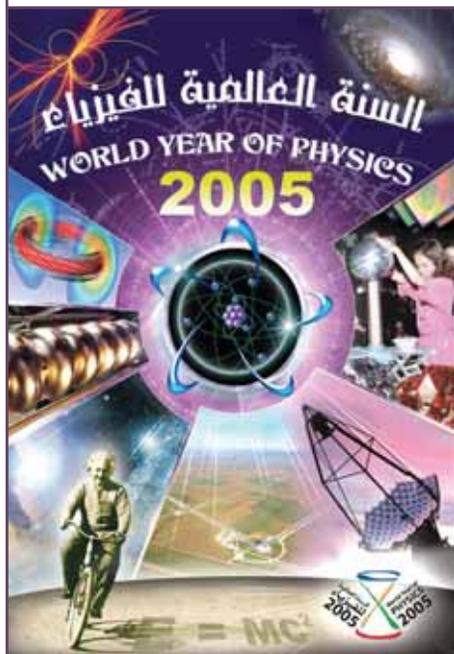
**Wasn't the declining number of young people studying physics one of the issues highlighted by the Year? Are countries taking any policy measures to redress the situation?**

**J.F.** In the USA, we ran a very successful program for secondary-level pupils in which more than 700 schools participated. In the USA, the American Institute of Physics keeps very good statistics about the number of pupils taking physics in secondary school and the number of undergraduate physics degrees awarded, as well as a great deal of additional data. The number of physics degrees awarded to undergraduates has been rising for the past five years or so, so it may be difficult to see the effect of the Year on top of this background increase. We shall nevertheless try to do so.

**M.D.** Many activities have sought to attract the attention of young people, but it is still too early to assess

## Would Einstein Have Approved?

the impact of these. In some countries, like France, there has already been an increase in the number of students enrolling in science at the university level, as observed



First prize poster in the age 13-16 category of SAW's poster competition. The artist is Asma Mimouni of Algeria.

active part in mobilizing physics teachers and pupils. More female pupils are getting involved in science at school. This is evident in the number of females (40 percent) who attended the Year launch ceremonies and took part in the Physics Talent Search and physics competitions we organized. Over 6 000 students and pupils took part in the talent search, which was organized at the district level right through to the regional and national levels. It is too early to talk about policy or to have data, but the Ghanaian Minister of Education and Sports has indicated in the media that he will be instituting financial incentives to motivate more pupils to take science in secondary school and at university.

**M.G.** Yes, that was the idea behind the Year. I am convinced that secondary-level physics will be more interesting for pupils from now on. But I am not so sure these same pupils will go on to study physics at university and take up a career in physics. The main problem is that, while they may find physics an interesting subject to study, many bright students think there is no future for them in physics. It may be a good idea to invite physical societies around the world to gather this information. The Indonesian Physical Society has encouraged

last September. The need to change teaching methods in science has already been felt in France and has led to the *La main à la pâte* program in primary schools, which is being extended to a number of European countries and beyond. Similar approaches are now being developed for physics teaching in secondary schools.

**F.A.** Yes, the declining number of physics students was one of the motivations behind the Year. The Ghana Institute of Physics is taking an

students to enroll in physics at university. For example, we already have an agreement with the dean of the Faculty of Mathematics and Science at the University of Indonesia to allow admission without sitting the regular university entrance test for students taking part in any international physics competitions. We are also exploring support from local governments and private companies for scholarships for bright pupils planning to enroll in physics at university.

**Do you think the Year has succeeded in generating a durable interest in physics among the general public and the media in your country?**

**J.F.** In the USA, there is no durable interest in almost anything. We shall have to maintain our efforts for the interest to survive. However, we have learned a lot about what efforts are most successful. I believe there were articles in most major newspapers. Science-oriented magazines and newsletters all gave the Year excellent coverage. It would be interesting to learn how many countries had at least one major public outreach event—we know this was the case for about 90 countries and perhaps more—and how many of these organized events they had never tried before. From the enthusiastic responses I have seen, many countries and physical societies will be continuing some of their more successful activities now that the Year is over. I know that the American Physical Society has added a staff person to continue our Physics Quest as an annual activity. This is aimed at middle school students (years 6-9 of schooling), an age group for which the American Physical Society has never had programs before. Activities during the Year depended heavily on national and international physical organizations and key individuals who volunteered a tremendous amount of their time. In fact, the large portion of volunteer time is a good measure of the importance of the Year for the international physics community. In addition, many organizations and governments contributed funding. Working together, IUPAP, UNESCO, and its Abdus Salam International Centre for Theoretical Physics were able to raise almost USD 500 000 for the World Conference on Physics and Sustainable Development in Durban last October, with contributions from more than 25 different organizations.

**M.D.** In France, and more generally in Europe, the impact on science communication has been tremendous: More than 500 public events were held in 2005 in France, 700 in Germany, 200 in Poland, etc. Throughout Europe, 37 countries participated actively in the Year, 18 of which received grants from the European Union. Public inter-

## A Discussion About the International Year of Physics

est in physics has definitely been raised. Our concern now is the durability of this interest. The tremendous momentum given to science communication should be carried on. On the media side, there has been a noteworthy interest, although this was more focused on Einstein himself than on physics. This has demonstrated that collaboration between science and communication can be done on a large scale.

**F.A.** The Year was very successful. Five commemorative stamps were issued. A weekly one-hour science program was initiated by a national radio station. Activities of the Ghana Institute of Physics have increased. Moreover, the Ghana Association of Science Teachers has requested that the outreach programs of Science on Wheels and the Physics Talent Search continue, which they are doing. With financial support from the Ministry of Science and Technology and the Ministry of Education and Sports, Science on Wheels visited various schools and colleges. Physicists from the Ghana Institute of Physics arranged science demonstration equipment on a van, both of which were provided by the Ghana Education Service. As for the talent search, it has raised awareness among students, parents, education planners, and the government of the importance of physics. As a result, for the first time, Ghanaian media and secondary school pupils are showing great interest in the solar eclipse we shall be able to observe in Ghana on 29 March 2006. On this occasion, the Ghana Institute of Physics and the Society of African Physicists and Mathematicians are organizing a conference at the University of Cape Coast. This will be webcast around the world and will showcase Ghanaian science.

**M.G.** The media—television, newspapers, and radio—gave all the events enthusiastic coverage, making the Year more popular. I was interviewed on a very good radio show along with teachers, parents, and others from different islands, among them Aceh, Kalimantan, and Bali. The show was broadcast all over Indonesia. There is a program called *Pesona Fisika*, or *Physics Edutainment*, which has been broadcast every Sunday evening for two years now on *Televisi Republik Indonesia* to very good viewer ratings. I think the Year was very suc-

cessful. Pictures of Einstein and of the Year's logo could be seen everywhere. People talked about the Year. Many pupils became more interested in physics than before. In my opinion, the International Physics Young Ambassadors' Symposium in Taipei, mentioned earlier by Prof. Allotey, was one of the Year's biggest achievements because it captured the spirit of solidarity. Many countries participated in the culminating event for the Year's Physics Talent Search, which targeted girls and boys ages 10–18 who were not enrolled in university. The symposium provided these gifted pupils with an authentic scientific and international experience, which enabled them to share their interests, work on experiments together, and create lasting friendships. 🌐

**Minella Alarcon** <[m.alarcon@unesco.org](mailto:m.alarcon@unesco.org)> is a physicist and UNESCO Coordinator of the International Year of Physics.

### About the Illustrations

The Science Across the World competition to mark the World Year of Physics 2005 was an overwhelming success, with nearly 2 000 entries—many of very high quality—from 34 countries, ranging from Algeria, Croatia, Iran, Mexico, Romania, Singapore, UK, to the USA. Winners were selected by members of the European Physical Society's Executive Committee at their General Meeting in Bern, Switzerland. Posters reprinted with permission. For more details see <[www.scienceacross.org](http://www.scienceacross.org)>.



*First prize poster in the age 8–12 category of SAW's poster competition. The artist is Nikita Herfet-Jones of the UK.*

# Nanotechnology

## Lessons from Mother Nature

by Alan Smith

*In an earlier article (Jan-Feb 2006 CI, p. 8), the author asked "Does Nanotechnology Have a Sporting Chance?" and reviewed briefly the hype surrounding the field. In this article, Smith illustrates how lessons from Mother Nature are resulting in the design of new nanotechnology applications. These applications, which relate to our everyday life, provide excellent examples that children and adults can relate to, and should be used to promote good science.*



Sunset over the Grenadines (Caribbean)—Palm Island. Photo credit: Alan Smith

**O**ver the last hundred years Nobel Prizes have been awarded in medicine, chemistry, and physics for work that would nowadays be described as nanotechnology. Nanotechnology is certainly not new; Mother Nature has been the best exponent since creation!

For those not familiar with the nanoscale, it is about as small as you can get, and down at that molecular or atomic level it has been found that properties of things can change. To help understand how small the nanoscale is, it would take 80 000 nanoparticles in a row to be just the diameter of a human hair, and if a gull landed on the deck of an aircraft carrier the ship would sink in the water by only one nanometre (a millionth of a millimetre).

Although scientists are developing exciting new products that make use of the new properties offered by nanotechnology, nature has been the leader in this science. Geckos hang upside down on the ceiling because of nanoscale "hairs" on each toe. Each "hair" grips with a miniscule force, but when there are millions of these "hairs" on each toe it is able to support its own weight when it is upside down. In fact, if it was 200 times its own weight it would still be able to hang there. Industry is looking at copying this ability by developing more-effective adhesives.

There is a beetle that lives in the scorching heat of the Namibian Desert that gets its water through

nanotechnology. Its back has a surface which repels water, but some bumps on its shell do not have this special surface. In the early mornings the water in the atmosphere condenses on those bumps and when the drop gets large enough it runs down the water repellent surface straight into the beetle's mouth. Such "hydrophobic" surfaces are now being used in textile applications; Hugo Boss sells suits that have self-clean surfaces based on nanotechnology coatings. Similar effects are being used by Gortex for wind and water-proofing. It is known as the lotus effect, since water just runs off lotus leaves.

Moths' eyes are antiglare and antireflective; if they were not then their predators would be able to pick them off much more easily. Scientists have copied the nanotechnology structure of those eyes and are able to produce antiglare and antireflective films, which could lead to digital camera screens that consumers can see on sunny days.

Many color effects in nature are the result of nanotechnology. The colors in butterfly wings or the pearl effects of shells are due to light being bounced off nanoscale layers in the structure of the wing or shell. Christian Dior has copied this effect with their Pure Poison perfume bottle, which looks like a pearl due to nano-layers on the inside of the bottle. Dior was not the first to produce nanotechnology color effects, the Romans left behind a glass cup known as Lycurgus' cup. Estimated to be 1600 years old, this piece in the British Museum looks jade green in natural light

but when a bright light shines through it, it becomes a spectacular red color. This is because of a minute amount of nanoparticles of gold and silver in the glass that reflect light in a novel way. The effect is similar to the reds and yellows one sees at sunsets, where the light bounces off nanoparticulates in the atmosphere. After Krakatoa exploded in 1883, there were incredible sunsets for decades, all due to nanoparticles.

Many sunscreen products use nanoparticles to bounce off the bad ultraviolet light and let through the good, tanning UV light. Each year, 1300 people in Australia die from skin cancer, so there should be some benefit from this nanotechnology.

Our own skeletons are self-assembling nanostructures. Again, scientists are copying such structures to make new materials that are stronger and lighter weight. These new nanocomposite materials are finding applications in many cars now, where replacement of heavy metal parts with these strong and lighter-weight materials, enables more miles per gallon. Ford, General Motors, BMW, and others are all reducing the weight of their car models. In addition, Mercedes has developed an antiscratch surface for its cars that is based on nanotechnology. Sporting goods manufacturers are also making use of nanotechnology structures to obtain different properties. Roger Federer's tennis racquet, Easton baseball bats, and Padraig Harrington's golf clubs are made from nanocomposite materials.

It is estimated that there are already over 700 "nano"-based products on the market. So, it is no wonder that governments worldwide are investing heavily in this technology. It has been said that if developed countries are not involved in nanotechnology, they will become third-world nations very quickly. The timescales for taking ideas through research to production are shorter now than they have ever been. Nanotechnology is particularly multidisciplinary and the speed at which products are being introduced exceeds most previous developments.

In addition to the energy saved by reducing the weight of cars, there are other applications that are beneficial to mankind. The UK company Oxonica has developed an additive based on cerium oxide nanoparticles that is added to diesel fuel at less than 5 parts per million. The ingredient helps catalyze the "burn" better; improving mileage by up to 15 percent and reducing polluting exhaust fumes.

At the nanoscale, it is possible to detect things faster and more sensitively; a sniffer dog can find a human after an earthquake or a trace of a drug in someone's luggage because it is working down at the molecular level. A great deal of research is being conducted to detect diseases using nanotechnology before they get a hold in the body. In this regard, the U.S. government is investing heavily in its Cancer Nanotechnology Plan. In terms of healthcare we are only seeing the tip of the iceberg.

Following the SARS outbreaks in the Far East, silver nanoparticles, which are commonly incorporated into wound dressings because of their antimicrobial properties, are now being used in other applications. Washing machines and refrigerators have been developed that use this technology to prevent mold. There are baby milk cartons, socks, and even underpants that use silver nanoparticles to reduce the possibility of infection.

The University of Leeds has a group of researchers using nanotechnology to develop nanofluids. By suspending nanoparticles in water or other liquids, these nanofluids can transfer heat up to 400 percent faster than other liquids. In a central heating system, nanofluids could increase efficiency without the need for a more powerful pump, thereby saving energy and providing major environmental benefits. Some researchers have theorized that nanofluids could be used during critical surgery to cool the brain so it requires less oxygen, thereby enhancing the patient's chance of survival and reducing the risk of brain damage. The technology could also be used to produce a higher temperature around tumors to kill cancerous cells without affecting nearby healthy cells.

I'll bet there is a creature somewhere that developed this technology long before the University of Leeds team applied it. We still have a lot to learn about nanotechnology from Mother Nature! 

*We still have a lot to learn about nanotechnology from Mother Nature!*

**Alan Smith <SmithAZT@aol.com> is an associate director of the UK government's Micro Nano Technology Network, which is coordinating activities in nanotechnology throughout the UK. He is a member of the IUPAC Bureau and a member of the Committee on Chemistry and Industry.**

# The IUPAC International Chemical Identifier: InChI—A New Standard for Molecular Informatics

by Alan McNaught

**T**he emergence of computerized information-handling systems has had an enormous impact on chemistry and chemists. The ease with which chemical information can be shuttled around the world is phenomenal. Nevertheless, we are only just beginning to exploit the huge potential of the computer for sharing and processing such information. A major stumbling block has been the lack of agreement on standard ways of structuring and encoding molecular information (i.e., chemical structures and properties). Progress in this area has been disappointingly slow. Although work towards a standard format for chemical structure files has been discussed extensively during the past decade, it has been inhibited by various technical and political factors. However, the widespread availability of the Internet and IUPAC's increasing interest in these problems have now helped create an environment where progress can be made.

There are many ways of specifying the identity of a chemical compound. Chemical identifiers can be information poor, carrying no information about molecular structure (e.g., a registry number), or information rich, allowing the structure to be deduced (e.g., a systematic name or a computerized representation of bonding). Naming systems are internationally agreed (through IUPAC), but hitherto there has been no successful attempt to establish an agreed unique computerized representation for any molecular structure. There are several file formats in common use offering various approaches to uniqueness, but these are proprietary, and generally geared to specific applications for their owners. Furthermore, as molecular structures of interest to researchers in chemistry become more and more complex, our ability to devise nomenclature systems giving compact and intelligible names is being severely challenged.

An IUPAC strategy meeting in March 2000 at the National Academy of Sciences in Washington, D.C., USA, brought together a broad spectrum of providers and users of chemical information to discuss future

requirements for nomenclature and other ways of designating chemical compounds. The need for a computerized equivalent of an IUPAC name (i.e., a standard chemical identifier) was recognized, and after some exploratory studies, including a September 2000 consultative meeting in Cambridge, UK, with representatives from a number of interested organizations, a project to develop such an identifier was launched early in 2001. The project is described in detail on the IUPAC website.<sup>1</sup>

The work on the Chemical Identifier was carried out under IUPAC auspices by Dmitrii Tchekhovskoi, Steve Stein, and Steve Heller at the US National Institute of Standards and Technology (NIST). Their approach is to express a chemical structure in terms of five layers of information (connectivity, tautomeric, isotopic, stereochemical, and electronic). In the final representation the unique connectivity layer is essential, but the user can choose which other layers to keep. The InChI algorithm converts input structural information into the identifier in a three-step process: normalization (to remove redundant information), canonicalization (to generate a unique set of atom labels), and serialization (to give a string of characters). The procedure generates a different Identifier for every compound, but always gives the same identifier for a particular compound regardless of how the structure is input. Of course, the procedure is equally applicable to both known and as yet unknown compounds.

