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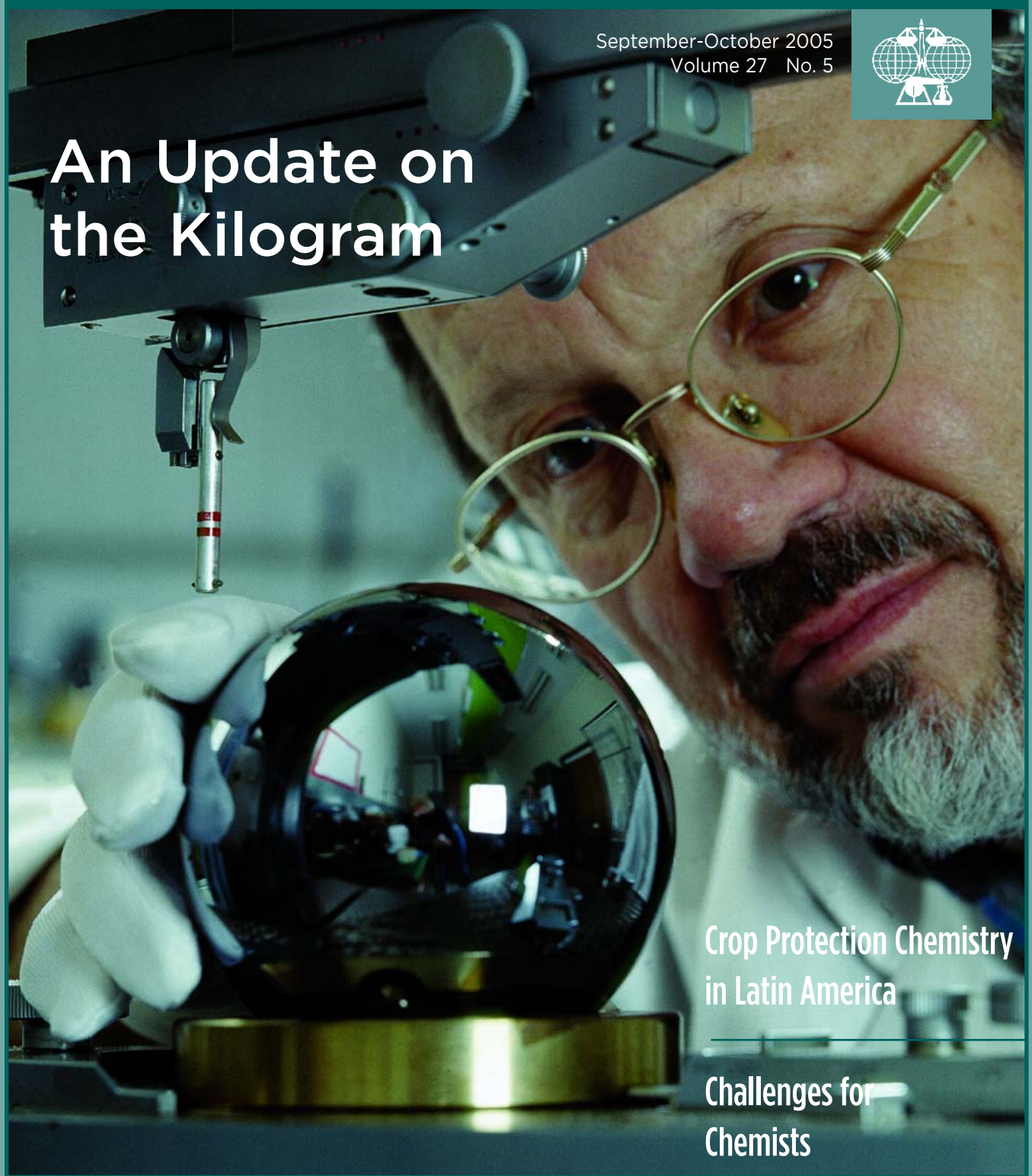

An Update on the Kilogram

Crop Protection Chemistry in Latin America

Challenges for Chemists

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

www.iupac.org/publications/ci

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From the Editor

If metrology has never before tickled your interest, this issue of *CI* may change your mind. Several features should help convince you of the importance of the "scientific study of measurement" and its impact not only on all disciplines of science, but also on the world at large.

First, Ian Mills reviews in detail (p. 12) the problems related to our current kilogram standard and prototype. Surely, changing the kilogram standard—as scientists are considering—will not make your favorite recipe turn out any different, nor will it cause your scale to reveal changes in your body weight. Instead, the proposed definition of the kilogram will reveal weights, and also related fundamental constants, with more accuracy and precision down to the parts per 10^8. Mills explains the importance of making the change and how it would benefit fields such as quantum metrology in which the unit of mass finally would be based on a standard "invariant of nature" and referenced to quantum properties, as are the units of length and time.

As we have come to appreciate, international trade, human health and safety, and environmental protection measures depend on metrology. From a qualitative point of view, there is also the need for a shared measurement terminology. In a position paper (p. 18), Paul De Bièvre shows how ambiguous terminology can create barriers to trade. Reviewing typical terms such as "quantity" or "measurand," he points out pitfalls that could lead to misunderstanding.

The importance of precision and accuracy in measurement is echoed by K. Racke et al. in their article on crop protection chemistry (p. 4). Results from a recent workshop held in Costa Rica highlight the importance of regulatory harmonization and control of residues and human exposure; these also depend on metrology.

So, as you can glance at C.P. Casey's article listing the challenges facing chemists (p. 8), perhaps you will add to your own list the challenge of being precise and accurate?

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Cover: Master optician Achim Leistner checks on an Avogadro's sphere. Such a perfectly spherical single crystal of silicon is needed for the X-ray crystal density experiment relevant to one of the proposed alternative definitions of the kilogram. See "An Update on the Kilogram" by Ian Mills, p. 12. (Image courtesy of CSIRO Industrial Physics, Lindfield NSW, Australia.)

International Union of Pure and Applied Chemistry

Advancing the worldwide role of chemistry for the benefit of Mankind

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

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Österreichische Akademie der Wissenschaften *(Austria)*
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The Royal Academies for the Sciences and Arts of Belgium *(Belgium)*
Brazilian Chemistry Committee for IUPAC *(Brazil)*
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Thieme Publishers and IUPAC in collaboration with the editors of SYNTHESIS · SYNLETT · SCIENCE OF SYNTHESIS · HOUBEN–WEYL announce the

2006 Thieme–IUPAC Prize in Synthetic Organic Chemistry

Call for Nominations

The Thieme–IUPAC Prize is presented every two years on the occasion of the International Union of Pure and Applied Chemistry – International Conference on Organic Synthesis (IUPAC–ICOS). The 2006 ICOS will be held in Mérida, México, on June 11–15. The prize is awarded to a scientist under 40 years of age whose research has had a major impact in synthetic organic chemistry.

Prize € 5000

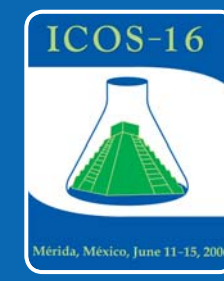
The Thieme–IUPAC Prize has been awarded to Stuart L. Schreiber in 1992, Paul Knochel in 1994, Eric N. Jacobsen in 1996, Andrew G. Myers in 1998, Alois Fürstner in 2000, Erick M. Carreira in 2002, and John Hartwig in 2004.

The prize will be awarded on the basis of scientific merit for independent research dealing with synthesis in the broadest context of organic chemistry, including organometallic chemistry, medicinal and biological chemistry, designed molecules, and materials. Candidates must be under 40 years of age as of January 1 of the year in which the prize is awarded.

Proposals must be accompanied by a biographical sketch of the nominee, a list of the candidate's ten most significant publications, and a statement of how the candidate's research has had a major impact on the field of synthetic organic chemistry. The material will be confidentially forwarded to an independent selection committee.

Deadline: December 9, 2005

For further information please visit www.thieme-chemistry.com



ICOS-16
June 11–15, 2006
Mérida, México

Nomination materials (8 copies)

should be submitted by December 9, 2005 to

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Achieving Important Goals with the Right Combination of "Hard Cash" and Volunteers

by Christoph Buxtorf

In financial terms, the biennium 2003–2004 has been a good one. Again, our reserves have increased—mainly due to some smart decisions made by the Financial Committee some years ago, moving a part of IUPAC capital from equity to bonds and making some changes in U.S.-dollar investments to bond investments in Euros just before the drop in the value of the dollar. As a result, our reserves have increased by 34% over this biennium.

Our income side is very much dependent on national subscriptions, publications, and earned interest. With the exception of some difficulties collecting national subscriptions from three National Adhering Organizations (one of them finally paid their arrears), operations went in an orderly manner. Expenses again were in line with budgets; hopefully we can achieve a similar result in the next biennium.

Can We Expect More Goods News?

Reading Bryan Henry's *Vice Presidential Critical Assessment* of the project system now established within IUPAC, one can appreciate the positive moves we have made over the last few years. As Henry noted, "Three years have passed, and it appears that the project system is functioning very well, perhaps even better than expected." It is my own impression that most of our "hard cash" is spent wisely and in a very professional manner. It underscores the thanks we owe to our many volunteers all over the globe who make a big impact on what we achieve at IUPAC. It is the combination of these two elements that creates a very powerful tool for "Advancing Worldwide Chemistry."

So the conclusion is clear—let us devote more funds to good projects. However, there is always room for improvement. Let us think of better ways to communicate our results to a broader outside world. For instance, I still have the feeling that many people in the chemical industry do not know enough about what we are doing and how we contribute to their success. If we could gain their understanding and their cooperation, we might be able to bring in additional "hard cash" for new projects. The generous Samsung donation (July-August 2005 *CI*, p. 14) is a shining, but rare, example of appreciation.

It is not the industry's fault that our name and work is not better known; we should work harder to present clearly what we do for their benefit. The Committee on Chemistry and Industry (COCI) has started a campaign to attract chemical companies to our Company Associates (CA) program. The new CA brochure describes IUPAC, what we do, and how we benefit industry. It also discusses how being a CA is an asset for companies, as it helps create new contacts and new initiatives. For instance, in collaboration with UNESCO, COCI coordinates a Safety Training Program that provides opportunities for young practitioners from developing countries to gain hands-on experience from IUPAC CAs.

The Safety Training Program has, in the past, allowed fellows from Egypt, Turkey, Nigeria, Kenya, China, and Uruguay to receive training at IUPAC CAs in Japan, South Africa, Sweden, and the USA. Such arrangements are very attractive—both for the fellows that receive them and for the host CAs. I personally give this initiative a lot of credit as I am convinced that joint projects with industry can be an avenue for demonstrating our high-quality work and generating support for IUPAC.

. . . the conclusion is clear—let us devote more funds to good projects.

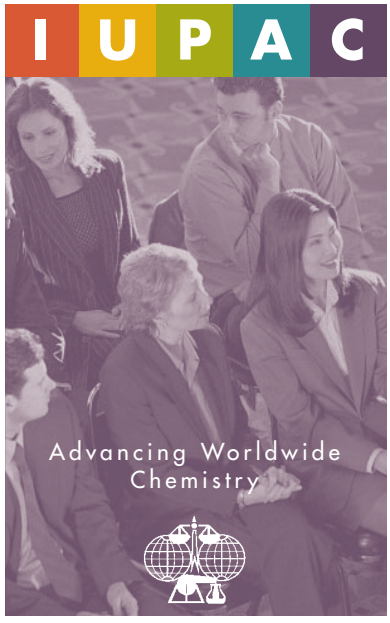
Our worldwide expertise is our most important strength, which, when combined with adequate funding, we can use in the following ways:

- developing our common language (nomenclature and structure)
- solving environmental problems
- enhancing education
- controlling chemical weapons
- improving human health
- promoting analytical and physical chemistry standards
- facilitating safety of plant operations

In a nutshell, it is of the highest importance that we continue to support these efforts to ensure public acceptance and appreciation of chemistry. Let us not underestimate our role in changing public views about chemistry. We distribute our know-how free of charge to any place in the world. Our homepage can be called on 24 hours a day, all year around. At our meetings and workshops, we achieve active, worldwide participation, and ideas are exchanged and further developed for the benefit of all. "Advancing Worldwide Chemistry" is much more than a phrase—it is an expression of what IUPAC actually does everyday. However, it is not good enough to just do good things—we need to talk about them more frequently and widely. This is especially important for countries that are trying to establish themselves economically. Our reputation as experts is not well known in these areas.

Let us use all of IUPAC's tools—global expertise in chemistry, combined with a powerful project system, highly skilled volunteers, and ample funding—to change the sometimes "not-so-brave new world" and help the human race to survive in a decent way. And in the very end, a big thank you—to all of you—for your hard work as highly skilled volunteers for IUPAC! Without your commitment and help, "hard cash" would not do it!

Christoph F. Buxtorf <ch.buxtorf@dplanet.ch> is the current treasurer of IUPAC and a member of the Executive Committee. He is retired from Novartis Crop Protection where he was head of the Production and Technology Division.



IUPAC Prize for Young Chemists

Supporting the future of chemistry

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

Call for Nominations: Deadline is **1 February 2006.**

For more information, visit www.IUPAC.org/news/prize.html or contact the Secretariat by e-mail at secretariat@iupac.org or by fax at +1 919 485 8706.

Advancement of Harmonized Approaches for Crop Protection Chemistry in Latin America

by K. Racke, E. Carazo, and G. Roberts

As a leading agricultural producer and exporter, Latin America constitutes one of the four largest global crop protection chemistry markets. In 2004, sales of agricultural chemicals in Latin America amounted to USD 5.6 billion, which is 20% of the global total in sales of agricultural chemicals—an increase of 25%–35% from sales experienced during the late 1990s. As the use of crop protection chemicals has increased, so have environmental, food safety, and regulatory concerns. Against this backdrop, the International Workshop on Crop Protection Chemistry in Latin America was held 14–17 February 2005 in San Jose, Costa Rica. It was organized around three priority topics related to crop protection chemistry: regulatory harmonization, environmental assessment, and residues and human exposure. Key observations from each of the three major workshop topics are summarized below, and future action items for IUPAC are also outlined.

Regulatory Harmonization

A fundamental assumption for the regulatory process is that chemical pesticides play an important role in sustainable agriculture, provision of the world's food supply, and protection of public health. Their use has contributed to efficient use of existing agricultural lands, thus minimizing further encroachment into natural areas. Pesticide use has had a major role in the tripling of world food production experienced during the past 50 years. For example, the use of pesticides in Costa Rica has resulted in a three-fold increase in production value during the past 5–10 years, while actually reducing the area of land under cultivation. Meanwhile, Costa Rica has been able to protect nearly one-quarter of its territory as national parks or private reserves.

Over the past decade, sales of crop protection chemicals in Latin America have grown significantly; the region is now one of the four largest global markets for such chemicals. Analysis of market trends indicates the potential for increased use of some categories of products, particularly those targeted for public health protection. Compared to other regions, Latin America has been faster to adopt products with new active ingredients. However, the cost of developing each new active ingredient has soared, and current estimates place the associated R&D expenses at between USD 180 and 200 million. For industry, this cost escalation has increased concerns about regulatory data and patent protection.

One major market trend is an overall increase in reliance upon generically produced, off-patent products. In light of this trend, lecturers from both industry and nongovernmental organizations emphasized the critical importance of quality control of approved sources of pesticide active ingredients and formulations. This is important for ensuring efficacy while supporting human and environmental safety, particularly with respect to the correct assay of active ingredients and the minimization of relevant impurities.

There are a number of international approaches available to support local regulatory evaluation and management of crop protection chemistry. These include the FAO Code of Conduct, the FAO/WHO product quality specification process, OECD test guidelines, and Codex maximum residue limits. In addition, crop protection chemistry will be affected by implementation of international treaties and conventions that have recently entered into force, including those related to persistent organic pollutants (Stockholm Convention, May 2004) and prior-informed consent (Rotterdam Convention, February 2004). It was suggested that most evaluation systems be redesigned to assess the *benefits* of pesticides as well as the risks. Currently, no internationally harmonized guidelines are in place to do this.

Some interesting regional approaches to harmonization have been initiated recently in Latin America. During the late 1990s, the five Andean countries agreed to adopt a common norm for evaluation and regulation of pesticides, and a technical manual of evaluation criteria and procedures was developed. Implementation is still at an early stage, but many valuable lessons have already been learned. One remaining gap concerns evaluation criteria and an agreed-upon procedure for establishing generic versions of existing active ingredients. Similarly, the CATIE/GTZ-NOQ project, in cooperation with the

Agricultural Regional Organization of Central America, has drafted a common set of regulatory evaluation guidelines specifically for microbial and botanical pesticides, which are currently not well covered by guidelines for traditional, synthetic pesticides. The proposals arose following evaluation of guidelines available from OECD and several major OECD countries. It is hoped that in the future the seven Central American countries plus the Dominican Republic will adopt this harmonized approach.

