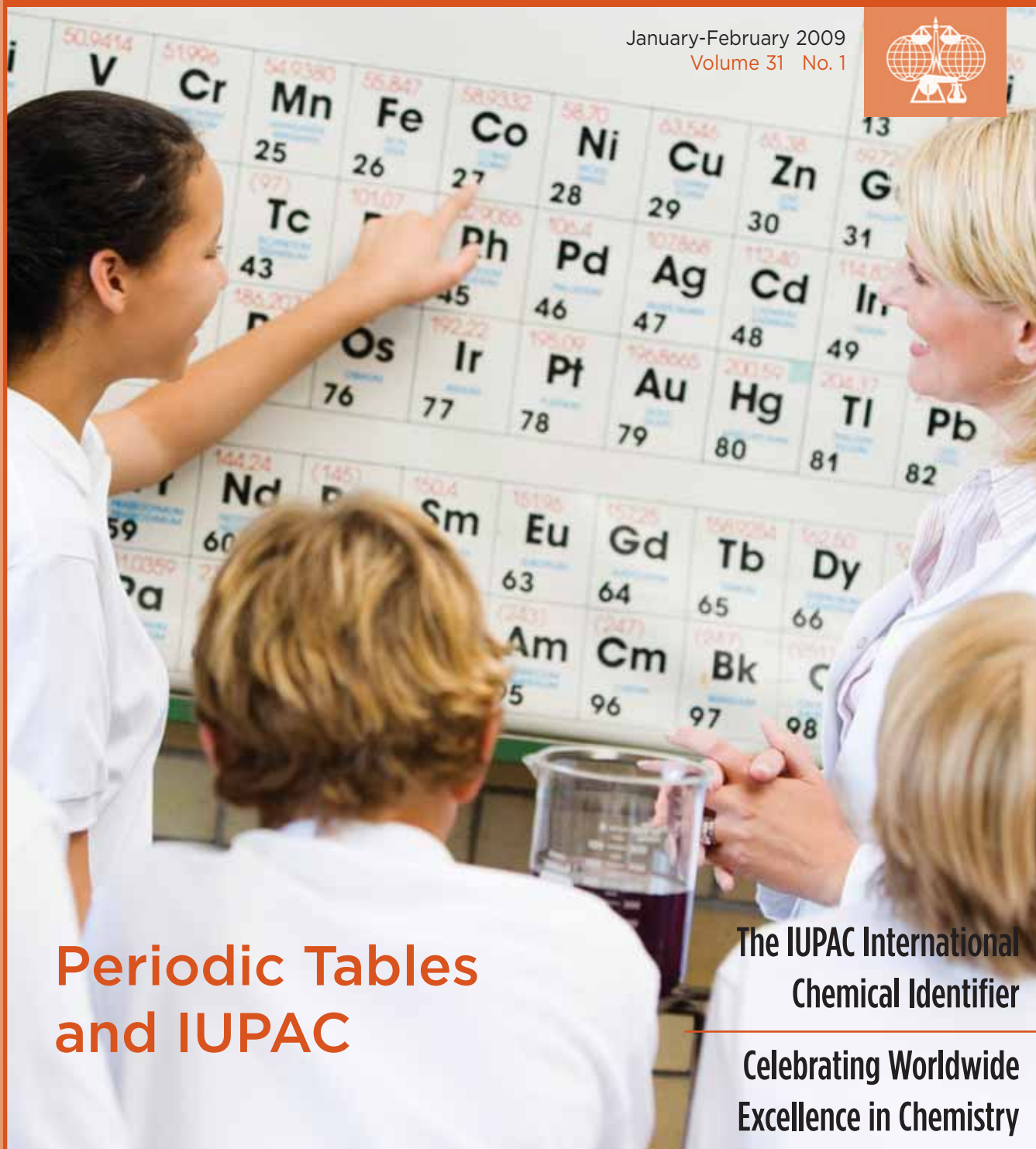


The News Magazine of the
International Union of Pure and
Applied Chemistry (IUPAC)

CHEMISTRY

International

January-February 2009
Volume 31 No. 1



**Periodic Tables
and IUPAC**

**The IUPAC International
Chemical Identifier**

**Celebrating Worldwide
Excellence in Chemistry**



From the Editor

CHEMISTRY International

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Applied Chemistry (IUPAC)

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Something old, something new, something borrowed, something blue... that recipe is for something else, yet it applies surprisingly well to the contents of this issue of *Chemistry International*.

Something old would be the description of IUPAC's position with regard to the periodic table. The feature article by Jeffery Leigh (page 4)



reminds the reader that "IUPAC's primary concern is with unequivocal and unambiguous communication," and in the context of a periodic table format, IUPAC's recommendation is only for the groups numbering from 1 to 18, and no more. Leigh demonstrates that one table does not fit all uses, and

the periodic table as we know it today is an icon often wrongly associated with IUPAC.

Something new would be the focus of Steve Heller and Alan McNaught's article (page 7) on InChI, known as "in-chee." The IUPAC International Chemical Identifier (InChI) continues to be developed and is becoming more widely used throughout the chemistry community. In striking contrast to the traditional nomenclature for which IUPAC is well known, InChI constitutes a contemporary tool that renders computer algorithms efficient at searching molecular representations.

Something borrowed would be the feature by Gábor Magyarfalvi (page 10) reporting on the 2008 International Chemistry Olympiad held in Hungary in July 2008. It is "borrowed" in the sense that the Olympiad continues to build on its success in generating enthusiasm among new generations of chemists, and that endeavor is applauded by IUPAC. IUPAC is proud to support the Olympiad, particularly by facilitating the participation of students from economically disadvantaged countries. Magyarfalvi, a former medalist at the 1989 Olympiad, takes the reader on a tour of what was a pretty exciting '08 event. In 2009, it will take place in the U.K.

Something blue—a symbol of hope—in this case would be the plethora of new applications engendered by nanotechnologies. In their article, Hilda Coulsey and Alan Smith (page 13) review the impact nanotech is having on drug development and consumer healthcare products.

So, here they are, the four items of a good-luck token. With that, I simply wish you all the best for 2009.

Fabienne Meyers

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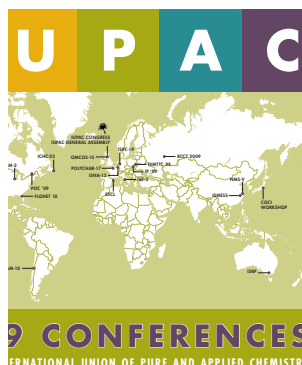
Cover: The periodic table is a familiar icon present in science classrooms around the world. IUPAC's only recommendation concerning the periodic table stipulates the Group numbering of 1 to 18.

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A complimentary map/2009
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Toward the Next Renaissance of Chemical Science in the 21st Century

by Jung-Il Jin



The public's opinions and attitudes towards chemistry are exceedingly negative. Many people do not appreciate that chemistry has contributed significantly to the quality of human life. They also cannot believe that chemistry continues to play a major role as a problem solver for such urgent global conundrums as energy, the environment, natural resources, human health, and personal and national security. Despite all this, I foresee with great positivity that a Renaissance of Chemical Science will blossom in the 21st century. This will occur because of chemistry's intrinsic creative nature and its ability to respond to societal needs.

However, we should not for a second harbor the belief that the next Renaissance of Chemical Science will inevitably envelop us. It can be achieved only through our incessant, diligent pursuit of it. It is true that crises generate chances, and challenges offer opportunities. It is particularly fortunate for us as chemists that most of the contemporary and near future challenges facing this planet can be solved through the power of chemistry. This power should be nurtured by all the chemical scientists throughout the world.

There is no doubt—or at least I strongly believe it—that IUPAC is the only organization that can pull together the ingenuity and creativity of all the world's chemists to cope with—and find answers to and remedies for—the scientific and technological demands necessary for the sustainable development of the world. If this statement elicits any doubt among IUPAC members, I would like to have them explain why. After all, it is the responsibility of all IUPAC members to explain to others how IUPAC can pull together chemists worldwide.

The year 2009 has special meaning and significance to IUPAC. It offers us a golden opportunity to

attract international attention to the importance of the chemical sciences and, at the same time, to the eminent historical role that IUPAC has played at the forefront of the world chemical community. The focal point of this attention is likely to be the news that 2011 will be the International Year of Chemistry; soon to be proclaimed by the United Nations General Assembly. The year 2011 will be the centenary of Marie Curie's receipt of the Nobel Prize in Chemistry. Also, we will be celebrating 100 years since the formation of the International Association of Chemical Societies (IACS), the predecessor to IUPAC. We have to make the most of these opportunities to achieve several important goals:

- improve the public appreciation of chemistry
- entice more of the promising younger generation into the fields of chemical sciences
- regain for chemistry the respect and admiration that it deserves for a century of unprecedented progress in technologies
- start building the groundwork for the second century of IUPAC

Progress in chemistry in the past century has brought us material abundance and improved health care and disease control. However, in the second half of the last century, public acceptance of chemistry and chemicals has deteriorated for various reasons that we all are very well aware of. Needless to say, a part of this negative public opinion is groundless and/or politically misguided, but it is a fact that we must overcome.

All of the present century's new slogans such as sustainable development, green growth, environmental protection and friendliness, innovative energy technologies, improved personal and national security, functional longevity, and more, can find technical solutions from the chemical sciences. International cooperation coupled with individual chemists' creativity and backed by constructive social consciousness, should lessen all the global anguish. Such a socio-scientific analysis of global issues, and synthetic efforts to find speedy answers to them, promptly and rightfully imply that IUPAC should assume the central position, should be the nexus, to which all the chemical scientists and local societies will network.

This brings us to the ultimate and most sensi-

I foresee with great positivity that a Renaissance of Chemical Science will blossom in the 21st century.

tive question: Is IUPAC ready and able to assume a leadership role in the world chemical community? Is IUPAC really communicating effectively with the world chemistry community and general public? Are we indeed addressing global issues in an authoritative and convincing manner? I am more than confident that IUPAC, with minor adjustments in communication, inner as well as outer, and administration, in style and philosophy, can fill these roles superbly.

Recently, I had wonderful meetings with Latin American representatives, American Chemical Society officers, and leaders of major Asian Chemical communities. Soon, I plan to meet with VIPs of African and Arabian chemical societies and representatives of the European Union countries' chemical societies. Bringing chemistry back to the center of the natural sciences and preparing globalized and successful celebrations of the International Year of Chemistry are the foci of my consultations with worldwide leaders. I

have thoroughly enjoyed the personal contacts with these individuals and have appreciated the valuable opportunities to hear their views on IUPAC, in general as well as in specific, and to understand the local issues for which IUPAC's assistance is essential. Many IUPAC officers have joined me in these meetings, for which I am most grateful.

As I wrote in *CI* a year ago, we have to be ready, before it's too late, to greet the second century of IUPAC, with hope and confidence. For this, constructing a solid groundwork is indispensable. We shall endeavor to make big strides in 2009 toward the next Renaissance of Chemical Science despite the global difficulties we hear about everyday.

I wish you all the best. 🏆

Jung-Il Jin <jijin@korea.ac.kr> has been IUPAC president since January 2008. Previously in IUPAC, he served as president of the Polymer Division. Jin is a professor at the Korea University in Seoul, Korea.



IUPAC strives to become the global leader in advancing knowledge and understanding of chemistry worldwide. Over the next decade IUPAC will continue its effort to increase membership by building partnerships among scientists around the world. Our goal is to celebrate IUPAC's centennial in 2019 with a truly global membership base of at least 100 countries. **Best wishes for a happy and successful 2009 from the IUPAC Officers and Secretariat!**



Periodic Tables and IUPAC

by G. Jeffery Leigh

In more than one IUPAC publication you will find a periodic table, sometimes referred to as an IUPAC Periodic Table. Invariably this version of the table is what was once known as the long form, in which the various Groups are numbered from 1 to 18 (figure 1). The so-called short form cannot display the 1-18 numbering, and has largely fallen into disuse. The implication is that this is an IUPAC-approved table (see, for example, Lavelle, 2008), and indeed a Google search of the Web will unearth several entries for "IUPAC approved Periodic Table." Figure 1 is based upon the periodic table that appears on the IUPAC website, though nowhere is it stated that that version is "approved." In fact, IUPAC has not approved any specific form of the periodic table, and an IUPAC-approved form does not exist, though even members of IUPAC themselves have published diagrams titled "IUPAC Periodic Table of the Elements." However, the only specific recommendation IUPAC has made concerning the periodic table covers the Group numbering of 1-18.

The usual presentation of the periodic table which we use (figure 1) is subject to continual updating as new elements are produced (Holden and Coplen, 2004). Nevertheless the conventional long form with the 1-18 group numbering, which goes back at least to the 1920s (Paneth, 1923), is certainly not ideal for every purpose. Teachers especially find that it does not fulfill all their requirements. For example, it is not strictly consistent with all our ideas about electronic structure.