A PC-based, executable version of an InChI test algorithm was released in March 2002. This version was developed to deal with well-defined, covalently-bonded organic molecules (both neutral and ionic). It was given to testers in a form that would accept structure input in a commonly used format, and deliver data as tagged text. No problems were reported, and the InChI was received enthusiastically when presented at the Chemical Abstracts Service/IUPAC Conference on Chemical Identifiers and XML for Chemistry, held in Columbus, Ohio, USA, in July 2002. A further version of the software, with applicability expanded to deal with inorganic, organometallic, and coordination compounds, was presented at a meeting with potential users at NIST in November 2003. The meeting was intended to obtain further comments on desirable output formats, and in light of the feedback, version 1 of the InChI software was released in April 2005. An updated version was released in August 2006 (see IUPAC Wire, p. 23), along with a validation protocol for software developers to check the validity of output from applications incorporating the InChI algorithm.

Figure 1 shows the InChI strings for two examples:

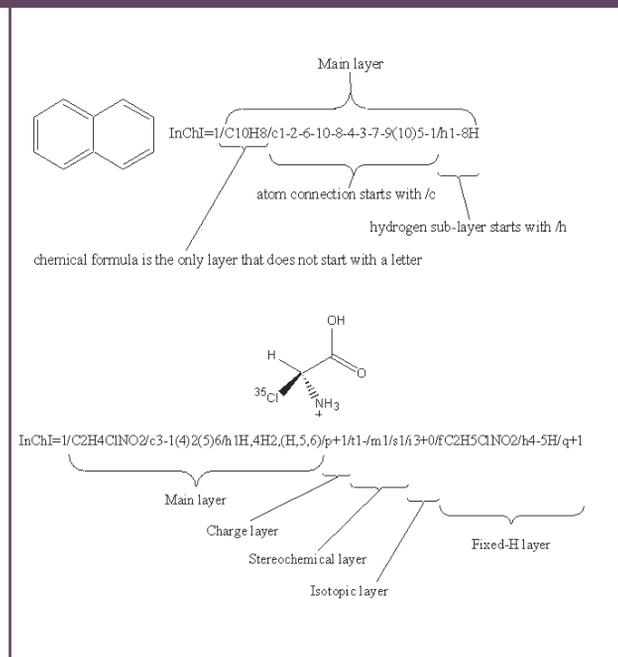


Figure 1. InChI strings for naphthalene and  $[^{35}\text{Cl}]$ chloro-L-glycinium.

the unsubstituted naphthalene molecule and the isotopically substituted cation  $[^{35}\text{Cl}]$ chloro-L-glycinium, with the component layers indicated. A full explanation of the way in which layers are specified is given in the *InChI Technical Manual* distributed with the InChI software and on the InChI website at the University of Cambridge (UK).<sup>2</sup> The manual is an invaluable source of answers to InChI-related questions. Figure 2 shows the software's InChI display window, containing the structure, canonical numbering, and identifier for cholesterol.

For the International Chemical Identifier to fulfill its potential, software developers need to incorporate it into their products. InChI files can already be generated easily by using the freely available structure-drawing program ChemSketch,<sup>3</sup> and the PubChem database of the US National Institutes of Health offers an online "InChI-generation-as-you-draw" facility.<sup>4</sup> The Identifier has also been included as an integral component of Chemical Markup Language.<sup>5</sup> The potential for using InChI in Internet searching is highlighted in a recent article,<sup>6</sup> and

other InChI-related articles are listed on the IUPAC website.<sup>7</sup> Anyone can easily obtain an InChI file at the desktop, or convert an InChI file back into a displayed structure.

The availability of this new standard will enable a wide variety of applications, such as:

- ordering chemicals from suppliers
- finding compounds in the chemical/patent/general literature via text-based search engines
- communication between databases
- merging data collections developed using different systems/protocols
- maintaining a laboratory chemical inventory or any broad-based local chemical collection
- passing the "identity" of a substance to a colleague for use in any of the above

Database providers have been among the first to recognize the enormous potential of InChI, and a list of these early adopters is provided on the IUPAC website.<sup>8</sup> As a result, millions of identifiers are available for searching on the web. At present, the largest collections are in the NIH/NCI database (~26 million), the NIH/PubChem database (~8 million), the Thomson/ISI database (~2 million), and the MDL/Elsevier database (>2 million). The freely accessible PubChem database of the US National Institutes of Health<sup>9</sup> also demonstrates the utility of InChI in structure searching, including both similarity and substructure searching<sup>10</sup>

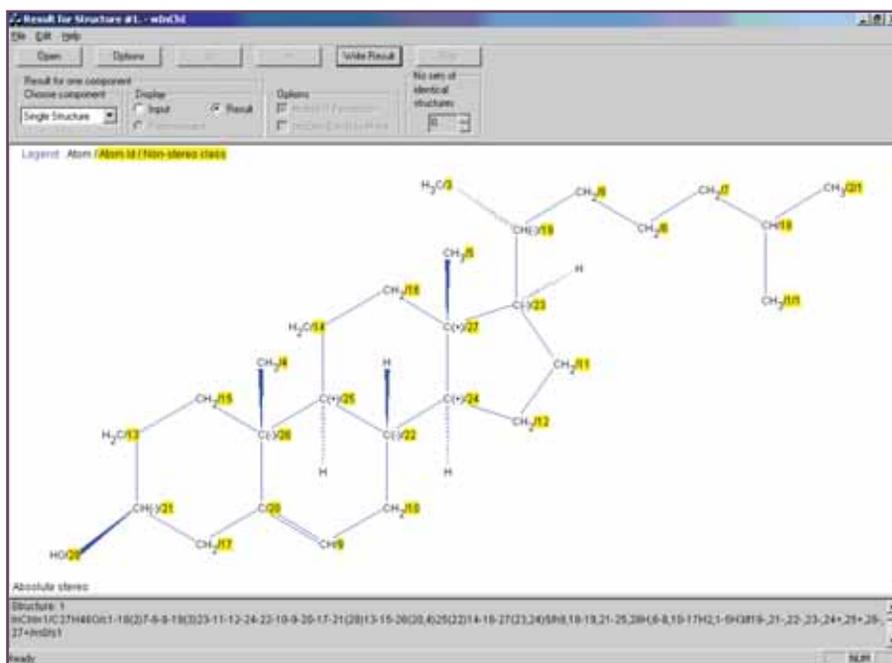


Figure 2. IUPAC International Chemical Identifier for cholesterol.

## Tools of the Trade

and a similar facility is provided by the National Cancer Institute's Chemical Structure Lookup Service, allowing the use of InChIs to search 78 databases containing a total of ~31 million entries.<sup>11</sup>

Publishers of all varieties of chemical information are recognizing the identifier as an essential way of "labelling" molecular data. We will all reap the benefits of a generally accepted convention for uniquely representing and communicating electronically the identity of any chemical substance.

### References

1. [www.iupac.org/projects/2000/2000-025-1-800.html](http://www.iupac.org/projects/2000/2000-025-1-800.html)
2. <http://wwwmm.ch.cam.ac.uk/inchifaq>
3. [www.acdlabs.com/products/chem\\_dsn\\_lab/chemsketch](http://www.acdlabs.com/products/chem_dsn_lab/chemsketch)
4. <http://pubchem.ncbi.nlm.nih.gov/edit>
5. [www.xml-cml.org](http://www.xml-cml.org)
6. "Enhancement of the Chemical Semantic Web through the Use of InChI Identifiers," Simon J Coles, Nick E Day, Peter Murray-Rust, Henry S Rzepa and Yong Zhang, *Org. Biomol. Chem.*, 2005, 3, 1832-1834. (doi: 10.1039/b502828k)
7. [www.iupac.org/inchi/articles.html](http://www.iupac.org/inchi/articles.html)
8. [www.iupac.org/inchi/adopters.html](http://www.iupac.org/inchi/adopters.html)
9. <http://pubchem.ncbi.nlm.nih.gov>
10. <http://pubchem.ncbi.nlm.nih.gov/search>
11. <http://cactus.nci.nih.gov/lookup>

Alan McNaught <[adm@rsc.org](mailto:adm@rsc.org)> has been involved with InChI since the beginning. He is past president of the IUPAC Division on Chemical Nomenclature and Structure Representation (Division VIII) and formerly was general manager, production, at the Royal Society of Chemistry in Cambridge, UK.

 [www.iupac.org/inchi](http://www.iupac.org/inchi)

## Using InChI

by Jeremy G. Frey

**T**he Southampton group has recently published several papers that make use of the IUPAC International Chemical Identifier (InChI). The InChI came along at a very convenient time for this group's research and became a key part of its e-Science Project<sup>1</sup> on computers to support the undertaking of chemical research<sup>2</sup> and new methodologies for dissemination of that research; bringing the Semantic Web or Web2.0 to the chemistry laboratory.

One of the major problems in chemistry is ensuring that chemical information is fully annotated to allow computers to facilitate the processing of this

information. This is especially difficult when chemistry researchers are confronted with data overload, an increasingly common issue. Because of rapid advances in high-throughput chemistry and analysis, traditional approaches to the dissemination of data, or even the wide range of chemical databases available now, can not keep pace with the rate at which new data is generated. Therefore, it is proving ever more difficult to assess the validity of the information.

The InChI provides an excellent way of calculating a unique computer-readable identifier from a structure file, admittedly it is not an identifier that a person would wish to employ, but we have IUPAC names for that. It is even possible to use the InChI in a Google search to locate articles pertaining to specific molecules.<sup>3</sup>

Increasingly, the value of depositing data along with publications is understood as a way to promote its subsequent re-use and the information, supporting the provenance and enabling re-analysis. Some of this material can be stored as supplementary data at a journal site, but this does not usually support a rich enough description to ensure that the data can be found and accessed in a digital form.<sup>4</sup> The InChI works well in providing a link to chemical information stored in a repository. At Southampton, we initially experimented with using data repositories for crystallography data,<sup>5</sup> but now we are using a greater range of experimental data within the Repositories for the Laboratory (R4L) project.<sup>6</sup> The ability to correlate information on the same molecular species via the InChI makes for a very powerful approach. The National Crystallography Service deposits structures in a local version of the ecrystals archive and routinely provides the InChI.<sup>7</sup>

We have been investigating ways in which to store semantically annotated chemical information, describing the data items as fully as possible. For example, describing that a molecule has a melting point, recorded by a given method, reported by specified people, measured with a given uncertainty, and all recorded in a computer readable form using RDF, which is an XML-like approach that fully incorporates the ideas of unique identifiers to link together related information.<sup>8,9</sup> This approach enables us to automatically link items recorded in the electronic laboratory notebook to properties information about this entity. A similar underlying technology is used to record the information on both processes and properties.<sup>10</sup> This rich labelling is carried forward to model building, undertaken using the annotated data. One use of this approach is to track the impact of information subse-

## Using InChI

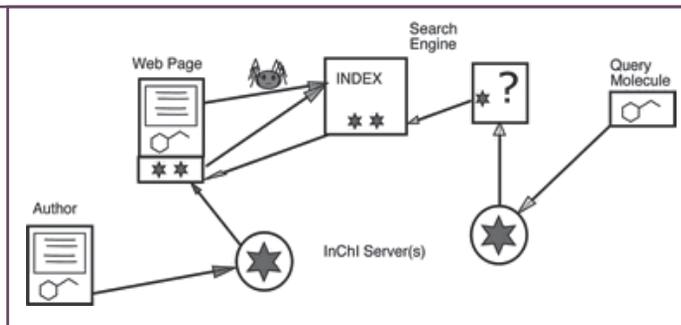
quently discovered to be inaccurate.

We have also found the InChI useful in more local contexts. The e-Malaria project<sup>11</sup> is a system we have developed to teach chemical concepts to 16-18 year-old students by allowing them to use drug-design software running on a cycle steeling computational grid. They sketch a molecule, which is then converted into 3D so they can test its suitability as an anti-malarial drug by looking up its docking score with Gold software.<sup>12</sup> One of the aspects that interests the students is to know if someone else has run their molecule before. We can simply compare the InChI of the new molecule with all the ones stored in the database. Interesting issues concerning different stereoisomers can then arise as the molecular mechanics and quantum calculations that turn a 2D sketch into a 3D molecule do not always lead to the same 3D stereochemistry. As the InChI is a structured URI, a more complex comparison between two InChIs can be made by determining to what degrees they may match.

The InChI may still have a few problems. One which has caused some concern is that it is defined by the InChI program rather than an explicit algorithm. However, this program is widely available and the InChI has proved extremely valuable in enabling the linking up of annotated chemical data, providing a very good example of the "network effect," and potentially increasing the usefulness of any single data item added to the web.

### References

1. [www.rcuk.ac.uk/escience](http://www.rcuk.ac.uk/escience)
2. [www.combechem.org](http://www.combechem.org)
3. Coles, S.J., Day, N.E., Murray-Rust, P., Rzepa, H.S. and Zhang, Y. (2005) "Enhancement of the Chemical Semantic Web through the Use of InChI Identifiers." *Org. Biomol. Chem.* 3(10), 1832-1834. (doi:10.1039/b502828k)
4. Rousay, E.R., Fu, H., Robinson, J.M., Essex, J.W. and Frey, J.G. (2005) "Grid-Based Dynamic Electronic Publication: A Case Study Using Combined Experiment and Simulation Studies of Crown Ethers at the Air/Water Interface." *Philosophical Transactions of the Royal Society A: Mathematical Physical and Engineering Sciences* 363, (1833), 2075-2095. (doi:10.1098/rsta.2005.1630)
5. <http://ecrystals.chem.soton.ac.uk>
6. <http://r41.eprints.org/about.html>
7. Coles, S.J., Frey, J.G., Hursthouse, M.B., Light, M.E., Milsted, A.J., Carr, L.A., De Roure, D., Gutteridge, C.J., Mills, H.R.,



**Molecules, as defined by connectivity specified via InChI, are precisely indexed by major web search engines so that Internet tools can be transparently used for unique structure searches.**

Reprinted from reference 3, by permission of the Royal Society of Chemistry.

- Meacham, K.E., Surridge, M., Lyon, E., Heery, R., Duke, M. and Day, M. (2006) "An E-Science Environment for Service Crystallographys from Submission to Dissemination." *J. Chem. Inf. Model.* 46(3), 1006-1016 (doi:10.1021/ci050362w); Coles, S., Frey, J.G., Hursthouse, M.B., Light, M.E., Meacham, K.E., Marvin, D.J. and Surridge, M. (2005) "ECSES—Examining Crystal Structures Using 'e-science': A Demonstrator Employing Web and Grid Services to Enhance User Participation in Crystallographic Experiments." *J. Appl. Cryst.* 38(5), 819-826 (doi:10.1107/S0021889805025197)
8. Taylor, K.R., Gledhill, R., Essex, J.W., Harris, S.W., De Roure, D.C. and Frey, J.G. (2006) "Bringing Chemical Data Onto the Semantic Web." *J. Chem. Inf. Model.* 46(3), 939-952. (doi:10.1021/ci050378m)
9. Taylor, K., Essex, J.W., Frey, J.G., Mills, H.R., Hughes, G. and Zaluska, E.J. (2006) "The Semantic Grid and Chemistry: Experiences with CombeChem." *Web Semantics* 4(2), 84-101. (doi:10.1016/j.websem.2006.03.003)
10. Hughes, G., Mills, H., De roure, D., Frey, J.G., Moreau, L., Schraefel, M.C., Smith, G. and Zaluska, E. (2004) "The Semantic Smart Laboratory: A System for Supporting the Chemical eScientist." *Org. Biomol. Chem.* 2(22), 3284-3293. (doi:10.1039/B410075A)
11. Gledhill, R., Kent, S., Hudson, B., Richards, W.G., Essex, J.W. and Frey, J.G. (2006) "A computer-Aided Drug Discovery System for Chemistry Teaching." *J. Chem. Inf. Model.* 46(3), 960-970. (doi:10.1021/ci050383q)
12. The Gold software was provided by Cambridge Crystallographic Data Centre (CCDC) for use with this teaching project.