Lecturers also emphasized the importance of education as a complement to regulation to support effective management of crop protection chemistry throughout the region. Health and environmental risks, especially those that may be associated with misuse, are largely a preventable problem. Safe pesticide use requires safe equipment and good systems for training and educating pesticide applicators and farm workers. In addition, good regulation and enforcement by a well-trained authority are essential. In Costa Rica, for example, the Ministry of Agriculture and Agricultural Pesticide Chamber trained nearly 130 000 people during the past 20 years in safe pesticide use practices. The appropriate management of an ever-expanding information base related to crop protection chemistry was also emphasized. The Internet in particular has become a vast resource for exchanging information on pesticide chemistry. Navigating this information, with respect to both availability and reliability, is an increasing challenge. Perhaps two quotes from classical scholars summarize well the present situation:

"The next best thing to knowing something is to know where to find it." — *Samuel Johnson, English author (1709–1764)*

"Man's most judicious trait is a good sense of what not to believe." — *Euripides, Greek philosopher (c. 480–406 BC)*

To this end, the recently initiated IUPAC project on global agrochemical information management was introduced as a means of improving the situation. In partnership with FAO and IAEA, this project aims to increase availability of reliable information on the most important pesticides and pesticide information sources.

Environmental Assessment

Environmental fate and ecological risk assessment were important areas of emphasis at the workshop, particularly in light of growing environmental awareness in the Latin America region. Although past IUPAC project (*PAC* **69**(6), 1349–1371 [1997]) conclusions highlighted the overall tendency for more rapid dissipation of pesticides under tropical or sub-tropical conditions, it was noted that much of the area in Latin America where pesticides are used heavily actually falls within the temperate climate zone (e.g., grain and soybean-growing regions of Southern Brazil and Argentina; fruit-growing regions of Argentina and Chile). The wide diversity of agricultural, soil, and climatic conditions present in both temperate and tropical areas of Latin America make it important to understand the processes governing fate and transport under these conditions. On the other hand, it was noted that testing has consistently revealed a similar level of sensitivity to pesticide exposure within major groups of non-target wildlife in temperate and tropical area species. Thus, it is possible to refer to standardized OECD test guidelines and organisms without having to implement specific tests on locally prominent species.

Attendees and speakers at the Workshop on Crop Protection Chemistry in Latin America.

The off-target movement of pesticide residues during and following application was emphasized as an important factor not to be neglected. Considerations of such movement include direct human exposure, deposition on sensitive non-target crops or plants, and contamination of surface water resources. Spray drift of fine particulates during application may be an inevitable process, but preliminary results of an ongoing IUPAC project (# 2001-023-1-600) indicate that a variety of drift mitigation practices are available.

Options for best management practices for drift mitigation include sprayer technology (e.g., drift-reducing nozzles, properly calibrated equipment), chemical technology (e.g., spray tank adjuvants), and operational practices (e.g., wind speed restrictions, no-spray zones). Pesticide labeling regulations and education are also important factors for ensuring that applicators understand their responsibilities and take appropriate precautions.

Although application spray drift and post-application surface water runoff/sediment erosion are perhaps the greatest contributors to offsite movement of pesticides from agricultural areas, volatilization was also noted as a potentially significant loss process for some chemicals in combination with favorable meteorological and soil conditions. Although research in Latin American countries is limited, work in other regions indicates that under some conditions, from 5% to 20% or more of applied residues for certain pesticides may volatilize from soil and foliar surfaces into the atmosphere, where they may constitute sources for exposure or redeposition into sensitive areas. Unique combinations of environmental conditions and agricultural practices may contribute in some regions to higher pesticide volatilization (e.g., frequent pesticide application, frequent precipitation/irrigation, high temperature, low organic carbon content soils). In some cases, minor use pesticides may also be major constituents of atmospherically derived residues depending on their particular solubility, sorption, persistence, and volatility properties.

Without a doubt the noisier workshop participants, these macaws, which are native to South and Central America, were eager to learn more about crop protection.

Lecturers and participants also discussed the impact of pesticides on water quality, including effects on aquatic organisms, humans, and livestock. Water monitoring has indicated the presence of trace concentrations of both highly persistent and more degradable pesticides in natural water areas adjacent to agricultural fields. For example, monitoring of irrigation return waters near the Palo Verde National Park area of Costa Rica displayed low ppb (μg/L) levels of both insecticides and fungicides. Similar observations of low concentrations of pesticides in both irrigation and natural waters have been reported from the fruit and vegetable areas of Mexico, the banana-growing areas of Central America, and the soybean and grain growing areas of Brazil.

The importance of effective water management in mitigating pesticide entry into natural areas was also emphasized. The movement of residues from agricultural areas following sprinkler/flood irrigation compared to the lack of detections where drip irrigation was employed was particularly noteworthy. Lecturers also stressed the need for accurate and reliable data from well-designed studies for regulatory compliance purposes and for determining the effectiveness of exposure mitigation practices. It was generally recognized that regional cooperation would be beneficial for implementing systematic monitoring of surface water residues from pesticides and other contaminants. Important quality control aspects for both chemical and biological monitoring of residues were highlighted (# 1999-017-1-600), including the establishment of monitoring objectives, design of sampling frequency and procedures, secure sample handling and preparation procedures, laboratory analysis using appropriate methods and procedures (e.g., accredited labs), and reporting of results with appropriate limits.

Finally, with respect to establishment and interpretation of limits for pesticide residues in water, conclusions and recommendations of a recently completed IUPAC project were highlighted. Key considerations include defining the purpose of the standard and type of water to which the standard will apply, explaining publicly and transparently the rationale for each limit, and developing analytical methods with limits of quantitation that can match concentrations relevant to biological effects. Arbitrary adoption of water standards from other regions without consideration of the basis or rationale for such standards could result in little real benefit to advancement of environmental and human health protection in the Latin American region.

Ecological risk assessment involves consideration of the inherent toxicity of a pesticide as well as the magnitude and likelihood of exposure. Although simple toxicity or hazard classification systems are available and may be suitable for purposes of handling, storage, and transportation, these may be entirely

inadequate and subject to misuse for purposes of environmental evaluation and regulation when not considered within the context of a full risk assessment. The importance of exposure considerations in determining potential harm was perhaps first well recognized some 500 years ago:

"All substances are poisons: there is none which is not a poison. The right dose differentiates a poison and a remedy." — Paracelsus, Swiss philosopher and medical expert (1493–1541)

A number of schemes have been developed, primarily in the United States and Europe, for supporting the regulatory evaluation of ecological risk posed by pesticides. Generally, these schemes involve tiered approaches whereby screening levels requiring limited data are used to identify those products and crop/use scenarios for which more detailed, data-intensive assessments are required. A recently initiated IUPAC project (# 2004-011-1-600) provided initial insight into how screening-level or comparative approaches may be employed as a first step in the pesticide evaluation procedure, particularly in countries where there are significant evaluation resource limitations. The EU's tiered approach to ecological risk assessment, involving standardized fate/exposure scenarios to represent different climatic/geographic areas across a region, was also highlighted. What made this approach particularly interesting for the Latin American situation was the collaborative manner, involving both government and industry, in which the FOCUS (FOrum for the Coordination of pesticide fate models and their USe) scenarios were developed. This might be a good model for Latin America to follow since the region has yet to achieve consensus on ecological risk assessment methods.

Finally, preliminary conclusions of an IUPAC project on environmental implications for the use of genetically modified crops (e.g., insecticide resistant and/or herbicide tolerant) were reviewed (# 2001-024-2-600). Such crop protection technology has growing importance in many parts of the world, including the soybean- and grain-growing areas of Argentina and Brazil, which together contain around one-fourth of the world's transgenic crops. Genetically modified, disease-resistant rice and banana varieties are currently under investigation in Central America. In general, data predict genetically modified crops are likely to have less environmental impact than traditional pest management practices.

Residues and Human Exposure

The topic of pesticide residues and human exposure was also included in the workshop. Latin America is an important agricultural producing and exporting region, and food safety considerations are of growing importance in today's regulatory arena. Mexico's vegetable and fruit exports to the USA, the worldwide export of bananas and other tropical fruits from the Central American and Andean countries, and the grain, soybean, meat, and fruit exports of Brazil, Argentina and Chile to the USA and EU are all major components of the increased international trade in agricultural commodities observed during the past 20 years.

The primary means of local management of pesticide residues in food is via establishment of maximum residue limits or MRLs:

Maximum residue limit (MRL) "Maximum concentration of a residue that is legally permitted or recognized as acceptable in, or on, a food, agricultural commodity or animal feedstuff as set by Codex or a national regulatory authority." (IUPAC 1996)

These MRLs are set to reflect the good agricultural practice (GAP) of a particular country or region, and when residues are present at or below the MRL, this is an indication that GAP has been followed. Most of the countries in Latin American, even those that may establish their own national MRLs, defer to the internationally harmonized MRLs established by Codex when it comes to the regulation of pesticide residues in imported foods. These Codex standards are specifically established to promote fair practices in food trade by ensuring that all relevant GAPs of producing countries are considered in establishing the MRLs. The suitability of these Codex standards for consumer protection is evaluated using chronic and, where appropriate, acute dietary intake assessment methods developed, in part, based on the recommendations of IUPAC. It should be noted that MRLs are *not* health standards per se, but are established based on GAPs and are evaluated for consumer safety. Thus, when an MRL in a food commodity is exceeded, it should not necessarily be viewed as a health concern, but primarily as an indication that GAP may not have been followed.

Monitoring results from tests on both locally produced and imported agricultural commodities in the EU, Japan, and the USA, generally show the vast

continued on page 24

Challenges for Chemists

This invited paper was presented in support and recognition of the Cuban chemical community at the 5th International Conference on Chemistry and Chemical Engineering, held 18–22 October 2004 in Havana, Cuba.

by Charles P. Casey

During my tenure as president of the American Chemical Society in 2004, I have tried to focus attention on the challenges that chemists and chemistry face. Some of these challenges were outlined in the National Research Council report *Beyond the Molecular Frontier: Challenges for Chemistry and Chemical Engineering* (National Research Council, The National Academies Press, Washington, D.C., 2003 <www.nap.edu/books/0309084776/html>). This report comes at a critical time, when the challenges that chemists and chemistry face continue to grow. More than two years in the making, the report had more than 170 contributors, and was prepared by a committee—co-chaired by Ronald Breslow and Matthew V. Tirrell—of 17 distinguished chemists and chemical engineers.

Beyond the Molecular Frontier is the latest in a series of reports from the National Research Council (NRC) on the future of chemistry or chemical engineering. While previous reports focused either on chemistry (Westheimer, 1965, *Chemistry: Opportunities and Needs*, and Pimentel, 1985, *Opportunities in Chemistry*) or chemical engineering (Amundsen, 1988, *Frontiers in Chemical Engineering: Research Needs and Opportunities*), it is significant that the latest report covers both areas and underscores the growing importance of interdisciplinary cooperation between chemists and chemical engineers. These earlier reports were important in setting the direction of chemistry in the United States, and I hope that *Beyond the Molecular Frontier* will also influence the direction of chemistry.

The report offers us a snapshot as well as a vision: a snapshot of where research in the chemical sciences stands today, and a vision of how advances that seem possible in the near term could contribute to a brighter future. Above all, it presents "grand challenges," as well as wonderful opportunities for chemistry professionals and for society.

I have outlined some of the challenges cited in *Beyond the Molecular Frontier*, and encourage readers to look at the full report and the reports of the workshops that helped to frame it.* The challenges and opportunities for each country will be different, depending on local problems and local resources, but many of the challenges will be common to many countries.

Challenges in Synthesis

Chemistry is one of the few sciences that creates new materials rather than simply studying the physical universe. Chemists are challenged to develop highly selective, energy efficient, and environmentally benign new synthetic methods. For example, synthetic chemists will need to devise ways to predictably carry out synthesis on the surfaces of semiconductor chips to enable the attachment of genes for use in diagnosis.

Chemists and chemical engineers will need to work together to develop new processes that are greener by design. Atom economy and energy efficiency will become crucial elements for ensuring sustainability of the chemical enterprise. The application of green chemistry principles will help to reduce or eliminate the use and generation of hazardous substances.

*NRC workshop reports: *Health and Medicine: Challenges for the Chemical Sciences in the 21st Century* (2004), *Energy and Transportation: Challenges for the Chemical Sciences in the 21st Century* (2003), *Information and Communications: Challenges for the Chemical Sciences in the 21st Century* (2003), *The Environment: Challenges for the Chemical Sciences in the 21st Century* (2003), *National Security and Homeland Defense: Challenges for the Chemical Sciences in the 21st Century* (2003), published by National Academies Press, Washington, D.C.

Alternatives to Fossil Fuels

Due to the finite supply of fossil fuels, and because of global warming from CO_2 emissions when they are burned, we are challenged to develop inexpensive and unlimited energy sources to enable a sustainable future. Inexpensive and more efficient photocells will be part of the solution. More efficient methods for nuclear fuel production and safer methods of handling radioactive waste will enable the use of nuclear energy.

Moving towards a hydrogen economy will enable the use of clean energy for transportation. Improved methods for transporting and storing hydrogen and improved fuel cells for utilization of hydrogen will need to be developed. Of course, we will still require new energy sources for the production of hydrogen.

Self-Assembly and Nanoscience

Self-assembly and nanoscience hold great promise for the development of interesting new materials. Properties change drastically in the nanometer range; this is the range between single molecules and bulk materials. As we move towards a revolution in nanoscience, we need to understand the structures of materials on a smaller and smaller scale, and of single molecules and self-assembled arrays of molecules on a larger and larger scale. Self-assembled arrays and self-optimizing systems offer the promise of exciting functionality and possibly behavior.

Physical Chemistry

Advances in physical chemistry should lead to an understanding of how molecules change and react over shorter and shorter time scales and across a full range of molecular sizes. The ability to follow reactions over the picosecond timescale will allow the direct observation of bond making and bond breaking. The ability to investigate and manipulate single molecules will open new avenues to the study of reactions. Bond-selective chemistry will result from selective laser activation of specific bonds. Computing and modeling of larger systems will open new vistas in biophysical chemistry.

Safety, Security, and Defense

Chemical plant security needs to be improved through the substitution of less toxic chemicals for use in processes. Designing processes that minimize the accumulation of hazardous materials would increase the inherent safety of plants. We are challenged to develop robust and selective sensors to help protect our nations against disease and terrorism.

A huge and obvious way in which countries can improve their security is by achieving energy independence. In my view, the root cause of terrorism is the gap between developing and developed countries. Transferring technology to enable developing countries to set up the most modern and efficient means for energy generation and materials synthesis will help to narrow this gap, as will the use of green insecticides and genetic engineering to increase world agricultural production.

Challenges at the Interface with Biology and with Medicine

As chemistry expands into the interfaces with biology, materials science, and environmental sciences, new challenges are presented that will require teamwork among scientists in many disciplines. Biological chemists are challenged to understand the complex interactions among cell components and to work on teams with biologists to understand the processes of life in molecular terms. Research will be needed at the interface between chemistry and biophysics to understand how protein sequence determines protein folding, and eventually protein function.

Medicinal chemists are challenged to find new drugs that will operate by mediating protein-protein interactions. Therapies for preserving memory, for slowing the aging process, and for controlling obesity will require fundamental advances. While pharmaceutical chemists have been largely successful in controlling bacterial infections, new drugs for treating viral diseases like AIDS and Ebola are sorely needed. Drugs to better prevent rejection of transplanted organs and biocompatible materials for organ replacement still need to be developed. New ways of delivering drugs to targeted cells would dramatically increase their efficacy.

The opportunity presented by the determination of the structure of the human genome will be followed by advances in proteomics and bio-informatics that promise to lead to new diagnostic methods and to new therapies.

Challenges at the Interface with Environmental Sciences

Chemists, in cooperation with other scientists, need to develop a better understanding of the atmosphere and the biosphere so that we can maintain a livable environment.

Challenges at the Interface with Materials Chemistry

These challenges include the design of molecular devices and new materials with predictable and tunable properties. Materials chemists are challenged to design and synthesize new electronic and optoelectronic materials, high-temperature superconductors, and new composites and ceramics.

Communication Challenges

As chemists, we all share the goal of communicating chemistry's tremendous contributions to society and the increasingly important role that chemistry must play in meeting challenges of the future. To recruit students into chemistry, we must convince them that they are *needed* to help meet the challenges of preserving the environment, developing renewable energy sources, discovering drugs, and synthesizing nanoscale materials. We will rely on chemistry teachers at all levels to inspire students to use their own potential to unlock chemistry's still hidden secrets. If we present these critical human needs and challenges to the best and brightest students, we can attract them into the chemical sciences.

If I have any criticism of the *Beyond the Molecular Frontier*, it is that it attempts to be too comprehensive and thus does not provide sufficient emphasis and focus. We can all find our favorite problems in the report, but how do we choose those that are the most important? By speaking about the challenges facing chemists and chemical engineers, I have tried to catalyze discussion of the most important problems. To avoid leaving off the readers's favorite challenge, I present lists of five challenges, with the fifth one being "your problem here." I have encouraged audiences to make their own short lists of priorities for chemical research and to share their ideas with me and their colleagues.

Setting Priorities

I urge all chemical scientists to make a list of five major societal problems that require advances in basic chemistry, five advances in basic chemistry that enable new opportunities for chemists, and five modern achievements of basic chemistry that have had major impacts on our science and our society. As you read this article, I hope you will think about your personal list and what you could do to contribute to advances in chemistry. Chemical scientists need these shorter and more focused lists of challenges when trying to increase public or government support for chemistry.