The periodic table was developed from considerations of chemical properties and atomic weights



Monument honoring Dmitri Mendeleev and the periodic table, in front of the Faculty of Chemical and Food Technology of the Slovak University of Technology in Bratislava, Slovakia.

and even then the latter arrangement was not without inconsistencies. Once the significance of atomic electronic configurations was realized, the table was adapted to be almost completely consistent with them. There are minor discrepancies, such as copper seeming to prefer the arrangement $d^{10}s^1$, rather than d^9s^2 as one might expect. As the long form places them, the lanthanoids and actinoids sit rather uncomfortably each in a single place, but should lanthanum and actinium be grouped directly with their congeners? Hydrogen is always a problem. In the conventional long form, hydrogen appears as in the first short period along with helium, as a kind of pseudo-alkali metal. Logically, however, one might consider it as having an outer shell lacking one electron for completion, so that it is also a kind of halogen, maybe a pseudo-halogen, though that term may confuse some readers. There is no absolutely satisfactory position for hydrogen (Scerri, 2007).

Some people have found the simple long-form periodic table unsatisfactory for aesthetic reasons. The possibility of producing a "best" form has been discussed recently (Scerri, 2008). Just as the d-transition elements were introduced into the old short form of the table to make a long form (figure 1), the actinoids and lanthanoids have been further inserted to make an even longer form (figure 2). A plethora of shapes have been proposed for the table, both two- and three- dimensional, and triangular or circular or square. For a selection see van Spronsen, 1969. None is ultimately the "correct" or "best" shape. Teachers have

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	57-71	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	89-103	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg							
57-71	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
89-103	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		

Figure 1. Periodic Table adapted from <www.iupac.org/reports/periodic_table>, accessed 19 September 2008.

Periodic Tables and IUPAC

A table showing the periodicity of the properties of many chemical elements, from the first English edition of Dmitrii Mendeleev's Principles of Chemistry (1891, translated from the Russian fifth edition).

Group numbering later propagated by IUPAC seemed (and still seems) to be the most generally useful. It is now widely accepted.

The 1990 edition of *Nomenclature of Inorganic Chemistry*, page 280, described quite clearly what was and still is IUPAC's position concerning forms of the periodic table and Group numbering:

"While it is neither the intent, nor the purpose of the IUPAC Commission on the Nomenclature of Inorganic Chemistry (since 2000 superseded by the IUPAC Chemical Nomenclature and Structure Representation Division) arbitrarily to set the format of the Periodic Table to be used in all parts of the world, it is the responsibility of the Commission to offer broadly useful nomenclature proposals where direct conflicts in usage occur. After extensive discussions and many public appeals for comment, the Commission concluded that the use of the 1 to 18 numbering for the 18 columns provides a clear and unambiguous labelling for reference. . . ."

This is still (2008) the opinion of the division. For references to this discussion see Fernelius and Powell, 1982; Fluck, 1988; Fernelius, 1986; and Emsley, 1985.

The long, long forms of the periodic table with 32 columns shown in figures 2 and 3 also show the 1-18 Group numbering. Continuous numbering from 1 to 32 across all 32 columns would not really meet IUPAC requirements.

. . . they should not amend the recommended 1-18 Group numbering unless and until they can propose something that meets both their own criteria and those of IUPAC for clarity, simplicity, and brevity.

Nevertheless, teachers and others should not hesitate to develop new forms of the periodic table, and to publish them if they so wish. However, they should not amend the recommended 1-18 Group numbering unless and until they can propose something that meets both their own criteria and those of IUPAC for clarity, simplicity, and brevity. Above all, they should refrain from approaching IUPAC for approval of a new form of periodic table unless these criteria are met. Until then, there is unlikely to be a definitive IUPAC-recommended form of the periodic table. 🏠

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The IUPAC International Chemical Identifier (InChI)

by Stephen R. Heller and Alan D. McNaught

The properties and behaviors of chemical substances are generally interpreted and discussed in terms of their molecular structures, and to convey structural information, chemists use diagrammatic representations supplemented by verbal descriptions. In order to have a means of specifying or describing a chemical structure in words, conventional chemical nomenclature was developed.

Systematic nomenclature provides an unambiguous description of a structure; a diagram of which can be reconstructed from its systematic name. However, there are other means of specifying molecular structures. Those based on "connection tables" (coded specifications of atomic connectivities) are more suitable than conventional nomenclature for processing by computer, as they are matrix representations of molecular graphs readily governed and handled by graph theory. In parallel with its continued development of conventional nomenclature, IUPAC has developed a structural identifier that can be readily interpreted by computers, or more precisely, by computer algorithms.

The IUPAC International Chemical Identifier (InChI) is a freely available, nonproprietary identifier for chemical substances that can be used in both printed and electronic data sources. It is generated from a computerized representation of a molecular structure diagram, produced by chemical structure-drawing software. Its use enables linking of diverse data compilations and unambiguous identification of chemical substances. A full description of the Identifier and software for its generation are available from the IUPAC website.¹ In addition, an unofficial, but helpful compilation of answers to frequently asked questions has been compiled by Nick Day of the Unilever Centre for Molecular Science Informatics as part of his Ph.D. project on the Chemical Semantic Web.² A full account of the InChI project is in preparation.³ Commercial structure-drawing software that generates the Identifier is available from several organizations, listed on the IUPAC website.¹

The conversion of structural information to the Identifier is based on a set of IUPAC structure conventions, and rules for normalization and canonicalization (conversion to a single, predictable sequence) of an

input structure representation. The resulting InChI is simply a series of characters that serve to uniquely identify the structure from which it was derived. This conversion of a graphical representation of a chemical substance into the unique InChI character string can be carried out automatically by any organization, and the facility can be built into any program dealing with chemical structures.

The InChI uses a layered format to represent all available structural information relevant to compound identity. InChI layers are listed below. Each layer in an InChI representation contains a specific type of structural information. These layers, automatically extracted from the input structure, are designed so that each successive layer adds additional detail to the Identifier. The specific layers generated depend on the level of structural detail available and whether or not allowance is made for tautomerism. Of course, any ambiguities or uncertainties in the original structure will remain in the InChI.

This layered structure design offers a number of advantages. If two structures for the same substance are drawn at different levels of detail, the one with the lower level of detail will, in effect, be contained within the other. Specifically, if one substance is drawn with stereo-bonds and the other without, the layers in the latter will be a subset of the former. The same will hold for compounds treated by one author as tautomers and by another as exact structures with all H-atoms fixed. This can work at a finer level. For example, if one author includes double bond and tetrahedral stereochemistry, but another omits stereochemistry, the latter InChI will be contained in the former.

The InChI layers are:

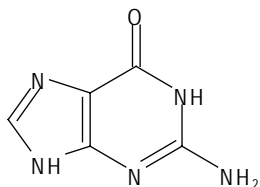
1. Formula
2. Connectivity (no formal bond orders)
 - a. disconnected metals
 - b. connected metals
3. Isotopes
4. Stereochemistry
 - a. double bond (Z/E)
 - b. tetrahedral (sp³)
5. Tautomers (on or off)

Charges are not part of the basic InChI, but rather are added at the end of the InChI string.

The IUPAC International Chemical Identifier (InChI)

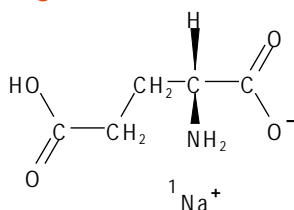
Two examples of InChI representations are given below. It is important to recognize, however, that InChI strings are intended for use by computers and end users need not understand any of their details. In fact, the open nature of InChI and its flexibility of representation, after implementation into software systems, may allow chemists to be even less concerned with the details of structure representation by computers.

guanine



InChI=1/C5H5N5O/c6-5-9-3-2(4(11)10-5)7-1-8-3/
h1H,(H4,6,7,8,9,10,11)/f/h8,10H,6H2

monosodium glutamate



InChI=1/C5H9NO4.Na/c6-3(5(9)10)1-2-4(7)8;/h3H,1-
2,6H2,(H,7,8)(H,9,10);/q;+1/p-1/t3-;/m1./s1/fC5H8NO4.
Na/h7H;/q-1;m

The layers in the InChI string are separated by the '/' character followed by a lowercase letter (except for the first layer, the chemical formula) with the layers arranged in predefined order. In the examples, the following segments are included:

InChI version number

/ chemical formula

/c connectivity-1.1 (excluding terminal H)

/h connectivity-1.2 (locations of terminal H, including mobile H attachment points)

/q charge

/p proton balance

/t sp³ (tetrahedral) parity

/m parity inverted to obtain relative stereo

(1 = inverted, 0 = not inverted)

/s stereo type (1 = absolute, 2 = relative, 3 = racemic)

/f chemical formula of the fixed-H structure if it is different

/h connectivity-2 (locations of fixed mobile H)

/q charge

/t sp³ (tetrahedral) parity

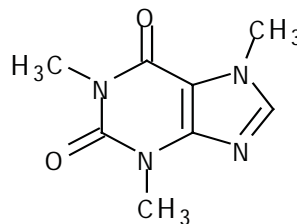
/m parity inverted to obtain relative stereo

(1 = inverted, 0 = not inverted, . = inversion does not affect the parity)

/s stereo type (1 = absolute, 2 = relative, 3 = racemic)

One of the most important applications of InChI is the facility to locate mention of a chemical substance using Internet-based search engines. This is made easier by using a shorter (compressed) form of InChI, known as InChIKey. The InChIKey is a 27-character representation that, because it is compressed, cannot be reconverted into the original structure, but it is not subject to the undesirable and unpredictable breaking of longer character strings by some search engines. The usefulness of the InChIKey as a search tool is enhanced by its derivation from a "standard" InChI, (i.e., an InChI produced with standard option settings for features such as tautomerism and stereochemistry). An example is shown below; the "standard" InChI is denoted by the letter "S" after the version number.

caffeine



InChI=1S/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/
h4H,1-3H3

First block (14 letters)
Encodes molecular
skeleton (connectivity)

Second block (8
letters), encodes
stereochemistry
and isotopes

Character indicat-
ing the number
of protons ("N"
means neutral)

InChIKey=**RYYVLZVUVIJVGH-UHFFFAOYSA-N**


Flag character ("S") indicates
standard InChIKey (produced from
standard InChI)

Flag character for
InChI version: "A"
for version 1

InChIKey also allows searches based solely on atomic connectivity (first 14 characters). Software for generating InChIKey is available from the IUPAC website.¹

The IUPAC International Chemical Identifier (InChI)

The enormous databases compiled by organizations such as PubChem,⁴ the U.S. National Cancer Institute, and ChemSpider⁵ contain millions of InChIs and InChIKeys, which allow sophisticated searching of these collections. PubChem provides InChI-based structure-search facilities (for both identical and similar structures),⁶ and ChemSpider offers both search facilities and web services enabling a variety of InChI and InChIKey conversions.⁷ The NCI Chemical Structure Lookup Service⁸ provides InChI-based search access to over 39 million chemical structures from over 80 different public and commercial data sources.

In the age of the computer, the IUPAC International Chemical Identifier is an essential component of the chemist's armory of information tools, enabling location and manipulation of chemical data with unprecedented ease and precision. 

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Alan McNaught <mcnaught@ntlworld.com>, retired from RSC, is one of the InChI's fathers; with broad expertise in publication and nomenclature, he has been involved in IUPAC activities for many years (including ICTNS, CPEP, and Div VIII) and with InChI since day one. Steve Heller <steve@hellers.com>, from NIST, is also a father of InChI, stimulating development and making the identifier known to the community.

 www.iupac.org/inchi/

Use of InChI and InChIKey in the XML Gold Book

The *IUPAC Compendium of Chemical Terminology* (aka Gold Book) is a valuable resource to all chemists. It contains definitions of many chemistry-related terms and, thus, drawings of many chemical structures. In producing the XML version of the Gold Book we use InChI both internally and as meta-data on Gold Book pages to enable search engines to index this information.

As early adopters of InChI, we started to include InChIs of molecules in pages of indi-

vidual terms in 2006. The InChIs are hidden from users, but are visible to search engines.

Thus, it is possible to reach appropriate Gold Book pages by searching for InChI or InChIKey code using any popular search engine.

To provide chemists with as many ways to navigate the website as possible, we created a few chemistry-related indexes. For this task, InChI was an invaluable tool that saved us much time and effort because it enabled us to



Google search for the InChIKey of thiolane, Gold Book ring index takes the first position.

compare structures in different entries using a simple text comparison.

Maybe the most interesting of the available chemical indexes in the Gold Book is the ring index. In this case, we not only used InChI to compare rings extracted from individual molecules using our in-house tools, but we used InChIKey to name files of individual rings. In this way, we solved a problem of giving the files useful and unique names while creating yet another way to make our structures visible to the outside.