Jeremy G. Frey <[j.g.frey@soton.ac.uk](mailto:j.g.frey@soton.ac.uk)> is a professor at the School of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK. He is a member of the IUPAC Physical and Biophysical Chemistry Division and is chairman of the Commission on Physicochemical Symbols, Terminology, and Units.

## The Canadian National Committee for IUPAC's Travel Awards Program—A Success Story

by Chris. I. Ratcliffe

The Canadian National Committee for IUPAC (CNC-IUPAC) runs a highly successful program of Travel Awards to enable top young Canadian scientists to attend and present their research at IUPAC-sponsored scientific conferences taking place outside of Canada and the USA.

The Travel Awards scheme has been operating for nearly 25 years and is made possible by funding from the Canadian Society for Chemistry's Gendron Fund and by CNC-IUPAC's Company Associates. The Gendron Fund had its origin in a highly successful IUPAC Congress held in Vancouver, Canada, in 1981. Surplus money generated from this Congress was put into a trust fund set up in June 1982 and administered by the Chemical Institute of Canada (CIC). The trust was named after Pierre Gendron, a prominent Canadian chemist.

Each year a competition is held for Travel Awards for the following year. Candidates who have obtained their Ph.D. within the last 10 years submit an application, which must include evidence of an independent research program, a publication record of high quality, and the ability to attract research funding, and indicate which IUPAC-sponsored conference they wish to attend. Preference is given to applicants who have not previously won an award. Applications are reviewed by a committee, whose members cover a broad range of expertise in chemistry, which then makes recommendations to CNC-IUPAC. Currently each award covers expenses up to a maximum of

### The 2006 Award Winners

**Garry Hanan**—associate professor at the Université de Montréal—went to the 37th International Conference of Coordination Chemistry in Cape Town, South Africa, in August 2006.

**Matthew Moffitt**—assistant professor at the University of Victoria—attended the World Polymer Congress: Macro 2006, in Rio de Janeiro, Brazil, in July 2006.

**Joelle Pelletier**—associate professor at the Université de Montréal—traveled to Dresden, Germany, to attend the First International IUPAC Conference on Green-Sustainable Chemistry, held in September 2006.

**Alison Thompson**—associate professor at Dalhousie University in Halifax—attended the 16th International Conference on Organic Synthesis (ICOS 16), 11-15 June 2006, Merida, Yucatan, Mexico.



[www.cnc-iupac.org/awards06\\_e.html](http://www.cnc-iupac.org/awards06_e.html)

CAN\$ 2 000. Normally, four or five awards are made per year. However, in 2003, in order to encourage the participation of young scientists at the IUPAC Congress in Ottawa, smaller awards were made to 10 individuals.

This is a nationwide competition and the awards are regarded as quite prestigious for young career chemists within the Canadian scientific community. The award winners are given considerable exposure, with short biographies published on the website of CNC-IUPAC and in the CIC magazine *Canadian Chemical News*. The Travel Awards program also increases awareness of IUPAC and CNC-IUPAC among young scientists and encourages their participation in IUPAC affairs. Winners who use their awards to attend an IUPAC Congress are also invited to become Young Observers at the IUPAC General Assembly that is held concurrently. Some Travel Award winners have gone on to play active roles within IUPAC or CNC-IUPAC. The incoming and outgoing chairpersons of CNC-IUPAC, Neil Burford (Dalhousie University) and Linda Johnston (National Research Council) respectively, were both recipients of Travel Awards early in their careers, as were other members of the committee.

CNC-IUPAC's Company Associates are also strongly linked to the Travel Awards scheme, as a large proportion (almost 90 percent) of their annual fees go directly to support this award. The awards give



exposure to our Company Associates (i.e., Boehringer Ingelheim (Canada) Inc., Merck Frosst Canada Inc., and Bruker Biospin Ltd.) who see this as a good way of helping the scientific community. They benefit from exposure in Canada, from announcements about the awards, and worldwide, through acknowledgements during presentations by the award recipients at IUPAC-sponsored conferences. Indeed, the Travel Awards program is a tangible incentive to become a Company Associate.

In addition to the benefits for awardees and Company Associates, the Travel Awards program also helps to spread awareness of the activities of CNC-IUPAC and IUPAC within Canada.

The Travel Awards program received a significant and welcome boost this year when the Pestcon Graduate Scholarship Fund, which was administered by CIC since 1986, was closed and folded into the

Gendron Fund. This could allow CNC-IUPAC to sponsor one more Travel Award each year in future competitions.

It appears that while most member countries of IUPAC have national committees that handle liaison with IUPAC, the Canadian National Committee for IUPAC is unique in promoting a travel awards scheme. All the parties involved benefit from CNC-IUPAC's Travel Awards program, including the award winners, the Company Associates, CNC-IUPAC, and IUPAC. Might this kind of program be worth trying in other countries?

**Chris. I. Ratcliffe** <Chris.Ratcliffe@nrc-cnrc.gc.ca> is CNC-IUPAC secretary. He is at the Steacie Institute for Molecular Sciences of the National Research Council in Canada

 [www.cnc-iupac.org](http://www.cnc-iupac.org)

## Emerging Issues in Developing Countries

*This series seeks to inform readers, explore new ideas, and promote discussion on themes related to developing countries and emerging analytical communities. Articles in this series are available from <[www.iupac.org/publications/ci/indexes/emerging-issues.html](http://www.iupac.org/publications/ci/indexes/emerging-issues.html)>.*

### Standardization of Analytical Approaches and Analytical Capacity-Building in Africa

*by Robert Maybury, Walter Benson, and David Moore*

The 2003 World Bank book entitled *Standards and Global Trade: A Voice for Africa* (edited by John S. Wilson and Victor O. Abiola; ISBN 0-8213-5473-6) reports that trade can be a powerful driver of a country's growth, but in many African countries there are severe barriers to exporting commodities. One such barrier is the poor performance of many African laboratories when testing commodities for export. For a commodity to be exported, its levels of pesticide, heavy metal residue, and other contaminants must be determined through analytical tests. The results of



The IOCD team's visit to the Uganda National Bureau of Standards (UNBS) in October 2005. Team members (rear, from left) Walter Benson, Albert Pohland, and Geoffrey Kamau, shown with (front left) Anthonia Nakamya (head of the National Drug Authority Quality Control Laboratory in the Uganda National Drug Authority) and Hope Kamusiime (head of the Chemistry Section at UNBS).

this testing must not only comply with various international standards, but the accuracy and reliability of the results must also be accepted internationally. Yet, few testing laboratories in Africa are able to obtain such trustworthy test results.

A project of the International Organization for Chemical Sciences in Development (IOCD)\*—in col-

\* See May-June 2002 CI or <[www.iocd.org](http://www.iocd.org)>. For the project announcement, see Mar-Apr 2005 CI or <[www.iupac.org/projects/2004/2004-017-1-500.html](http://www.iupac.org/projects/2004/2004-017-1-500.html)>.

## Up for Discussion

laboration with IUPAC and several other international partners—is assisting analytical laboratories in Africa, initially in Uganda and Kenya, with upgrading their performance in testing export commodities.



*The IOCD team during a visit to the Chemistry Department of Makerere University: (from left) Hope Kamusiime, Patrick Wilson, Geoffrey Kamau, Al Pohland, and B.T. Kiremire, professor of chemistry.*

The project work plan has three phases:

### **Phase I: Gathering local information relevant to the export of commodities**

In this phase, local personnel first determine which export commodities require analytical testing. Then they must determine which local laboratories can perform the testing.

### **Phase II. Diagnosis of a laboratory's problems and inadequacies**

In this phase, IOCD scientists visit the African country and hold discussions with the manager and scientists of each laboratory to diagnose the particular problems and inadequacies that hinder the reliability and accuracy of the lab's analytical tests. IOCD and the laboratory personnel then agree on appropriate remedial measures and schedule their implementation.

### **Phase III: Delivery of appropriate remedial measures to build analytical capacity**

During the third phase, IOCD collaborates with IUPAC and other partners to implement remedial measures.

The remedial measures involve human capacity building and laboratory upgrading. Capacity building

efforts include fellowships awarded to African scientists or managers to work and learn at laboratories in developed countries, visits by foreign consultants to African laboratories, and workshops organized at African laboratories on relevant analytical chemistry topics. Laboratory improvement efforts include customizing international analytical methods to the needs of African laboratories, organizing a laboratory's participation in a proficiency testing exercise with an accredited laboratory, and acquiring better equipment.

### **Review of the Project's Implementation to Date**

IOCD received modest initial funding for the project, including a grant of USD 25 000 from the US National Academy of Sciences and USD 10 000 from IUPAC. With these funds, IOCD initiated work in phases I and II.

IOCD initiated this project in early 2003 after consulting with a World Bank trade development officer who helped IOCD contact trade-development offices and government authorities in Uganda and Kenya. In early 2004, IOCD received approval of a project proposal it had submitted to the Uganda Ministry of Tourism, Trade, and Industry (MTTI).

After some early difficulties, the project began in earnest in October 2005, when a team of IOCD scientists spent one week visiting eight Ugandan laboratories suggested by the director of the Uganda National Bureau of Standards. Team leader Walter Benson, chairman of the IOCD Working Group on Analytical Chemistry and associate member of the IUPAC Chemistry and the Environment Division was accompanied on the visit by Patrick Wilson (U.S. Food and Drug Administration, Office of International Affairs), Albert Pohland (FDA retired, and AOAC International, USA), and Geoffrey Kamau (University of Nairobi, Kenya).

### **Summary of the IOCD Team's Visit to Uganda**

During its visit, the IOCD team determined the following:

- The two private laboratories test exports and are operated competently using official methods. The few problems they had were addressed on the spot.
- Three laboratories do not analyze products for export.
- The remaining three of the eight laboratories, have the potential to undertake export testing after improving their quality assurance, or good

## Emerging Issues in Developing Countries

laboratory practice: the Uganda National Bureau of Standards (UNBS), the **Government Chemist Laboratory**, and the **Uganda Industrial Research Institute**.

The **UNBS** laboratory has space and a well-trained chemistry laboratory director, but lacks all of the following: space for expansion, additional trained personnel, modern equipment, and a complete quality assurance system. The UNBS lab is performing a few basic tests, but it does not have a means to repair its equipment rapidly and inexpensively. The laboratory for testing microbiological contamination of samples is certified and has a good reputation, but it was closed for repairs while we were visiting.

The **Government Chemist Laboratory** has spacious grounds and facilities, trained chemists, functioning equipment, adequate office space, adequate funding, an advanced pesticide laboratory, and plans to expand. It mainly performs analyses on local samples from the police and local clients. It has a good grasp of the regulatory requirements and use of official methods. In our judgment, it has potential to expand into analyzing products for export.

The **Uganda Industrial Research Institute** (UIRI) is a parastatal, government laboratory that could perform export testing. Its laboratories are large and stocked mainly with analytical equipment in need of repair; they lack staff and funds. We saw little evidence of quality assurance. The Chinese government sent a scientist to UIRI for four years, together with laboratory equipment. A modern nitrogen analytical system for proteins appeared to function correctly. UIRI seems to have little contact with Ugandan industry, but performs some analyses for UNBS.

### Conclusions

- All the laboratories have problems with repairing their equipment and ordering chemicals in a timely manner.
- Competition between government laboratories and between industry and government became evident during our visit. This may keep them from cooperating with each other.
- Universities must offer courses and carry out research so that they train chemists in areas needed by government and industry.



*Ugandan National Drug Authority laboratory.*

The task group believes that IUPAC scientists who would visit Uganda during phase III could have a major impact by offering training in quality assurance, quality control, good laboratory/manufacturing practice, and accreditation to Uganda's industrial, government, and university chemists and microbiologists.

IOCD is waiting for a request from the Ugandan government to start the next phase of the project. Work in Kenya will commence once work in Uganda has been completed.

IOCD has learned an important lesson in carrying out a project that seeks to assist government-operated laboratories in a developing country. As a private nongovernmental organization, we must be mindful of our status as a body outside the government domain. Hence, we must recognize that a government agency is an instrument for carrying out a particular mission, which has been set by legislation or executive order. Those individuals charged with implementing this mission are expected to respect hierarchical lines of authority and we must respect this ordering of responsibility when we interact with them.

Robert Maybury <[iocd@igc.org](mailto:iocd@igc.org)> is IOCD executive director, Walter Benson <[wbenson270@aol.com](mailto:wbenson270@aol.com)> is task group chairman for the joint IOCD/IUPAC project, and David Moore <[moored@lanl.gov](mailto:moored@lanl.gov)> is former president of the IUPAC Analytical Chemistry Division and also a task group member on this project.

 [www.iupac.org/projects/2004/2004-017-1-500.html](http://www.iupac.org/projects/2004/2004-017-1-500.html)

## Young Chemists to the 41st IUPAC World Chemistry Congress

The 41st IUPAC Congress will be held 5–11 August 2007 at the Lingotto Conference Centre in Torino, Italy. The theme of the Congress is “Chemistry—Protecting Health, Natural Environment, and Cultural Heritage.” It will include the following sessions: Chemistry Protecting Natural Environment, Chemistry Protecting Health, Chemistry Protecting Cultural Heritage, Materials Chemistry and Nanotechnologies, Theoretical Chemistry and Computer Chemistry, Inorganic Chemistry, Analytical Chemistry, Organic Chemistry, Biological and Biophysical Chemistry, and Advances in Chemical Education.



To encourage young chemists to participate in this unique congress, the organizers have established two different programs, both offering travel assistance. The first program is especially targeted to young scientists from developing and economically disadvantaged countries; the second is open to chemists from any country.

About 50 awards will be given to qualified candidates as a contribution toward their registration fees and

travel costs.

Applications from candidates under age 40 are welcomed. Scientists from academia, government, or industry may submit applications directly to the address below. Award winners will be expected to submit an abstract of a poster or paper to be presented at the Congress. These abstracts will be subject to adjudication as will all other submissions for presentation at the meeting.

There is no specific application form, but applicants are required to provide:

- a letter of application
- a brief curriculum vitae
- a confirmation of their current status and affiliation
- a publication list
- a letter of support from the appropriate department head, dean, or laboratory supervisor

Estimates of the economy airfare to and from the Congress should also be provided.

The deadline for receipt of applications is **31 January 2007**. Applications should be sent to:

Prof. Roberto Gobetto  
Dept. of IFM Chemistry  
Via P. Giuria 7, 10125 Torino (Italy)  
E-mail <[iupac-2007.youngchemists@unito.it](mailto:iupac-2007.youngchemists@unito.it)>

 [www.iupac.org/news/archives/2006/41stCongress-yc.html](http://www.iupac.org/news/archives/2006/41stCongress-yc.html)

### Observers at the IUPAC General Assembly

In sync with this program, and to also facilitate the participation of young scientists at the concurrent **IUPAC General Assembly**, IUPAC and some NAOs offer additional travel support. The Young Observer programs provide an excellent opportunity for young scientists to establish international collaborations, gain knowledge of global research activities, and participate in IUPAC activities.

For more details about these programs, including application procedures, age limits, criteria for selection, and timelines/deadlines, please inquire with one of the following individuals, depending on your current location:

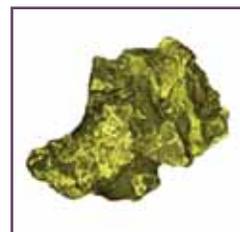
- In the USA, contact Katherine Bowman at the National Research Council <[iupac-us@nas.edu](mailto:iupac-us@nas.edu)> (deadline is 15 January 2007).
- In the UK, contact Stanley Langer at the Royal Society of Chemistry <[langers@rsc.org](mailto:langers@rsc.org)> (deadline is 15 January 2007).

For all other countries represented in IUPAC by a National Adhering Organization, invitations will follow the awards made to Young Chemists by the Congress itself. Those interested should therefore apply first to the Congress program by 31 January 2007.

 [www.iupac.org/general/Young-Observer](http://www.iupac.org/general/Young-Observer)

### The XML Gold Book Online

The IUPAC Gold Book—the *Compendium of Chemical Terminology*—is now available in an all-new format, making this key resource computer and Net friendly. The new version takes full advantage of new technologies based on eXtensible Markup Language (XML) and provides efficient ways of browsing, searching, and simply using this reference. The XML *Gold Book* is a milestone in chemical referencing.