Below is my own list of the five most important societal problems that will require advances in basic chemistry. When I present this to audiences, I have found that there is general agreement with the list and a variety of suggestions for a fifth problem. Suggestions have included enabling human space travel, developing useful molecular machines utilizing nanoscience, attacking global warming by development of CO_2 sequestration, understanding chemical communication mechanisms, promoting technology transfer to developing countries so that they can use the safest and most modern means of energy generation, and materials synthesis.

Casey's List of Five Major Societal Problems that Require Advances in Basic Chemistry

1. conquer disease: anti-viral drugs, drugs to prevent or cure Alzheimer's, malaria, tuberculosis, etc.
2. solve our energy problems by developing sustainable energy sources: solar, nuclear energy; fuel cells for transportation (H_2, CH_4 and CH_3OH)
3. clean the environment: materials from renewable or recycled resources; environmentally benign pesticides and fertilizers
4. deter terrorism: sensors to detect biological and chemical warfare agents
5. your problem here

We all find it much more difficult to think of advances in basic chemistry that will enable new opportunities. Consider how hard it would have been 50 years ago to conceive of the advances in structure determination that would be enabled by the development of nuclear magnetic resonance spectroscopy! In response to my second list, I've received other suggestions, including development of techniques to directly observe very low concentrations of reactive intermediates, which would revolutionize mechanistic chemistry and our understanding of the molecular basis of life processes. The later would require an understanding of the self-assembly of complex systems, self replication, and systems for energy generation; these advances could lead to an understanding of the molecular origin of life on earth.

Casey's List of Five Advances in Basic Chemistry that Enable New Opportunities

1. selective catalysts for direct oxidation of hydrocarbons by molecular oxygen: revolutionary routes to oxygenated materials
2. computations accurate and powerful enough to predict non-covalent interactions: predict protein folding and protein-protein interactions
3. nanoscience and molecular self assembly: multiproperty nanoscale materials; molecular organization in complex systems
4. better understanding of electron transport leading to improved photovoltaic devices and fuel cells
5. your advance here

Casey's List of Five Modern Achievements of Basic Chemistry with Major Impacts on our Science and our Society

1. organometallic catalysts: olefin metathesis, single site polymerization, enantioselective catalysts
2. new pharmaceuticals for mental illness, blood pressure, etc.
3. nuclear magnetic resonance and mass spectrometry for structure determination of biomolecules
4. atomic microscopy and single molecule spectroscopy
5. your suggestion here

For chemists, it's easy to think of many modern achievements of basic chemistry that have had major impacts on society. The difficult task is to limit the list to five. As an organometallic chemist, I had an easy job in filling the top of my list. Other suggested achievements included the introduction of chlorofluorocarbons to resolve stratospheric ozone depletion; advances in computational chemistry, including density functional theory for handling larger molecules; laser chemistry; the development of higher temperature superconducting materials; and the determination of the structure of the human genome.

I am convinced that if chemists focus their creative energies on today's challenges, they can turn them into opportunities for tomorrow's achievements.

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Your Lists of Five Challenges

Major societal problems that require advances in basic chemistry	Advances in basic chemistry that enable new opportunities	Modern achievements of basic chemistry that have had major impacts on our science and our society
1.	1.	1.
2.	2.	2.
3.	3.	3.
4.	4.	4.
5.	5.	5.

An Update on the Kilogram

by Ian Mills

We need a new definition for the kilogram! The present definition (see highlight below) was sanctioned by the first General Conference on Weights and Measures (CGPM, Conférence Général des Poids et Mesures) in 1889, with a minor revision to the words in 1901, and remains unchanged after 116 years. It is the only base unit of the International System of Units (the SI) that is still defined in terms of a prototype artifact, the International Prototype of the Kilogram (IPK), which is kept in a safe at the International Bureau of Weights and Measures (the BIPM, Bureau International des Poids et Mesures) in Sèvres, near Paris.

Present definition of the kilogram:

The kilogram is the unit of mass; it is equal to the mass of the international prototype of the kilogram.

The definitions of the base units play a key role in modern metrology, a subject of ever greater importance in our society. International trade, macro-engineering such as the construction of aircraft wings made in Britain to fit a hull made in France, micro-engineering such as the manufacture of integrated electronic chips with many thousands of elements, the measurement of drug concentrations in medicine, the measurement of pollutants in the environment—all these, and many more, demand reliable measurements to an appropriate level of accuracy for the purpose concerned, and with a known and appropriate uncertainty. In defining the units of the SI upon which this subject is built, we endeavor today to choose definitions that are referenced to quantum properties of atoms or to fundamental constants, a subject known as quantum metrology. Thus, our unit of length (the metre) is defined in terms of the speed of light, and our unit of time (the second) in terms of the period of the hyperfine frequency of a caesium atom. These are believed to be "invariants of nature," available to anyone, anywhere, at any time, and thus are appropriate references for the internationally agreed units of our system.

The present definition of the kilogram in terms of the IPK does not fulfill this requirement, and moreover there are good reasons for believing that the mass of the IPK, along with all its official copies, may be "drifting" in relation to a true invariant such as the mass of a carbon atom, by perhaps as much as 100 μg (0.1 ppm, or a part in 10^7) over 50-year periods. The IPK, a cylinder of platinum-iridium alloy measuring 39 mm high by 39 mm diameter, has been weighed against its various copies three times since it was made: in the 1890s, in the late 1940s, and most recently in the late 1980s. The conclusion from these periodic reviews is that the various kilogram artifacts may well be changing in mass. This is believed to be due to surface contamination (they are stored and weighed in air), wear and tear from handling, and the possible leaching out of gases occluded in the artifact when it was manufactured.

We would like a new definition, and we would like one that would fix the kilogram in terms of what we believe to be an invariant of nature, such as a fundamental constant or the mass of an atom. Draft wording for two possible new definitions of the kilogram that have been discussed for the past fifteen years or more are shown below.

First alternative—draft definition of the kilogram to fix the Planck constant *h*:

The kilogram is the mass of a body at rest such that the value of the Planck constant *h* is exactly $6.626\ 069\ 311 \times 10^{-34}$ joule second.

Second alternative—draft definition of the kilogram to fix the mass of the carbon 12 atom $m(^{12}C)$, and also to fix the atomic mass constant m_u and the value of the Avogadro constant N_A:

The kilogram is the mass of exactly $(6.022\ 141\ 527 \times 10^{23} / 0.012)$ unbound carbon 12 atoms at rest and in their ground state.

It may not be obvious that fixing the value of the Planck constant defines the kilogram: it does so, because $h = 6.626\ldots$ J s = $6.626\ldots$ kg m^2 s^{-1}, and since the metre and the second are already defined in terms of invariants, the value of the kilogram is fixed once the numerical value in this expression is fixed. Similarly $m(^{12}C) = (0.012 / 6.022\ldots \times 10^{23})$ kg, and fixing the numerical value in this expression has the effect of determining the value of the kilogram in the second alternative definition.

There are two experiments that are relevant to these two alternative definitions. The first is the watt balance experiment, in which a weight is measured against the electrical force generated by a coil carrying a current

suspended in a magnetic field. The electrical measurements are made using the Josephson and quantum hall effects. The second is the X-ray crystal density experiment, in which a perfectly spherical single crystal of silicon (see photo on cover of this issue) is weighed against a kilogram standard, and its lattice spacing is measured by X-ray diffraction, allowing a calculation of the number of atoms in the crystal from its diameter. The watt balance leads to a measurement of the Planck constant h in terms of the kilogram, and the X-ray crystal density experiment leads to a measurement of the Avogadro constant N_A in terms of the kilogram. However, if we were to fix the value of h, it would define the kilogram, and the watt balance could then be used to realize the definition. Similarly, if we were to fix the value of N_A it would define the kilogram, and the silicon crystal density experiment could be used to realize the definition. Both experiments are complex, and both are expensive and difficult to perform with high accuracy. The present relative uncertainty of measurement in these experiments is about 0.08 ppm for the watt balance experiment, and about 0.4 ppm for the X-ray crystal density experiment.

The kilogram, kept by the Bureau International des Poids et Mesures.

Either of the two alternatives would give us a definition referenced to an invariant of nature, in place of the somewhat uncertain platinum-iridium prototype used in the present definition. Either could be realized by the experiments described in the previous paragraph, and would also give us a reference available to anyone, anywhere, at anytime, unlike the prototype reference that remains locked in a safe in Sèvres. However, a recent paper by Mills, Mohr, Quinn, Taylor, and Williams, *Metrologia* 2005, **42**, 71–80, has drawn attention to the fact that there are further important considerations involved in changing the definition.

All mass measurements are relative. We measure the mass of one object against another. Our ability to make such measurements has improved dramatically in the last 100 years, and even during the last 10 years. To discuss the uncertainties in such experiments we have to consider two distinctly different kinds of mass measurement. On the one hand, we may be concerned with measuring the mass of macroscopic objects, measured in grams or kilograms, usually using a balance of some kind. This, to most of us, is the kind of mass measurement that immediately springs to mind; we might call it "macroscopic mass metrology." The reference standard for such measurements is (at present) the prototype kilogram—the IPK—used in the current definition of the kilogram. The IPK has proved a convenient reference for making macroscopic mass measurements, and even if we change the definition to one of the alternatives, it is likely to remain an important intermediate step in relating mass standards around the world for macroscopic mass measurements.

On the other hand, physicists and chemists are concerned with the masses of atoms and fundamental particles, which may be compared with each other by mass spectrometry, for example. The reference standard for these measurements is the unified atomic mass unit, symbol u, defined as one-twelfth of the mass of a carbon 12 atom, also known as the atomic mass constant m_u.* We might call such measurements "microscopic mass metrology." It is also a fact that the best estimates of the values of many of the fundamental constants of physics, such as the Planck constant h and the elementary charge e are strongly correlated with the atomic masses, so that whenever we discuss the masses of the atoms we have also to consider the values of the fundamental constants.

The present situation is that relative mass measurements within either the field of macroscopic or microscopic masses can be made with very much higher precision than that with which we are able to compare masses between the two fields. For example, it is possible to compare the mass of two kilogram artifacts,

*This unit is also known as the dalton, symbol Da. The latter name and symbol is widely used by biochemists and others concerned with the mass of large molecules that may be measured in kilodaltons, kDa, or megadaltons, MDa. Thus 1 Da = 1 u = m_u = $m(^{12}C)$ / 12.

Some of the fundamental constants whose values depend on the kilogram

Atomic mass constant	m_u	Josephson constant	K_J
Electron mass	m_e	Proton gyromagnetic ratio	γ_p
Planck constant	h	Faraday constant	F
Avogadro constant	N_A	Bohr magneton	μ_B
Elementary charge	e	Nuclear magneton	μ_N

using the best modern balances, to better than a part in 10^9, a relative uncertainty of less than 0.001 ppm, or less than a microgram in a kilogram. Similarly, the mass of an electron m_e can be determined relative to the unified atomic mass constant m_u with a relative uncertainty of 4.4 parts in 10^{10}, 0.00044 ppm. However, when it comes to measuring the mass of any of the fundamental particles in terms of the present SI kilogram, the uncertainty is about 2 parts in 10^7, 0.2 ppm, a relative uncertainty more than two orders of magnitude greater. Such measurements are dependent on either the watt balance or the silicon crystal density experiment. The present uncertainty in our best measurement of m_e/kg, for example, is 0.17 ppm, and there is a similar uncertainty in all atomic and particle masses when they are expressed in the present SI kilogram. Moreover, most of the fundamental constants of physics depend on the kilogram (see table above). The best estimates of these constants are revised at intervals by the CODATA (Committee on Data for Science and Technology) task group established for this purpose. The most recent 2002 revision was published earlier this year (Mohr and Taylor, *Rev. Mod. Phys.* 2005, **77**, 1–107). This review shows that the present relative uncertainties in the fundamental constants, when expressed in SI units, are mostly around 0.2 ppm. In every case the dominant contribution to this uncertainty is simply the uncertainty in relating atomic or particle masses to the macroscopic reference kilogram, the IPK.

The present situation regarding redefining the kilogram is, therefore, as follows. If we were to change to a new definition using a fundamental constant or an atomic mass as a reference, it would follow immediately that all particle masses and fundamental constants would be known with an uncertainty reduced by two orders of magnitude—because their values expressed in SI units would no longer involve a knowledge of the bridge between macroscopic and microscopic masses. Both the elementary charge e and the Josephson constant K_J would also be more accurately known by a similar factor, so that all electrical measurements made using these constants would be similarly improved. These are important advantages. The effect on the values of the fundamental constants is illustrated in the table on page 15. However, the mass of the IPK would no longer be 1 kg by definition, but would have to be determined by experiment. Although the constant appearing in the new definition would be chosen so that the mass of the prototype would initially still be exactly 1 kg, it would be subject to the uncertainty of about 0.2 ppm that applies to all atomic masses under the present definition, and it is also possible that future measurements would lead us to revise the mass of the IPK so that it might be slightly different from 1 kg. Although it is unlikely that this change would ever be greater than 0.2 ppm, this is seen as a disadvantage of changing the definition by those concerned with macroscopic mass metrology. Mills et al. suggest that, after changing the definition, macroscopic mass measurements could continue to be made in terms of the mass of the IPK, with a correction factor being applied in those rare occasions when it is really necessary.

If, however, we retain the present definition, then the values of the fundamental constants expressed in SI units will remain uncertain to about 0.2 ppm, just as they are at present. The mass of the IPK will remain equal to 1 kg by definition—although this would not dispel doubts arising from the uncertainty of the mass of the IPK compared to an invariant of nature. The magnitude of this uncertainty is not known, but it is believed to be of the order 0.05 ppm, or possibly as much as 0.1 ppm.

There is little doubt that the definition of the kilogram will eventually be changed to one of the two alternatives . . .

In this brief review it is not possible to cover all the problems of redefining the kilogram, and readers are referred to the paper by Mills et al. for further details. However, there is one further point to note here, which concerns the timing of any possible change. Changes to the base units of the SI are made by the CGPM, on the advice of the CIPM (International Committee for Weights and Measures) and its various consultative committees. The CGPM meets at four-year intervals,

Value and relative standard uncertainty, for the mass of the IPK, *m*(*K*), and for a small selection of fundamental constants, for three different definitions of the kilogram (abstracted from Mills et al., *Metrologia* 2005):

Key to Definitions	
a.	*m*(*K*) fixed (present definition)
b.	*h* fixed (first alternative definition)
c.	N_A fixed (second alternative definition)

	value	**relative uncertainty**
mass of international prototype *m*(*K*)		
a.	1.000 000 00 kg	(exact)
b.	1.000 000 00	0.17 ppm
c.	1.000 000 00	0.17 ppm
Planck constant *h*		
a.	$6.626\ 069\ 3 \times 10^{-34}$ J s	0.17 ppm
b.	6.626 069 311	(exact)
c.	6.626 069 311	0.0067 ppm
Avogadro constant N_A		
a.	$6.022\ 141\ 5 \times 10^{23}$ mol^{-1}	0.17 ppm
b.	6.022 141 527	0.0067 ppm
c.	6.022 141 527	(exact)
electron mass m_e		
a.	$9.109\ 382\ 6 \times 10^{-31}$ kg	0.17 ppm
b.	9.109 382 551	0.0067 ppm
c.	9.109 382 551	0.00044 ppm
elementary charge *e*		
a.	$1.602\ 176\ 53 \times 10^{-19}$ C	0.085 ppm
b.	1.602 176 532	0.0017 ppm
c.	1.602 176 532	0.0050 ppm

and the next two meetings will be in October 2007 and in October 2011. There is little doubt that the definition of the kilogram will eventually be changed to one of the two alternatives, but there are different opinions about when to make the change.

The argument for making the change as soon as possible is that once we change to one of the proposed alternative definitions, we shall know the values of the fundamental constants with much reduced uncertainty, and, moreover, future CODATA reviews can only lead to zero or very small changes in their values. We shall also be using a kilogram defined by reference to an invariant of nature. This has to be set against the fact that improved watt balance results in a few year's time might perhaps lead to small changes in our estimate of the mass of the IPK, which will almost certainly continue to be used as an intermediate reference standard in macroscopic mass measurements. But such changes are unlikely to be greater than the believed uncertainty arising from the drift in the mass of the IPK compared to a true invariant.

On the other hand, the possible advantage in postponing the change is that new watt balance results in the next few years *cannot* lead to any change in the mass of the IPK, which will always be 1 kg by definition, although, of course, doubts about the drift of its true mass will remain. However, we would lack the advantage of lower uncertainties in the fundamental constants, and new watt balance measurements might lead to significant changes in the fundamental constants in future CODATA reviews. This would be an inconvenience to atomic and molecular physicists, and to electrical metrologists who make use of the Josephson constant and the elementary charge. The choice is between redefining the kilogram now—so that it is referenced to an invariant of nature, and the fundamental constants are more exactly known and will not be subject to significant future changes—or postponing the decision until new experiments have reduced the uncertainty in the relation between the atomic masses and the IPK to some chosen value, perhaps 2 or 3 parts in 10^8, and putting up with the disadvantages in the meantime.