For questions/comments, please contact Bedrich Kořata <Bedrich.Kosata@vscht.cz>.

 <http://goldbook.iupac.org/>

The blue rectangle highlights InChIs and InChIKeys (shown here in the beta-test version of the 25 characters) that are normally invisible to the user.

Celebrating Worldwide Excellence in Chemistry

by Gábor Magyarfalvi

The 40th International Chemistry Olympiad (IChO) returned to one of the countries that founded the event. In July 2008, the competition was held for the fourth time in Hungary. The world and the Olympiad have changed considerably since that event 20 year ago. The change is even more pronounced when we compare it to the very first IChO in Prague in 1968, a rather local meeting of 18 students from three Central European countries. We were happy to have a Hungarian mentor and a student from that first Olympiad as special guests during the Olympiad.

Participation and diversity have greatly increased since the early IChOs. This year, 257 students from 66 countries participated. The map on page 11 shows the countries affiliated with the Olympiad. Three countries were observing in preparation for joining. Sadly, Africa is underrepresented on the map, especially since the Egyptian team could not participate this year.

This year, for the first time, a generous grant of USD 10 000 from IUPAC helped economically disadvantaged countries participate in the Olympiad. The Steering Committee of the IChO allocated the money to help with the travel expenses and participation fees of seven Central Asian and Latin American nations.

In his welcoming message, George A. Olah, Nobel laureate patron of the event, said "There are only a few meetings in chemistry that have such a wide participation, reaching almost to 80 percent of the population of the globe." Indeed, one of the main purposes of the meeting is to provide students with

international experience and help them develop a network of friends from around the world who share the same interest. The core goals of the Olympiad are to motivate participants to excel and build their self-confidence as they solve interesting and challenging chemistry problems. Many former participants are working their way towards prominence in our science.

The schedule and rules for the Olympiad are largely unchanged from the practices described earlier in an earlier *CI* article by Jan Apotheker (Jul-Aug 2005 *CI*, p. 3). The five-hour practical and theoretical exams are spread over two days. The rest of the schedule was devoted to sightseeing and exploring Hungary and Hungarian culture. There was time for team-building

games and a chemistry demonstration lecture. A team of 80 Hungarian students, many of whom spoke the languages of the visitors helped ensure that the participants relaxed and enjoyed their time.

The accompanying mentors had considerably less time for tourism. Finalizing, translating, and correcting the exams kept them busy during the 10 days of the Olympiad. They exchanged souvenirs and e-mail addresses like the students, but the exchange

of teaching experiences and chemistry problems was equally important.

Although the form of the Olympiad has not changed, the style and content of the exams was slightly altered this year. Sometimes, the Olympiad problems necessarily extend beyond the secondary school curriculum of most countries. A syllabus and rule set guides the organizers when preparing the exams for acceptance by the International Jury. This syllabus was reorganized this year to make preparation for the Olympiad easier. Solving chemical problems requires the knowledge of basic chemical concepts and skills together with factual data. The new syllabus tries to define the factual knowledge and strictly limits the number of advanced topics the students should be familiar with.

The organizers' intentions were to move the focus toward challenging students' creativity and thinking rather than assessing familiarity with recent scientific achievements or university-level materials. Students



Students from the world over participated in the International Chemistry Olympiad, which features theoretical and practical exams designed to challenge students' creativity.



were not expected to memorize formulas or facts, but they were asked to apply well-known concepts to solve problems. This meant that the problem topics were interesting, but a little less prominent than usual, with less state-of-the-art science included.

The advanced topics were announced and demonstrated in a 40-problem preparatory set that was published in January. The set, which illustrates the style and difficulty of the problems, is intended to assist students during preparation for the test. Officially, two weeks of special preparation are allowed. The topics and competition problems are available on the Olympiad website.

The Science Committee began working on the problems in 2006. Most team members were affiliated with Eötvös Loránd University of Budapest, the main organizing institution and the venue for the exams. Hungary is fortunate enough to have many individuals with Olympiad experience, so other major Hungarian universities and a research institute were represented on the board. A core team of 12 persons worked in secrecy on the problems. By the time of the Olympiad, this group had been expanded to 37, including young colleagues and graduate and undergraduate students who could help run the exams and evaluate the answers. The latter was no small feat considering the 257 papers and the one-day deadline. The team's most important contribution was to test the exams two weeks before the Olympiad and then correct each

other's work. The thorough checking allowed organizers to eliminate virtually all ambiguities in the questions and the marking scheme. The equipment and procedure of the practical tasks was also finalized after testing and organizers obtained a good set of statistical data on the variability of the results.

All this work made the task of the International Jury easier. There were no major alterations of the exams when discussed by the delegations. The usually exhausting jury discussions on the problems and marking were over in two hours and left the mentors contented. As each student can work in a language of his or her choice, all problems had to be formulated so that the answers were nonverbal (multiple choice or numerical).

The laboratory portion of the exam poses more difficulties. Setting up 270 identical work desks required all student laboratories of the Chemistry Institute and the assistance of all technicians. To illustrate the scale of the logistical effort, there were more than 12 pallets of equipment that arrived from just the main supplier. When preparing the tasks, organizers had to consider the cost, but their main consideration was that most



Sixty-six countries participated in the 2008 International Chemistry Olympiad. Unfortunately, Africa was under represented.

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secondary school students have very little laboratory experience. It has happened in previous Olympiads that carrying out the explicitly detailed procedures in the five hours of the exam would have been difficult even for trained chemists. Organizers kept the three types of tasks that typically comprise the exam (qualitative and quantitative analysis, preparative work), so the challenge was not in the running of the experiments, but their planning and interpretation.

The simple synthesis task was the acetylation of glucose and isomerisation of the β isomer into the α form. This latter step was to be followed by thin-layer chromatography. Performance on this task was marked based on the yield, while the titration task was graded according to accuracy. The quantitative results led to the determination of the composition of the precipitate

that forms in the reaction of zinc ions and potassium hexacyanoferrate(II). The most difficult task proved to be the simplest. Students were given eight colorless solutions, indicator paper, a heat gun, test tubes, and a solubility table. It took a lot of effort for them to identify the two ions present in each solution from the long list of possible answers.

The theoretical problems as usual, involved a wide range of chemical subdisciplines (organic, inorganic, analytical, and physical chemistry). However, unlike in recent years, there was no spectroscopy, nor quantum chemistry among the topics. The problem sets usually include references to the scientific achievements of the host country. These references were mainly relegated to the preparatory problems, but still the chemistry of carbocations (George A. Olah) and the synthesis and metabolism of vinpocetine (an original drug discovered in Hungary) were the subjects of a task.

Organizers tried to include relatively easy problems together with questions that challenged even the best students. Probably three tasks out of the nine belonged to the first category: a pH calculation with a twist, the chemistry of thallium iodides, and the synthesis of azulene from naphthalene. In one problem, students had to find out that during the photolysis of aqueous cerium(III) solutions water is split into hydrogen and oxygen. In another problem, they worked out the crystal structure of methane and chlorine hydrates. The favorite task of many mentors was a kinetics prob-

lem. From relatively simple measurements students were able to find out the mechanism and the molecular level processes of the oxidation of dithionate ions. Another task that solicited a lot of emotion (praise and shock equally) was based on the chemistry of some barium salts, but their identification was rather difficult based on the information given.

The distribution of the scores was encouraging. Hardly any students came away without at least partial

marks. The highest scores in both the theoretical and practical tasks were achieved by Yongping Fu of China, with 87 percent of the total score. Although the competition is strictly between individuals, the list of the best students is dominated by participants from Asian countries and former Soviet republics. Sixty percent of participants returned home with a medal.

Hopefully, all participants were left with a sense of achievement and a memory of a unique experience.

The organization of the Olympiad was centered at the Eötvös Loránd University, with the Hungarian Chemical Society as a co-organizer. Most of the considerable cost of the event was carried by the Hungarian Ministry of Education, with significant support coming from the chemical and pharmaceutical industry. Gedeon Richter Ltd. was the main corporate sponsor; Servier, EGIS, and MOL were sponsors; and Sigma-Aldrich, Microsoft, Cerbona, and Heidolph were partners. The participation fee paid by the countries is mainly a nominal contribution.

The next Olympiad, which will take place in Cambridge, United Kingdom, will be a cooperative effort between the Universities of Cambridge and Oxford and the Royal Society of Chemistry. Japan, Turkey, USA, and Singapore will host events in the coming years, so the future of the Olympiads seems to be bright and secure. 🏆

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👉 www.icho.hu

For information about the 2009 event, see <www.icho2009.co.uk>.



Nanotechnology in Good Health?

by Hilda Coulosey and Alan Smith

The business environment for large pharmaceutical companies is changing. Profits from blockbuster drugs are under threat due to expiring patents. Healthcare will change because of the ever-increasing cost to develop drugs. The only way forward, to become more efficient in cost and patient care, will be through nanotechnology.

For those not familiar with nanometres (nm), they are one millionth of a millimetre. To appreciate this more easily, a human hair is about 80 000 nanometres in diameter; red blood cells are about 5 000-nm across; the AIDS virus is approximately 100-nm long; and DNA is less than 3 nm. At the nano-scale, properties change and the reason for this can be understood if one considers a cube of just about any substance, which would have one in 10 million of the atoms on the surface. However, for a one-nanometre cube, 80 percent of the atoms are on the surface. This increased surface area can be beneficial for many technologies and products. For several years now, car exhaust catalysts have relied on nanotechnology and the increased surface area it provides to break down exhaust fumes.

A project on emerging nanotechnologies at the Woodrow Wilson International Center for Scholars has to date cataloged over 500 manufacturer-identified, nanotechnology-based products.¹ These include numerous sun-screen products in which the nanoparticles of titanium dioxide let the “good” ultraviolet light through but reflect the “bad” UV. In addition, there are an increasing number of products—ranging from socks and towels to refrigerators and food storage containers—that incorporate silver nanoparticles, which provide antimicrobial properties. Many wound dressings now contain silver nanoparticles to aid faster recovery. The earliest applications for nanotechnology products have been in sporting goods (see Jan-Feb 2006 *CI*, p. 8), where the margins are high; for example Federer’s tennis racket, lighter weight materials in Formula One racing cars, and Floyd Landis’s cycle frame. Once established in those markets, the technology moves down to commodity products, which is certainly what is happening with most automotive companies.

For consumer healthcare products, we are seeing many new types of toothpaste on the market that are based on nanotechnology. Guaber in Italy makes BlanX, containing NANOREPAIR, which is treated nanoparticulate hydroxyapatite for filling the minute cracks that occur in the enamel of teeth. A similar system is available for hair-damage repair, which is called TANAGRA,

and contains “nano-molecular” keratin to block cracked or rough hair. L’Oreal has the largest number of patents relating to nanotechnology in health and personal care,² many of which are for

antiaging products. Their significant R&D expenditures on nanocapsule technology are directed at delivering agents such as vitamin A and retinol into the skin.

However, the most promise for nanotechnology will come from “nanomedicine,” which has been described as the application of nanotechnology to achieve breakthroughs in healthcare.³ Nanomedicine promises to impact all stages of healthcare:

- preventative medicine
- diagnosis
- therapy
- follow-up care

Proponents of nanomedicine hold that it will lead to earlier detection of diseases and novel therapies that will minimize discomfort for the patient, and hence provide cost savings all around. The European Strategic Research Agenda for nanomedicine³ has set priorities based on a number of parameters:

- mortality rate
- level of suffering
- burden on society
- prevalence of the disease
- ability of nanotechnology to diagnose and overcome illnesses

The strategy is to attack the diseases that are the greatest burden on society first:

- cardiovascular diseases
- cancer
- musculoskeletal disorders
- neurodegenerative diseases and psychiatric conditions
- diabetes
- bacterial and viral infections

According to the World Health Organization,⁴ cardiovascular diseases are the most frequent cause of death in the European Union. However efforts to reduce heart-related problems by encouraging more



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exercise and a reduction in cholesterol levels are paying off, and cancer instead may soon become the leading cause of death. In the United States, nanotechnology solutions for cancer therapy are receiving high priority. A Cancer Nanotechnology Plan⁵ is being spearheaded by the National Cancer Institute, which acknowledges that “nanotechnology offers the unprecedented and paradigm-changing opportunity to study and interact with normal and cancer cells in real time, at the molecular and cellular scales, and during the early stages of the cancer process.”