Turn to page 28 for a more detailed presentation of the new format and feature, or to simply see for yourself, go to <<http://goldbook.iupac.org>>.

## IUPAC Elections for the 2008–2009 Term

Every two years, IUPAC holds an election for its officers and committee members. About 120 individuals are to be elected or reelected either as Titular Members, Associate Members, or National Representatives. Information concerning the voting process and the role of each kind of member is contained in the Union bylaws.

Any qualified individual who is interested in being nominated is invited to contact his/her National Adhering Organization (NAO) and/or the current committee officers. The next election will cover a two- or four-year term that will start in 2008. The following division committees and standing committees will all have vacancies: Physical and Biophysical Chemistry, Inorganic Chemistry, Organic and Biomolecular Chemistry, Polymer, Analytical Chemistry, Chemistry and the Environment, Chemistry and Human Health, Chemical Nomenclature and Structure Representation, CHEMRAWN, Chemistry and Industry, Chemistry Education, Interdivisional Committee on Terminology, Nomenclature and Symbols, and Committee on Printed and Electronic Publications.

As part of the nomination procedure, NAOs are invited to submit curriculum vitae for each nominee to the IUPAC Secretariat no later than 1 December 2006. Elections for each division committee will then take place during the first half of 2007. The 2008–2009 memberships for all committees will be finalized during the next General Assembly in August 2007.

Individuals interested in becoming officers on the IUPAC Bureau should contact his/her NAO. Nominations for officers have a different timeline and can only be made by an NAO. Elections will take place at the Council Meeting during the next General Assembly.

Contact information for all NAOs and division and standing committee officers is available on the IUPAC website, or upon request at the IUPAC Secretariat (e-mail <secretariat@iupac.org>; tel.: +1 919 485 8700; fax +1 919 485 8706).

 [www.iupac.org/news/archives/2006/elections.html](http://www.iupac.org/news/archives/2006/elections.html)

## Industry and IUPAC Meeting Halfway



A world chemistry leadership meeting has been proposed to bring together senior academic and industrial figures to discuss the changing regulatory environment for chemistry in the world. The meeting, which would take place during the 41st IUPAC World Chemistry Congress in Torino in August 2007, was suggested during discussions at the IUPAC Committee on Chemistry and Industry (COCI), held in Chicago, Illinois, USA, from 20–21 July 2006.

IUPAC has an obvious interest in the development of the chemical sciences and the regulatory environment in which they are deployed by industry. The purpose of the meeting would be to identify IUPAC-sponsored or supported research projects that would benefit both science and industry. IUPAC has previously organized such large projects, including a study on endocrine disrupting chemicals that helped move the science forward significantly and provided new perspectives. This project will aim to share views on health and environment issues facing both science and industry in the context of the Strategic Approach to International Chemicals Management (SAICM),<sup>1</sup> Registration, Authorization, and Evaluation of Chemicals (REACH),<sup>2</sup> and industry responses through the Global Product Strategy and Responsible Care initiatives. In particular, it may be very useful to develop aligned or joint perspectives on the safety and use (both intentional and unintentional) of chemicals.

Another important area of focus could be bio-monitoring, where IUPAC is concerned that the results from analytical science are correctly presented and interpreted, and that international standards for the use of biomonitoring techniques are established. The establishment of such international frameworks would be very useful in ensuring that biomonitoring can be a bona fide tool for the risk assessment of chemicals in the body.

For more information contact the IUPAC secretariat <secretariat@iupac.org> or COCI officers—visit <[www.iupac.org/standing/coci.html](http://www.iupac.org/standing/coci.html)>.

<sup>1</sup> [www.chem.unep.ch/saicm](http://www.chem.unep.ch/saicm)

<sup>2</sup> [http://ec.europa.eu/environment/chemicals/reach/reach\\_intro.htm](http://ec.europa.eu/environment/chemicals/reach/reach_intro.htm)

### IUPAC President Attends the International Chemistry Olympiad

In early July, Bryan Henry became the first IUPAC president to participate in the International Chemistry Olympiad (ICHO) held 2–11 July 2006 in Gyeongsan, South Korea. Henry presented IUPAC Gold Books to the gold medalists at the closing ceremonies and delivered a brief talk and general overview of IUPAC at a farewell dinner that evening.

Organizers of the 38th IChO awarded a total of 28 gold, 56 silver, and 81 bronze medals in Gyeongsan, which is south of Seoul. More than 250 students from 68 countries competed in theoretical and practical exams that each lasted five hours.

All four members of China's team won gold medals. Taiwan, the Russian Federation, and the host country each won three gold medals and one silver medal. Poland ranked fifth, earning two golds, one silver, and one bronze. Cheng-Yi Kao of Taiwan won an individual award for performance on the practical test, while Lichao Cai of China received recognition for excellence on the theoretical component. Hande Boyaci from Turkey earned the award for Best Female Student. Students also participated in several cultural tours and activities in South Korea.

Henry's visit, from 5–11 July, was arranged by the IChO-2006 Organizing Committee and Duckwan Lee in particular. Kook Joe Shin, a past president of the Korean Chemical Society, (KCS) served as Henry's host during his entire stay and organized his itinerary.

The first three days of his visit took place in Seoul, where he had the opportunity to meet many members of the Korean chemical community. On 6 July he met with Eun Lee, the current president of the Korean Chemical Society, and Young Bok Chae, president of the Korean Federation of Science and Technology



A medalist is awarded at the closing ceremonies of the 38th International Chemistry Olympiad.

Societies. That evening he attended a dinner with Korean chemists who are associated with IUPAC in various roles. Korea is very active within IUPAC with 43 Fellows, 10 individuals who are either chairs or members of task groups, 20 subcommittee members, 4 national representatives, and 7 titular members. Notable among this group is Jung-il Jin who is a member of the Bureau and president of the Polymer Division.

On 8 July, Henry traveled to Gyeongsan, in the southeastern region of South Korea, where he had a traditional Korean dinner with several member of the IChO Organizing Committee, including Daewoon Lee, the committee chair. Over dinner, Henry learned about the history of the Chemistry Olympiad movement and its impressive growth.

According to Henry, 10 July was the highlight of the trip. It began with a visit to Yeungnam University, in Gyeongsan, which was the venue for IChO. After visiting the Department of Chemistry and meeting with the University President, he was treated to a guided tour of the fascinating university museum with its anthropological focus on the indigenous culture. Next, he met with Jin Soon Cha, the next president of the KCS. He ended the day at the Olympiad. "The closing ceremonies were nothing short of incredible," said Henry.

The International Chemistry Olympiad was detailed in the July-Aug 2005 *CI* <[www.iupac.org/publications/ci/2005/2704/1\\_apotheker.html](http://www.iupac.org/publications/ci/2005/2704/1_apotheker.html)>. The next Chemistry Olympiad will be held in Russia at Moscow State University in July 2007 under the theme "Chemistry: Art, Science, and Fun." The official website of the 39th IChO is <[www.icho39.chem.msu.ru](http://www.icho39.chem.msu.ru)>.



From left: Eun Lee (president of the Korean Chemical Society), Bryan Henry (IUPAC president), and Kook Joe Shin (KCS past president).

For more details about the 2006 event, see <<http://icho2006.kcsnet.or.kr>>.

## InChI 1.01

The IUPAC International Chemical Identifier, InChI version 1, was released in August 2006. The whole package, available at [www.iupac.org/inchi](http://www.iupac.org/inchi), includes:

- InChI version 1 software version 1.01 documentation, and Windows and Linux (i386) executable programs
- InChI version 1.01 source code and Application Program Interface (API)
- InChI validation protocol
- What's new in InChI software version 1.01

This release includes the following new features:

- InChI validation protocol to establish whether software that includes the InChI algorithm produces valid InChI
- InChI reversal: InChI to structure conversion (connection table, bond orders, charges, stereochemical parities; the resultant structures have no coordinates; success rate on average is 99.7 percent)
- Several bug fixes that eliminate known InChI failures
- Several minor additional features

For more detail, see the *Whats\_New.pdf* included in the package.

We express our gratitude to those who discovered and helped fix various problems with the software and validation protocol.

**Q&A—Q:** Why is the InChI version in this package 1, not 1.01?—**A:** The version of the chemical identifier (as a string of characters derived from a chemical structure) is the same, only the software and documentation were updated. Therefore, the InChI version is still version 1.



See Tools of the Trade on page 12 for more information on InChI.

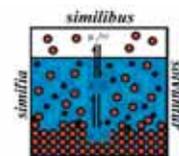
 [www.iupac.org/projects/2004/2004-039-1-800.html](http://www.iupac.org/projects/2004/2004-039-1-800.html)

## Dewen Zeng Receives the 2006 Franzosini Award

At the 5th Annual Meeting of the IUPAC Subcommittee on Solubility and Equilibrium Data, the Franzosini Award was presented to Dewen Zeng in appreciation of his scientific contributions to the Solubility Data Project.

Zeng received his Ph.D. in 2003 at TU Bergakademie Freiberg, Germany. During his Ph.D. project he worked under the supervision of Wolfgang Voigt (Institute of Inorganic Chemistry) on the thermodynamic modelling of salt-water systems. Zeng is a very active scientist who became an expert in thermodynamics and phase diagrams. After one year as a post-doc he returned to China and continued to work on modelling and evaluating solubilities and vapor pressures of salt-water systems.

At the 12th International Symposium on Solubility Phenomena, held in Freiberg, Germany, 24–28 July 2006, Zeng presented research conducted with Hongyan Zhou and Wolfgang Voigt on “Thermodynamic Consistency of Solubility and Vapour Pressure of a Binary Saturated Salt-Water System: II.  $\text{CaCl}_2 + \text{H}_2\text{O}$ .” See page 31 for a report on the symposium.



Dewen Zeng would like to contribute with his scientific experience to the activities of the solubility data group, particularly in respect to the oceanic salt project. Since Zeng is a native Chinese writer and speaker, he can provide access to Chinese literature on solubility phenomena, which is becoming more and more important to the solubility data group.

Zeng is a professor in the College of Chemistry and Chemical Engineering at Hunan University, Changsha, China.

 For more info about the Franzosini Award, its origin, and previous awardees, see [www.iupac.org/divisions/V/502/Franzosini-Award.html](http://www.iupac.org/divisions/V/502/Franzosini-Award.html).

## Biophysico-Chemical Processes Involving Natural Nonliving Organic Matter in Environmental Systems

Little is known about the fundamentals of physico-chemical and biological interfacial reactions and their impact on nonliving natural organic matter (NOM) in nature. To advance the frontiers of knowledge on the subject matter would require a concerted effort of scientists in relevant physical and life sciences such as chemistry, mineralogy, geochemistry, microbiology, ecology, and soil, atmospheric, and aquatic sciences. Environmental science is indeed the fusion of physical and life sciences. Scientific progress in advancing the understanding of NOM in the environment is based ultimately on unification rather than fragmentation of knowledge.

The overall goal of this project is to provide the scientific and professional communities with an up-to-date and critical evaluation by world-leading scientists of the biophysico-chemical processes of NOM in various environmental compartments. The specific objectives are to address (1) the fundamentals and the impact of mineral-organic matter-biota interactions on the formation, nature and properties, transformation, turnover, and storage of NOM in various environmental systems, and (2) state-of-the-art analytical methods for investigating the biophysico-chemical processes involving NOM in nature.

### New IUPAC-Sponsored Wiley Book Series Biophysico-Chemical Processes in Environmental Systems

Series Editors: P.M. Huang and N. Senesi

The IUPAC Chemistry and the Environment Division recently approved the creation of an IUPAC-sponsored book series entitled Biophysico-Chemical Processes in Environmental Systems, which will be published by John Wiley & Sons, Hoboken, NJ. This series addresses the fundamentals of physical-chemical-biological interfacial interactions in the environment and the impacts on: (1) the transformation, transport, and fate of essential nutrients, inorganic and organic pollutants and pathogens, (2) food chain contamination and food quality and safety, and (3) ecosystem health including human health. With rapid developments in environmental physics, chemistry and biology, it is becoming much harder, if not impossible, for scientists to follow new developments outside their immediate area of research by reading the primary research literature. This book series will present a distilled and integrated version of new developments in biophysico-chemical processes in environmental systems.

Volume 1: Biophysico-Chemical Processes of Metals and Metalloids in Soil Environments (for details, see [www.iupac.org/projects/2004/2004-003-3-600.html](http://www.iupac.org/projects/2004/2004-003-3-600.html))

The outcomes of this project will be published as volume II of a recently approved book series to be published by Wiley (see box). The book will also identify gaps in knowledge on the subject matter, thereby providing future directions for research on biophysico-chemical interfacial reactions in natural habitats. This in turn may lead to the subsequent development of innovative management strategies to sustain environmental quality and ecosystem health on a global scale.

In contrast to classical books, which largely focus on separate physicochemical and biological aspects, this book aims to integrate the frontiers of knowledge on NOM in soil, sediment, water, and air.

The book will be co-edited by N. Senesi, B. Xing, and P.M. Huang.

For more information, contact Task Group Chairman Nicola Senesi <[senesi@agr.uniba.it](mailto:senesi@agr.uniba.it)>.

 [www.iupac.org/projects/2006/2006-014-1-600.html](http://www.iupac.org/projects/2006/2006-014-1-600.html)

## Trace Elements Analysis: Role of Grain Size Distribution in Solid Reference Materials

Existing guidelines do not report indications for the selection of the most appropriate particle size distribution for reference material. In the case of solid reference material, particle size distribution plays a vital role in the homogeneity of the material and in the minimum representative test portion required for performing trace element analysis. Commonly, matrix reference materials originating from different producers show different particle size distributions. In the case of soil and sediment, particle size distribution ranges from <120  $\mu\text{m}$  to <20  $\mu\text{m}$ .

Finer particles can increase the homogeneity of the material, but the reference material can significantly differ from the real samples routinely analyzed in the laboratories. In the case of contaminated soils, the analyses are usually carried out on test samples with particle sizes of <2 mm, while the related reference materials have particle sizes of <90  $\mu\text{m}$ . The effect of particle size on extractable trace metals in soil reference materials already has been observed (A. Sahuquillo et al., "Certified Reference Materials for Extractable Trace Metals in Soils: Effect of the Particle Size," 1998, *Fresenius J. Anal. Chem.* 304-307). In addition, it is also necessary to point out that the production of reference materials with fine size particle

distribution also has a relevant impact on the production costs.

This proposed project, to be carried out within the Analytical Chemistry Division (V), aims to investigate:

1. the influence of grain size distribution on the homogeneity of solid reference materials
2. the influence of grain size distribution on the minimum sample intake for the analysis of different analytes
3. the influence of grain size distribution on the stability of the reference materials
4. the cost associated with the production of reference materials with different particle size distribution

The project, funded by the different participants, began in October 2006. It is being coordinated by the Italian Environmental Protection Agency and involves representatives from the International Atomic Energy Agency, Austria; Institute for National Measurement Standards, Canada; University of Barcelona, Spain; and the National Institute of Standards and Technology, USA.

For more information and to submit comments, please contact Task Group Chairman Maria Belli <maria.belli@apat.it>.

 [www.iupac.org/projects/2005/2005-035-2-500.html](http://www.iupac.org/projects/2005/2005-035-2-500.html)

## The Chemistry Clearing House as a Way to Better Chemistry Teaching

With the support of the Russian Academy of Sciences, the Chemistry Clearing House was organized at Mendeleyev's University of Chemical Technology of Russia in order to disseminate information about chemistry and chemical education throughout Russia and the Commonwealth of Independent States. The objective of the Clearing House is to improve the professional skills of teachers in secondary schools, high schools, colleges, and polytechnic schools by disseminating IUPAC-sourced educational and reference materials to educational institutes. The Clearing House helps teachers select the right materials, adapt them to their curricula, and translate them if necessary.

One of the goals of this project was to eliminate the gap in the teaching of chemistry between fundamental science and curricula by adopting educational materials and practices approved by the IUPAC Committee on Chemistry Education (CCE).

Information about the Chemistry Clearing House has

been incorporated into the website of Mendeleyev's University of Chemical Technology of Russia. The website (in Russian) <<http://gh.muctr.ru>> includes the following:

- project information, head coordinators, and participant information
- list of the Education Ministry of Russian Federation documents regarding chemical education and the integration of science and education
- translation of CCE reports
- translations of IUPAC materials regarding chemical terminology
- presentations of new methods and techniques for scientific education

The Chemistry Clearing House achieved its goal of contributing to the public understanding of chemistry and the scientific method. Future curricula will promote the public appreciation of chemistry and the benefits brought to society by the discovery and application of chemical knowledge.