In writing this short article, I have tried to present the various arguments objectively, without taking sides. However, I must conclude by saying that I personally find the arguments for making the change as soon as possible to be compelling. I would also prefer the new definition chosen to fix *h* rather than N_A, although the difference is small, because of the central place that the Planck constant has as the fundamental constant of quantum physics.

Ian Mills <i.m.mills@reading.ac.uk> has been the IUPAC Representative on BIMP since 1996. He is a professor at the University of Reading.

Lida Schoen Made Knight of the Order of Orange-Nassau

In The Netherlands, on the occasion of the celebration of the Queen's birthday, a number of citizens are appointed to knighthood by her Majesty the Queen as a result of their valuable contributions to society, science, art, or sports. On 29 April 2005, one of these royal awards—Knight of the Order of Orange Nassau—went to Dr. Lida Schoen for her numerous efforts to promote education in and public understanding of chemistry, not only in The Netherlands but also globally. The Order of Orange-Nassau is conferred on people who have rendered outstanding service to the community for a considerable period, often people who carry out voluntary work for all manner of civil society organizations.

Before receiving honors in her homeland, Schoen was busy being an ambassador for chemistry. On 16–17 April 2005, she participated in the 5th Arab Conference on Teaching and Learning where she presented the Young Ambassador of Chemistry (YAC) project, outlining its aim of enhancing the public understanding of chemistry with the help of young students. One of the recommendations to emerge from the event was to hold an interactive discussion with teachers at the 6th Arab conference next year to discuss their ideas for organizing YAC events in Egypt.

Lida Schoen after receiving her royal medal, engraved with the motto "JE MAINTAINDRAI." Congratulations to Dr. Schoen, who proudly wore her YAC badge for the occasion!

Then, less than a month later, Schoen went to Argentina, where she helped organize a YAC event from 9-15 May. The event was held at and hosted by ESSARP, the English Speaking Scholastic Association of the River Plate <www.essarp.org.ar>, which is located in the heart of Buenos Aires.

Lida Schoen graduated with a degree in chemistry from the University of Amsterdam. She worked as a teacher trainer and during the last 10 years as an educational consultant, mainly for international projects. She is a team member of and trainer for the Science Across the World program and is a titular member of IUPAC's Committee on Chemistry Education. Her main interest is in communication and public understanding of science.

Curious about YAC? See link below.

www.iupac.org/projects/2003/2003-055-1-050.html

Address to Younger Chemists

IUPAC President Leiv Sydnes will address for a second time Europe's largest assembly of young chemists when they convene for their fifth conference this September in Brno, Czech Republic. Sydnes gave a similar address at the 2004 conference in Torino, Italy.

This series of annual Conferences for Europe's Younger Chemical Researchers was initiated, with the aid of European Community support, by SET for EUROPE in 2000. (SET stands for Science, Engineering, and Technology, and "younger" covers the age range of 21 to 35 years old). Previous conferences were held in London, UK (July 2001); Heidelberg, Germany (October 2002); Grenoble, France (August 2003); and Torino, Italy (August 2004).

The central objective of the conferences is to bring together younger European chemists, chemical engineers, and chemical technologists to exchange ideas, new results and discoveries, and to learn from each other not only about European chemistry research and R&D, but also about Europe. Chemistry is interpreted broadly at these conferences, and the scientific scope ranges from fundamental molecular-level chemistry to large-scale chemical processing technology. The conferences, which are intended to be multidisciplinary and interdisciplinary in nature, often include areas such as biology and the biosciences, the environment, materials science, medicine, and nanotechnology.

In Torino, IUPAC President Leiv Sydnes gave a 45-minute address on IUPAC's role and function. This time, he hopes to further enlighten attendees about the IUPAC of today, which too many people think is "just something to do with nomenclature." In addition, the IUPAC Executive Committee recently approved sponsorship of a lecture at this conference.

Leiv Sydnes (right) enjoying the company and humor of young participants at the 4th conference in Torino, August 2004. (CI note—We like to think that Torino's air is the reason for this "bonne ambiance" . . . a good sign for the next IUPAC GA/Congress, to be held in Torino in August 2007!)

The conference will be held 30 August to 4 September 2005 in Brno, Czech Republic, in association with Masaryk University and the Czech Chemical Society. For more information, contact Eric Wharton <ericw@setforeurope.org>.

www.setforeurope.org/brno05

In Memorium: Jacques-Emile Dubois (1920–2005)

The international chemistry community lost a pioneer when Jacques-Emile Dubois died of cancer in Paris on 2 April 2005. Dubois was known for his advances in handling chemical structural information.

Prof. Dubois received many civic and scientific awards, including the French Resistance Medal, French Legion of Honour, Ramsay Fellowship in London, and Herman Skolnik Award of the ACS Division of Chemical Information.

He was a member of many French scientific bodies and director and member of numerous academic research institutes and laboratories. He also held a number of responsible positions within the French government, including scientific advisor in the Ministry of National Education, deputy director of Higher Education, and director of Research for Defense.

Dubois chaired the IUPAC Interdivisional Committee on Machine Documentation in the Chemical Field (1969–1977) and was a member of the IUPAC Working Party on NMR Computerized Data Banks in the late 1980s and early 1990s. He was president (1994–1998) of CODATA (Committee on Data for Science and Technology) of the International Council of Scientific Unions .

Perhaps his greatest contribution to science, and more specifically to chemical information science and technology, was the invention of DARC (Documentation and Automated Research of Correlations), a topological chemical information system conceived after World War II, when the amount of published chemical information dramatically increased and needed to be appropriately coded, classified, organized, and retrievable to answer specific queries. Computer hardware and software, however limited and primitive, became available and it was obvious to a forward-thinking individual such as Dubois that they needed to be harnessed to counteract the information crisis. The DARC system, conceived in the early 1960s, became operational in 1977 as part of EURECAS, the online chemical substructure search service utilizing CAS files.

Dubois authored over 1000 articles and presentations in fast kinetics, thermodynamics, and chemical information. He also edited a number of scientific books, primarily in the field of scientific and technological information.

He obtained a Ph.D. in Physical Sciences in 1947 in Grenoble, and began his scientific career as an advisor to the cultural attaché of the French Embassy in London. The academic path included readership in chemistry at the University of Grenoble, founding professorship of the Trilingual Chemistry Institute at the University of Saar, and chair of physical and organic chemistry at the University of Paris.

He was respected by his colleagues, students, and friends for his competence in numerous scientific fields, his promotion of multidisciplinary endeavors, and his pioneering work in developing modern tools in chemical information science.

Emerging Issues in Developing Countries

This series, coordinated by Jan-Åke Jönsson, seeks to inform readers, explore new ideas, and promote discussion on themes related to developing countries and emerging analytical communities. If you wish to contribute to this series, please contact Jan-Åke Jönsson <jan_ake.jonsson@analykem.lu.se>. Articles in this series are available from <www.iupac.org/publications/ci/indexes>.

Can Ambiguous Terminology Cause a Barrier to Trade?

by Paul De Bièvre

Trading in and between developed and developing countries is an exchange process in which both parties must have a clear understanding about the value of the goods being traded. A primary means of establishing the quality of goods is through measurement. However, there should be mutual trust in the measurement results to sustain a successful trading partnership. This obvious requirement can often cause problems for developing countries when they are trying to export raw materials, food products, or manufactured or processed goods that have to satisfy high import standards in order to "protect the consumers." This is especially true in trade with developed countries that may believe, rightly or wrongly, that they have more sophisticated measurement methods and better trained staff.

Analytical laboratories in countries trading with one another must be able to express their measurement results using concepts and terms that are identical and unambiguous, irrespective of language. This requires a common, globally accepted, vocabulary in measurement, such as the ISO "International Vocabulary of Basic and General Terms in Metrology" (VIM),[1] which is used in physics and engineering. Such a rigorous approach has not yet been fully followed in chemical terms, although a highly laudable initial work using English as the medium has already been done by IUPAC in its "Color Books."[2] Dybkaer also produced a more fundamental approach for measurements in clinical chemistry and clinical biochemistry.[3]

The end goal must be to have the definitions of all basic concepts in all major languages of the world. For that, there must be worldwide agreement on chemical measurement concepts and terms in a single language because terms are in reality labels for underlying concepts. Thus, the concept must be unambiguously defined first, then a term must be allocated to the concept.

The need for agreed terms in chemical measurement results has now arrived in full at the analytical chemist's doorstep, in both developing and developed countries. Any ambiguity can have commercial and financial consequences in intercontinental trade. Additionally, lives may depend on clinical measurement results in case they are obtained from laboratories in different countries. For example, what if from one lab to another the glucose level of a diabetic patient reads differently. Identical understanding of the same concepts must be ensured at the time that chemical measurements are entering the VIM in its ongoing revision.[1]

Typical Examples of Technical Barriers to Understanding

A few typical terms causing problems are quantity, measurand, concentration, measurement result, and traceability.[4]

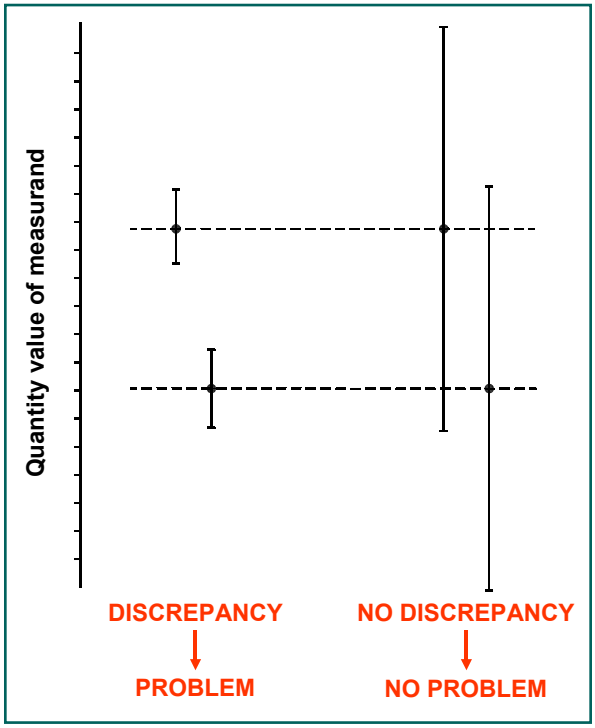
"Quantity" is defined as "attribute of a phenomenon, body or substance that may be distinguished qualitatively and determined quantitatively."[1] Thus, in chemical measurement, "quantity" is "concentration," "content," "amount-of-substance fraction," or "mass fraction." But "quantity" is also used by chemists colloquially to mean "amount." Thus we often talk ambiguously about a "quantity of sample." If we want to express "how much of a substance there is," then the term "amount" should be used to avoid confusion.

The definition of **"measurand"** is "quantity subject to measurement."[1] This could be interpreted in many chemical measurements as meaning "electric current" because that is the output of the instrument. It has been proposed in VIM3 that measurand should be defined as "quantity intended to be measured." This will be more suitable for chemical measurements as the analytical chemist aims to determine a "concentration," not just the electric current from the spectrometer.

"Measurement result" poses particular problems. Is it a numerical value times a unit? Is the inherent uncer-

tainty of the measurement result also part of that result? If a measurement result contributes to an important decision, its definition is very important. Discrepancy problems are mostly caused by lack of full evaluation of measurement uncertainty. It is important when comparing measurement results from developed and developing countries, that the measurement uncertainty associated with each result is evaluated in the same way. Otherwise results that are equivalent may appear to differ, casting doubt on the reliability of one of the laboratories. That may lead, in the worst case, to customs officials refusing the entry of what should be acceptable goods or produce. Common evaluation procedures (according to the ISO Guide on the Expression of Uncertainty in Measurement, i.e., GUM) should be used in the evaluation of all measurement results by all laboratories, whether located in developed or developing countries.

The term **"traceability"** was almost unheard of several years ago, but it has dramatically invaded oral and written language as one of the newer buzzwords. However, what does it really mean? Does it refer to traceability of the sample, of the accompanying document, of the accompanying certificate, or of a measurement result, the really important feature in measurement? "Metrological traceability" is proposed in VIM3 as a more specific term for the traceability to a common metrological reference: to a value embodied in a certified reference material, to a common measurement unit, or to an internationally agreed measurement procedure.



Importance of measurement uncertainty when reporting and comparing measurement results: (left) measurements claimed with a small but incomplete measurement uncertainty, leading to the incorrect conclusion of "discrepancy"; and (right) better measurement results claimed with larger but complete measurement uncertainty, and leading to the correct conclusion of "no discrepancy."

This relationship is important when a comparison between measurement results from different countries is made, as measurement results are only comparable when their metrological traceability has been established beforehand. Only then can we decide if the results obtained on one sample from a material batch indicate a larger concentration of a given substance than the results obtained on a sample from another similar material batch. For example, is one used-car exhaust catalyst revealed to contain a larger concentration of a valuable platinum metal (Rh or Pt) than that concentration in another car-exhaust catalyst, and can the first material therefore be priced higher? Similarly, the concentration of cholesterol for a person traveling in different countries may seem to be different, but is not (see figure). This can lead to incorrect treatment.

The difficulty for developing countries is also that they can be at a disadvantage in trade as their measurement results may be considered dissimilar to those from other countries because even the term "comparability" is used ambiguously: Most of the time it means "being of the same size" rather than "can be compared because traceable to the same reference," regardless of size.

All of this generates confusion, and even more so for the non-native English-speaking person.

Certified reference materials required for the comparisons may also be prohibitively expensive in developing economies and, hence, difficult to justify. Worse, commercial organizations may offer reference materials embodying values that are "traceable to an institute," but that does not show by itself that these values are metrologically traceable to a common, internationally agreed metrological reference needed for any scientifically valid, intercontinental comparison of measurement results.

Although the UK and the USA are often said to be countries "*divided* by a common language," this is no

longer acceptable in the analytical chemistry laboratories of developed and developing countries. In order to have "fair trade," they must be *united* by a common [measurement] language and by common understanding of the concepts and terms labeling these concepts in that language. Only after this is accomplished is it worth putting time and effort into translating these terms into 30–40 (or more?) of the world's other languages, an obvious necessity.

Acknowledgements

Useful comments by René Dybkaer are gratefully acknowledged. The author also thanks the series editor Jan Åke Jönsson, as well as Roger M. Smith, secretary of the IUPAC Analytical Chemistry Division, for their comments and input. This contribution was approved for publication on 20 May 2005, World Metrology Day—a salute to all interested in Metrology!

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1 BIPM, IEC, IFCC, ISO, IUPAC, IUPAP, OIML, *International Vocabulary of Basic and General Terms in Metrology*, 2nd edition, VIM2, ISO Genève (1993); a revised edition (leading up to VIM3) is expected shortly.
2 The IUPAC Color Books is a series of references on IUPAC nomenclature, terminology, and symbols. For instance, the so-called "Gold Book" is the *Compendium of Chemical Terminology*, the "Green Book" is the *Quantities, Units, and Symbols in Physical Chemistry*, the "Orange Book" is the *Compendium of Analytical Nomenclature*, etc. References to this collection are available online at www.iupac.org/publications/books/seriestitles/nomenclature.html.
3 R. Dybkaer, *Eur J Clin Chem Clin Biochem* 35 (1997) 141–173
4 P. De Bièvre, "The Terms We Use and the Words We Choose: International Terminology Needed for Measurements in Chemistry," *VAM Bulletin*, LGC, Teddington, 2004

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Simples and Compounds: Another Opinion

by Tomislav Portada and Vladimir Stilinovic

Although we do agree with Giomini et al. about the necessity of making a clear-cut distinction between elements and elementary substances,[1] in our opinion it is superfluous to introduce new terms for these concepts. We believe that the problem originates in the current IUPAC definition of "chemical element."[2] We suggest limiting the definition of chemical element to "A species of atoms; all atoms with the same number of protons in the atomic nucleus."

We also suggest introducing "elementary substance" as a separate term defined as "A pure chemical substance composed of atoms of the same element." The current problems would be circumvented by using these terms strictly according to the above-suggested definitions.

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2 IUPAC: *Compendium of Chemical Terminology* (The Gold Book), 2nd edition, Blackwell Science, 1997.

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Erratum: Wolfram vs. Tungsten

The editor apologizes for having inadvertently edited the last paragraph of Damhus' reply (July-August *CI*, p. 28) and consequently rendered the conclusion illegible. It should have read as follows:

To summarize, Profs. Goya and Román have highlighted an example of having to make non-trivial choices when devising nomenclature recommendations. We believe that if one wishes to control proliferation of alternatives, be as systematic as possible, and at the same time not ignore prevailing usage in English—the language in which we have agreed to provide our recommendations—we have made the right choices regarding tungsten/wolfram and names derived from these. At the same time, the Spanish, the Danes and many other nationalities may happily continue to use wolfram in their locally adapted IUPAC nomenclatures.

Terminology for Biomedical (Therapeutic) Polymers

Like most of the materials used by humans, polymers and polymeric materials have been tested and used by surgeons and pharmacists to treat trauma and diseases. Polymers are also used when studying living systems in the environment. Each domain has developed specific terminologies, which have been the source of misunderstanding, confusion, and misperception among scientists, surgeons, pharmacists, journalists, and policy makers.