It is worth listing part of the vision statement for the Cancer Nanotechnology Plan, which says that nanotechnology will be the enabling technology for:

- early imaging agents and diagnostics that will allow clinicians to detect cancer at its earliest, most easily treatable, presymptomatic stage
- systems that will provide real-time assessments of therapeutic and surgical efficacy for accelerating clinical translation
- multifunctional, targeted devices capable of bypassing biological barriers to deliver multiple therapeutic agents at high concentrations, with physiologically appropriate timing, directly to cancer cells and those tissues in the micro-environment that play a critical role in the growth and metastasis of cancer
- agents capable of monitoring predictive molecular changes and preventing precancerous cells from becoming malignant
- surveillance systems that will detect mutations that may trigger the cancer process and genetic markers that indicate a predisposition for cancer
- novel methods for managing the symptoms of cancer that adversely impact quality of life
- research tools that will enable investigators to quickly identify new targets for clinical development and predict drug resistance.

Nanomedicine can be divided into four main areas:

- drug delivery
- molecular diagnostics
- tissue engineering
- cell/gene therapy

Drug Delivery

In addition to all this proposed new work, the challenge for the traditional pharmaceutical companies is to deliver the right therapeutic to the right target with no, or minimal, side effects, and at reduced cost. Drug delivery using nanostructures offers considerable potential to accomplish this. Some early successes have come from the Elan Corporation, a neuroscience-based biotechnology company headquartered in Dublin, Ireland. They have developed proprietary NanoCrystal technology for active pharmaceuticals that have poor water solubility. This technology reduces the particle size and increases the surface area of drugs leading to an increased dissolution rate. The nanoparticles are processed into finished dosage forms for all methods of administration. There have been four commercial approvals for products that have incorporated this type of technology:

- *Rapamune*, Wyeth’s immunosuppressant, now in tablet form. Previously it was available as a refrigerated product that was available in packets or in bottles.
- *Emend*, which was developed as a new chemical entity by Merck for cancer treatment.
- *TriCor*, a reformulated drug for lowering cholesterol from Abbott. Previously it had to be taken with a meal.
- *Megace ES*, an appetite enhancer for AIDS sufferers from Par Pharmaceuticals, who have licensed the Megace name from Bristol-Myers Squibb. NanoCrystal technology improves the rate of dissolution and bioavailability of the original unpalatable oral suspension.

In the United States, the company Esprit Pharma markets *Estrasorb* (from Novavax), which is an emulsion containing nanoparticles that is rubbed onto the legs to reduce hot flashes. There are two other cancer therapy drugs that are now nanotechnology-based: *Abraxane* for fighting metastatic breast cancer (Abraxis BioScience and AstraZeneca) and *Doxil* for ovarian cancer (Ortho Biotech).

A NanoMarkets report⁶ suggests that \$65 billion per annum in drug revenues are accounted for by active agents with low bio-availability, which can lead



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to inefficient treatment, higher cost and risk of toxic side effects; hence the drive to develop reformulations based on nanotechnology. The report estimates that nano-enabled drug delivery systems will reach \$1.7 billion in 2009.

For cancer therapy, the goal is to target cancerous cells while leaving healthy cells intact. With nanotechnology, it is possible to specifically target the cancerous cells and then activate the nano-structures to kill just those cells. Naomi Halas and Jennifer West are working on gold nanoshells that can be tailored to absorb near infrared light, which passes harmlessly through soft tissue. When nanoshells are activated under near infrared light, enough heat is generated to burst the walls of cancerous cells.⁷ This breakthrough has led to the set up of spin-off company Nanospectra Biosciences, which will begin trials with the nanospheres in humans.

Molecular Diagnostics

As indicated earlier, biological structures exist at the nano-scale, and nanomaterials are being used for both *in vivo* and *in vitro* biomedical research, especially for diagnostic devices. Some technologies are now mimicking the effectiveness of “sniffer” dogs at airports, which are able to rapidly detect minute amounts of drugs or explosives very quickly. Such sensitivity has recently been reported,⁸ from the University of Manchester where gas sensors are being developed that use graphene to detect single gas molecules. The promise for molecular diagnosis is that diseases will, in the future, be easily and quickly detectable before they have gained a foothold on the body, resulting in less severe and expensive therapy.

Hand-held lab-on-a-chip devices are already being used in hospitals to detect whether someone is having a heart attack. A similar development is being used to distinguish among several different narcotics in the bloodstream.

An area that has seen huge growth in the last decade is medical imaging. Here, nanotechnology applications are beginning to appear for both imaging tools and marker and contrast agents. It is expected, in the foreseeable future, that nano-imaging will lead to the detection of single cells in very complicated environments.

In 2005, the molecular diagnostics market was about \$5.5 billion, and the nano-diagnostics share was about \$1 billion. It is estimated that by 2015, the nano-diagnostics market will be worth \$9.5 billion and will predominate the molecular diagnostics market.⁹

Tissue Engineering

Tissue engineering uses materials engineering and life science developments to provide biological substitutes to reproduce or to repair damaged tissue. Tissue engineering stimulates cell proliferation using nanomaterial scaffolds, which are porous or solid. It is expected that in the future, tissue engineering will enable the replacement of artificial implants and organ transplants.

Nanotechnology is already contributing to commercially available products. *NanOss* and *Vitoss* are basically fillers for damaged bone. *NanOss*, from Angstrom Medica, Inc. in the United States, was the first nanotechnology medical device to receive approval from the U.S. Food and Drug Administration. It is an innovative structural biomaterial, based on nanocrystalline calcium phosphate technology, that is highly osteoconductive and remodels over time into human bone. The material has applications in sports medicine and trauma, spine, and general orthopaedics markets. *Vitoss*, from Orthovita, is also based on calcium phosphate and comes in blocks that can be shaped with a scalpel and gently tamped into place, or in granules that can be packed into irregularly shaped voids in the defect site. A third product, *TiMesh*, from GP Surgical, is described as a soft-tissue reinforcement implant for hernia repair, and is based on titanised polypropylene.

The market described as tissue engineering,⁹ was worth \$6.9 billion in 2005 and is predicted to rise to \$23.2 billion in 2015.

Cell/Gene Therapy

This type of therapy repairs or replaces damaged tissue by using cells from the patient or a donor that have been multiplied and sometimes altered outside the body. A good example of this is stem cells, which can be grown and transformed into specialized cells, such as nerves and muscles, through cell culture.

SiBiono Gene Tech, based in China, was the first company to commercialize gene therapy. Its product *Gendicine* makes use of the fact that over 50 percent of tumors have a dysfunctional gene that makes protein p53, a cellular anti-cancer agent. Effectively, *Gendicine* works by inserting the p53 gene into a virus, which is then injected into patients. The gene is naturally present in healthy cells but is “turned off” or mutated in many cancer patients. When reinserted into tumor cells by the virus, it causes them to self-destruct. *Gendicine* is finding success among sufferers of head and neck squamous cell carcinoma. The only other commercially available gene therapy is from

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Shanghai-based Sunway Biotech, which has a virus that kills tumors. The product, called *Oncorine*, is a genetically modified virus that selectively replicates inside tumor cells with dysfunctional p53 genes.

Nanomedicine is moving forward at a rapid pace, and we are only just seeing the tip of the iceberg. The best is yet to come. 🧪

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 www.nanotechia.co.uk

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

Stamps International

Inverted Methane

Methane, the simplest hydrocarbon, is a colorless, odorless, and flammable gas widely distributed in nature. It is the main component of natural gas, which contains about 70–90% CH₄, and it is found in large clathrate deposits underneath ocean floors. It is also formed on a regular basis by methanogenic bacteria present in wetlands and the guts of humans and ruminants. In addition to being the final product in the decay of organic matter, methane is a well-known greenhouse gas and thus plays a key role in the global carbon cycle.

The main use of methane is as a fuel, either for electricity generation in power plants or for domestic heating and cooking. In the chemical industry, methane is an essential feedstock in the production of the so-called synthesis gas (a mixture of carbon monoxide and hydrogen) by steam reforming of natural gas. In turn, synthesis gas is the critical intermediate in the preparation of pure hydrogen, used in a huge industrial scale in the synthesis of ammonia via the Haber-Bosch process, and also in the production of methanol, which

can be converted to acetic acid, formaldehyde, and many other important organic chemicals.

The stamp shown in this note was issued by Monaco in 1986 to recognize its fledgling plastics industry, a puzzling choice since the economy of the wealthy principality relies primarily on tourism and banking. More questionable is the stamp designer's choice of methane as a direct source of gasoline for automobiles, as the illustration seems to suggest, although compressed (or liquefied) natural gas is a relatively common transportation fuel in countries such as Argentina and Brazil. Perhaps most aggravating to chemists is that the structural formula of methane is given as C₄H: definitely an item for chemical philately's "Hall of Shame"!

Interestingly, the linear butadiynyl radical does exist and has been unequivocally identified by spectroscopic methods in interstellar space, but that's not exactly what I would call a readily available alternative source of energy . . .

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



Yuan Tseh Lee to Be President of the International Council for Science

Yuan Tseh Lee, a Nobel Prize-winning chemist from Taipei, China, has been elected president of the International Council for Science (ICSU). A world leader in the field of chemical dynamics, Lee was elected by representatives of ICSU's 114 National Members and 29 International Scientific Unions at the 29th General Assembly in Maputo, Mozambique, 21-24 October 2008. He will take up the appointment in April 2010 and will succeed the current president, Catherine Bréchnagnac, in October 2011.

Lee was born and educated in Taipei before moving to the USA where he obtained a Ph.D. in chemistry from the University of California, Berkeley, in 1965. In the ensuing years, his career flourished, both as a creative scientist and an inspiring teacher. In 1986, he was awarded the Nobel Prize in Chemistry for his seminal



Yuan Tseh Lee.

contribution to the development of reaction dynamics—a new field of research in chemistry at the time. His use of crossed molecular beams allowed the study of complex reaction mechanisms beyond the capability of previous methods. Lee returned home in 1994, taking up the position as president of the Academy of Sciences in Taipei. Under his 12-year leadership the institution was transformed into a world-class research center, attracting scholars and creative young scientists from around the world.

His achievements have been recognized with many awards and professional memberships, which include the U.S. National Academy of Sciences and the

Academy of Sciences for the Developing World. He has been involved with ICSU for 15 years and served on the Standing Committee on Freedom in the Conduct of Science from 1996 to 2005.

“I am honored and excited to be elected the next president of ICSU, an organization that has been at the forefront of international science for more than 75 years,” said Lee. “As a child I was inspired by Madame Curie who believed that scientific knowledge belonged to all mankind.* It is my strong belief that ICSU will pave the way in ensuring that scientific knowledge is available to all—a critical factor in providing the solutions for sustainable development, climate change mitigation, global human health issues, and alleviating poverty.”

 www.icsu.org

*An interview with Lee was published in the November 2008 issue of *Chemical Education International*. See page 21 for more information.

Leading Scientific Organization Affirms Freedom, Responsibility, and the Universality of Science

In light of recent high-profile cases of scientific misconduct, the General Assembly of the International Council for Science (ICSU) reaffirmed the universal values that should guide the conduct of science. The assembly also explicitly recognized the key social responsibilities of the scientific community as laid out in a new booklet, *Freedom, Responsibility, and Universality of Science*, which will be made widely available to scientists across the world.

Ultimately the integrity of science depends on scientists themselves and all scientists have a duty to expose fraudulent information and/or misconduct. Given the unique position of scientists as the gatekeepers of new knowledge in today's knowledge societies, respect for these values is critically important if confidence in science is to be maintained.

The booklet asserts that “all scientists have a responsibility to ensure that they conduct their work with honesty and integrity; to ensure that methods and results are reported in an accurate, orderly, timely, and open fashion.” The booklet goes on to say that scientists are expected to be impartial, fair, respectful and considerate in relation to fellow human



beings, animals, and the environment, and to acknowledge risk and uncertainty. By extending its consideration of the long-established Principle of the Universality of Science to explicitly include responsibilities as well as freedoms, ICSU emphasizes that this balance is critical both for science and society.

"In many ways, what the booklet says is simple, but actually reaching agreement on these issues was surprisingly complicated," explained Bengt Gustafsson, chair of the ICSU Committee on Freedom and Responsibility in the conduct of Science, which produced the booklet. "Hopefully now we have a starting point for the different parts of the scientific community to establish their own more specific guidelines, codes or practices, where these are lacking."

The booklet and more on the ICSU General Assembly are available at <www.icsu.org/3_mediacentre/GA_29.html>.

About ICSU

Founded in 1931, ICSU is a nongovernmental organization with a global membership of national scientific bodies (114 members, representing 134 countries) and International Scientific Unions (29 members). The council is frequently called upon to speak on behalf of the global scientific community and to act as an advisor in matters ranging from the environment to conduct in science. ICSU's activities focus on three areas: planning and coordinating research, science for policy, and strengthening the Universality of Science.

 www.icsu.org

Remembering Dana Knox

Dr. Dana E. Knox, professor of Chemical Engineering in the Otto H. York Department of Chemical, Biological, and Pharmaceutical Engineering and associate provost for undergraduate programs at the New Jersey Institute of Technology, died on 24 September 2008 at the age of 53. He was the chairman of the IUPAC Subcommittee on Solubility and Equilibrium Data.