In the future, the Clearing House hopes to work more closely with CCE on educating Russian science teachers. However, it is not enough to simply deliver information regarding IUPAC activities. Instead the system must allow for two-way communication and feedback.



The Chemistry Clearing House is a vital component of Russian chemistry education because it helps teachers adopt foreign science teaching methods and take part in an international exchange of information and educational experience.

Other countries should consider developing their own chemistry clearing houses in order to accomplish the following:

- improve chemical education overall
- advance public understanding of chemistry and the scientific method
- exchange information on teaching methods among colleagues around the world
- adapt curricula to technology and industry problems

For more information contact Task Group Chairman Elena S. Gryzlova <[nrcr@geokhi.ru](mailto:nrcr@geokhi.ru)>.

 [www.iupac.org/projects/2001/2001-003-5-050.html](http://www.iupac.org/projects/2001/2001-003-5-050.html)

## The Project Place

### Teaching High-Temperature Materials Chemistry at the University Level

The growth of high-temperature materials chemistry (HTMC) into an increasingly important field of scientific and technological research is due to the continuous demand for new materials and the need for systematic knowledge of their physical and chemical behavior in the conditions required by the new technologies (e.g., space and energy technologies). These materials (e.g., oxide and nonoxide modern multifunctional ceramics, intermetallics), which offer interesting technical applications for such things as surface coatings, electronic components, and advanced turbines, are prepared through high-temperature processing (e.g., transport reactions, CVD, combustion synthesis, laser ablation, and deposition) and must be stable under extreme thermal and chemical conditions.

HTMC now encompasses many fields of science and technology. Its advancement has involved a synergic interchange between basic and applied research, with the application of thermodynamics, kinetics, and a variety of physical, chemical, and modeling techniques to investigate processes and behaviors of materials at

temperatures as high as 3 000K to 5 000K.

More than 50 years of studies have demonstrated that the general behavior of materials and reactions at high temperatures often differs dramatically from what we are educated to expect at room temperature. HTMC topics are rarely addressed in chemistry and materials science programs at the university. Therefore, it is important to introduce to students of chemistry and materials science the concepts underlying the behavior of materials and chemical bonding at high temperatures.

The proposed project will provide a resource book of topics in the area of properties and behavior of high-temperature materials for those teaching materials science or physical or inorganic chemistry at various levels. The recommended topics will be accompanied by a bibliography of helpful references and a short introduction or explanation, including the areas of application.

For more information contact Task Group Chairman Giovanni Balducci <[giovanni.balducci@uniroma1.it](mailto:giovanni.balducci@uniroma1.it)>.

 [www.iupac.org/projects/2000/2000-024-2-200.html](http://www.iupac.org/projects/2000/2000-024-2-200.html)

## Provisional Recommendations

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

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

### Standard Definitions of Terms Relating to Mass Spectrometry

This document contains recommendations for nomenclature, definitions of terms, and acronyms in mass spectrometry. In 1974, the IUPAC Commission on Analytical Nomenclature issued recommendations on mass spectrometry terms and definitions. In 1978, the Commission on Molecular Structure and Spectroscopy updated and extended the recommendations and made further recommendations regarding symbols, acronyms, and abbreviations. The Physical Chemistry Division Commission on Molecular Structure and Spectroscopy's Subcommittee on Mass Spectroscopy revised the recommended terms in 1991 and appended terms relating to vacuum technology. Some additional terms related to tandem mass spectrometry were

added in 1993 and accelerator mass spectrometry in 1994. Due to the rapid expansion of the field, particularly in mass spectrometry of biomolecules, a further revision of the recommendations has become necessary.

#### Comments by 31 January 2007

Prof. Kermit K. Murray  
Louisiana State University  
Department of Chemistry  
331 Choppin Hall  
Baton Rouge, LA 70803, USA  
Tel: +1 225-578-3417  
Fax: +1 225-578-3458  
E-mail: [kkmurray@lsu.edu](mailto:kkmurray@lsu.edu)

 [www.iupac.org/reports/provisional/abstract06/murray\\_310107.html](http://www.iupac.org/reports/provisional/abstract06/murray_310107.html)

## Standards, Calibration, and Guidelines in Microcalorimetry. Part 2. Calibration Standards for Differential Scanning Calorimetry (IUPAC Technical Report)

Giuseppe Della Gatta, Michael J. Richardson, Stefan M. Sarge, and Svein Stølen  
*Pure and Applied Chemistry*  
Vol. 78, No. 7, pp. 1455-1476, 2006  
doi:10.1351/pac200678071455

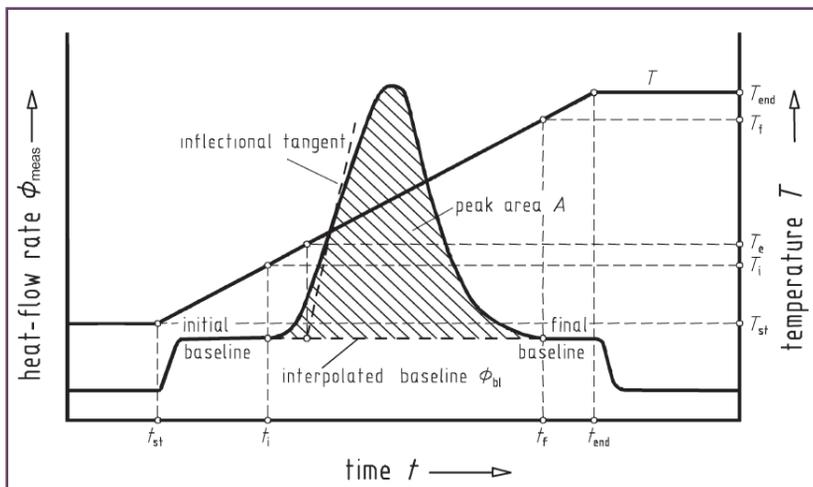
Differential scanning calorimeters are widely used for temperature, heat capacity, and enthalpy measurements in the range from subambient to high temperatures. The aim of this report is to describe calibration procedures and to review reference materials (RMs) for temperature, heat capacity, and enthalpy measurements made by differential scanning calorimetry in the temperature regions from subambient to high. The

report focuses on the calibration of the response of the instrument and on the estimation of the measurement uncertainty. The procedures for temperature, enthalpy, and heat-flow rate calibration are given in detail. Calibration on cooling has also been considered. Recommended RMs are listed, and the relevant properties of these materials are discussed. The paper should be helpful to those who wish to participate in laboratory accreditation schemes—involvement with such schemes is now often essential before a work program can be agreed upon. Key components on the route to accreditation are well-defined operating procedures and their validation using certified reference materials.

"Part 1. Standards in Isothermal Microcalorimetry," *Pure Appl. Chem.* **73**(10), 1625-1639 (2001).

 [www.iupac.org/publications/pac/2006/7807/7807x1455.html](http://www.iupac.org/publications/pac/2006/7807/7807x1455.html)

Definition of terms for describing measured curves with the peak representing a transition or reaction in the sample (subscript m denotes measured quantities) in a plot of heat-flow rate and temperature against time.



## Feature Articles Wanted

CI is currently seeking feature articles

Please note that articles should be submitted no later than two months before the issue date. Contact the editor for more information at [edit.ci@iupac.org](mailto:edit.ci@iupac.org).

# Internet Connection

## Chemical Terminology at Your Fingertips

by Miloslav Nic, Jiri Jirat, and Bedrich Kosata

The *IUPAC Compendium of Chemical Terminology*, commonly known as the **Gold Book**, is one of IUPAC's major contributions to communication among chemists. It collects terms and definitions from primary specifications and provides single-point access to them. With more than 6 500 entries, it is a real treasure for every chemist.

The first edition was published in 1987 and updated in 1997. Both editions are now out of print. Fortunately, the second edition is also available as a series of PDF files at <[www.iupac.org/publications/compendium](http://www.iupac.org/publications/compendium)>. In addition, there is a searchable version via the Muscat interface at <[www.chemsoc.org/goldbook](http://www.chemsoc.org/goldbook)>.

If users are looking for a reliable definition of a term, access to such information via the book or PDF indexes is sufficient. But very often their wishes are not so simple. The readers may be unsure under which heading the required information is hidden or they may have only a vague notion of what they are looking for.

A few years ago, the only strategy in such cases was to browse through a few books and rely on good luck in finding some clues. Nowadays, we have computers which can browse millions of pages and look up relevant information in a few seconds.

But nothing is perfect in this world. Computers are very fast, but they do not possess human intelligence. Humans can identify important points from context, they can see through irregular structures, inaccuracies, usage of uncommon words, and other pitfalls of text browsing. Computer programs rely on regularity and possibility to consult internal vocabularies and other sources, but they do not cope well with the unexpected. So far, no solution has been found that can compete with a trained human in understanding text.

Chemistry represents a particularly difficult area for computers to compete in. Chemists communicate

with combination of texts, structural formulas, pictures, and equations, and so automatic understanding of chemical texts is especially demanding. The Muscat search of the Gold Book gives a realistic picture of what an advanced, generalized automatic process can provide. This search engine not only properly understands similar words, but it even clusters results that share some common features. It definitively offers an important improvement over standard full text searches, yet its capabilities are restricted. It does not understand chemical formulas and mathematics, it does not understand some clues any undergraduate student would pick up on, it may even run entirely astray if some textual similarity perplexes its algorithms. It is important to keep in mind that the search relies on generic analysis of text, not on chemical knowledge.

But the situation is not so bleak as it may sound from the preceding paragraphs. The art of communication with computers resides in their ability to organize text and other data into many small sections and annotate these parts in a way that makes it much easier to convey some sense to the computer.

There now exist technologies based on XML (eXtensible Markup Language) that are very good at such partitioning and further processing of the marked information. Research into the efficient markup of chemical text and in finding the optimal structure of information is in its infancy, and the XML Gold Book represents a milestone in this development.

The Gold Book includes chemical formulas, mathematical symbols, units, and other features. Its structuring and

further transformation has required enormous effort over five years, but the work finally paid off. Relevant information is now captured in a way that makes it accessible using standard software techniques.

It happens too often that the usefulness of excellent books is spoiled by mediocre indexing. The new version of the Gold Book does not suffer such a fate. The fact that all information contained in the book is meticulously marked in XML enabled the creation of many indexes that are difficult to find in similar publications.

Some indexes extract chemical meaning so that entries can be selected based on the compounds they



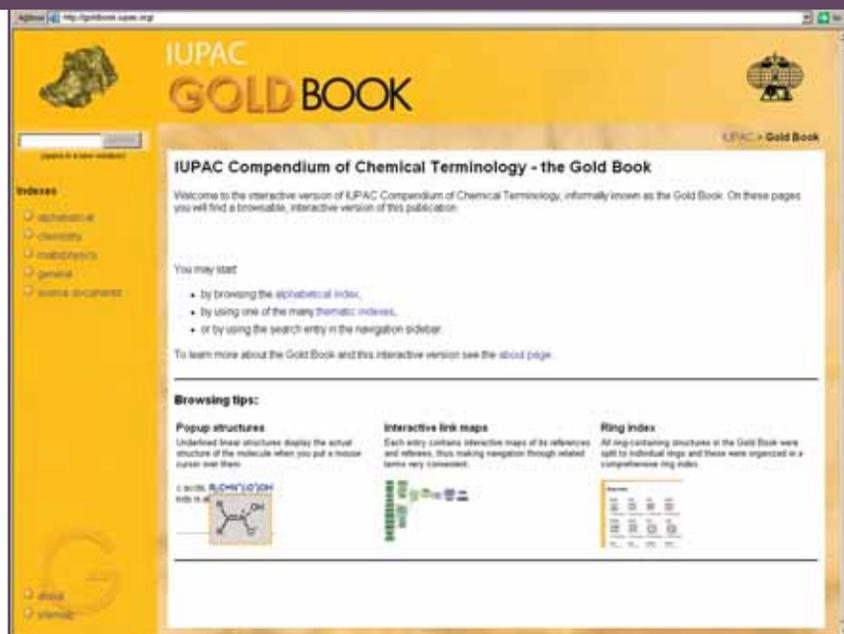
contain (index of structures, chemical formulas, ring index), while others summarize information about physical constants, units, and quantities. Other indexes list images and offer selections of acronyms and abbreviations. All indexes are generated automatically from the available source text, so there is no need for manual intervention. Any upgrades and additions automatically appear in the indexes. One InChI identifier was generated for each compound to make chemical information accessible for search engines and data mining.

The XML version's "link maps," which are also generated automatically, are very useful as well. Every entry is accompanied by a map that graphically displays the relation of the entry to other terms and definitions. These maps often reveal relationships that are difficult to decipher by other means.

Full text incremental searching is also available. This search does not rely on an Internet connection and can be used directly from the CD-ROM.

The Gold Book is a very useful resource on its own, but its usefulness does not end here. Concurrently, software has been developed that enables automatic incorporation of Gold Book data into other resources. One of the features of this software is its ability to recognize Gold Book entries in various texts from independent sources. The software automatically links these entries to the Gold Book, so that in the near future anyone reading materials from IUPAC literally will be a click away from finding proper definitions of terms he/she does not understand.

As with any major undertaking, the XML Gold Book required the cooperation of many people. The activity started as part of the IUPAC project "Standard XML Data Dictionaries for Chemistry" (2002-022-1-024) under the leadership of Steve Stein from NIST. Miloslav Nic, Jiri Jirat, and Bedrich Kosata from the Laboratory of Informatics and Chemistry at ICT Prague did the XML work and other programming. Jiri Znamenacek from ICT Press wrote the search engine and also implemented the graphic design created by Ladislav Hovorka. Eva Dibuszova, the head of ICT Press, provided valuable editorial advices. Cheryl Wurzbacher, the production editor for *Pure and Applied Chemistry*, proofed very thoroughly the XML version against the



original printed version of the book, which resulted in the correction of many errors and mistakes that sneaked in during the initial XML conversion. Aubrey Jenkins continues to update the Gold Book with new entries and to correct the old ones. Alan McNaught, Steve Heller, Leslie Glasser, and Jack Lorimer were also instrumental.

As mentioned at the beginning of the article, the new version of the Gold Book is a very important step in improving the availability of IUPAC materials to chemists and the general public. Further developments will transform IUPAC materials from a collection of independent sources to an integrated information resource. Many articles have been recently published about Semantic web both in the scientific and popular press. With this new development, IUPAC again will be a pioneer in a new territory, showing how to manage and distribute complex scientific information.

Miloslav Nic <Miloslav.Nic@vscht.cz> is the head of the Laboratory of Informatics and Chemistry at ICT Prague and the coordinator of the B.Sc. and M.Sc. study programs "Informatics and Chemistry" and "Applied Informatics in Chemistry." He is an invited observer on the IUPAC Committee on Printed and Electronic Publication. Jiri Jirat <Jiri.Jirat@vscht.cz> is a lecturer at ICT Prague (chemical informatics, XML technologies) and a researcher at the Laboratory of Informatics and Chemistry at ICT Prague. Bedrich Kosata <Bedrich.Kosata@vscht.cz> is a lecturer at ICT Prague (chemoinformatics, programming) and a researcher at the Laboratory of Informatics and Chemistry at ICT Prague. He is the author of the open source molecular editor BKChem <<http://bkchem.zirael.org/>>.

 <http://goldbook.iupac.org>

## Internet Connection

The following review is the third in a series of articles surveying free online resources of potential interest to chemists. The first article appeared in the July-Aug 2006 CI, p. 26, and the second in the Sep-Oct 2006 CI, p. 29.

# Free Information Resources for Chemists—Part 3

by Leslie Glasser

## Chemical Journals

While subscriptions are generally required to access the chemical literature, many journals permit free Internet access after a period. For example, all reports and recommendations in IUPAC's *Pure and Applied Chemistry* <[www.iupac.org/publications/pac](http://www.iupac.org/publications/pac)> are available immediately upon publication, while the remaining material is available for free a year after the complete publication of a volume.

IUPAC's news magazine *Chemistry International*, <[www.iupac.org/publications/ci](http://www.iupac.org/publications/ci)> offers free access from the time it is published.