This project aims to define specific terms used by people active in the biomedical, pharmacological, environmental, and journalistic fields. ASTM, ECS (European Committee for Standardization), and normalization bodies of different countries will be consulted so that the definitions can be accepted worldwide at last.

For more information and comments, contact the Task Group Chairman Michel Vert <vertm@univ-montp1.fr>.

www.iupac.org/projects/2004/2004-043-1-400.html

Teaching School Children About Pesticides and Health

Infants and children are particularly vulnerable to pesticides and other toxic chemicals because their bodies are smaller and still developing. Children also face greater exposures than adults due to their hand-to-mouth behaviors. Children living in farming areas or whose parents work in agriculture suffer greater pesticide exposure than other children. The aim of this joint project (between IUPAC and the World Health Organization [WHO]) is to educate children about protecting themselves from the harmful effects of pesticides and hazardous chemicals, and to develop a safety culture for the future. The training material shall include general facts about chemistry; risk assessment; POPs (persistent organic pollutants); pesticides; safe handling; preventing contamination; protecting oneself, others, and the environment from harmful effects; and how chemicals, especially POPs and pesticides, can affect human health and the environment.

The training materials will be prepared as CD-ROMs, booklets, and flip charts for use in countries with different levels of development. The materials might serve as the first part of a series "Toxicology in the Classroom" for use in chemistry classes.

The project, as proposed, will provide a foundation of knowledge about pesticide use and safety in developing countries. Educating young people about pesticides and POPs as well as how to protect themselves from exposure is important worldwide. The main focus will be on pesticide modes of action, safe handling, and personal protection, with a minor focus on when and where they are appropriate. It may be more effective to emphasize a range of options about how to avoid exposure (use of protective equipment, better personal hygiene, etc.) and the potential dangers of not doing so.

Training programs shall include the whole family—parents and adolescent children—all of whom may be involved in the farming operations. Since the parents are responsible for both their children and for the misuse of pesticides they need to be made aware of the consequences.

A specific plan for promoting and distributing the material will be developed. The task group will seek advice on the compounds of greatest concern and most relevant risk as identified by the national poison control centers of developing countries and the WHO. Training tools will make use of available and scientifically sound information from government, industry, and other reliable sources. The Internet provides access to an enormous amount of information on environmental health science, including homework resources and online activities for students, lesson

Kick-off meeting of task group in Berlin, in May 2005. From left to right: Axel Hahn, Fritz Schweinsberg, Lutz Rexilius, Nida Besbelli, Wayne Temple, and Birger Heinzow.

resources and classroom activities for teachers, and presentation materials for scientists. The task group will compile materials that might be suitable for use.

The educational material will be designed primarily for developing countries in Asia, South America, and Africa. The basic material will be written in English, but in a simple and easily translatable fashion.

The material will be targeted to 9–13 year olds, because this age group is in transition from guarded childhood to more independence and might be at higher risk. Also, children in this age group are often responsible for looking after their sisters and brothers and they influence the behavior of younger children. The project is not intended to train the students in safe handling, but to educate them about the risks and necessary precautions associated with pesticides (as well as their benefits) and hazardous compounds. The project will mainly develop pictograms for students and explanatory text (descriptions, definitions) for teachers.

Comments and recommendations are welcome. For more information contact Task Group Chairman Wayne A. Temple <wayne.temple@otago.ac.nz>.

www.iupac.org/projects/2004/2004-045-1-700.html

Towards Defining Materials Chemistry

The last 10–15 years have seen the emergence and rapid growth of "materials chemistry" as a distinct discipline within the broad family of chemical sciences. This was a combination of noun and adjective that had not previously formed part of the chemists' vocabulary. Now a significant portion of all publications in chemistry claim to form part of this new field. In particular, two international journals (*Chemistry of Materials*, published by the American Chemical Society, and the *Journal of Materials Chemistry*, published by the Royal Society of Chemistry in the UK) are achieving high-impact factors and publish work emanating from every continent of the world. Yet, there remains no definition of the phrase "materials chemistry" that is agreed upon by the global chemical community. As IUPAC is the most appropriate body to sponsor such a debate, the project proposed here aims to address this deficit.

Part of the difficulty in defining the scope of materials chemistry arises from the fact that it transcends the divisions separating the traditional branches of chemistry (e.g., organic and inorganic) or between continuous-lattice and molecular solids. To address these difficulties it appears necessary to assemble a small, multi-national and multi-disciplinary task group, representing different aspects of the subject, to harness these experts' experience in compiling lists of relevant published material (books, reviews, chapters, Web sites, etc.). The goal of the project is to produce a set of brief statements summarizing the current consensus on the scope of materials chemistry.

For more information and comments, contact Task Group Chairman Peter Day <pday@ri.ac.uk>.

www.iupac.org/projects/2005/2005-001-1-200.html

Thermodynamics of Ionic Liquids, Ionic Liquid Mixtures, and the Development of Standardized Systems

Ionic liquids (ILs) represent a new class of liquid solvents having some characteristics of molten salts. Recently synthesized compounds are moisture, air, and temperature stable. Their melting points are distinctly below room temperature. Most of these ionic liquids consist of cations based on alkylimidazolium or alkylpyridinium ions and anions such as BF_4^-, PF_6^-, $N(CF_3SO_2)_2^-$, $CF_3SO_3^-$. Chloroaluminate anions are also important, provided moisture can be excluded. A large number of ionic combinations are possible for designing compounds with specific properties.

ILs have attracted considerable interest during the last few years. They have no detectable vapor pressure and therefore exhibit favorable solvent properties for new homogeneous catalytic reactions and other chemical production processes with respect to "green chemistry." An increasing number of successful applications are described in the literature. The utilization of ionic liquids in industrial chemistry requires a systematic study of their thermodynamic and thermophysical properties, which are required for chemical process design. The most important properties are as follows:

- thermodynamic and transport properties of the pure ionic liquids
- solubility of gases in ionic liquids
- miscibility gaps of ionic liquids with organic liquids

and water (liquid-liquid equilibria)
- densities, activity coefficients and excess properties of ionic liquids + organic substances (and water)
- viscosities, diffusion coefficients, and electrical conductivities of ionic liquids + organic substance (and water)
- data required by theoreticians for predicting properties using computer simulation and/or *ab-initio* calculation methods

Prior to 2003, a number of workshops and special sessions on ILs were held, but they were primarily directed towards the use of ionic liquids as solvent systems for chemical reactions, with an emphasis on kinetics and homogeneous organometallic catalysis. There has been minimal emphasis on thermophysical property information. Of the little duplicate thermophysical property data published, agreement was generally poor.

The objectives of this project are as follows:
- encourage systematic studies of thermodynamic and thermophysical properties of ionic liquids based on the needs of industrial chemical processes
- recommend a reference ionic liquid and make reference quality measurements on selected thermophysical properties of both the pure ionic liquid and its mixtures
- establish recommended equations for the properties measured and provide recommendations on measurement methods
- suggest directions of future research and encourage cooperation to avoid unnecessary duplication of measurements
- organize workshops and special sessions devoted to the thermophysical properties of ionic liquids
- provide software for submission of data to the ionic liquids database

The project, which was initiated in March 2003, is expected to be completed by the end of 2005. Software for submission of data to the ILs Database (see project # 2003-020-2-100; right) is in the testing stage and should be made available from the NIST Web site.

For more information and comments, contact Task Group Chairman Kenneth N. Marsh <ken.marsh@canterbury.ac.nz>.

www.iupac.org/projects/2002/2002-005-1-100.html

Ionic Liquids Database

Progress in utilizing ionic liquids has been hampered by the lack of an open-access, public-domain, comprehensive data retrieval system scoped to cover information pertaining to ionic liquids. Development of such a database infrastructure encompasses a number of complex issues related to data submission, processing, mining, quality control, management, critical evaluation, and dissemination. It is also obvious that such a system should provide coverage for various types of data such as synthesis, catalysis, structure, manufacturing, and modeling, as well as thermophysical and thermochemical property data. Because of the great diversity of the data types listed above, it is envisioned that the users will have a distributed information system with access to various types of data managed independently by different research groups and linked together via the main Web outlet. An international effort is now developing such an information system under the auspices of IUPAC.

This project objective is simply to create an open-access, free, online, comprehensive database for storage and retrieval of metadata and numerical data for ionic liquids, including their syntheses, structure, properties, and uses; lack of this information is impeding progress in a burgeoning field of significant current interest.

The project team has made substantial progress since their first meeting held in January 2004. To date, the NIST team has modified the Thermodynamics Research Center's SOURCE database and the Guided Data Capture application to facilitate the storage and retrieval of ionic liquids property data and have created a Web-based properties retrieval system by using an Oracle Java Application Development Frame. Presently, search functionality within the properties database is undergoing rigorous internal testing. An external launch of the property database, named ILTHERMO, is anticipated in December 2005.

For more information and comments, contact Task Group Chairman Kenneth R. Seddon <k.seddon@qub.ac.uk>.

www.iupac.org/projects/2003/2003-020-2-100.html

continued from page 7

majority of samples contain no detectable residues or residues at levels well below relevant MRLs. For example, U.S. Department of Agriculture monitoring of residues between 2001–2003 of the commonly used insecticide chlorpyrifos on bananas imported from Latin America revealed only one detection (at 0.007 mg/kg or ppm) in more than 1400 samples. In other cases, detections may be more frequent, but in general the vast majority fall well within established MRLs. Monitoring data from Brazil during the past 10 years reveals a generally low incidence of residues exceeding MRLs in fruits and vegetables (1%–2%), but between 5% and 19% of the samples in recent years have contained residues of pesticides for which use is no longer permitted. These illegal residues, primarily involving chlorinated hydrocarbon pesticides banned for use after 1995, may be present due to either lingering environmental contamination or illegal use.

Recent food residue monitoring results from Costa Rica have highlighted some interesting differences. Whereas during 2003, approximately 98% of food items imported into or exported from the country had no detectable residues or residues below the relevant MRL (i.e., 2% MRL violation rate), only 52% of food items grown for local consumption fell within established MRLs (i.e., 48% MRL violation rate). Findings such as these from Brazil and Costa Rica highlight the need for consideration of both extraneous MRLs (i.e., residues which may result from historic use and environmental contamination) and continued surveillance and education concerning adherence to approved GAP. Concerning the implementation of such monitoring programs, it was recognized that adherence to good laboratory practices concerning both sampling and analysis may be important considerations for ensuring reliability of reported results. Sampling programs, in particular for monitoring of pesticides with acute toxicity considerations that may be present on foods eaten as individual units, must be designed to accommodate the considerable unit-to-unit variability that may occur. For example, recent testing of Brazilian-grown eggplant, mango, papaya, and summer squash revealed variability factors of 2–3 (residue level in the 97.5th percentile of individual unit divided by the mean of the population). It was noted that this data was consistent with an IUPAC recommendation to use a general variability factor of 3 when estimating acute dietary intakes of pesticides through consumption of this type of commodity (project # 1999-009-1-600).

Despite availability of internationally harmonized Codex MRLs for many pesticide/crop combinations, the Codex promise of promoting fair practice in international food trade through worldwide adoption of its voluntary standards has not been fully realized. This is in part due to the slowness in developing a full set of Codex MRLs, but also to the implementation of divergent national MRL systems by the world's most influential food-importing regions (EU, Japan, USA). These competing MRL systems are posing significant challenges for pesticide management in Latin American export crops. In addition to Codex standards, which have been historically respected by the countries in Latin America, growers and exporters also must now consider EU, Japan, and USA MRLs that have not generally been established with the GAPs of Latin American producers in mind.

The emergence of "private" food-quality standards developed by retailers and food importers primarily in the EU, some more restrictive than those set by governments, is posing an additional challenge. Some of these private standards go so far as to mandate no allowable use of particular pesticides that are not favorably viewed, regardless of whether any detectable residues are present in the commodity at harvest. Minor crops, for which MRLs may often be nonexistent due to a lack of available field trial data, are particularly susceptible to trade disputes related to pesticide residue detections. Although these crops may be too "minor" in the sense of overall dietary contribution and/or economic value to justify the cost of registration studies, in some instances (e.g., spices, herbs, tropical fruits, tea) they may nevertheless have high economic importance for growers and their regions. Initial findings were reviewed at the workshop from an ongoing IUPAC project on MRLs for minor crops (# 2001-039-1-600). The project aims to develop scientifically justified recommendations for a tiered approach to establishing MRLs for pesticide uses on minor crops without the need for comprehensive field trials.

Finally, worker exposure during handling and application is also an important consideration from a safety standpoint. A tiered system of exposure assessment has been recommended, which may involve application of generic estimates from established databases of available exposure studies to the conduct of new studies to measure external or absorbed residues (i.e., biomonitoring).

Future Plans

Although the workshop in San Jose was a great success in terms of participation and the level of scientific information exchange involved, it only represented the second of three objectives for the "Crop Protection Chemistry in Latin America" IUPAC project (# 2003-013-1-600). The project also aims to develop recommendations for future advancement of crop protection chemistry in Latin America. Although the results of the workshop are still being evaluated, three preliminary areas of emphasis and future action have so far been proposed.

First, the importance of pesticide **product specifications** as a means of controlling the quality of locally available products was emphasized. The harmonized FAO/WHO process has been well documented and supported by a past IUPAC project (# 640/20/87), but satisfactory application of the process in some Latin American countries would be greatly assisted by specific training of the personnel involved. Therefore, a hands-on training session involving several key international experts and perhaps 15 to 20 or more of the key regulatory experts and analysts from the region has been proposed.

Second, the importance of **ecological risk assessment** methods for the safety evaluation of pesticide products was emphasized. The ongoing IUPAC project on development of simplified methods for ecological risk assessment will be of great assistance in this regard (# 2004-011-1-600), but further dissemination of the outcomes of this project and also development of additional levels of refinement to address the inevitable "problem cases" must be addressed. In addition, it is vitally important that the various Latin American stakeholders for crop protection chemistry, government, industry and academia, develop a consensus regarding the tiers of assessment to be employed and the risk mitigation and management approaches to be endorsed. Therefore, the formation of a Latin America ecological risk assessment working group has been proposed.

Third, the importance of **education** in achieving scientifically sound and harmonized approaches for regulation was recognized. Of primary importance is outreach to the key leaders and influencers within the Latin America crop protection chemistry field, including regulatory officials, industry leaders, technical specialists, agricultural consultants, and researchers. One issue currently slowing advancement in this area is a shortage of comprehensive and affordable crop protection chemistry information resources in the Spanish language. Two action steps were proposed to help address this issue. First, the IUPAC *Glossary of Terms Related to Pesticides*, currently being updated as part of an ongoing IUPAC project (# 2004-002-1-600), will be translated into Spanish with the cooperation of the FAO and IAEA. Second, the excellent textbook *Pesticides and the Environment*, co-authored by workshop lecturer Gerry Stephenson of the University of Guelph, will be reviewed and edited by the IUPAC Subcommittee on Crop Protection Chemistry and subsequently translated into Spanish. Particular emphasis will be placed on Latin American considerations.

For Further Information

The IUPAC workshop in Costa Rica was the sixth in a developing series of such crop protection chemistry-related workshops organized by the DCE since 1988. Past workshops have been held in Brazil, China, Korea, Taiwan, and Thailand. The papers from the Costa Rica workshop proceedings are available at the Web site listed below.

Ken Racke <kracke@dow.com>, a global regulatory leader with Dow AgroSciences in Indianapolis, Indiana, USA, was chair of the international organizing committee for the workshop. Dr. Racke is currently president of the IUPAC Division of Chemistry and the Environment (DCE), and has been active with the Subcommittee on Crop Protection Chemistry for several years. His interests include environmental considerations related to pesticide use and establishment of international standards for pesticide management.

Elizabeth Carazo <ecarazo@cariari.ucr.ac.cr>, a professor at the University of Costa Rica in San Jose and director of the Centro de Investigación en Contaminación Ambiental, was chair of the local organizing committee for the workshop and project leader on behalf of IUPAC. Carazo has been active with the DCE Subcommittee on Crop Protection Chemistry for several years, and has a particular interest in the environmental aspects of pesticides and other contaminants.

Graham Roberts <grarob@bigpond.net.a>, a scientist with the Department of Primary Industries in Victoria, Australia, was a member of the international organizing committee for the workshop. Roberts has been active with the DCE Subcommittee on Crop Protection Chemistry for several years, and has a particular interest in food residue considerations for pesticides and human dietary intake. He has also served on the Australian delegation to the Codex Committee on Pesticide Residues for a number of years.

To access IUPAC projects visit <www.iupac.org/divisions/VI/cp6.html>.

www.iupac.org/projects/2003/2003-013-1-600.html

Chemical Structure and Physical Properties of Cyclic Olefin Copolymers (IUPAC Technical Report)

Ju Young Shin, Ji Yong Park, Chenyang Liu, Jiasong He, and Sung Chul Kim
Pure and Applied Chemistry
Vol. 77, No. 5, pp. 801–814 (2005)

The modification of general-purpose polyolefin materials in order to enable their use as engineering plastics is currently a relevant topic for industrial as well as academic research. Cyclic olefin copolymers comprise one of the new classes of polymers based on cyclic olefin monomers and ethene. Because of the bulky cyclic olefin units randomly or alternately attached to the polymer backbone, the copolymer becomes amorphous and shows the properties of high glass-transition temperature, T_g, optical clarity, low shrinkage, low moisture absorption, and low birefringence.