Knox was born in upstate New York and received B.S. (1977), M.S. (1978), and Ph.D. (1982) degrees from the Rensselaer Polytechnic University in Troy, New York, USA. He began his career on the faculty at NJIT, based in Newark, New Jersey, USA, in 1983. He joined the Provost's Office at NJIT in 2004. This year he would have celebrated his 25-year anniversary at NJIT.

Knox was an expert in thermodynamics of fluids and fluid mixtures. He was widely published in the technical literature and extremely active in research. In 2002, he received the Franzosini Award from IUPAC in appreciation of his continuous contributions to the Solubility Data Project. He was extremely active in the American Institute of Chemical Engineering, often organizing and chairing sessions at the national meetings. He was also a frequent contributor to annual meetings of ASEE.

He was beloved as a colleague across the NJIT campus, as a dedicated advisor for many students who received their degrees from NJIT, and he was currently serving as co-advisor for the NJIT student chapter of AIChE. He received awards for excellence in teaching and for excellence in advising from the Newark College of Engineering. In 1994 he received the university-wide Robert W. Van Houten Award bestowed by the NJIT alumni to recognize teaching excellence. In 2002, he was appointed to the rank of master teacher at NJIT.

Chemical Heritage Foundation Fellowships

The Chemical Heritage Foundation, an independent historical research center, library, and museum in Philadelphia, Pennsylvania, USA, is accepting applications for long-term and short-term fellowships in residence at CHF's Beckman Center for the History of Chemistry for the academic year 2009-2010. These fellowships are for scholars working in some area of the history and social studies of alchemical, chymical, chemical, and molecular sci-

ences, technologies, crafts, or industries (broadly construed) in all chronological and geographical areas. To get a better sense of the kinds of research CHF supports, visit its website and review the work being done by current and past fellows.

The deadline for applications is 15 February 2009. CHF has an online application procedure that should streamline the process. Each applicant will select whether they are applying for a nine-month post-doctoral, nine-month dissertation, or short-term (with a specific number of months) fellowship. They will fill out the online form, attach the necessary supporting documents, and contact information for their references. Fellows will be selected by a peer review selection committee and awardees should be notified in April 2009.

 www.chemheritage.org/research/research.html

The Royal Society of Chemistry and ChemSpider to Develop InChI Resolver

An InChI Resolver, a unique free service for scientists to share chemical structures and data, will be developed through a collaboration between ChemZoo Inc., host of ChemSpider, and the Royal Society of Chemistry. Using the InChI—an IUPAC standard identifier for compounds—scientists can share and contribute their own molecular data and search millions of others from many web sources. The RSC/ChemSpider InChI Resolver will give researchers the tools to create standard InChI data for their own compounds, create and use search engine-friendly InChIKeys to search for compounds, and deposit their data for others to use in the future.

“The wider adoption and unambiguous use of the InChI standard will be an important development in the way chemistry is published in the future, and the further development of the semantic web,” said Robert Parker, managing director of RSC Publishing.

The InChI Resolver will be based on ChemSpider’s existing database of over 21 million chemical compounds and will provide the first stable environment to promote the use and sharing of compound data. “ChemSpider hosts the largest and most diverse online database of chemical structures sourced from over 150 different data sources” added Antony Williams of

ChemSpider. “We have embraced the InChI identifier as a key component of our platform and the basis of our structure searches and integration path to a number of other resources. We have delivered a number of InChI-based web services and, with the introduction of the InChI Resolver, we hope to continue to expand the utility and value of both InChI and the ChemSpider service.”

So Why Do We Need an InChI Resolver?

Whereas the InChI itself contains the chemical structure of the compound, the InChIKey cannot itself be used to derive the compound. If the InChI and InChIKey are published together, there is no ambiguity, but to avoid confusion there is a need for an InChIKey resolver, to allow anyone to submit an InChIKey and have returned the full InChI which describes the compound. InChI generation can be done in different ways, and an agreed “standard” generation protocol is imminent.

Frequently asked questions about the InChI are answered at www.rsc.org/Publishing/Journals/ProjectProspect/InChIFAQ.asp.

See feature on page 7 for more on InChI.

 www.rsc.org

IUPAC Executive Director—Expression of Interest

The IUPAC Executive Director, Dr. John W. Jost, has indicated his intention to retire towards the end of 2010. IUPAC would like to appoint a successor early in 2010 in order to provide important overlap and continuity. I am therefore calling for any confidential expression of interest, either directly to myself or to one of the other members of our Search Committee, Professor Bryan Henry, Professor Jung-Il Jin, Professor Nicole Moreau, Professor John Corish, or Dr. Mark Cesa. Further information, including a duty statement, will be available upon request. It is intended that the position will be advertised formally in the first quarter of 2009, with the aim of making an appointment around mid-2009, to provide ample time for the appointee to commence work very early in 2010.

— Professor David Black, IUPAC Secretary General

Glossary of Terms Related to Kinetics, Thermodynamics, and Mechanisms of Polymerization (IUPAC Recommendations 2008)

Stanisław Penczek and Graeme Moad

Pure and Applied Chemistry, 2008

Vol. 80, No. 10, pp. 2163–2193

doi:10.1351/pac200880102163

This document presents recommended definitions of basic terms related to polymerization processes. Recent developments relating to the kinetics, thermodynamics, and mechanisms of polymerization have necessitated the introduction of new terms and some revision or augmentation of terms previously defined in the *Compendium of Chemical Terminology* (the Gold Book), the “Glossary of Basic Terms in Polymer Science.” [PAC 68, 2287 (1996)], and the “Basic Classification and Definitions of Polymerization Reactions” [PAC 66, 2483 (1994)]. In most cases, the previously given definitions have been retained, but, in a few cases, the development of the field has required changes. Those definitions from the Gold Book and the glossary that have been changed are provided in appendices to the present document.

 <http://dx.doi.org/10.1351/pac200880102163>

Protocols on Safety, Efficacy, Standardization, and Documentation of Herbal Medicine (IUPAC Technical Report)

M. Mosihuzzaman and M. Iqbal Choudhary

Pure and Applied Chemistry, 2008

Vol. 80, No. 10, pp. 2195–2230

doi:10.1351/pac200880102195

“Health for all” is a dream and a goal which humanity at large shares and strives for. Unfortunately, it has now been proven without doubt that modern pharmaceuticals are, and will remain, out of reach for a large proportion of the human population for the foreseeable future. This has created an appreciation and a need for the use of other sources of human knowledge to provide common health benefits. Alternative and traditional medicines, largely herbal in nature, are now regarded as important but under-utilized tools against disease. The World Health Organization recognized this fact in the early 1970s and encouraged governments to effectively utilize local knowledge of herbal medicines for disease prevention and health promotion. Herbal medicines, however, suffer from a range of shortcomings. These include insufficient and unacceptable evidence of safety, efficacy, standardization, and inconsistent production practices.

This technical report compiles and analyzes the current scientific knowledge on herbal medicine and highlights the practical ways for ensuring the safety of herbal preparations and evaluating their claimed efficacy. Emphasis has been given to the methods for standardization of herbal medicine and the ways and means for moving forward to achieve the difficult goal of preparing herbal medicines of consistent quality and effects. Pragmatic approaches have been recommended to overcome the difficulties in 1. protecting intellectual property rights; 2. producing safe, potent, standardized, and affordable herbal medicine; and 3. documenting the knowledge base on herbal medicine in an easily accessible format.

 <http://dx.doi.org/10.1351/pac200880102195>

Greetings to those of you whose work or interest is related to terminology. Following is a prescient extract of *Through the Looking Glass*, by Lewis Carrol, 1871:

“When I use a word,” Humpty Dumpty said in rather a scornful tone, ‘it means just what I choose it to mean—neither more nor less.’

‘The question is,’ said Alice, ‘whether you CAN make words mean so many different things.’

‘The question is,’ said Humpty Dumpty, ‘which is to be master—that’s all.’”

Online text available at Project Gutenberg <www.gutenberg.org/files/12/12-h/12-h.htm>.



Solubility Data Series Volume 85: Transition and 12–14 Main Group Metals, Lanthanide, Actinide, and Ammonium Halates

H. Miyamoto, et al

J. Phys. Chem. Ref. Data, 2008, Vol. 37, No. 2,
pp. 933–1118

doi: 10.1063/1.2804088

This paper is the fourth and final volume in the halate solubility series. The solubility data for halates of transition metals, lanthanides, actinides, ammonium, and metallic elements of the main groups 12–14 are reviewed. Where appropriate, binary, ternary, and multicomponent systems are critically evaluated. Most of the solubility results were obtained in water or aqueous solutions of electrolytes. The solubility in organic solvents and aqueous-organic solvent mixtures is also collected in this volume.

All these data were critically examined for their reliability. The best values were selected on the basis of critical evaluations and presented in tabular form. Fitting equations and graphical plots are also provided. When numerical data were not reported in an original publication, they were read out from figures and digitized by the compilers. The quantities, units, and symbols used in this volume are in accord with IUPAC recommendations. Authors of this paper always reported the original data and, if necessary, transferred them into the IUPAC recommended units and symbols. The literature on the solubility data was researched through 2002.

The halates of these metals play a role in industrial processes. For example, some halates are essential as catalysts, heat stabilizers, and bleaching reagents for manufacturing polymer products such as textiles and resins. Some iodates are used in pyrotechnic compounds for weather modification and colored smoke generation. The nonlinear halate crystals are important in construction of optical devices.

 www.iupac.org/publications/sds/2008/85_abstract.html

Solubility Data Series Volume 86: Ethers and Ketones with Water

Andrzej Maczynski et al.

J. Phys. Chem. Ref. Data, 2008 (6 part series)

The mutual solubilities and related liquid-liquid equilibria of various systems with water are exhaustively and critically reviewed. These systems include:

- C2–C5 ethers (part 1)
- C6 ethers (part 2)
- nine binary systems of C7–C14 ethers (part 3)
- six binary systems of C4 and C5 ketones (part 4)
- eight binary systems of C6 ketones (part 5)
- 25 binary systems of C7–C12 ketones (part 6)

All data are expressed as mass percent and mole fraction as well as the originally reported units. In addition to the standard evaluation criteria used throughout the Solubility Data Series, a method based on the evaluation of all experimental data for a given series of ketones was used. This completes a six-part series of papers which compile and evaluate mutual solubility data of ethers and ketones with water.

 www.iupac.org/publications/sds/2008/86_abstract.html

Now Available

Chemical Education International Volume 8, Issue 1 November 2008

In the latest issue of the online journal *Chemical Education International*, Yoshito Takeuchi provides a transcript of his interview with Yuan Tseh Lee, winner of the 1996 Nobel Prize in Chemistry.

This issue of CEI also offers articles based on presentations by Viktor Obendrauf, Onno De Jong, E. Steenberg and J.D. Bradley, and Ameen F.M. Fahmy and J.J. Lagowski at the 19th International Conference on Chemical Education (Seoul, Korea, August 2006).

www.iupac.org/publications/cei

Bookworm

Future Energy—Improved, Sustainable, and Clean Options for Our Planet

Trevor M. Letcher (editor)

Elsevier, 2008 (ISBN-13: 978-0-08-054808-1)

The book *Future Energy* was produced to enable readers to make reasonable, logical, and correct decisions on our future energy as a result of two of the most serious problems that the civilized world has had to face: the looming shortage of oil (which supplies most of our transport fuel) and the alarming rise in atmospheric carbon dioxide over the past 50 years, which threatens to change the world's climate through global warming.

Future Energy focuses on all the types of energy available to us. It is unique in the genre of books of a similar

title currently on sale since each chapter has been written by an expert, scientist, or engineer, working in the field.

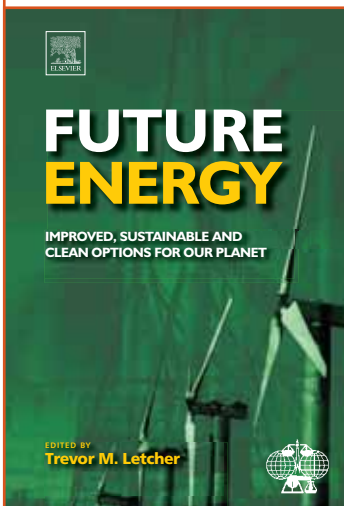
The book is divided into four parts:

- Fossil Fuel and Nuclear Energy
- Renewable Energy
- Potentially Important New Types of Energy
- New Aspects to Future Energy

Each chapter highlights the basic theory, implementation, scope, problems, and costs associated with a particular type of energy. The traditional fuels are included because they will be with us for decades to come—but, we hope, in a cleaner form. The renewable energy types include wind power, wave power, tidal energy, two forms of solar energy, biomass, hydroelectricity, and geothermal energy. Potentially important new types of energy include pebble bed nuclear reactors, nuclear fusion, methane hydrates, and recent developments in fuel cells and batteries. In conclusion, the final section highlights new aspects of future energy usage with chapters on carbon dioxide capture and storage, smart houses of the future. The book ends with a chapter on possible scenarios for electricity production and transport fuels to the year 2050.