Currently, the Open Access Publishing movement is urging a move towards free public access to publicly funded, original research publications <<http://bmj.bmjournals.com/cgi/content/full/328/7430/1>>, with the author paying the publication costs. An important new site for this movement is "Open Access Central" <[www.openaccesscentral.com](http://www.openaccesscentral.com)>, which is the portal for three open-access sites: the well-established "BioMed Central," which lists over 150 peer-reviewed open access journals covering all of biology and medicine; "Chemistry Central" <[www.chemistrycentral.com](http://www.chemistrycentral.com)>, which currently features chemistry-related articles from BioMed Central, including the new online *Beilstein Journal of Organic Chemistry* <<http://bjoc.beilstein-journals.org>>; and the forthcoming "PhysMath Central" <[www.physmathcentral.com](http://www.physmathcentral.com)>. Links to the many current or recent journals that offer free full-text articles appear in English on the Belorussian site <[www.abc.chemistry.bsu.by/current/fulltext.htm](http://www.abc.chemistry.bsu.by/current/fulltext.htm)>. The U.S. National Science Digital Library provides links to a wide range of resources <[www.nsd.org](http://www.nsd.org)>.

## General Software

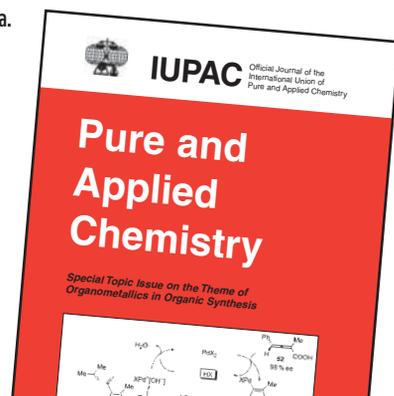
Application software (which must be installed in your computer system) when mentioned below is for the widely-used commercial Windows operating system (in its various guises); no effort has been made to include Linux-based software, although this free operating system is of growing importance.

Free software of a general nature is available from many sites—for example, tu cows <[www.tucows.com/downloads/Windows](http://www.tucows.com/downloads/Windows)>, Download.com <[www.download.com](http://www.download.com)>, ZDNet <[downloads-zdnet.com.com/2001-20-0.html?legacy=cnet](http://downloads-zdnet.com.com/2001-20-0.html?legacy=cnet)>, and so on. A useful chemical application is a Java-based checker for consistency in experimental data, as is typically presented in an article for publication <[www.rsc.org/Publishing/ReSource/AuthorGuidelines/AuthoringTools/ExperimentalDataChecker/index.asp](http://www.rsc.org/Publishing/ReSource/AuthorGuidelines/AuthoringTools/ExperimentalDataChecker/index.asp)>.

## Update (to part 1)

eMolecules, <[www.emolecules.com](http://www.emolecules.com)>, is the new incarnation of the chemical search engine Choogle, which had to alter its name for legal reasons (see *Chemistry World*, July 2006, p.10).

Leslie Glasser <[leslieglasser@yahoo.co.uk](mailto:leslieglasser@yahoo.co.uk)> is chairman of the IUPAC Committee on Printed and Electronic Publication (CPEP). He is a professor in the Department of Applied Chemistry, Nanochemistry Research Institute, of the Curtin University of Technology, in Perth, Australia.



The image is a screenshot of the Chemistry Central website. The header features the 'Chemistry Central' logo. Below the header, there are several sections: 'Home' with a list of links like 'About Chemistry Central', 'Contact Us', 'Submit a manuscript', 'Sign up for article alerts', 'Institutional membership scheme', 'Starting a journal', 'News and updates', and 'Sign up for updates'. The 'Research highlights' section includes 'New microbial community compartments found' and 'Navigating metabolomics data'. The 'Welcome to Chemistry Central' section provides information about the service and its goals. At the bottom, there is a 'Journals' section listing 'Beilstein Journal of Organic Chemistry', 'IUPAC Biochemistry', and 'IUPAC Chemical Biology'.

# Conference Call

## Solubility Phenomena

by Heinz Gamsjaeger and Wolfgang Voigt

The 12th International Symposium on Solubility Phenomena and Related Equilibrium Processes was held 24–28 July 2006 at the TU Bergakademie Freiberg in Germany under the auspices of IUPAC. As initiated at the 10th ISSP in Varna, this symposium continued the practice of offering a workshop on a special topic related to solubility.

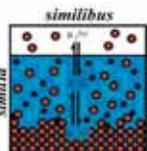
The Subcommittee on Solubility and Equilibrium Data (SSED) of the IUPAC Analytical Chemistry Division (Division V) met over the two days prior to the symposium, with Heinz Gamsjäger (Austria) as the chair. The joint organizers of the symposium were the TU Bergakademie Freiberg, the German Chemical Society, and SSED. Sponsors of the symposium, in addition to the TU Bergakademie Freiberg, were the German Research Foundation and the Federal Ministry of Economics and Labour. The symposium was chaired by Wolfgang Voigt, with assistance from Daniela Freyer, conference secretary, and members of the local organizing committee. The symposium was reported on by the TU Bergakademie Freiberg websites, Journal of Solution Chemistry, Nachrichten of the German Chemical Society, Molten Salts Bulletin, and several international conference information websites.

One hundred and twenty-four participants from 30 countries took part in the symposium. One hundred and three participants registered for both the symposium and the workshop, whereas 8 attended the workshop only.

The opening ceremony was presided over by the Rector of TU Bergakademie Freiberg, Georg Unland. Welcoming remarks were also given by Heinz Gamsjäger, the representative of IUPAC, Matthias Otto, dean of the Faculty of Chemistry and Physics in Freiberg, and Wolfgang Voigt, symposium chair.

Six plenary and two invited lectures highlighted a wide spectrum of solubility phenomena. Gerd Maurer (Germany) gave the opening plenary address on “Gas Solubility in Aqueous and Non-Aqueous Solutions,” a topic of pressing importance. His lecture demonstrated that classical thermodynamics, as well as molecular simulations, are needed for predicting gas solubilities in “complex” systems. The concluding plenary address was given by Petros G. Koutsoukos (Greece), whose stimulating lecture on “Solubility of Salts in Water: Key

Issues for Crystal Growth and Dissolution Processes” elucidated the role of supersaturation, substrate/water interface, and fluid dynamics on solubility phenomena. The other keynote lectures dealt with: limitations of Li-air batteries due to solubilities (M. Salomon, USA), fundamentals and applications of gas hydrates (E.D. Sloan, USA), radioactive-waste disposal (H. Wanner, Switzerland), high-pressure investigations (S. Sawamura, Japan), high-temperature *in situ* pH measurements of metal oxide solubilities (D.J. Wesolowski, USA), and preferential crystallization in the region of two solid phases (A. König, Germany). These plenary and invited lectures are to be published in



*Pure and Applied Chemistry* under the editorship of Earle Waghorne (Ireland).

Thirty-one short communications and 59 posters were presented during afternoon and morning sessions. Thirty minutes were assigned to short communications, which turned out more convenient than the usual 15 to 20 minutes, a fact that should be considered for future ISSPs. The oral and poster contributions ranged from fundamentals of phase equilibria to new experimental data and modelling of solubility processes to applications in industry and environment. The delegates continued their scientific discussions over lunch in the historical restaurant “Schwanenschlösschen.” Throughout the conference a stimulating atmosphere prevailed.

At the one-day workshop on “Quality Assurance in Thermodynamic Databases for Performance Assessment Studies in Waste Disposal,” run in parallel to the conference, invited speakers presented updates on thermodynamic database projects. Speakers included R. Rarey, Dortmund Databank; H. Wanner, OECD Nuclear Energy Thermochemical Database Project; M. Gaune-Escard, Molten Salt Database; P. Cloke, Yucca Mountain Project Database; Th. Vercouter, Common Thermodynamic Database Project; E. Bastrakov, FreeGs Thermodynamic Database Project; S. Hagemann, THEREDA German Database for Waste Disposal Assessment Studies). Ken Marsh introduced the XML-based IUPAC standard “ThermoML,” designed for exchange of thermo-physical data.

The three IUPAC poster prizes were given to Alexander S. Lileev (N.S. Kurnakov Institute of General and Inorganic Chemistry of Russian Academy of Sciences, Russia) for his poster “Non-Additivity of Contributions into the Dielectric Constant of Saturated Solutions and Ion-Ion interactions in Ternary Water-Salt Systems,” to Sven Hagemann (Gesellschaft für

## Conference Call

Anlagen- und Reaktorsicherheit, Germany) for his poster "A New Simple Method for the Investigation of Hydrogen Sulfide Solubilities in Aqueous Solutions," and Georgia Wollmann (Institute of Inorganic Chemistry, TU Bergakademie Freiberg, Germany) for her poster "Solubilities Related to Substituted Polyhalites."

The 13th ISSP will be held in July 2008 in Dublin, Ireland.

Heinz Gamsjäger <gamsjaeg@unileoben.ac.at>, a professor at the Montanuniversität Leoben in Austria and an active member of IUPAC, served as the IUPAC representative at the meeting. Wolfgang Voigt <Wolfgang.Voigt@chemie.tu-freiberg.de> was the symposium chair.

 [www.issp.tu-freiberg.de](http://www.issp.tu-freiberg.de)

---

## Green Chemistry: A Tool for Socio-Economic Development and Environmental Protection

by *Pietro Tundo and Kenneth R. Seddon*

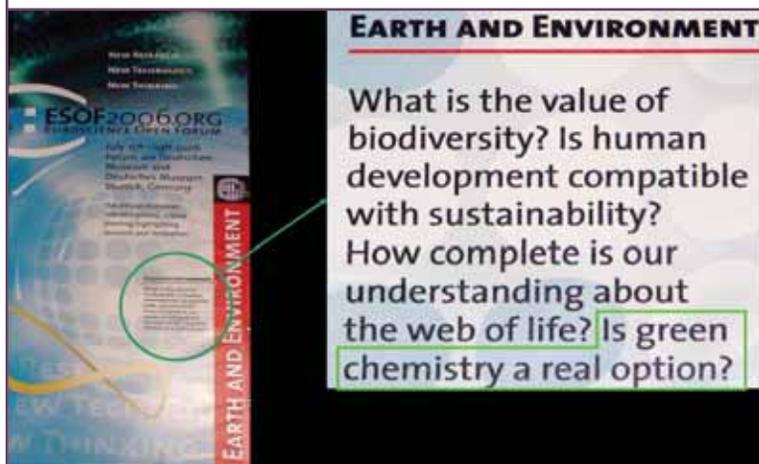
The European Science Open Forum (ESOF 2006), the 2nd Pan-European General Science Meeting, was held in Munich, Germany, at the Forum am Deutschen Museum and the Deutsches Museum from 15–19 July 2006. The purpose of the forum—similar to the British Association—is to promote the public understanding of science, particularly by encouraging dialogue between scientists and the general public. Seven scientific themes were chosen to reflect the sessions:

- Combining Cultures
- Dealing with Disasters
- Earth and Environment
- Particles and Planets
- Science and Society
- Fabric of Science
- Workings of Life

Even though Green Chemistry is associated with the 2005 Nobel Prize for Chemistry, it has not had widespread public recognition. However, within the forum's Earth and Environment theme, Green Chemistry was put forward as one of the main options for environmental protection. Moreover, the session on Green Chemistry at this meeting was the *only* session on chemistry. In fact, the ESOF meeting featured Green Chemistry on its advertising posters, thereby placing it on the same level as other more popular scientific disciplines. The poster provocatively asked: "Is Green Chemistry a Real Option?" This question was clearly answered by the panellists Pietro Tundo, Martyn Poliakoff, Ken Seddon, Marian Mours, and Leiv Sydnes during a two and one-half hour session on "Green Chemistry: A Tool for Socio-Economic Development and Environmental Protection" (The idea for this session initiated with the Italian Interuniversity Consortium [INCA] <[www.unive.it/inca](http://www.unive.it/inca)>).

The session was the latest in a series of initiatives that are placing Europe in the lead in Green Chemistry. The crowded event (more than half the audience members were nonscientists) was expertly moderated by freelance science journalist Barbara Schwerdtfeger. Among the participants were Francesco Fedi, president of EU COST Actions; Howard Moore, consultant to the ICSU (International Council for Science) and the *Berliner Zeitung*. All wanted to know (as became clear in the important question and answer session) why Green Chemistry is an option, and why they should care.

Poliakoff (University of Nottingham, UK) gave a clear and entertaining exposition of exactly what is meant by Green Chemistry, and how the chemical industry is now adopting its principles and introducing green production techniques, hand-in-hand with academic researchers. Tundo (University of Venice, and chairman of the G8-sponsored International Green Network [IGN]) then stressed the importance of an international effort, including India, China, and the developing nations of Africa and



## Conference Call



*The G8 Science Ministers of the Carnegie Group, the sponsors of the International Green Network, meeting in Venice, 4 December 2004: From the left: Arthur Carty (Canadian Ministry for Research), Janez Potocnik (European Commission), John Marburger (Scientific Advisor USA President, OSTP), Letizia Moratti (Italian Minister for Research), Edelgard Bulmahn (German Minister for Research), David King (Chief Scientific Adviser of HM Government, UK), Andrey Fursenko (Russian Minister for Research), William Golden (Founder of the Carnegie Group), François D'Aubert (French Vice Minister for Research), and Hiroyuki Abè (Council for Science and Technology, Cabinet Office, Japan).*

South America. According to Tundo, MEGREC (the Mediterranean Green Chemistry Network), which constitutes a platform for the development of research and training in green chemistry in the countries of the Mediterranean basin (with a focus on water management, exploitation of local natural resources, production and use of fertilizers, monitoring, and reducing the presence of toxic compounds in the food chain) has a crucial role to play here. Seddon (of the Queen's University of Belfast and director of QUILL) described the most recent and important truly international network, the International Green Network, founded by the G8 ministers of scientific research, which is about to start, thanks to national government funding of its activities. Mours (CEFIC) offered the industrial perspective on green chemistry, and Sydnes demonstrated how green chemistry is needed in order to address some of the major concerns affecting humanity, such as poverty, lack of resources in the developing nations, and widespread pollution. The presentations were followed by an hour-long discussion based on questions from the audience. Both science policy and research issues were addressed, as well as possible actions on how to improve the public understanding of chemistry.

Later, Quentin Cooper, a BBC radio science journalist, hosted an informal and highly entertaining summary of the day's sessions. Seddon and Poliakoff were two of the five speakers at this session. They were targeted with numerous questions from the audience, which clearly showed the high level of public interest in Green Chemistry.

At the end of the day, though, what was the answer to the question: "Is Green Chemistry a Real Option?" The answer is no, it is not an "option" as the word is defined: the power or freedom to choose. There is no freedom to choose here: Green Chemistry is a necessity, not an option, if we are to achieve a sustainable earth.

Pietro Tundo <tundop@unive.it> is from the Consorzio Interuniversitario Nazionale "la Chimica per l'Ambiente" INCA Italy. Kenneth R. Seddon <k.seddon@qub.ac.uk> is from the QUILL Research Centre, The Queen's University of Belfast, Belfast, Northern Ireland, UK.

 [www.esof2006.org](http://www.esof2006.org)

---

## Polymers and Organic Chemistry

*by Shinichi Itsuno*

The 12th International Conference on Polymers and Organic Chemistry 2006 (POC'06) attracted more than 120 participants from Canada, China, Czech Republic, Egypt, England, Germany, Hong Kong, India, Korea, Poland, Qatar, Scotland, Slovenia, Spain, Switzerland, Taiwan, USA, and Japan. The conference was held at the Okazaki Conference Center in Okazaki, Japan, from 2–7 July 2006. The conference, which was the 12th meeting in the series on Polymers in Organic Chemistry, was coorganized by the Toyohashi University of Technology and the Institute for Molecular Science.

During the opening session, Mitsuo Sawamoto (Kyoto University, Japan), a member of the IUPAC Polymer Division, discussed IUPAC's objectives and gave an overview of the activities of the Polymer Division.

The main topics of the conference included polymer supported reagents, polymer catalysts, poly-

*continued on page 37*

# Where 2B & Y

## Polymers for Advanced Applications

20-23 November 2006, Stellenbosch, South Africa



The **9th Annual UNESCO/IUPAC Conference on Macromolecules** will be held from 20-23 November 2006 in Stellenbosch, South Africa. The conference will be centered around "Polymers for Advanced Applications." Four themes have been selected that will be covered in eight plenary lectures:

- hydrogels
- polymer brushes
- vesicles
- synthetic/biopolymer hybrids

Speakers who already have accepted invitations include K. Matyjaszewski (Carnegie Mellon University, Pittsburgh, USA), W. Hennink (Utrecht University, The Netherlands), S. Brocchini (Univ. London, UK), and H. Maeda (Sojo University, Japan).