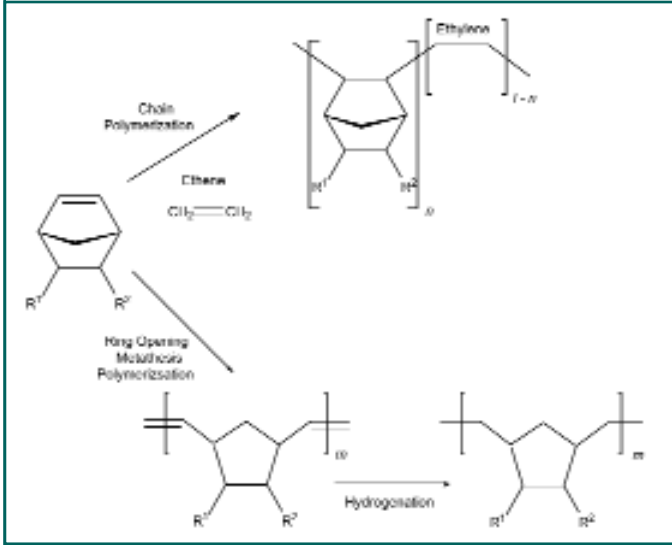
With these properties, the application of cyclic olefin copolymer has now been extended to production of plastic lenses and optical storage media, and is currently being produced by Mitsui Chemical Co., Ticona (formerly Hoechst Celanese), Japan Synthetic Rubber, and Zeon Chemicals Co.

There are several types of commercial cyclic olefin copolymers based on different types of cyclic monomers and polymerization methods. Cyclic olefin copolymers are produced by chain copolymerization of cyclic monomers such as 8,9,10-trinorborn-2-ene (norbornene) or 1,2,3,4,4a,5,8,8a-octahydro-1,4:5,8-dimethanonaphthalene (tetracyclododecene) with ethene, Ticona's TOPAS, Mitsui Chemical's APEL, or by ring-opening metathesis polymerization of various cyclic monomers followed by hydrogenation (Japan Synthetic Rubber's ARTON, Zeon Chemical's Zeonex and Zeonor).

Recently, a considerable amount of work has been reported on the physical properties and microstructure of cyclic olefin copolymers. Most of these reports correlated the composition, microstructure, and thermal properties of ethene-norbornene copolymer. A few studies have been made on the influence of chemical structure on the thermal properties of cyclic olefin copolymers. There is no report on the surface characteristics of these polymers.

This paper analyzes the chemical structure of the currently commercialized cyclic olefin copolymers by ^{13}C NMR, and investigates their glass-transition temperatures and surface characteristics. It was observed that the glass-transition temperature of cyclic olefin copolymers depended on the bulkiness of the main chain, and the number of rings had an important role in increasing the bulkiness of cyclic olefin copolymers. Cyclic olefin copolymers with polar substituents such as ester or ether groups showed high surface energy per area and peel strength.

www.iupac.org/publications/pac/2005/7705/7705x0801.html

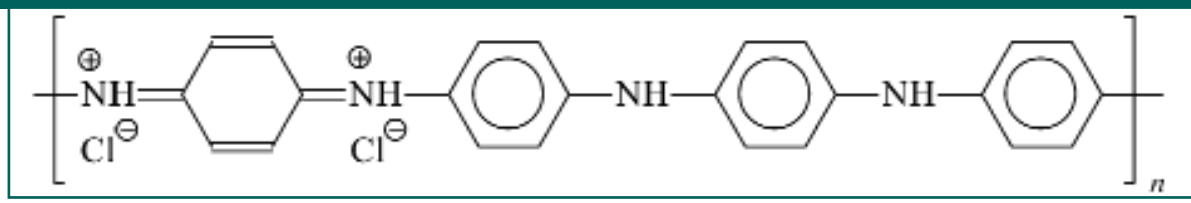


Typical polymerization scheme for a cyclic olefin polymer.

Polyaniline: Thin Films and Colloidal Dispersions (IUPAC Technical Report)

Jaroslav Stejskal and Irina Sapurina
Pure and Applied Chemistry
Vol. 77, No. 5, pp. 815–826 (2005)

Polyaniline (PANI) is one of the most important and widely studied conducting polymers. It is easily prepared (e.g., by the oxidation of aniline with ammonium peroxydisulfate in acidic aqueous medium) and obtained as a precipitate. Such synthesis has recently been investigated within IUPAC project 1999-024-1-400, "Polyaniline: Preparation of a Conducting Polymer," and a report has been published in *PAC* **74**, 857–867 (2002).



Polyaniline (emeraldine) hydrochloride (one of the possible presentations).

Polyaniline protonated with inorganic acids is difficult to process because it cannot be dissolved or melted below the decomposition temperature in the conducting state. The protonation of PANI with organic acids having a bulky hydrocarbon component has been used to increase the solubility of PANI in organic solvents and the plasticity. The uses of dodecylbenzenesulfonic acid, dinonylnaphthalenesulfonic acid, or diesters of sulfosuccinic acid may serve as examples. Various surfactants have also been used as a component of the reaction mixture for the same purpose. Alternative processing strategies consist in coating of the surfaces of various substrates with a conducting PANI film and in the preparation of PANI colloids. The latter forms, produced in situ during the polymerization of aniline, are discussed in this paper.

An authority on conducting polymers has pointed out that "there are as many different types of PANI as there are people who synthesize it." The purpose of this collaborative study was to test this statement, by having various researchers follow the same preparative protocol. Two supramolecular PANI forms, thin PANI films on glass and colloidal PANI dispersions stabilized with poly(N-vinylpyrrolidone) (PVP), were prepared independently in several laboratories. In this study, the films and colloids were characterized with respect to film thickness, film conductivity, and colloidal particle size.

The average thickness of the films, assessed by optical absorption, was 125 ± 9 nm, and the conductivity of films was 2.6 ± 0.7 S cm^{-1}. Films prepared in 1 mol l^{-1} HCl had a similar thickness, 109 ± 10 nm, but a higher conductivity, 18.8 ± 7.1 S cm^{-1}. Colloidal polyaniline particles stabilized with a water-soluble polymer, poly(*N*-vinylpyrrolidone) [poly(1-vinylpyrrolidin-2-one)], have been prepared by dispersion polymerization. The average particle size, 241 ± 50 nm, and polydispersity, 0.26 ± 0.12, have been determined by dynamic light scattering. The preparation of these two supramolecular polyaniline forms was found to be easily reproducible.

www.iupac.org/publications/pac/2005/7705/7705x0815.html

Terminology in Soil Sampling (IUPAC Recommendations 2005)

Paolo De Zorzi, Sabrina Barbizzi, Maria Belli, Giovanni Ciceri, Ales Fajgelj, David Moore, Umberto Sansone, and Marcel Van Der Perk

Pure and Applied Chemistry
Vol. 77, No. 5, pp. 827–841 (2005)

Recently, there have been a growing number of efforts to overcome confusion, ambiguity, and contradictions in the usage of terms and clarification of their definitions in the field of sampling. The IUPAC Recommendations, "Nomenclature for Sampling in Analytical Chemistry," published in 1990 (*PAC* **62**, 1193–1208), and the ISO standard 11074-2, "Soil Quality—Vocabulary—Part 2, 1998," are the most widely used terminology documents related to soil sampling. However, recent developments and studies of various sampling aspects (i.e., uncertainty quantification, method validation, comparison of sampling tools, and strategies) require new concepts to be developed and also some new terms to be introduced for their description.

One of the outcomes of the SOILSAMP international project, funded and coordinated by the Italian Environmental Protection Agency (APAT, Italy) and aimed at assessing the uncertainty associated with soil sampling in agricultural, semi-natural, urban, and contaminated environments, was an updated terminology in sampling.

This paper is the result of that effort, and is intended to present terms and definitions to be used in soil sampling and sampling uncertainty. A set of geostatistical terms, of interest in the context of soil sampling and sampling uncertainty estimation, is also illustrated together with the recommended definitions.

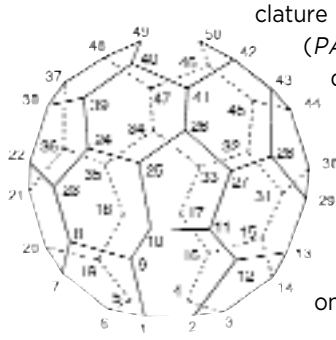
www.iupac.org/publications/pac/2005/7705/7705x0827.html

Numbering of Fullerenes (IUPAC Recommendations 2005)

F. Cozzi, W. H. Powell, and C. Thilgen

Pure and Applied Chemistry
Vol. 77, No. 5, pp. 843–923 (2005)

In 1995, a preliminary survey on numbering and nomenclature for fullerenes was prepared (*PAC* **69**, 1411–1434 [1997]). It described two types of names for fullerenes, one proposed by some workers in the field and another one used by the Chemical Abstracts Service (CAS); and two systems for numbering fullerene skeletons, one proposed in a publication by R. Taylor (*J. Chem. Soc., Perkin Trans.* **2**, 813–824 [1993]), and one published by CAS (*J. Chem. Inf. Comp. Sci.* **35**, 969–978 [1995]). In addition, alternative methods for naming derivatives of fullerenes were discussed. More recently, a document appeared reporting IUPAC recommendations for the nomenclature for the C_{60}-I_h and C_{70}-$D_{5h(6)}$ fullerenes and their derivatives (*PAC* **74**, 629–695 [2002]). This report was limited to these fullerenes because there are only a small number of known derivatives of only a few other fullerenes.



One numbering system, exemplified in this report, for compounds (C_{50}-D_{5h})[5,6]fullerene.

This paper contains recommendations for the numbering of fullerenes other than (C_{60}-I_h)[5,6]fullerene and (C_{70}-$D_{5h(6)}$)[5,6]fullerene and contains recommendations for numbering a wide variety of fullerenes of different sizes, with rings of different sizes, from C_{20} to C_{120}, and of various point group symmetries, including low symmetries such as C_s, C_i, and C_1, as well as many fullerenes that have been isolated and well characterized as pristine carbon allotropes or as derivatives. These recommendations are based on the principles established in the earlier publication and aim at the identification of a well-defined and preferably contiguous helical pathway for numbering. Rules for systematically completing the numbering of fullerene structures for which a contiguous numbering pathway becomes discontiguous are presented.

www.iupac.org/publications/pac/2005/7705/7705x0843.html

Gaseous Fluorides of Boron, Nitrogen, Sulfur, Carbon, and Silicon and Solid Xenon Fluorides in All Solvents

H. Lawrence Clever (editor)
IUPAC-NIST Solubility Data Series. 80.
Journal of Physical and Chemical Reference Data,
Vol. 34, No. 1, pp. 201–438, 2005

This volume provides a compilation of data from a literature search through 2002 June for solubility data on the gases BF_3, NF_3, N_2F_4, SF_6, CF_4, CHF_3, CH_2F_2, CH_3F, C_2F_6, CHF_5, 1,1,1,2-$C_2H_2F_4$, 1,1,1-$C_2H_3F_3$, 1,1-$C_2H_4F_2$, CH_5F, C_3F_8, c-C_4F_8, C_2F_4, 1,1-$C_2H_2F_2$, C_2H_3F, C_3F_6, C_3F_6O, and SiF_4, and the solids XeF_6, XeF_4, and XeF_2 in all solvents. Where feasible, evaluations have been carried out. The evaluations were mostly carried out for water as a solvent, as the water systems are the most extensively studied. For other systems there is often only one or two sets of measurements, which do not agree well. Evaluation of such systems will have to wait for further experimental measurements.

www.iupac.org/publications/sds/2005/80_abstract.html

Polymers in Novel Applications

H. Pasch and R.D. Sanderson (editors)
Macromolecular Symposia, Vol. 225
Wiley-VCH, 2005, pp. 1–237
ISBN 3-527-31328-1

The UNESCO School and Conference on Macromolecules & Materials Science is held annually in different locations in South Africa. World authorities in various fields of macromolecular science are invited to give tutorials at the UNESCO School and informative plenaries at the conference. The exposure to new ideas and advanced concepts in macromolecular science is of great importance to South African students and senior staff of various universities and research institutions.

This volume contains abridged versions of a number of papers presented at the 7th UNESCO/IUPAC Conference (April 2004), which focused on polymers in medicine, nanotechnology, degradation, and stabilization. These papers—and papers from previous UNESCO conferences—are available at <http://academic.sun.ac.za/unesco/>.

www.iupac.org/publications/macro/2005/225_preface.html

Bio-Based Polymers: Recent Progess

S.S. Im, Y.H. Kim, J.S. Yoon, and I.-J. Chin (editors)
Macromolecular Symposia, Vol. 224
Wiley-VCH, 2005, pp. 1–376
ISBN 3-527-31327-3

Most people would agree that we live in an "age of plastics." Packaging is one of the areas where plastics are favorably used. In particular, as the geographical separation between the producers and the consumers has been widened, efficient packaging became essential to retain the nutrients and freshness of produce and to reduce the amount of preservatives used.

There is an ever-increasing demand for manufacturing plastics out of sustainable resources, because raw materials derived from fossil fuels are rather limited. Bio-based polymers can make excellent candidates for such materials. It was, therefore, very timely that the 8th World Conference on Biodegradable Polymers and Plastics (BDPP8) was held to discuss current issues and the most recent advances in biodegradable and bio-based polymers and plastics. The conference series began in 1991 as the International Scientific Consensus Workshop on Degradable Materials, and thereafter has been held almost every two years. The BDPP8 emphasized the industrial aspects of biodegradable plastics, and representatives of the major producers of biodegradable plastics were invited to present the most recent developments. Government policies and regulatory issues of several countries were also addressed. The list of participants shows a broad spectrum in terms of countries represented, areas of interest, and types of organizations.

This volume contains selected papers on six different topics: microbial poly(hydroxy alkanoate)s, poly(lactic acid)s, biodegradable polyesters and polyurethanes, hydrogels and biomedical applications, blends and processing, and microbial degradation.

www.iupac.org/publications/macro/2005/224_preface.html

Macromolecules

by Jean-Pierre Vairon and Jean-François Joanny

The **40th International Symposium on Macromolecules (World Polymer Congress—Macro 2004)** sponsored by IUPAC, was held at the Convention Center of Paris, 4–9 July 2004. It was organized by the Centre National de la Recherche Scientifique with the participation of the Université Pierre et Marie Curie, and the Ecole Supérieure de Physique et de Chimie de la Ville de Paris.

The congress was sponsored by the French Ministère de la Recherche, Ville de Paris, Académie des Sciences, and the Union des Industries Chimiques. It was held under the auspices of European Polymer Federation, Groupe Français des Polymères (a Division of the Société Française de Chimie and of the Société Française de Physique), Société de Chimie Industrielle, Société Française de Métallurgie et Matériaux, Groupe Français de Rhéologie, and the International Polymer Processing Society. P.-G. De Gennes and J.-M. Lehn were co-chairmen of the congress.

The congress was part of the series of regular biennial "IUPAC Macro Meetings" of the IUPAC Polymer Division. These meetings are the most important events in the activities of the Polymer Division, and are by far the world's largest gathering of polymer scientists. They provide a venue where young scientists and more experienced researchers have the opportunity for close, friendly contacts with the leading specialists in the various domains of polymer science.

E. Giacobino (Director of the Research, Ministry of Research) opened the Congress on behalf of Minister François D'Aubert, before an audience of more than 2300 attendees. Her address was followed by those of Bryan Henry, president-elect of IUPAC, and R.F.T. Stepto, president of the Polymer Division, who respectively stressed the eminent roles played by the Union and its Polymer Division.

The unified character of the now mature polymer science was deliberately emphasized and appeared as an essential feature (and success) of this congress. The Paris MACRO 2004 meeting was largely open to other disciplines, such as polymer and soft matter physics, mechanics, rheology, and polymeric materials processing. It involved 10 plenary lectures devoted to contemporary topics (including those of two Nobel Prize winners) and more than 280 invited lectures, together with about 350 contributed oral presentations, and more than 1300 posters.

The conference embraced fundamental and applied aspects of major frontier topics in polymer science. Special emphasis was placed on new concepts and developments in both basic research and industrial applications. The furthering of polymer education and international cooperation in polymer science are also major concerns of the IUPAC Polymer Division. Two specific symposia were devoted to these issues.

This one-week congress was organized around three half-day plenary sessions devoted to trends in polymer science, and around parallel sessions associated with 21 thematic symposia. For the opening plenary session, the choice was made to move progressively from cutting-edge interfacial aspects of chemistry toward pure polymer science. This was superbly realized by Kurt Wütrich (Nobel, 2002, "NMR with Biopolymers-From Structural Biology to Proteomics"), Jean-Marie Lehn (Nobel, 1987, "Dynamic Molecular and Supramolecular Polymers") and Dame Julia Higgins ("Polymers Blends: Mixing and De-Mixing Them").