Looking at the whole spectrum of options in the book, the reader will gain a good understanding of the options that best suit us now and in the future.

 www.iupac.org/web/ins/2007-015-2-100



Biophysical Chemistry of Fractal Structures and Processes in Environmental Systems

Series on Analytical and Physical Chemistry of Environmental Systems—Vol. 11

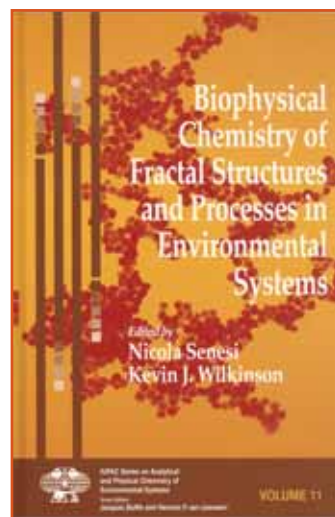
Nicola Senesi and Kevin J. Wilkinson (editors)

John Wiley & Sons, 2008 (ISBN 978-0-470-01474-5)

This book employs fractal geometry concepts to understand the properties and processes of diverse environmental systems. The interpretation of complex environmental systems using modern fractal approaches is compared and contrasted with the more classical approaches. The book provides the fundamental knowledge necessary for solving practical environmental problems. Furthermore, it examines how the fractal approach has been applied in order to understand the structure and reactivity of natural environmental systems, including flocs, sediments, soils, microorganisms, and humic substances.

The IUPAC Series on Analytical and Physical Chemistry of Environmental Systems provides a critical evaluation of the state-of-the-art on physicochemical properties and processes in environmental systems, as well as on the analytical techniques required to study and monitor them. The series is aimed at promoting rigorous analysis and understanding of physicochemical functioning of environmental and bioenvironmental systems.

 www.iupac.org/web/ins/2003-014-2-600



Macromolecular Symposia—recent volumes

Nanostructured Polymers and Polymer Nanocomposites

Libor Matějka (ed.)

Volume 267, pp. 1–133 (June 2008)

Research in nanoscale science and technology contributes to the development of multifunctional materials composed of nanostructured polymers and nanocomposites. Polymer nanocomposites are systems containing three-dimensional heterogeneities of the size 1–100 nm (in one dimension). The unique behavior of the nanocomposites is mainly caused by a large interfacial area between the polymer and nanofiller. The interfacial interaction, resulting in immobilization of the polymer at the interface, plays a crucial role in the structure formation and behavior of the nanostructured polymers. In addition, the filler-filler interaction and a potential nanofiller percolation in the polymer matrix must be taken into account.

The nanostructured polymers exhibit the interfacial interaction on the nanoscale level. However, the supramolecular structuring, including self-assembling and nanodomains ordering in the polymer matrix, are also of high importance. Block copolymers, liquid crystalline and supramolecular polymers, and gels are examples of organized polymer systems with a hierarchical structure.

Polymer nanocomposites often contain inorganic nanofillers, and hence the systems based on the organic-inorganic polymers are an important class of nanomaterials. Two main procedures of the formation of nanostructured polymer systems are used. The top-down approach consists in disintegration of large “filler” particles into nanoparticles within the polymer matrix, while the bottom-up procedure is based on formation of “filler” nanodomains in a polymer starting from molecular level of inorganic components or precursors. The former approach is typical of clay (layered silicates) nanocomposites where the dispersion of nanoparticles is a main problem and goal of the research. The controlled formation of nanostructures in the case of the bottom-up approach could be achieved by using *in situ* generation of nanodomains by the sol-gel process or by application of well defined nanobuilding blocks, such as polyhedral oligomeric silsesquioxanes or other inorganic functional clusters. Moreover, the prospective class of nanocomposites is based on organic-organic nanostructured polymers containing carbon nanotubes, fullerenes, and others.

The 2007 Prague Meetings on Macromolecules, held in Prague from 8–12 July 2007, contributed to the understanding of nanostructured polymers and polymer nanocomposites and the general relationships between synthesis, structure, and properties of the nanomaterials. The approaches to characterization of hierarchical structure of nanostructured polymers by using novel experimental

techniques are described including procedures for determination of dynamics of the nanostructured systems or interface interactions. An important part of contributions is devoted to application of nanomaterials, such as opto-electronic and magnetic materials, coatings, membranes, and many others.

 www3.interscience.wiley.com/journal/120756038/issue

Advanced Polymer Materials for Photonics and Electronics

Vera Cimrová (ed.)

Volume 268, pp. 1–128 (July 2008)

This issue contains papers presented at the conference on Advanced Polymer Materials for Photonics and Electronics which took place in Prague, 15–19 July 2007.

 www3.interscience.wiley.com/journal/120835641/issue

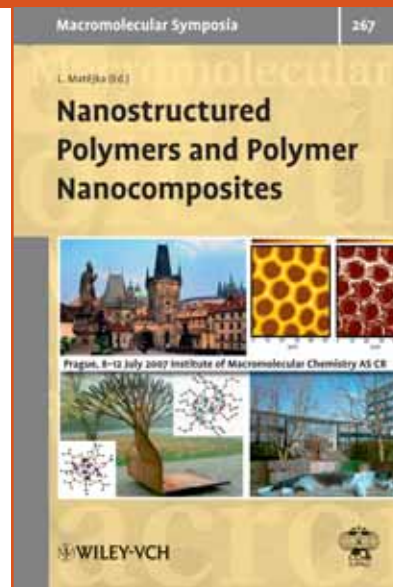
Macromolecular Complexes

Naoki Toshima (ed.)

Volume 270, pp. 1–201 (August 2008)

This issue of *Macromolecular Symposia* contains plenary and invited lectures delivered at the 12th IUPAC International Symposium on Macromolecular Complexes (MMC-12), that was held in Fukuoka, Japan, from 27–31 August 2007.

 www3.interscience.wiley.com/journal/121392665/issue



Conference Call

Chemical Education

by Morton Z. Hoffman and Ponnadurai Ramasami

The island of Mauritius (*Île Maurice, en français*), a tiny dot in the Indian Ocean at 20° S latitude and 57° E longitude, is located about 1 000 km east of Madagascar off the southeastern coast of Africa. Home to about 1.2 million people and the University of Mauritius, it was the site of the **20th International Conference on Chemical Education (ICCE)**, which was held on 3–8 August 2008 at Le Méridien Hotel in Pointe aux Piments. With about 200 attendees from 40 countries, the conference, which had “Chemistry in the Information and Communications Technology (ICT) Age” as its theme, featured 140 oral presentations and 50 posters.

Welcoming remarks were made by Peter Mahaffy (Canada), chair of the IUPAC Committee on Chemistry Education (CCE); Dharambeer Gokhool, minister of Education and Human Resources in Mauritius; I. Fagoonee, vice chancellor of the University of Mauritius;

- Roald Hoffmann (USA), “Chemistry’s Essential Tensions: Different Ways of Looking at a Science”
- Peter Mahaffy (Canada), “Communicating the Chemistry of Climate Change with ICT and Paraffin”
- Loretta Jones (USA), “How Technology Can Help Students to Visualize the Molecular World without Inducing Misconceptions about Chemistry”
- Henry Schaefer III (USA), “Lesions in DNA Subunits: Foundational Studies of Molecular Structures and Energetics”
- Arthur Olson (USA), “Back to the Future: Grasping Molecular Biology with Tangible Interfaces”
- Peter Atkins (UK), “The Future of the Book”
- Vandana Hunma (Mauritius), “Chemistry Education for Socially Responsible and Sustainable Development: What Are the Challenges for a Developing Country?”
- John Bradley (South Africa), “Substances, Molecules, and Symbols in the ICT Age”
- Shalini Baxi (India), “Community-Based Collaborative ICT Strategies for Science Education”

The parallel oral sessions centered around the following themes: teaching chemistry at the secondary and tertiary levels, chemistry education research, the use of modern technologies, green chemistry, involvement of the arts, public understanding of chemistry, and chemistry teacher education. In addition, symposia were held on best practices in professional development, process-oriented guided inquiry learning (POGIL), increasing the popularity and relevance of school chemistry, structural models and chemical understanding, and the systemic approach to teaching and learning chemistry (SATL). Workshops were offered on the teaching of advanced chemistry courses, electrochemical model experiments, air and water environment, and strategies to assist students with learning chemistry.

The organization of the program gave participants time to interact and develop connections. In addition to morning and afternoon coffee/tea breaks and daily group lunches, evening events included a welcoming reception, an entertainment evening with local singers and dancers, the conference banquet at a Chinese restaurant in Port Louis, the Mauritian capital city, and participants night with national songs and performances. The day-long conference tour in the middle of the week to sites of interest on the island provided a delightful break.



Peter Mahaffy (left) and Ponnadurai Ramasami.

Ambassador Kalimi Mugambi Mworia (Kenya), director of the International Cooperation and Assistance Division of the Organization for the Prohibition of Chemical Weapons, which was a financial sponsor of the conference. The ICCE was organized by a local committee headed by Conference President Henri Li Kam Wah and Conference Chair Ponnadurai Ramasami of the Department of Chemistry of the University.

Plenary lectures were given by nine distinguished chemists and educators:



Roald Hoffmann and Morton Hoffman.

The 20th ICCE also featured a virtual conference, held 1–25 July 2008, at which 45 papers were presented and 371 participants from 44 countries participated in the discussion. Loretta Jones and her group presented the keynote address entitled “Designing Effective Visualizations of Molecular Structure and Dynamics. The presentation entitled “Chemistry in Daily Life: Good Reasons to Opt for Chemistry” by second-year

B.Sc. (Hons) chemistry students from the University of Mauritius was well appreciated. Participants expressed their satisfaction about the virtual conference and many of them acknowledged that this was their first participation in an online conference.

A post-conference satellite meeting held at the University of Nairobi, Kenya, drew 20 registrants. See box below for a summary of this event.

Mei-Hung Chiu, Lida Schoen, and Erica Steenberg conducted a successful Young Ambassadors for Chemistry (YAC) course from 31 July to 2 August 2008 at the University of Mauritius. Thirty local chemistry teachers attended the workshop. On 2 August they showed hundreds of students how to conduct demonstrations for the public. (A report about this YAC will appear in the March 2009 issue.)

The ICCE was the occasion of the annual meeting of the IUPAC Committee on Chemistry Education (CCE), which consists of titular members, divisional representatives, and national representatives. The CCE approved the minutes of its last meeting at the IUPAC

The Relevance of Chemistry in a Globalized Society: A Satellite Meeting of the 20th ICCE

by John Bradley

The satellite meeting, organized by Shem Wandiga on behalf of the Kenya Chemical Society, was held at the University of Nairobi. The approximately 60 delegates who registered were university staff and students and secondary school teachers of chemistry. While the majority were from Kenya, there was a significant number of attendees from Uganda and Tanzania.

Most of the meeting's first day was devoted to three plenary lectures and general discussions:

- “ICT as a Tool for Collaborating in Chemistry,” Joseph M. Mwaniki
- “Low-Cost Experiments in Chemistry,” John D. Bradley
- “Public Image of Chemistry,” Shem O. Wandiga

After the presentations, the participants split into three groups to discuss further one of the topics presented. Each group was chaired by a plenary speaker and a rapporteur was elected. I chaired the Low-Cost Experiments group, for which JI Jondiko (Maseno University) was rapporteur. A lively discussion ensued that extended well beyond the expected closing time.

There was enthusiasm among group members for the microscale chemistry concept and awareness of the activities to introduce it in Kenya during the past few years. Although some teachers were conservative and reluctant to change, this attitude was also justified by the Kenya National Exams Council (KNEC) policy regarding practical exams. They specified only traditional equipment and no alternatives. The Kenya Institute of Education had approved microscale equipment, but in spite of this the KNEC policy remained. The consensus was that the situation was unsatisfactory and that concerted

representations should be made by all stakeholders. It was also suggested that a pilot implementation project should be advocated.

On the second day, the Low-Cost Experiments group spent 1.5 hours in practical activities with microscale equipment. The activities, which were the same as those presented at the main conference in Mauritius, exemplified how microscale equipment can be used to understand the air and water environment. Participants were able to complete two or three of the five activities available in the session, and there was general success and satisfaction.