One of the above mentioned topics will be discussed per day. The morning session will largely be dedicated to synthesis and characterization of the materials. The focus of the afternoon session will be more on applications of the indicated classes of materials. However, there will be flexibility in the program to accommodate contributions in the field of "Polymers for Advanced Applications" that do not exactly fit in the indicated four areas.

The conference will be held in the town of Stellenbosch, which is located about 30 minutes from the airport of Cape Town. Stellenbosch is surrounded by mountains and is in the middle of the well-known wine district of South Africa. November is the beginning of the summer in South Africa, which means that the weather will be very pleasant.

See **Mark Your Calendar** on page 36 for contact information.

 <http://academic.sun.ac.za/unesco/Conferences/Conference2006/HOMEPAGE2006.htm>

## NanoTech Insight '07

10-17 March 2007, Luxor, Egypt

The **International Conference on Nanotechnology: Science and Application (NanoTech Insight '07)** will be held 10-17 March 2007 in Luxor, Egypt. The time for small is now. The nanoscale challenges all we know and imagine knowing. From the smallest parts come a universe of discovery. As with every scientific leap, we need new ways of thinking and exploring the problems at hand. With creativity, dedication, and open minds, we can turn yesterday's nanotech "science fiction" into today's reality.

NanoTech Insight aims to stimulate a worldwide dialogue on the planned advancement of nanotechnology. Interdisciplinary communication is the foundation of nanoresearch. This conference promotes this by covering the main topics in nano from a wide range of disciplines. The idea is not to build generalists but rather to guide the specialists to effectively use their knowledge and expertise to enrich the nano research domain.

In addition to the breathtaking and inspirational environment that Egypt provides for social networking, NanoTech Insight provides the chance for students and educators from developing countries

to learn and be inspired by the world's leading researchers. In addition, the conference will provide special financial support for attendees from developing nations. "Responsible nanotechnology" dialogue must include all global players to ensure the risks and benefits of the new technology are fully understood. The conference emphasizes applications of nanotechnology for sustainable development, with special sessions on nano ethics, environmental applications, and nanotechnology for industry.

Topics include:

- Bio-applications
- Fabrication
- Medical and Pharmaceutical Applications
- Nano Applications for Clean and Renewable Energy
- Nano Ethics / Environmental Impact
- Nanomaterials and Structures
- NanoTech For Industry
- NanoTechniques
- Optoelectronics and Photonics
- Simulation and Molecular Dynamics
- Single Molecules

 [www.nanoin sight.net](http://www.nanoin sight.net)

## Heterocyclic Chemistry

15–20 July 2007, Sydney, Australia

The **21st International Congress for Heterocyclic Chemistry (ICHC21)** will be held from 15–20 July 2007 in Sydney, Australia. The congress, which is an activity of the International Society of Heterocyclic Chemistry, will cover all aspects of heterocyclic chemistry, with particular focus on the following areas:

- new heterocyclic structures
- industrial developments in heterocyclic chemistry
- heterocycles in biomolecular chemistry
- new synthetic methodology

- heterocycles in green chemistry
- heterocycles in new materials and polymers
- heterocycles in new devices and sensors

The program will include plenary and invited lectures, contributed oral presentations, and poster sessions. A call for abstracts will be made in November 2006—check the conference website.

See **Mark Your Calendar** on page 36 for contact information.

 [www.ichc21.com.au](http://www.ichc21.com.au)

## Biophysics

3–7 March 2007, Baltimore, Maryland, USA

The **Biophysical Society Annual Meeting** is held each year in February or March. With over 6 000 attendees, the meeting is the largest gathering of biophysicists around the world. More than 3 000 abstracts are submitted each year, which are programmed into poster and platform sessions. The meeting includes

symposia, workshops, subgroup programs, and the national lecture. The meeting also features nearly 200 exhibits, exhibitor demonstrations, satellite meetings, and programs developed by the society's committees. The 51st annual meeting will be held in Baltimore, Maryland, USA.

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

## Visas

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

## How to Apply for IUPAC Sponsorship

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

[<www.iupac.org/symposia/application.html>](http://www.iupac.org/symposia/application.html).

# Mark Your Calendar

Upcoming IUPAC-sponsored events  
See also [www.iupac.org/symposia](http://www.iupac.org/symposia) for links to  
specific event websites

## 2006

 IUPAC poster prizes to be awarded

**20-23 November 2006 • Polymers for Advanced Applications • Stellenbosch, South Africa**   
*9th Annual UNESCO/IUPAC Conference on Macromolecules: Polymers for Advanced Applications*  
Prof. Ron D. Sanderson, Department of Chemistry and Polymer Science, University of Stellenbosch  
Private Bag X1, Matieland, 7602, South Africa, Tel.: +27 21 808 3172, Fax: +27 21 808 4967  
E-mail: [rds@sun.ac.za](mailto:rds@sun.ac.za)

## 2007

**1-2 March 2007 • Clinical Laboratory • Barcelona, Spain**   
*Fourth European Symposium on Clinical Laboratory and In Vitro Diagnostic Industry*  
Dr. Josep M. Queralto, Hospital de la Santa Creu i Sant Pau, Servei de Bioquímica, Av. S. Antoni M. Claret, 167  
Barcelona, 08025, Spain, Tel.: +34 932919022, Fax: +34 932919196, E-mail: [jqueralto@santpau.es](mailto:jqueralto@santpau.es)

**11-14 March 2007 • Heterocyclic Chemistry • Gainesville, Florida, USA**  
*8th 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)

**15-21 April 2007 • Phosphorus Chemistry • Xiamen, China**  
*17th International Conference on Phosphorus Chemistry*  
Prof. Yufen Zhao, Xiamen University, Department of Chemistry, Xiamen, China 361005, Tel.: +86 5922185610  
Fax: +86 5922186292, E-mail: [yfzhao@xmu.edu.cn](mailto:yfzhao@xmu.edu.cn)

**21-25 May 2007 • Mycotoxins and Phycotoxins • Istanbul, Turkey**   
*XIth International Symposium on Mycotoxins and Phycotoxins*  
Dr. Hamide Z. Senyuva, Tubitak-Atal, Konya Yolu No. 67, Besevler, 06530, Ankara, Turkey,  
Tel.: +90 312 2124620/ext.14, Fax: +90 312 2123749, E-mail: [hamide.senyuva@tubitak.gov.tr](mailto:hamide.senyuva@tubitak.gov.tr)

**26-30 June 2007 • Advanced Materials • Kharkiv, Ukraine**  
*Modern Physical Chemistry for Advanced Materials (MPC'07)*  
Prof. Yuriy Kholin, Materials Chemistry Department, V.N. Karazin Kharkiv National University, Svobods Square 4,  
Kharkiv 61077, Ukraine, Tel.: +380 57 707 51 26, Fax: +380 57 705 12 61, E-mail: [kholin@univer.kharkov.ua](mailto:kholin@univer.kharkov.ua)

**15-20 July 2007 • Heterocyclic Chemistry • Sydney, Australia**  
*21st International Congress of Heterocyclic Chemistry*  
Dr. Kate Jolliffe, School of Chemistry, The University of Sydney, Sydney NSW 2006, Australia,  
Tel.: +61 2 9351 2297 | Fax: +61 2 9351 3329, E-mail: [jolliffe@chem.usyd.edu.au](mailto:jolliffe@chem.usyd.edu.au)

**16-20 July 2007 • Solution Chemistry • Perth, Australia**   
*30th International Conference on Solution Chemistry*  
Prof. Glenn Hefter, School of Mathematical and Physical Sciences, Murdoch University, Murdoch, WA 6150  
Australia, Tel.: +61 8 9360 2226, Fax: +61 8 9360 1711, E-mail: [g.hefter@murdoch.edu.au](mailto:g.hefter@murdoch.edu.au)

**22-27 July 2007 • Novel Aromatic Compounds • Awaji City, Japan**  
*12th International Symposium on Novel Aromatic Compounds (ISNA-12)*  
Prof. Yoshito Tobe, Division of Frontier Materials Science, Osaka University, Toyonaka, Osaka University, Japan,  
Tel.: +81 6 6850 6225, Fax: +81 6 6850 6229, E-mail: [tobe@chem.es.osaka-u.ac.jp](mailto:tobe@chem.es.osaka-u.ac.jp)

**2-6 August 2007 • Organometallic Chemistry • Nara, Japan**  
*14th International Symposium on Organometallic Chemistry Directed Towards Organic Synthesis (OMCOS-14)*  
Prof. Koichiro Oshima, Department of Material Chemistry, Graduate School of Engineering, Kyoto University,  
Kyoto-daigaku katsura, Nishikyō-ku, Kyoto 615-8510, Japan, Tel.: +81-75-383-2437, Fax: +81-75-383-2438, E-mail:  
[oshima@orgrxn.mbox.media.kyoto-u.ac.jp](mailto:oshima@orgrxn.mbox.media.kyoto-u.ac.jp)

**4-12 August 2007 • IUPAC 44th General Assembly • Torino, Italy**  
IUPAC Secretariat, Tel.: +1 919 485 8700, Fax: +1 919 485 8706, E-mail: [secretariat@iupac.org](mailto:secretariat@iupac.org)

**5-11 August 2007 • IUPAC 41st Congress • Torino, Italy**   
*Chemistry Protecting Health, Natural Environment, and Cultural Heritage*  
E-mail: [IUPAC.2007@unito.it](mailto:IUPAC.2007@unito.it) <[www.iupac2007.org](http://www.iupac2007.org)>



2-7 September 2007 • Ionic Polymerization • Kloster Banz, Germany 

*International Symposium on Ionic Polymerization*

Prof. Axel Müller, MC II/NW II, Universität Bayreuth, D-95440 Bayreuth, Germany, Tel.: +49 921 553399, Fax: +49 921 553393, E-mail: ip07@uni-bayreuth.de

23-28 September 2007 • Transactinide Elements • Davos, Switzerland

*Third International Conference on the Chemistry and Physics of the Transactinide Elements (TAN'07)*

Prof. H.W. Gäggeler, Paul Scherrer Institut, Radio- und Umweltchemie, CH-5232 Villigen, Switzerland, Tel.: +41 (0)56 310 24 01, Fax: +41 (0)56 310 44 35, E-mail: heinz.gaeggeler@psi.ch

2008

 IUPAC poster prizes to be awarded

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

## Conference Call

*continued from page 33*

mers in medicine and biochemistry, supports for fast chemistry, polymers for separations, electro- or light-sensitive functional polymers, polymers for environmental protection, processes within functional polymers, and novel functional polymers. The first plenary lecture, titled "Polysaccharide Derivatives for Efficient Enantioseparation by HPLC," was delivered by Yoshio Okamoto. J.M.J. Frechet delivered the second plenary lecture on "Functional Polymers as Therapeutic Carriers."

The program also included 11 invited lectures by the following internationally well-known keynote speakers:

- D.E. Bergbreiter, "Facilitating Organic Reactions with Soluble Polymers as Phase Anchors"
- Kuiling Ding, "Self-Supported Chiral Catalysts for Heterogeneous Enantioselective Reactions"
- S. Kobayashi, "Renaissance of Immobilized Metal Catalysts"
- Y.-S. Lee, "Novel Polymer-Supported Catalysts and Reagents for Oxidation Reaction and Carbon-Carbon Coupling"
- H. Wennemers, "Peptides as Asymmetric Catalysts"
- P.K. Dhal, "Polymeric Drugs for Treating Obesity"
- T. Inoue, "The Future Direction of Research

and Development of Polyesters-From High Performance to Environment Friendly"

- E. Yashima, "Helical Polymers: Synthesis, Function, and Assembly"
- P.A.G. Cormack, "Functional Polymers in Analytical Chemistry"
- H. Stover, "Synthesis and Study of Reactive Onion-Type Polymer Microspheres"
- K. Nozaki, "Asymmetric Hydroformylation Catalyzed by a Rhodium Complex Immobilized to Highly Cross-Linked Polystyrene"

Some of the invited lectures will appear in a future issue of *Pure and Applied Chemistry*. Julian Zhu of the Department of Chemistry at the University of Montreal will organize the 13th Conference on Polymers and Organic Chemistry, which will be held in Montreal, Canada, in 2008 or 2009.

 [www.tutms.tut.ac.jp](http://www.tutms.tut.ac.jp)

Prof. Shinichi Itsuno <[itsuno@tutms.tut.ac.jp](mailto:itsuno@tutms.tut.ac.jp)>, a professor in the Department of Materials Science at Toyohashi University of Technology, served as the conference cochairman of POC'06 along with Prof. Yasuhiro Uozumi.

**Bookworm**

- Biological and Synthetic Polymer Networks and Gels*, 31(1)  
*Fundamental Toxicology*, 24(4)  
*Macromolecular Symposia*—recent volumes, 24(4)  
*Magnituds, Unitats i Símbols en Química Física*, 31(1)  
*Obsessive Genius: The Inner World of Marie Curie*, reviewed by S. Penczek, 30(5)  
*Organometallics in Organic Synthesis*, 27(3)  
*Philosophy of Chemistry: Synthesis of a New Discipline*, reviewed by S. Weininger, 33(5)  
*Special Topic Articles Featuring the 2005 Winners of the IUPAC Prize for Young Chemists*, 25(3)  
*The International System of Units (SI)*, 8th edition, 30(5)  
*Volume G: Definition and Exchange of Crystallographic Data*, 32(5)

**Conference Call**

- Advanced Materials and Polymer Characterization, by Michael Hess, 39(5)  
 Advanced Materials—WAM III, by Piet Steyn and John Corish, 35(1)  
 Analytical Chemistry and Chemical Analysis, by Vladimir Zaitsev, 34(2)  
 Analytical Spectroscopy, by René Van Grieken, 37(5)  
 Carotenoids by George Britton, 38(2)  
 Chemical Thermodynamics, by Andrey Ya. Borschevsky and Svetlana S. Melkhanova, 28(3)  
 Chemistry for Agriculture, by Adam Pawelczyk, 35(5)  
 Chemistry in Kenya—Its Contribution to a Healthy Environment and Socio-Economic Development, by Sidney F.A. Kettle, 33(3)  
 European Science Education Research, by Roser Pintó, 31(4)  
 Food and Drug Administration—100 Years of Service, by Laure Joumel, 41(5)  
 Green Chemistry: A Tool for Socio-Economic Development and Environmental Protection, by Pietro Tundo and Kenneth R. Seddon, 32(6)  
 Green/Sustainable Chemistry by M. Kidwai, 37(5)  
 Heterocyclic Chemistry, by Girolamo Cirrincione and Anna Almerico, 31(3)  
 Innovation in Chemistry, by Xibai Qiu, 32(1)  
 Ionic Polymerization, by S. Sivaram, 30(4)  
 Macromolecule-Metal Complexes, by Francesco Ciardelli and Giacomo Ruggeri, 34(2)  
 Molecular Mobility and Order in Polymer Systems, by Anatoly Darinskii, 32(3)  
 New Directions in Teaching, Learning, and Evaluating the Chemical Sciences at the Tertiary Level, by

- Neelakanthi E. Gunawardena, 32(4)  
 New Science Education Assessment: The Challenge by Laure Joumel, 34(4)  
 Novel Materials and Synthesis, by Yuping Wu, 35(2)  
 Photodynamics, by Jesus Rubayo Soneira, 36(5)  
 Polymer Gels and Networks, by Miroslava Duskova and Michal Ilavsky, 30(4)  
 Polymers and Organic Chemistry, by Shinichi Itsuno, 33(6)  
 Polymers for Advanced Technologies, by György Bertalan, György Marosi, and Andrea Toldy, 28(3)  
 Polymers for Africa, by Dhanjay Jhurry, 36(2)  
 Solubility Phenomena, by Heinz Gamsjaeger and Wolfgang Voigt, 31(6)  
 Solution Chemistry, by Vojko Vlachy, 34(1)  
 ThermoML, by Michael Frenkel, 38(5)  
 Young European Chemists, by Leiv K. Sydnes, 36(1)