The topics of the seven other plenary lectures were balanced in order to merge together different polymer communities that normally meet separately, and thus to focus on the unity of polymer science. This was achieved through the cutting-edge lectures of first-rank scientists who kindly agreed to play the game. Following is a selection of lecturers and their topics. A complete list of lectures can be found online at <www.upmc.fr/macro2004>.

From Polymer Chemistry

- Jean Fréchet, "Functional Polymers: From Organic Electronics to Therapeutics"
- Kris Matyjaszewski, "From Precise Macromolecular Synthesis to Macroscopic Materials Properties"

From Polymer Physics

- Masao Doi, "Motion of Micro Particles with Complex Shape: Application to Separation"
- Helmut Möhwald, "Smart Polyelectrolyte Capsules as Microcontainers and Reactors"
- Ludwik Leibler, "From Nanostructured Plastics to Green Supramolecular Rubbers: Joys of Self-Assembling"

From Polymer Mechanics and Processing

- Han Meijer, "Multi-Scale Analysis of Mechanical Properties of Amorphous Polymers"
- Chris Macosko, "Polymer-Polymer Reactions with Applications to Compatibilization, Adhesion, and Solvent-free Block Copolymer Synthesis"

The general program covered nine broad topics, each of them generally divided into several more specific symposia:

- Polymer Chemistry: Reactions and processes
- Macromolecular Architectures and Organized Materials
- New Tools and Polymer Characterization Techniques
- Polymer-Based Complex Systems
- Polymers for Advanced Applications
- Polymer Processing and Induced Properties
- New Developments in Commercial Polymers
- Polymer Education
- International Cooperation in Polymer Science

Each symposium was organized and chaired by two or three eminent specialists from all over the world who defined the contents of the sessions, proposed the corresponding invited speakers, and selected the oral short presentations and posters. All the contributions submitted to MACRO 2004 followed a regular review procedure (acceptation/revision/rejection) by the chairpersons of the 21 thematic symposia.

A selection of the contributions (invited lectures and selected oral/poster presentations) will appear soon as full papers in the regular polymer journals of several publishers (Wiley-VCH, Elsevier, Springer-EDP Science, and VSP-Brill). Almost 2000 proceedings of all the contributions mentioned above can be found at the Web site of *e-Polymers* <www.e-polymers.org/paris>. A special issue of *Progress in Polymer Science* devoted to "Trends in Polymer Science" will feature full papers based on the plenary lectures.

Several prizes were presented during the Congress:

- The "IUPAC MACRO 2004 Distinguished Polymer Scientist Award," sponsored by Union des Industries Chimiques and Atofina (now Arkema), was presented to Axel Mueller (Bayreuth) and Ludwik Leibler (Paris).
- The "Samsung-IUPAC Polymer Division Young-Scientist Award," sponsored by Samsung General Chemicals, was presented to Timothy J. Deming (Santa-Barbara).
- The "Best Poster Award in Polymer Chemistry," sponsored by Wiley-VCH, was presented to Frederic Pelascini (Freiburg).
- The "Best Poster Award in Polymeric Materials," sponsored by Elsevier, was presented to Rafael Munoz-Espi (Mainz).

R.F.T. Stepto, president of the IUPAC Polymer Division, addresses the audience at Macro 2004.

- The "Best Poster Award in Polymer Physics," sponsored by Springer, was presented to Moon Jeong Park (Seoul).

World Polymer Congress Macro 2004 was the largest WPC to-date.This large gathering provided the dynamism and the creativity of a mature—but still young—polymer science that is developing in a multitude of directions. Participants came from 54 countries, roughly distributed between Europe (63%), Far East-Pacific (20%), North America (9%), Africa-Middle East (5%), and South America (3%). It should be noted that, due to attractive offers (reduced registration fees, as well as free lodging for some), more than 300 Ph.D. students attended and participated actively. Similarly, reduced fees or partial contributions toward lodging, or both, were allocated to about 200 regular participants from less favored countries. This was made possible thanks to the sponsorship of UNESCO and many industrial companies.

It is not our task to provide here scientific analyses or evaluations of the different symposia, themes, and trends, but the general opinion expressed by the scientific community was that, with respect to its size, its scientific coverage, and its scientific level, MACRO 2004 was one of the best polymer meetings ever held. Interesting and well-balanced reports on the Congress have already been published in *Nature Materials*, 2004, 3, 586–587, and *Polymer News*, 2004, 29, 355–357.

The polymer community is invited to join the next IUPAC WPC Macro 2006, 41st International Symposium on Macromolecules, to be held in Rio de Janeiro, 16–21 July 2006. See Where 2B & Y on page 38 or <www.abpol.com.br/macro2006.htm>.

Jean-Pierre Vairon <vairon@ccr.jussieu.fr>, a professor at the Université Pierre et Marie Curie, was chairman of Marco 2004. Jean-François Joanny, also a professor at the Université Pierre et Marie Curie, was vice-chairman.

Fats, Oils, and Oilseeds Analysis and Production

by Richard Cantrill

One of the goals of IUPAC and part of the mission of the American Oil Chemists' Society (AOCS) is to deliver technical information to audiences in regions of the world where access to the latest information may be limited. To this end, the two organizations held the **IUPAC-AOCS Workshop on Fats, Oils, and Oilseeds Analysis and Production** in Tunis, Tunisia, 6–8 December 2004. This workshop was the first time AOCS brought its expertise to the North African region. The program was tailored to the needs of the region, with a strong emphasis on oil processing and the requirements of the olive oil industry. Tunisia is the fourth largest olive-oil producing country after Italy, Spain, and Greece.

Plenary Lectures

The workshop was opened by Souilem El Fehri, the chairman and general manager of the Office National de l'Huile (ONH) of Tunisia; Patrick Dysseler of the Institut Meurice, Brussels, Belgium, representing IUPAC; and Richard Cantrill, AOCS technical director. Each speaker stressed the importance of holding this timely workshop in Tunis and thanked the organizing committee for developing such a relevant and integrated program.

The plenary session was opened by Habib Essid, the executive director of the International Olive Oil Council headquartered in Madrid, Spain, who described the world production, consumption, and trade in olive oil. He was followed by Dysseler who presented new and advanced methods for oil analysis, and Delia Amaya from the University of Campinas, Brazil, who outlined some of the principles and expectations of vitamin fortification of lipid-based foods. The session was rounded out by Gerrit van Duijn, Unilever Research (Vlaardingen, Netherlands), who described the quality control points in the oil processing system.

Oil Refining

In the short course on oil refining, many of the discussions centered on minor components that may be modified or lost at different stages in the process. An important factor in oil stability is the presence of tocopherols and minor sterol components; these may be lost or modified during deodorization. Their retention aids stability, whereas their removal enhances the economic value of the deodorizer distillate. These factors were clearly demonstrated for vegetable oils by Roland Verhé (University of Ghent, Belgium). Both Verhé and Wim de Greyt (De Smet, Zaventem, Belgium) highlighted the differences in deodorizer distillates obtained in the chemical and physical refining processes. Fereidoon Shahidi (Memorial University of Newfoundland, St. John's, Canada) also pointed out the relationship between triglyceride molecular structure and edible oil stability in native and structured lipids of marine, single cell organisms and plants. Andrew Logan, Alfa Laval (Soborg, Denmark), and Klaus-Peter Eickhoff, Westfalia Separators (Oelde, Germany), discussed degumming and alkali refining and how the chosen processes predetermine the plant layout and use of separation equipment. Roberto Berbesi, Oil-Dry Corporation (Chicago, Illinois), described the use of different sorbent materials, conditions of use, and expectations in the bleaching step of oil refining.

Analytical Techniques

Session III discussed many of the analytical techniques used by laboratories to determine oil quality and the extent to which unwanted materials are removed and advantageous components retained during processing. Regina Lago, EMBRAPA (Rio de Janiero, Brazil) presented discussed methods of fat extraction and the different compositions of the resulting material and its relationship to oil extraction in an industrial setting. In a presentation prepared by Michael Kennedy, Cargill (Minneapolis, Minnesota, USA), Cantrill described the AOCS Official Methods for ensuring vegetable oil-quality during refining. Chris

Dayton, Bunge Foods Corporation (Bradley, Illinois, USA), described how many classical wet chemistry methods provide the basis for correlations used in the development of rapid physical methods that can be applied in real-time monitoring of oil processing. Florence Lacoste, ITERG (Institute for Fats and Oils, Bordeaux, France), described the determination and limits set for the presence of contaminants and undesirable components in edible oil. The session was concluded by Wolfgang Burk, Bruker (Karlsruhe, Germany), who described the use of "Time Delay" (low resolution) NMR equipment in the measurement of solid fat content and other parameters.

Oil Processing

In the short course on oil processing, the use of bleaching earths and activated charcoal to remove unwanted compounds was discussed by Michel Remuzat, Süd Chemie (Choisy le Roi, France). De Greyt outlined the differences between chemical and enzymatic interesterifications and how these techniques are being used to produce oils with melting curves and solid fat contents useful for blending into margarines without resorting to using hydrogenated oils. Ignace Debruyne (Brussels, Belgium), a consultant to the American Soybean Association, detailed the conditions which can give rise to the development of off-flavors in refined oils and steps that can be taken to minimize them. He reminded the audience that a major premise is "good beans make good oil."

Jesper Hansen, Gerstenberg Schröder (Copenhagen, Denmark) presented the latest trends in the production of *trans* fatty acid-free margarines, challenges in their production, and the incorporation of functional ingredients and phytosterols. The fractionation of the triglyceride portion of oils according to their melting points was described by Véronique Gibon, Fractionnement Tirtiaux (Fleurus, Belgium). Olein and stearin fractions can be produced from oils according to their molecular structures using sophisticated cooling and separation protocols. The process can be monitored using a number of analytical techniques. Peter Johnsen, NCAUR (National Center for Agricultural Utilization Research, Peoria, Illinois, USA), concluded the session with an outline of studies undertaken by a group of United States Department of Agriculture scientists. An example of this successful program was the development of mid-oleic sunflower oil with the National Sunflower Association, based in Bismarck, North Dakota, USA.

Classification and Adulteration

The closing session of the workshop focused on the classification of olive oil, and the detection of adulteration by official analytical methods. Details on olive-oil processing and olive-pomace-oil extraction were jointly presented by Samira Sefi and Tarek Amamou, ONH, (Tunis). Mention was made of the traditional and industrial methods used for the extraction and treatment of different classes of olive oil and their effects on the composition of minor components. The identification, analysis, and potential health benefits of minor components in olive oil were the subject of the presentation by Apostolos Kiritsakis, Technological Educational Institute (Thessaloniki, Greece). His presentation highlighted the importance of retention of these high-value components and prompted much discussion with earlier speakers.

The methods of analysis recognized by the IOOC and Codex Alimentarius for the establishment of the purity of olive oil were presented by Efi Christopoulou, Ministry of Development (Athens, Greece). There are two categories of such methods: those required to measure quality parameters and those required to determine the purity of the oil. Their use in the detection of adulterated olive oil was discussed by Lanfranco Conte, University of Udine (Italy). He outlined progress in the development of analytical methods to meet increasing levels of sophistication on the part of those involved in adulteration. Conte also discussed the use of sensory evaluation in the analysis of virgin olive oil. He speculated on the use of sensory fingerprints to confirm the specific geographic origins of extra-virgin olive oils.

Richard Cantrill <Richard.Cantrill@aocs.org> is technical director for AOCS. He was a member of the task group heading the corresponding IUPAC project #2002-011-2-600 (see Web below). The presentations from the meeting can be accessed on the AOCS Web site at <www.aocs.org/archives/analysis/papers.asp>.

This report originally appeared in *inform* (the *International News on Fats, Oils, and Related Materials*), March 2005, and is reprinted with permission.

www.iupac.org/projects/2002/2002-011-2-600.html

Carbohydrates

by Elizabeth Hounsell

Known to most as an important food type, carbohydrates are critically involved in nutrition and metabolism. They also have profoundly important roles in the exciting new area of nutraceuticals, and in materials science. Carbohydrates possess greater potential diversity than proteins and this enormous variety of structure and activity has led to their use in fields as diverse as cancer therapy and toothpaste manufacture. Carbohydrates are already a multimillion dollar business, but their importance in research, medicine, agriculture, and industry will grow enormously in the future.

Carbohydrates are the "next frontier" in biomedicine. Cell surfaces are made up of proteins and lipids, but attached to these are carbohydrates. These form a critical interface by which the cell communicates with the outside world. It is the cell's 'telephone line'-alerting, for example, the body's defenses to an infection or, unfortunately, telling an invading cancer cell where a new home might be found. Other examples include organ transplantation, auto-immunity, allergy, and blood transfusion. No surprise then to discover that carbohydrates have already been involved in making vaccines, anti-inflammatory drugs, and drugs effective against HIV. This is just the tip of the iceberg.

These exciting developments and much more were the focus of the **22nd International Carbohydrate Symposium**, which was held 23–27 July 2004 at the Scottish Exhibition and Conference Center (SECC), Glasgow, Scotland, UK.

The symposium began with a sponsored reception at the Science Center just across the river Clyde from the SECC. This location offered a commanding view of the SECC and the University of Glasgow campus and provided a good orientation to the layout of Glasgow and the close-by student and hotel accommodations. The reception was a convivial and intellectually stimulating venue for introductions and meetings with old friends.

The first day of the symposium started with the opening ceremony, followed by the presentation of the Whistler Award to Anne Imberty (Grenoble) and Thomas Peters (Lubeck). The opening ceremony was presided over by Bob Stick (Perth), chairman of the International Carbohydrate Symposium. Hans Vliegenthart (Utrecht) gave a presentation in his role as representative of IUPAC. The president elect and chair of ICS-22, Elizabeth Hounsell (London), introduced the Deacon Convener of Glasgow City Chambers, who gave, on behalf of Glasgow's Lord Provost, a welcoming speech from the city.

The meeting covered new and emerging trends, with particular emphasis on synthetic methodology and applications in the design and synthesis of bioactive organic compounds. The program, which included relevant aspects of biologically active natural products and materials chemistry, catered to a wide range of interests in contemporary carbohydrate chemistry, biochemistry, and medicine, and offered a visionary perspective on future challenges and opportunities.

The program consisted of a mix of plenary, keynote, and shorter contributed lectures, as well as two formal poster sessions on the themes: "Carbohydrate Chemistry and Enzymology," "Carbohydrates in Medicine and Biology," and "Carbohydrate Materials and Biopolymers."

The scientific committee for the meeting consisted of the immediate past presidents of the RSC Carbohydrate Group: David Crout (Warwick), Rob Field (Norwich), and Hounsell (chair). They consulted widely within the groups mentioned above for choices for the plenary and invited keynote speakers (10 and 22, respectively). The symposium featured 67 oral presentations—selected from 128 abstracts that were submitted—and 491 poster presentations. A highlight was a buffet lunch sponsored by Elsevier for the student poster presenters to meet with the speakers and the editorial advisory board of Carbohydrate Research.

The meeting attracted 764 scientific contributors and 74 accompanying guests. Attendees were geographically diverse: Japan (110), Australia and New Zealand (29), South Korea (14), Taiwan (13), UK (161), Germany (55), and USA (55). There were 238 registered students, which reflected the availability of inexpensive student accommodations and the overall low registration fee, a result of having the meeting in Glasgow.

Elizabeth Hounsell <e.hounsell@bbk.ac.uk> is a professor of biological chemistry at Birkbeck College (London, UK). She was the chair of ICS-22.

Polymer-Based Materials

by Philippe Dubois

Approximately 300 scientists from 35 countries attended the first joint meeting of the **8th European Symposium on Polymer Blends and Eurofillers 2005**, which was held in the historical city of Bruges, Belgium, from 9–12 May 2005. The meeting featured 16 plenary/keynote lectures, 44 oral communications, and more than 200 poster presentations.

"Materials Design, Performance, and Problem Solving" was the general theme of this meeting, organized by laboratories of four Belgian universities active in polymer-based materials. The chairing committee was composed of Philippe Dubois, University of Mons-Hainaut; Gabriel Groeninckx, Catholic University of Leuven; Robert Jérôme, University of Liège; and Roger Legras, Catholic University of Leuven, Louvain-la-Neuve.

The purpose of this international joint symposium was to stimulate dialogue between specialists in complementary fields, including physicists, chemists, and engineers, with expertise in both organic and inorganic materials. Congress topics included the following.

In the field of Polymer Blends:

- innovations in generation and control of phase morphology, including theoretical approach and numerical simulation
- reactive processing—reactive compatibilization, dynamic crosslinking, polymer chemistry in the melt
- interfaces and interphases—control, characterization, and modeling
- structure-mechanical performance relationships
- specific polymer blends (including recycling) and their applications

In the field of Fillers and Filled Polymers:

- preparation and characterization of (nano)fillers of all shapes and functions
- formulations of (nano)fillers with polymers: nanocomposites, natural fiber composites, organic-inorganic hybrid materials
- adhesion between (nano)fillers and polymers
- structure-property relationships of (nano) composites, including confined crystallization issues
- industrial applications of filled polymers in automotive, electronic, biomedical and packaging area

Philippe Dubois

Based on the scientific success and interest of the meeting held in Bruges, both steering committees also agreed on the point that other joint meetings should be reorganized in the near future. It emerged from this first joint meeting that problems faced in "filled polymers" and "polymer blends" domains are most often very similar to each other and therefore should deserve attention and discussion from both scientific communities.