In the second and final session of the day, rapporteurs from each group presented a review of the discussions and experiences, and there was an opportunity for further questions. Shem Wandiga closed the meeting at lunchtime. The satellite meeting proved to be successful and provided a worthwhile stimulus for chemistry education in the region.

Conference Call

General Assembly in Torino in August 2007, received the minutes of its strategy meeting held at the Chemical Heritage Foundation in Philadelphia earlier in 2008, and heard reports from subcommittees.



The Subcommittee on Chemistry for Development reported on the two-day conference on “Improving Chemical Education in the Philippines” that was held at the University of Santo Tomas in Manila, 17-18 April 2008. This was a project of the Flying Chemists Program in which education experts collaborate with academic institutions and governmental officials in particular countries to help them improve the teaching of chemistry (see Jul-Aug 2008 *CI*, page 29). The activities of the Network for Inter-Asian Chemistry Educators (NICE) were also described (see page 30 of this issue for details on the coming 2009 symposium to be held 29-30 July 2009 at Tokyo Gakugei University).

The current effort of the Subcommittee on the Public Understanding of Chemistry is to work with IUPAC and its National Adhering Organizations toward the proclamation of 2011 as the International Year of Chemistry by UNESCO and the UN. Through very hard work by Ethiopia and the support of Algeria, Benin, China, Côte d'Ivoire, Cuba, Democratic Republic of the Congo, Egypt, France, India, Japan, Kuwait, Madagascar, Malaysia, Morocco, Niger, Nigeria, Republic of Korea, Russian Federation, Senegal, South Africa, Togo, Uganda, and the United Republic of Tanzania, and Zambia, the Executive Board of UNESCO approved the resolution.

CCE recognized the devoted efforts of Lida Schoen (Netherlands) to implement the successful Young Ambassadors for Chemistry (YAC) program. The committee discussed ways in which this outstanding project could be sustained.

The next meeting of CCE will take place at the 42nd IUPAC General Assembly and Congress (“Chemistry Solutions”) to be

held 2-7 August 2009 in Glasgow, Scotland. The 21st ICCE, “Chemistry Education and Sustainability in the Global Age,” will be held 8-13 August 2010 in Taipei, Taiwan; details are available at <icce2010.gise.ntnu.edu.tw>.

Morton Z. Hoffman <hoffman@bu.edu> is the U.S. National Representative to the IUPAC Committee on Chemistry Education and the liaison with the American Chemical Society Division of Chemical Education. He is a retired professor from Boston University, Massachusetts, USA. Ponnadurai Ramasami <ramchemi@intnet.mu> is an associate professor in the Department of Chemistry at the University of Mauritius. He was chair of the conference organizing committee.

Physical Organic Chemistry

by *Charles L. Perrin*

The **19th International Conference on Physical Organic Chemistry** (ICPOC2008), which was sponsored by IUPAC, was held 13-18 July 2008 at The Royal University of Santiago de Compostela in Galicia, Spain. This follows ICPOC18, held in August 2006 in Warsaw, Poland. The 2008 conference attracted 344 registrants, including 53 students. It was truly international, with participants from 43 countries.

Santiago de Compostela is in the northwest of Spain, a region of green forests, ocean bays, and cooling summer breezes. The imposing cathedral (below) is the destination of an important pilgrimage route, dating from medieval times. The University of Santiago de Compostela, founded in 1495 by Lope Gómez de Marzoa, is one of the oldest universities in the world. It now enrolls 45 000 students across several campuses. It was an excellent venue for a conference, close to the city center, well equipped for lectures and computer access, and with dining facilities and cafes serving abundant and tasty local food.

The scientific program featured 11 plenary speakers, 22 invited speakers, 89 oral communications, and 180 posters. The plenary lecturers showcased the diversity of physical organic chemistry, including instrumental methods, biochemical applications, and studies of the relationship between molecular structure and reactivity. A key topic was nanotechnology and surface science, which included lectures on the following topics:

- nanoscale switches and motors (B.L. Feringa, Univ. of Groningen, Netherlands)
- metal nanoparticles (J.C. Scaiano, Univ. of Ottawa, Canada)
- selective heterogeneous catalysis for green chemistry (Avelino Corma, Univ. of Valencia, Spain)



Conference Call

- reactive species through site isolation on surfaces (Christophe Copéret, Univ. of Lyon, France)
- the remarkable observation of intracage vapor bubbles arising by solvent loss from self-assembled trigonal prisms (Josef Michl, Univ. of Colorado, USA)

Another important topic was catalysis, which included the following lectures:

- NMR spectroscopy and ion pairing (Paul Pregosin, ETH, Switzerland)
- dynamic and thermodynamic contributions to enzymatic transition states (Vern Schramm, A. Einstein College of Medicine, USA)
- late transition-metal complexes as polymerization catalysts (Kyoko Nozaki, U Tokyo, Japan) transition-metal-free hydrogenation and hydrogenolysis (Leo Radom, U Sydney, Australia)
- investigations of some unusual structures, including divalent carbon(0) compounds (Gernot Frenking, U Marburg, Germany)
- symmetry of hydrogen bonds (Charles L. Perrin, UC San Diego, USA).

Following is a sampling of the many other oral presentations at the conference:

- aromaticity lag in proton transfer (Claude Bernasconi, UC Santa Cruz, USA)
- photochemistry of tetrazoles (María de Lurdes Cristiano, U Algarve, Portugal)
- methylglyoxal synthase (AnnMarie C. O'Donoghue, UK)
- solvolysis of benzhydryl derivatives (Olga Kronja, Croatia)
- isotope effects in methyl transfers from σ -methyl

cobalt(III) phthalocyanine to amines (Włodzimierz Galezowski, Poland)

- resonance-assisted hydrogen bonds (Manuel Yañez, Spain)
- conformations of N-nitroso-N,O-dimethylhydroxylamine (Howard Maskill, UK)
- photostimulated intramolecular SRN1 reactions (Roberto A. Rossi, Argentina)

Full details of the conference program, including a list of speakers and lecture titles, are available on the conference website <www.icpoc2008.org>.

This biennial conference, the nineteenth in an ongoing series, was sponsored by the IUPAC Organic and Biomolecular Chemistry Division under the auspices of its Subcommittee on Structural and Mechanistic Chemistry. The local organizers, especially José Ramon Leis and Amelia Huzum, of Universidad de Santiago de Compostela, and Arturo Santaballa, of Universidad de A Coruña, are to be commended for the excellence of their planning and implementation of this conference and for obtaining adequate funding from numerous sponsors.

The Subcommittee on Structural and Mechanistic Chemistry has recommended that the 2010 Conference be held in Busan, Korea.

Charles L. Perrin <cperrin@ucsd.edu>, professor of chemistry at the University of California, San Diego, is a member of the IUPAC Subcommittee on Structural and Mechanistic Chemistry and was the organizer of the 16th International Conference on Physical Organic Chemistry, held 4–9 August 2002 in La Jolla, CA.

Molecular Order and Mobility in Polymer Systems

by *Tatiana Birshtein*

The **6th International Symposium on Molecular Order and Mobility in Polymer Systems**, held 2–6 June 2008 in Saint-Petersburg, Russia, was the extension of the symposia series organized by the Institute of Macromolecular Compounds of the Russian Academy of Science (RAS). The symposium involved a very wide range of participants, not only in terms of the countries, universities, and laboratories they represented, but also in the positions they held in polymer science and their ages and qualifications.

The co-organizers of the symposium, dedicated to the 60th anniversary of the institute, were the Department of Chemistry and Material Science and the Scientific Polymer Council of RAS. The symposium was



The Cathedral Santiago de Compostela.

Conference Call

supported and sponsored by the IUPAC, the Russian Foundation for Basic Research, Saint-Petersburg Research Center of RAS, and ZAO L'Oreal.



The main aim of the symposium was to discuss the physics and chemistry involved in complex stimuli-responsive polymer systems with nano-structure organization and “soft” order preserving a pronounced molecular mobility. The experimental data and the results of theory and simulation were presented. The equilibrium properties of polymer systems also received attention.

Symposium topics were as follows:

- linear macromolecules, branched and star polymers, and dendrimers in solutions
- copolymers and polymer blends
- polymer brushes
- polymer micelles and complexes of different topologies
- polymer networks
- liquid crystalline polymer systems



At the opening ceremony participants remembered the well-known researchers P.-G. de Gennes, Nobel laureate, and V. Kabanov and N. Plate, academicians of RAS, who died last year and who actively participated at former symposia.

The conference involved 18 invited lectures, 63 oral communications, and 266 poster presentations. Lecturers were from Russia, Germany, France, The Netherlands, Greece, Bulgaria, Chile, Mexico, Finland, USA, Canada, and other countries. Thirty-five young scientists received financial support from IUPAC to attend the event.

Symposium papers will be published in a volume of *Macromolecular Symposia*. The next conference in the series is planned for 2011.



Tatiana Birshtein <birshtein@imc.macro.ru> was symposium chairman. She is a professor at the Institute of Macromolecular Compounds of the Russian Academy of Sciences, St. Petersburg, Russia.

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/conferenceSponsorship

Where 2B & Y

Trace Elements in Food

1-3 April 2009, Rome, Italy

The diet is the main source of trace elements for most of the world's people. Insufficient intake of essential trace elements has a direct impact on the health of hundreds of millions worldwide. In countries where malnutrition is widespread, deficiencies of iron, zinc, iodine, and selenium leave people vulnerable to a variety of diseases, with very serious consequences. On the other hand, the impact of toxic element species, such as inorganic arsenic and methylmercury, on whole populations is also a priority for the scientific community and health authorities.

The different facets of trace elements, from essentiality to toxicity, will be addressed at the **3rd International IUPAC Symposium on Trace Elements in Food**, which will take place 1-3 April 2009 in Rome, Italy. Advancements in the different areas will be discussed and special attention will be placed on preventing adverse health effects in those individuals and populations most vulnerable to trace-element inadequacies, excesses, or imbalances. The meeting



will consist of two and a half days of oral and poster presentations.

The objective of this interdisciplinary symposium is to gather experts with different backgrounds to discuss all aspects of trace elements in relation to food, with special emphasis on biological effects of elements. The topics covered include essentiality, toxicity, bioaccessibility, bioavailability, speciation, sources and transfer in the food chain, effects of processing, food fortification, supplementation, international legislation and standards, analytical developments, analytical quality assurance, and reference materials. Special emphasis will be placed on research and development efforts which have taken place in the last few years as well as on emerging issues.

Previous meetings were organized in Brussels, Belgium in 2004 and in Warsaw, Poland, in 2000. As with the two previous meetings, this symposium aims to provide a comfortable forum for new ideas and experiences to be exchanged among researchers.

See **Mark Your Calendar** on page 31 for contact information.

 www.tef3-2009.it

Chemical Thermodynamics

29 June- 3 July 2009
Kazan, Russia

Conferences on chemical thermodynamics have been held in Russia on a consistent basis (with one exception) since 1961. Before 1977, they were called "All-Union conferences on calorimetry." Between 1979 and 1991 the title was changed to "All-Union conference on calorimetry and chemical thermodynamics." The 17th conference in this series, now called the **International Conference on Chemical Thermodynamics in Russia**, will be held 29 June-3 July 2009 in Kazan, Russia.

The conferences typically attract up to 400 leading experts in various areas of chemical thermodynamics, including around 150 foreign scientists. The meetings are traditionally held at leading Russian scientific centers.

The choice of Kazan for the 17th conference is not casual. It is a large educational, scientific, and petrochemical center, located at the intersection of Europe and Asia. Kazan is home to a world-famous

chemistry school that has produced such luminaries as K.K. Klaus, N.N. Zinin, A.M. Butlerov, V.V. Markovnikov, A.M. Zajtsev, F.M. Flavitsky, A.E. Arbuzov, and B.A. Arbuzov.

The chief organizer of the forthcoming conference is the Kazan state technological university. The conference will investigate the following themes:

- technologies of petrochemical manufacturing
- technologies of synthetic rubber
- technologies of electrochemical processes
- technologies of organic and inorganic polymers
- mathematical modeling of chemical technology processes
- heat exchange and mass transfer
- chemistry of hetero-organic compounds
- theoretical chemistry
- special chemistry

See **Mark Your Calendar** on page 31 for contact information.

 <http://rcct2009.kstu.ru>

Where 2B & Y

Aromatic Compounds and π -Systems

19–24 July 2009, Luxembourg, Grand-Duchy of Luxembourg

The **13th International Symposium on Novel Aromatic Compounds** will be held from 19–24 July 2009 in Luxembourg City. The goal of this conference is to further elucidate the fundamental principles of synthesis and properties of novel aromatic and other interesting π -conjugated systems, to discuss recent experimental and theoretical insights into the concept of aromaticity, and to explore modern applications of such systems as advanced materials and tailor-made functional modules in supramolecular chemistry and optoelectronics. As such, the meeting is expected to encourage discussion and interaction among various communities connected to aromatic and other π -conjugated systems.