**Features**

- Art and Science: Looking in the Same Direction, by Maria Clara F. Magalhães and Rosa Maria Oliveira, 4(2)  
 Beyond Classical Chemistry: Subfields and Metafields of the Molecular Sciences, by Jesper Sjöström 9(5)  
 Chairing Scientific Symposia, by Roger Fenwick and Leiv K. Sydnes, 4(5)  
 Chemists' Understanding of the Public, by Peter Mahaffy, 14(4)  
 China's Petrochemical Technologies, by Jiming Wang, 4(3)  
 Frontier Science in the Middle East, by John M. Malin, 9(2)  
 GEOTRACES—Chemistry Takes Center Stage in Marine Science, by David Turner, 4(6)  
 GreenFacts: Communicating Science Information Clearly, by Manuel Carmona Yebra, 12(2)  
 Introducing EuCheMS, The European Association for Chemical and Molecular Sciences, by Gábor Náray-Szabó, 8(3)  
 Nanotechnology: Lessons from Mother Nature, by Alan Smith, 10(6)  
 Science Across the World: Exploring Science Locally and Sharing Insights Globally, by Marianne Cutler, 8(4)  
 The Ice that Burns: Burning Questions About Gas Hydrates, by Barbara Maynard, 3(4)  
 The Irrationality of Being: Fear of All Snakes, Spiders, . . . and Chemicals, by David A. Evans, 12(4)  
 Tools of the Trade: The IUPAC International Chemical Identifier (InChI): A New Standard for Molecular Informatics, by Alan McNaught, 12(6)

Using InChI, by Jeremy G. Frey, 14(6)  
 Tools of the Trade: The IUPAC Stability Constants Database, by Leslie D. Pettit, 14(5)  
 Would Einstein Have Approved?—A Discussion About the International Year of Physics, Minella Alarcon's Interview with Judy Franz, Martial Ducloy, Francis Allotey, and Masno Ginting, 6(6)

#### Internet Connection

Chemical Terminology at Your Fingertips, by Miloslav Nic, Jiri Jirat, and Bedrich Kosata, 28(6)  
 Free Information Resources for Chemists, by Leslie Glasser, Part 1, 26(4); Part 2, 29(5); Part 3, 30(6)  
 TOXNET—Information Resources and Services in Toxicology, by John Duffus, 27(4)

#### IUPAC Wire

2006 IUPAC Prizes for Young Chemists, 17(4)  
 37th International Chemistry Olympiad 2005, 19(1)  
 ACD/Labs' Free Naming Software Service Generates 200 000 IUPAC Names via the Web, 21(2)  
 Alexandra Navrotsky Awarded the 2006 Rossini Lecture, 18(2)  
 Capacity Building in Science, 18(5)  
 Choogle Search Engine Integrates ChemSketch, 21(2)  
 COCI Corner, 17(4)  
 David W.C. MacMillan is to be Awarded the 2006 Thieme-IUPAC Prize, obc(3)  
 Dewen Zeng Receives the 2006 Franzosini Award, 23(6)  
 Essential to You, 20(1)  
 Four Awards, One Passion: Chemistry, 19(5)  
 In Memoriam—Allan Ure, 21(5)  
 In Memoriam—Dale B. Baker, 22(2)  
 InChI 1.01, 23(6)  
 Industry and IUPAC Meeting Halfway, 21(6)  
 IUPAC Elections for the 2008-2009 Term, 21(6)  
 IUPAC President Attends the International Chemistry Olympiad, 22(6)  
 Malcom F.G. Stevens is Awarded the First IUPAC-Ritcher Prize, 18(5)  
 Memorandum on Cooperation with UNESCO, 19(4)  
 Permanent Access to Scientific Information in Southern Africa, 19(4)  
 Safety Training Program—Call for Host Companies, 21(5)  
 Safety Training Program—Call for Applicants, 20(2)  
 Strengthening International Science—A Recurring Catchphrase from ICSU, 21(1)  
 The XML Gold Book Online, 20(6)

The Year of . . . 19(2)  
 Two New CAs Join IUPAC, 20(1)  
 Young Chemists to the 41st IUPAC World Chemistry Congress, 20(6)

#### Making an impact

Atomic Force Microscopy and Direct Surface Force Measurements, 32(2)  
 Evaluated Kinetic Data for Combustion Modeling, 30(1)  
 Guidelines for NMR Measurements for Determination of High and Low pKa Values, 24(3)  
 Guidelines for Terminology for Microtechnology in Clinical Laboratories, 24(3)  
 How to Access Structure and Dynamics of Solutions: The Capabilities of Computational Methods, 21(3)  
 JCAMP-DX for Electron Magnetic Resonance, 23(3)  
 Measurement and Interpretation of Electrokinetic Phenomena, 29(1)  
 Nonspecific Sensor Arrays ("electronic tongues") for Chemical Analysis of Liquids, 32(2)  
 Postgenomic Chemistry, 29(1)  
 Reference Data for the Density and Viscosity of Liquid Aluminum and Liquid Iron, 20(3)  
 Standards, Calibration, and Guidelines in Microcalorimetry. Part 2. Calibration Standards for Differential Scanning Calorimetry, 27(6)  
 Supramolecular Assemblies with DNA, 33(2)  
 The International Harmonized Protocol for the Proficiency Testing of Analytical Chemistry Laboratories, 20(3)  
 Uncertainty Estimation and Figures of Merit for Multivariate Calibration, 23(3)  
 XML-Based IUPAC Standard for Experimental, Predicted, and Critically Evaluated Thermodynamic Property Data Storage and Capture, 22(3)

#### Mark Your Calendar

Listing of IUPAC Sponsored Conferences and Symposia, 42(1), 43(2), 38(3), 39(4), 43(5), 36(6)

#### Officers' Columns

A Balance—Difficult to Keep, Christoph Buxtorf, 2(4)  
 Chemistry—A Core Science with a Political Dimension, Leiv K. Sydnes, 2(5)  
 Encouraging Involvement Among Chemists, David StC. Black, 2(2)  
 IUPAC Within and Without, Bryan Henry, 2(6)  
 IUPAC: An Optimistic Future, Bryan R. Henry, 2(1)  
 The IUPAC Project System Revisited, Gus Somsen, 2(3)

**The Project Place**

- Adjustment, Estimation, and Uses of Equilibrium Reaction Constants in Aqueous Solution, 27(5)
- Analysis and Remediation of Arsenic Contamination in Groundwater, 14(3)
- Biophysico-Chemical Processes Involving Natural Nonliving Organic Matter in Environmental Systems, 24(6)
- Calibration of Organic and Inorganic Oxygen-Bearing Isotopic Reference Materials, 29(2)
- Chemical Education: Responsible Stewardship, 23(2)
- Defining a Data Standard for Near-Infrared Spectroscopy and Chemometrics, 12(3)
- Design of Polymer Education Materials for French-Speaking Countries, 27(5)
- Determination of Selenomethionine in Selenized Yeast Supplements, 24(5)
- Developments and Applications in Solubility, 22(1)
- Distance Learning in Toxicology, 25(1)
- Distance Learning in Toxicology: Effective Teaching through Technology, 20(4)
- e-Quiz for Promoting Chemical Education, 22(1)
- Flying Chemists Program—A Visit to India, 24(1)
- Global Climate Change—Translation and Dissemination of a Monograph for Secondary Schools, 25(1)
- Glossary of Terms Related to Solubility, 22(1)
- Herbal Medicine—Development of Methodologies and Protocols for Documentation, Evaluation of Safety and Efficacy, and Standardization, 17(3)
- International Funding for Chemical Research, 20(4)
- IUPAC Stability Constants Database Update, 26(1)
- Microstructure and Properties of Thermotropic Liquid-Crystalline Polymer Blends and Composites, 28(2)
- Nomenclature of Phosphorus-Containing Compounds of Biochemical Importance, 23(5)
- Putting Experimentation Back into Science Education, 22(4)
- Raising Awareness of the Chemical Weapons Convention and the Multiple Uses of Chemicals, 18(3)
- Selection and Use of Proficiency Testing Schemes for Limited Number of Participants (Chemical Analytical Laboratories), 24(5)
- Solubility and Thermodynamic Properties Related to Environmental Issues, 23(5)
- Solubility Data Series: Transition and 12 to 14 Main Group Metals, Actinide, and Ammonium Halates, 23(1)

- Teaching High-Temperature Materials Chemistry at the University, 26(6)
- Terminology for Self-Assembly and Aggregation of Polymers, 23(5)
- The Chemistry Clearing House as a Way to Better Chemistry Teaching, 25(6)
- Trace Elements Analysis: Role of Grain Size Distribution in Solid Reference Materials, 24(6)
- Validation of Qualitative and Semi-Quantitative (Screening) Methods by Collaborative Trial, 29(2)
- Young Ambassadors for Chemistry in Korea, 25(5)
- Young Ambassadors for Chemistry, 25(2)

**Provisional Recommendations**

- Definitions of Terms Relating to the Structure and Processing of Inorganic and Polymeric Gels and Networks, 19(3) and 23(4)
- Explanatory Dictionary of Key Terms in Toxicology, 30(2) and 19(3)
- Glossary of Terms Relating to Pesticides, 30(2) and 19(3)
- Glossary of Terms Used in Photochemistry, 28(1) and 31(2)
- Glossary of Terms Used in Toxicology, 23(4) and 28(5)
- Guidelines for Potentiometric Measurements in Suspensions—Practical pH Measurements in Soil Suspension, 23(4) and 28(5)
- JCAMP-DX for Electron Magnetic Resonance, 27(1)
- Nomenclature for Rotaxanes, 31(2)
- Quantities, Units, and Symbols in Physical Chemistry, 28(1) and 31(2)
- Standard Definitions of Terms Relating to Mass Spectrometry, 26(6)
- XML-Based IUPAC Standard for Experimental, Predicted, and Critically Evaluated Thermodynamic Property Data Storage and Capture (ThermoML), 27(1)

**Up for Discussion**

- “Inner Chemical Life” of Solids by Joachim Maier, 4(1)
- Can Ambiguous Terminology Cause a Barrier to Trade? letter by William Horwitz and reply by Paul De Bièvre, 15(2)
- Chemistry Enrollment in Germany: Bucking the Trend, by Terry Mitchell, 18(1)
- Emerging Issues in Developing Countries: Maintenance of Scientific and Technical Equipment—Challenges Faced by African Institutions, by Dzenko Mzengeza, 16(5)

## Emerging Issues in Developing Countries:

Standardization of Analytical Approaches and Analytical Capacity-Building in Africa, by Robert Maybury, Walter Benson, and David Moore, 17(6)

IUPAC in Beijing—Division Roundups Part II, 13(1)

Nanotechnology: Does It Have a Sporting Chance? by Alan Smith, 8(1)

Spectroscopic Data: The Quest for a Universal Format, by Robert Lancashire and Tony Davies, 10(1)

The Canadian National Committee for IUPAC's Travel Awards Program—A Success Story, by Chris. I. Ratcliffe, 16(6)

The Tyranny of the Chemist, by Eric Scerri, 11(3)

What Is Butadiene? by Karl-Heinz Hellwich, 17(2)

**Where 2B & Y**

Advanced Materials, 17–22 April 2006, Nara, Japan, 39(1)

Advanced Polymeric Materials, 11–15 June 2006, Bratislava, Slovakia, 40(2)

Advanced Polymers for Emerging Technologies, 10–13 October 2006, Busan, Korea, 40(1)

Bio calorimetry, 30 April–4 May 2006, Rio de Janeiro, Brazil, 39(2)

Biophysics, 3–7 March 2007, Baltimore, Maryland, USA, 35(6)

Chemical Biology, 9–13 September 2006, Antalya, Turkey, 36(3)

Chemical Thermodynamics, 30 July–4 August 2006, Boulder, Colorado, USA, 40(2)

Combustion, 6–11 August 2006, Heidelberg, Germany, 40(1)

Environmental Best Practices, 7–10 August 2006, Olsztyn, Poland, 36(4)

Environmental Best Practices, 7–10 August 2006, Olsztyn, Poland, 35(3)

Gas Analysis, 14–16 February 2007, Rotterdam, The Netherlands, 37(4)

Heterocyclic Chemistry, 15–20 July 2007, Sydney, Australia, 35(6)

Inorganic Chemistry—Metal-Nucleic Acids Interactions, 12–17 November 2006, Athens, Greece, 37(4)

Inorganic Materials, 23–26 September 2006, Ljubljana, Slovenia, 42(2)

Ionic Polymerization, 2–7 September 2007, Bayreuth, Germany, 37(3)

Macro and Supramolecular Architectures and Materials, 28 May–1 June 2006, Tokyo, Japan, 39(2)

Modern Physical Chemistry for Advanced Materials, 26–30 June 2007, Kharkiv, Ukraine, 38(4)

NanoTech Insight '07, 10–17 March 2007, Luxor, Egypt, 34(6)

Occupational Health and Safety Management, 27–29 September 2006, Nairobi, Kenya, 36(3)

Particle Separation, 9–12 July 2007, Toulouse, France, 38(4)

Phosphorus Chemistry, 15–21 April 2007, Xiamen, China, 41(1)

Physical Organic Chemistry, 20–25 August 2006, Warsaw, Poland, 41(2)

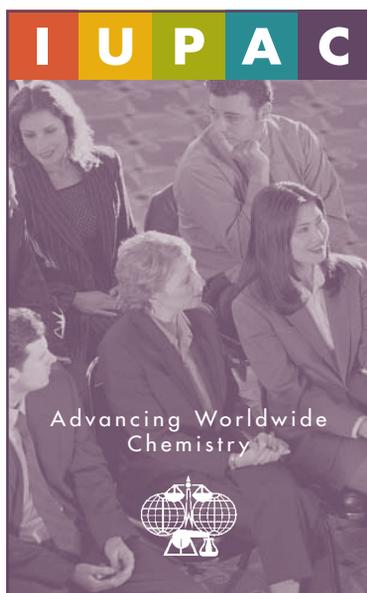
Polymers for Advanced Applications, 20–23 November 2006, Stellenbosch, South Africa, 34(6)

Radical Polymerization, 3–9 September 2006, Il Ciocco, Italy, 41(2)

Raman Spectroscopy, 20–25 August 2006, Yokohama, Japan, 35(5)

Supramolecular Assemblies with Nucleic Acids, 16–17 October 2006, Bordeaux, France, 36(4)

Theoretical and Computational Chemistry, 6–10 August 2006, Kunming, China, 39(1)



## IUPAC Prize for Young Chemists

*Supporting the future of chemistry*

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

**Call for Nominations:** Deadline is **1 February 2007**.

**For more information, visit [www.IUPAC.org/news/prize.html](http://www.IUPAC.org/news/prize.html)** or contact the Secretariat by e-mail at [secretariat@iupac.org](mailto:secretariat@iupac.org) or by fax at +1 919 485 8706.



# IUPAC Compendium of Chemical Terminology (Gold Book)

The screenshot shows the IUPAC Gold Book homepage. At the top, there is a search bar and the IUPAC logo. The main heading is "IUPAC GOLD BOOK". Below this, there is a navigation sidebar on the left with "Indexes" and "Source documents" sections. The main content area is titled "IUPAC Compendium of Chemical Terminology - the Gold Book" and contains a welcome message, a "You may start" section with three bullet points, and a "Browsing tips" section with three sub-sections: "Popup structures", "Interactive link maps", and "Ring index".

**Indexes**

- alphabetical
- chemistry
- math/physics
- general
- source documents

**You may start**

- by browsing the alphabetical index,
- by using one of the many thematic indexes,
- or by using the search entry in the navigation sidebar.

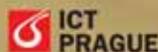
**Browsing tips:**

**Popup structures**  
Undefined linear structures display the actual structure of the molecule when you put a mouse cursor over them.

**Interactive link maps**  
Each entry contains interactive maps of its references and references, thus making navigation through related terms very convenient.

**Ring index**  
All ring-containing structures in the Gold Book were split to individual rings and these were organized in a comprehensive ring index.

This block contains a collage of four screenshots from the IUPAC Gold Book website. The top-left screenshot shows the "Ring index" page with a grid of icons for various ring types (C<sub>3</sub>H<sub>4</sub>, C<sub>4</sub>H<sub>6</sub>, C<sub>5</sub>H<sub>8</sub>, C<sub>6</sub>H<sub>10</sub>, etc.). The top-right screenshot shows a detailed entry for "Aliphatic & Aromatic" with chemical structures and text. The bottom-left screenshot shows an "Interactive link map" with a complex network of nodes and arrows. The bottom-right element is a CD-ROM with the IUPAC Gold Book logo, the text "Version 1.0.0", and the website URL "http://goldbook.iupac.org".



Created in the Laboratory of Informatics and Chemistry  
of the ICT Prague.

[http:// goldbook.iupac.org](http://goldbook.iupac.org)

CD INSIDE