In addition to an Opening Plenary Lecture and the Nozoe Memorial Lecture, the scientific program will include invited lectures, oral communications, and a



poster session. The main topics are:

- aromaticity and novel π -conjugated systems—theory and experiment
- aromatic polymers and oligomers and their optoelectronic properties
- supramolecular aromatic devices, switches, and machines
- aromatics on surfaces including graphene
- fullerenes and concave aromatics
- optoelectronics

Situated in the heart of Europe and bordered by Belgium, France, and Germany, Luxembourg is a convenient destination for business travel. The city has a cosmopolitan flair that is surprising in view of its size. Despite the political and economic developments involved in European unification, this multilingual country has maintained an atmosphere of contemplative tranquility.

See **Mark Your Calendar** on page 31 for contact information.

 www.isna13.lu

NICE '09

29–30 July 2009, Tokyo, Japan

The purpose of the **NICE—Network of InterAsian Chemistry Educators**—symposium is to promote communication among inter-Asian chemistry educators, to exchange chemistry teaching strategies and materials in different countries, and to share the fruitful results.

The tentative topics for this year's event are as follows:

- students' conceptions and conceptual change
- instructional strategies, use of audio-visual instruments in classes
- chemistry in daily life, attitudes toward chemistry
- lab activities, sharing/exhibiting of products of science fairs
- representation of textbooks
- chemistry for excellence, preparation for the International Chemistry Olympiad

 www.chemistryeducator.org

Other Conferences of Note

Reference Material, 7–10 July 2009

12th Biological and Environmental Reference Material (BERM) Symposium, Oxford, UK
www.berm12.com

History of Chemistry, 2–5 August 2009

The 7th International Conference on History of Chemistry, Sopron, Hungary
www.chemhist2009.mke.org.hu

Solution Chemistry, 21–25 August 2009

31st International Conference on Solution Chemistry, Innsbruck, Austria
www.icsc2009.org

Thermal Conductivity, 29 August to 2 September 2009

30th International Thermal Conductivity Conference, Pittsburgh, Pennsylvania, USA
www.thermalconductivity.org

2009

 IUPAC poster prizes to be awarded

15-17 February 2009 • Radical Polymerization • Melbourne, Australia

Materials of the Future-Science of Today: Radical Polymerization

Dr. Graeme Moad, CSIRO Molecular Science, Bag 10, Clayton South, Victoria, 3787, Australia

Tel.: +61 3 9545 2509, Fax: +61 3 9545 2446, E-mail: graeme.moad@csiro.au

8-11 March 2009 • Heterocyclic Chemistry • Gainesville, FL

10th Florida Heterocyclic Conference

Prof. Alan R. Katritzky, University of Florida, Department of Chemistry, Gainesville, FL 32611-7200, USA, Tel: +1

352-392-0554, Fax: +1 352-392-9199, E-mail: katritzky@chem.ufl.edu

1-3 April 2009 • Trace Elements in Food • Rome, Italy

3rd International Symposium on Trace Elements in Food (TEF-3)

Dr. Francesco Cubadda, National Centre for Food Quality and Risk Assessment, Istituto Superiore di Sanità, Viale Regina Elena 299, I-00161 Rome, Italy

Tel.: +39 06 4990 3643, Fax: +39 06 4990 2540, E-mail: francesco.cubadda@iss.it

16-17 April 2009 • Clinical Laboratory Diagnostics • Barcelona, Spain

5th European Symposium on Clinical Laboratory and Diagnostic Industry: Standardization and Tumor Markers

Dr. Xavier Filella, Hospital Clínic, Department of Biochemistry & Molecular Genetics, C/ Villarroel 170, E-08036 Barcelona, Spain, Tel: +34 93 227 54 00 x 3141, Fax: +34 93 337 93 76, E-mail: xfilella@clinic.ub.es

20-24 April 2009 • Advanced Materials • Rouen, France 

POLYCHAR-17: World Forum on Advanced Materials

Allisson Saiter, University of Rouen, Laboratory L'E.C.A.P., Avenue de l'Université, B.P. 12, F-76801 St-Etienne du Rouvray Cedex, France, Tel.: +33(0)2 32 95 50 86, Fax: +33(0)2 32 95 50 82, E-mail: allison.saiter@univ-rouen.fr

7-9 June 2009 • Frontiers in Polymer Science • Mainz, Germany

Frontiers in Polymer Science—International Symposium Celebrating the 50th Anniversary of the journal Polymer

Prof. Axel Müller, University of Bayreuth, Macromolecular Chemistry II, D-95440 Bayreuth, Germany, Tel.: +49 921 55 3399, Fax: +49 921 55 3393, E-mail: axel.mueller@uni-bayreuth.de

22-24 June 2009 • Vacuum Microbalance and Thermoanalytical Techniques • Lublin, Poland

32nd International Conference on Vacuum Microbalance and Thermoanalytical Techniques (IVMTTC 32)

Prof. Piotr Staszczuk, Maria Curie-Skłodowska University, Dept. of Physicochemistry of Solid Surfaces, Sienkiewicza 1123, PL-20 031 Lublin, Poland, Tel.: +42 81 5375 646, Fax: +42 81 5333 348, E-mail: piotrs@hektor.umcs.lublin.pl

28 June-1 July 2009 • Self-Healing Materials • Chicago, Illinois, USA

2nd International Conference on Self-Healing Materials

Dr. Solar Olugebefola, University of Illinois, Beckman Institute 3309, 405 N. Mathews Ave, Urbana, IL 61801 United States, Tel.: +1 217 333-2578, Fax: + 217 244-0181, E-mail: solar@illinois.edu

29 June-3 July 2009 • Chemical Thermodynamics • Moscow, Russia

XVII International Conference on Chemical Thermodynamics in Russia (RCCT 2009)

Prof. J.D. Tretjakov, Moscow State University, Department of Inorganic Chemistry, Leninskiy Gory, GSP-2, RF-119991 Moscow, Russia, Tel.: +7 8 495 939 2074, Fax: +7 8 495 939 0998, E-mail: rcct2009@kstu.ru

5-9 July 2009 • Polymers and Organic Chemistry • Montréal, Canada 

13th International IUPAC Conference on Polymers & Organic Chemistry (POC-'09)

Prof. Will Skene, Université de Montréal, CP 6128, Succ. Centreville, Montréal, QC H3C 3J7, Canada

Tel.: +1 514 340-5174, Fax: +1 514 340-5290, E-mail: wskene@umontreal.ca

19-24 July 2009 • Novel Aromatic Compounds • Luxembourg City, Grand Duchy of Luxembourg

International Symposium on Novel Aromatic Compounds (ISNA-13)

Prof. Carlo Thilgen, ETH Zürich, Laboratorium für Organische Chemie, Wolfgang-Pauli-Strasse 10, CH-8093 Zürich, Switzerland, Tel.: +41 1 632 2935, Fax: +41 1 6321109, E-mail: thilgen@org.chem.ethz.ch

Mark Your Calendar

26–31 July 2009 • Ionic Polymerization • Lodz, Poland

19th IUPAC International Symposium on Ionic Polymerization (IP '09)

Prof. Stanislaw Penczek, Polish Academy of Sciences, Centre of Molecular and Macromolecular Chemistry, Sienkiewicza 1123, PL-90 363 Lodz, Poland, Tel.: +48-42-681 9815, Fax: +48-42-684 7126, E-mail: ip09@bilbo.cbmm.lodz.pl

26–31 July 2009 • Organometallic Chemistry • Glasgow, UK

15th International IUPAC Conference on Organometallic Chemistry Directed Towards Organic Synthesis

Prof. Pavel Kocovsky, University of Glasgow, Department of Chemistry, Glasgow, G12 8QQ, United Kingdom, Tel.: +44 141 330 4199, Fax: +44 141 330 4888, E-mail: pavelk@chem.gla.ac.uk

26–31 July 2009 • Plasma Chemistry • Bochum, Germany

19th International Symposium on Plasma Chemistry (ISPC-19)

Prof. Achim von Keudell, Ruhr University Bochum Universitstrasse 150, D-44780 Bochum, Germany, Tel.: +49 234 322 3680, Fax: +49 234 321 4171, E-mail: Achim.vonKeudell@rub.de

31 July–6 August 2009 • IUPAC 45th General Assembly • Glasgow, UK

IUPAC Secretariat, Tel.: +1 919 485 8700, Fax: +1 919 485 8706, E-mail: secretariat@iupac.org
www.iupac.org/symposia/conferences/ga09/

2–7 August 2009 • IUPAC 42nd Congress • Glasgow, UK

Chemistry Solutions

IUPAC 2009, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK, Tel.: +44 (0) 1223 432380, Fax: +44 (0) 1223 423623, E-mail: iupac2009@rsc.org
www.iupac2009.org

2–7 August 2009 • Heterocyclic Chemistry • St. John's, Newfoundland and Labrador, Canada

22nd International Congress on Heterocyclic Chemistry (ICHC-22)

Prof. Mohsen Daneshmand, School of Pharmacy, Memorial University of Newfoundland, St. John's, NL A1B 3V6, Canada, Tel.: +1 709-777-6958, Fax: +1 709-777-7044, E-mail: mohsen@mun.ca

14–18 September 2009 • High Temperature Materials • Davis, CA, USA

High Temperature Materials Chemistry Conference–XIII (HTMC-XIII)

Alexandra Navrotsky, University of California at Davis, One Shields Avenue, Davis, CA 95616 USA
Tel.: +1 530 752-3292, Fax: +1 530 752-9307, E-mail: ANavrotsky@UCDavis.edu

28 September–2 October 2009 • Frontiers of Polymers • Santiago, Chile

10th International Conference on Frontiers of Polymers and Advanced Materials

Prof. Guillermo González, Department of Chemistry, Universidad de Chile, Las Palmeras 3425, Santiago, Chile
Tel.: +562 978-7404, Fax: +562 271-3888, E-mail: ggonzale@uchile.cl

10–14 October 2009 • Molecular Environmental Soil Science • Hangzhou, China

International Symposium of Molecular Environmental Soil Science at the Interfaces in the Earth's Critical Zone

Prof. Jianming Xu, Zhejiang University, College of Environmental & Resource Sciences, Hangzhou, 310029, China, Tel.: +86 571-8697-1955, Fax: +86 571-8697-1955, E-mail: jmxu@zju.edu.cn

2010

 IUPAC poster prizes to be awarded

4–8 July 2010 • Pesticide Chemistry • Melbourne, Australia

12th IUPAC International Congress of Pesticide Chemistry

Dr. Elizabeth Gibson, RACI, 1/21 Vale Street, North Melbourne, VIC 3051, Australia, Tel.: +[61] 0 3 9328 2033, Fax: +61 0 3 9328 2670, E-mail: elizabeth@raci.org.au

8–13 August 2010 • Chemical Education • Taipei, Taiwan

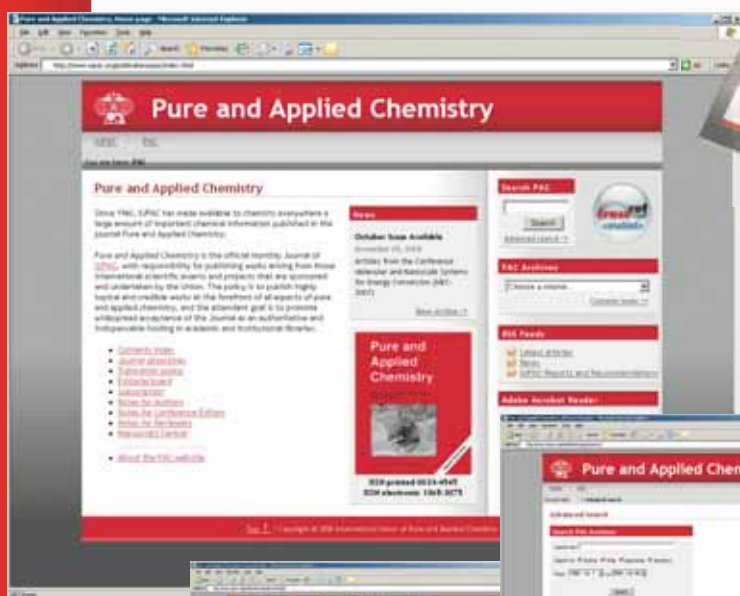
21st International Conference on Chemical Education (ICCE-21)—Chemistry Education and Sustainability in the Global Age

Prof. Mei-Hung Chiu, National Taiwan Normal University, No. 88, Ding-Zhou Road, Section 4, Taipei, 116, Taiwan
Tel.: + 886 2-2932-2756, Fax: + 886 2-2935-6134, E-mail: mhc@ntnu.edu.tw

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