More information (detailed program, pictures of speakers, participants, exhibitors, poster sessions, and ceremony of best poster awards) can be found on the congress Web site at <www.polymerblends-eurofillers2005.com>.

The next meetings will be organized as follows:

- The 8th European Symposium on Polymer Blends, which will be held in Palermo, Italy, is being organized by Prof. F. La Mantia (most likely mid-September 2007).
- Eurofillers 2007, which will be held the last week of August 2007 in Budapest, Hungary, is being organized by Prof. B. Pukansky.

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Fine Chemistry and Novel Materials

17–20 October 2005, Shanghai, China

The **15th International Symposium on Fine Chemistry and Functional Polymers (FCFP-XV)** and the 1st International Symposium on Novel Materials and Synthesis (NMS-I) will be jointly held 17–20 October 2005 at Fudan University in Shanghai, China. The meeting, which is being organized by Fudan University and the Institute of Chemistry of the Chinese Academy of Sciences, is sponsored by IUPAC, the National Natural Science Foundation of China, and Shanghai Key Laboratory of Molecular Catalysis and Innovative Materials. It is anticipated that 150–200 delegates from 26 countries and areas will attend. The official language of the conference is English.

The aim of the conference is to review recent achievements in experimental thermodynamics and explore likely future developments. The program is focused on the following fields: (1) preparation, characterization, and properties of fine chemicals and functional polymers; (2) application of the chemicals to special drugs, perfumes, agricultural chemicals, electrical materials, coloring matters, and fine ceramics, etc.; (3) application of functional polymers to catalysis, separation, medical use, electric and ionic conductors, liquid crystals, photosensitive materials, and others; (4) other novel materials and their properties, and novel synthesis methods.

The scientific program comprises plenary lectures, invited lectures, oral presentations, and poster sessions. There will also be an exhibition of products, instruments, and equipments.

All correspondence should be sent directly to the general secretary of the symposiums, Prof. Yuping Wu.

See Mark Your Calendar on page 41 for contact information

Water Contamination by Arsenic

12–14 December 2005, Dhaka, Bangladesh

The **Bangladesh Workshop on Origins and Remediation of Groundwater Contamination by Arsenic** is planned for 12–14 December 2005 in Dhaka, Bangladesh. This meeting will address the pressing problem of arsenic contamination in water. Naturally occurring arsenic in groundwater contaminates thousands of tube wells in Bangladesh. It is seriously affecting the health of more than 60 million people, as it ultimately leads to a slow and painful death for many. This problem also affects regional water supplies in a number of countries, including Argentina, Chile, China, France, India, and the United States.

The workshop will be supported by CHEMRAWN, IUPAC, and the American Chemical Society. The workshop will address the following questions:

- By what mechanism(s) does arsenic enter the groundwater in Bangladesh and elsewhere?
- What low-cost methods are available to determine arsenic concentrations in groundwater? What new methods need to be developed?
- What procedures exist or can be devised to remove arsenic economically?
- What is an economically practical action plan for implementing appropriate remediation technologies?

See Mark Your Calendar on page 41 for contact information

www.iupac.org/projects/2003/2003-050-1-021.html

Humic Science

22-24 March 2006, Boston, USA

The **Humic Science & Technology Conference IX** will be held 22-24 March 2006 at Northeastern University, Boston, USA. Conferences in this series focus on the structures, properties, and uses of humic science. This conference is dedicated to Dr. E. Michael Thurman of the Universidad de Almería, Spain. The honorary chair is Dr. Jerry A. Leenheer of the U.S. Geological Survey in Denver.

The deadline for abstracts is 31 December 2005. Please visit <www.hagroup.neu.edu> or call 1-617-373-2834 for further information.

Green and Sustainable Chemistry

10–13 January 2006, Delhi, India

The **Second International Symposium on Green/Sustainable Chemistry** will be held 10–13 January 2006 in Delhi, India. This conference aims to promote the activities of green and sustainable chemistry worldwide. It is becoming widely recognized that the development of sustainable technologies and prevention of pollution is the smarter and more effective way of managing the environment. Technologies and methods are being pursued to identify cleaner products and processes that can be implemented proactively. It has been said that "the revolution of one day becomes the new orthodoxy of the next." Most importantly, we need the relevant communities—scientific, engineering, educational, and others—to work together for a sustainable future through green chemistry.

The main themes of the conference will be:

- collaborations among academia, government, and industry, and scientists for green and sustainable chemistry
- the status of green chemistry activities in industry
- education to promote green and sustainable chemistry
- new approaches to products and processes for green and sustainable chemistry
- the role of biocatalysts in chemical synthesis
- green chemicals, processes, and technologies in pharmaceutical, agrochemical, and food product industries
- alternative synthesis (ionic liquids, super critical solvents, microwave, water based, solid phase, and photochemical)

See Mark Your Calendar on page 43 for contact information

www.greenchemistryindia.com

Photochemistry

2–7 April 2006, Kyoto, Japan

The IUPAC Symposium on Photochemistry is a biennial international conference with topics encompassing the entire spectrum of photochemistry. The series of symposia was initiated by George Hammond, with the first one held in Strasbourg in 1964. Since then, the symposia have been held every two years in Europe. The **XXIst Symposium on Photochemistry** will be held 2–7 April 2006 in Kyoto, Japan—the first time the symposium will be held outside Europe.

As with previous symposia in this series, a number of internationally known scientists will give lectures covering traditional as well as modern photochemistry and the latest developments in the field. Science and technologies related to photochemistry, such as materials for photonics, nanotechnology, and photobiology, will also be discussed in the symposium. The technical program will feature plenary lectures, invited lectures, workshops, oral communications, and posters. The workshops will deal with topics of electron transfer, organic light emitting diodes, and photocatalysts.

Attendees will have the chance to appreciate one of the most attractive spots in Japan. Kyoto is an ancient capital of Japan, and it retains a traditional

Japanese atmosphere. April in Kyoto is the best season to visit because of blooming cherry blossoms and a relatively mild climate.

See Mark Your Calendar on page 43 for contact information

www.pac.ne.jp/photoiupac2006

Organic Synthesis

11-15 June 2006, Mérida, Yucatán, Mexico

The **16th International Conference on Organic Synthesis**, co-sponsored by IUPAC, Academia Mexicana de Ciencias, and the Division of Organic Chemistry of the American Chemical Society, will take place in Mérida, Yucatán, Mexico, 11–15 June 2006.

Hoping to match the fantastic success achieved at previous conferences in this series, ICOS-16 has secured the participation of seven outstanding plenary speakers: Luiz C. Diaz (Brazil), Eric N. Jacobsen (USA), Paul Knochel (Germany), Shu Kobayashi (Japan), Stephen F. Martin (USA), Dieter Seebach (Switzerland), and Joaquín Tamariz (México). The 2006 Thieme-IUPAC Prize winner—who has yet to be selected—will also be a plenary speaker; see Call for Nomination on the back cover of this issue. Also scheduled are 15 renowned invited speakers: Carsten Bolm (Germany), Margaret Brimble (New Zealand), Cathleen Crudden (Canada), Gregory Fu (USA), Thoru Fukuyama (Japan), Miguel A. García-Garibay (USA), Cesare Gennari (Italy), Minoru Isobe (Japan), Eun Lee (Korea), Shengming Ma (China), Carmen Nájera (Spain), Régis Réau (France), Philippe Renaud (Switzerland), and Margarita Suárez (Cuba).

In addition, 36 invited experts will partake in 6 selected symposia in the areas of medicinal chemistry, organocatalysis, enantioselective synthesis of ß-amino acids (Ferenc Fulop, chair), organolithium compounds in synthesis (William F. Bailey, chair), industrial asymmetric synthesis, and applications of microwave in organic synthesis (Nicholas E. Leadbeater, chair).

The participation of attendees in the academic program is strongly encouraged. Thus, up to 600 poster presentations will be scheduled. Ample space for chemical exhibitors will also be available.

In the interest of facilitating interaction between participants, several social events are being planned, including an excursion to the archeological site of Uxmal, a banquet at a local hacienda, and a performance by the Yucatán's Folkloric Ballet at Mérida's Main Theater.

Yucatán is located in the southeast of México. The state´s capital is Mérida, which contains an international airport. Travelers can also fly from many countries to the city of Cancún and then to Mérida. The Yucatán area offers a variety of attractions for tourists, such as colonial cities, archeological sites, beaches, ecological reserves, haciendas, and more.

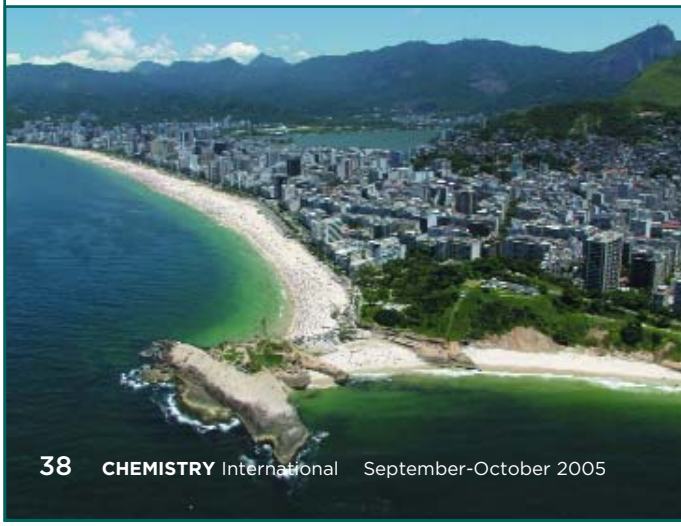
See Mark Your Calendar on page 43 for contact information

www.relaq.mx/RLQ/IUPAC_ICOS-16.html

Macromolecules

16–21 July 2006, Rio de Janeiro, Brazil

The Brazilian Polymer Association (ABPol) is pleased to invite professionals and students to attend the **World Polymer Congress—MACRO 2006**, the **41st International Symposium on Macromolecules**, which will be held 16–21 July 2006 at the Convention Center of the Intercontinental Hotel in Rio de Janeiro, Brazil. The symposium, organized under the general theme "Polymers-Promoting Life Quality," is an international forum for discussion of scientific and technological themes in the polymer field. More than 1500 participants from the academic sector, research and development institutions, and important industries in the polymer field are expected.



Oral presentations and poster communications will cover a wide variety of themes, such as biopolymers, polymer blends, characterization, polymer gels, nanocomposites, polymer processing, polymers for controlled drug release, recycling and synthesis, as well as polymer education. There will be special sessions on market-oriented themes and specific themes of industrial interest. The congress will feature around 10 plenary lectures and 230 invited lectures, which will be given by renowned scientists from different countries. The congress will feature the following sessions:

- polymer chemistry and reaction processes
- polymer characterization
- polymer processing

- structure and properties of polymers
- thermodynamics of polymers solutions
- polymer blends and composites
- modelling and simulation
- novel applications for polymers
- biomaterials and environment
- recycling
- advances in commercial polymers
- polymer education
- international cooperation

During the congress, there will also be an industrial exhibition of products and equipments from different companies.

The deadline for abstract submission is 10 March 2006.

See Mark Your Calendar on page 43 for contact information

www.macro2006.com.br

Other Upcoming Conferences

Green Chemistry
<www.gdch.de/vas/tagungen/tg/5559.htm>
10–15 September 2006, Dresden, Germany

Heterogeneous Catalysts
<www.cata.ucl.ac.be/9prep.htm>
10–14 September 2006, Louvain-la-Neuve, Belgium

Equifase Symposium
<termo.esiqie.ipn.mx/english/equifase2006/>
21–25 October 2006, Morelia, Michoacán, Mexico

Biotechnology and Sustainability
(contact Prof F.W. Bai <fwbai@dlut.edu.cn>)
12–17 October 2008, Dalian, China

Chemistry and Chemical Engineering

16–20 October 2006, Havana City, Cuba

The **27th Latin American Congress on Chemistry** and the **6th International Congress on Chemistry and Chemical Engineering** will take place 16–29 October 2006 at the Convention Center of Havana. The Congress is being organized by the Cuban Chemical Society and the Latin American Federation of Chemistry.

The congress will address the following topics: teaching, history, analytical, organic, inorganic, industrial, environmental, medicinal and pharmaceutical chemistry, chemical engineering, nanoscience, and new materials. Within the congress, the 3rd International Symposium on Biochemistry and Molecular Biology, 6th International Workshop on Natural Products, and the IVth International Conference on Biomaterials will take place.

Distinguished scientists have been invited to participate as lecturers. Among them are the Nobel Laureates Paul Crutzen (MPI of Chemistry-Mainz, Germany), Harry Kroto (University Sussex, UK), Jean-Marie Lehn (University Strasbourg, France) and Mario Molina, (MIT, USA), as well as Héctor D. Abruña (Cornell University, USA), Peter Atkins (Lincoln College Oxford, UK), Simon Campbell (President Royal Society of Chemistry, UK), Roberto Cao (University Havana, Cuba), Raymundo Cea (UNAM, Mexico), María A. Chávez (University Havana, Cuba), Robert Corriu (University. Montpellier, France), Eusebio Juaristi (CINVESTAV-IPN, Mexico), Andrés Menez (University Gif-sur-Yvette, France), Eloy Rodríguez (Cornell University, USA), and Henrique Toma (University Sao Paulo, Brazil).

Both Spanish and English are the official languages of the congress.

The president of the Cuban Chemical Society, Dr. Alberto Nuñez <alberto@cqf.co.cu> is the chair of the Organizing Committee. Dr. Roberto Cao <cao@fq.uh.cu> is the chair of the Scientific Committee and Dr. Irma Castro <irmac@infomed.sld.cu> is co-chair.

See Mark Your Calendar on page 44 for contact information

www.loseventos.cu/XXVIIclaq

GDCh
Gesellschaft Deutscher Chemiker

IUPAC

INCA

International IUPAC Conference on Green Chemistry

SEPTEMBER 10-15, 2006 • DRESDEN, GERMANY

TOPICS:

- Benign Syntheses Routes
- Future Green Energy Sources
- Use of Renewables
- Benign Process Technology
- Education in Green Chemistry

CHAIRMEN:

Prof. Dr. P. Tundo, Venice
(Chairman)
Prof. Dr. W. Hölderich, Aachen
(Co-Chairman)
Prof. Dr. W. Reschetilowski, Dresden
(Co-Chairman)

INFORMATION:

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Phone: +49-(0)69-7917-358 /-366
Fax: +49-(0)69-7917-475
E-mail: tg@gdch.de

www.gdch.de/vas/tagungen/tagungen2006/5559.htm

Mark Your Calendar

Upcoming IUPAC-sponsored events
See also www.iupac.org/symposia
for links to specific event Web site

2005 *(later than 1 September)*

IUPAC poster prizes to be awarded

4–9 September 2005 • Analytical Spectroscopy • Antwerp, Belgium
Colloquium Spectroscopicum Internationale XXXIV
Prof. Rene Van Grieken, Department of Chemistry, University of Antwerp, B-2610 Antwerp, Belgium, Tel.: +32 3 820 2362, Fax: +32 3 820 2376, E-mail: rene.vangrieken@ua.ac.be

5–9 September 2005 • Nanostructured Advanced Materials • Stellenbosch, South Africa
3rd IUPAC Workshop on New Directions in Chemistry—Workshop on Nanostructured Advanced Materials (WAM III)
Prof. R.D. Sanderson, University of Stellenbosch, Department of Chemistry & Polymer Science, Private Bag X1, Matieland 7602, South Africa, E-mail: rds@sun.ac.za

10–13 September 2005 • Macromolecule-Metal Complexes • Tirrenia (Pisa), Italy
11th IUPAC International Symposium on Macromolecule-Metal Complexes (MMC-11)
Prof. Francesco Ciardelli, Chemistry and Industrial Chemistry Department, University of Pisa, via Risorgimento, 35, I-56126 Pisa, Italy, Tel.: +39 0502219229, Fax: +39 0502219320, E-mail: fciard@dcci.unipi.it

11–15 September 2005 • Boron Chemistry • Sendai, Japan
12th International Meeting on Boron Chemistry
Prof. Yoshinori Yamamoto, Department of Chemistry, Graduate School of Science, Tohoku University, Sendai, Japan 980-8578, Tel.: +81 22 217 6581, Fax: +81 22 217 6784, E-mail: yoshi@yamamoto1.chem.tohoku.ac.jp

12–18 September 2005 • Analytical Chemistry • Kiev, Ukraine
International Congress on Analytical Chemistry and Chemical Analysis (AC&CA-05)
Prof. Vladimir Zaitsev, Chemistry Department, Kiev National University, 60 Vladimirskaya, Kiev 01033, Ukraine, Tel.: +380 44-2393345, Fax: +380 44-2393345, E-mail: zaitsev@univ.kiev.ua

13–16 September 2005 • Polymers for Advanced Technologies • Budapest, Hungary
8th International Symposium Polymers for Advanced Technologies
Prof. Gyorgy Marosi, Budapest University of Technology and Economics, Department of Organic Chemical Technology, Muegyetem rkp. 3, H-1111 Budapest, Hungary, Tel.: +36 1 4633654, Fax: +36 1 4631150, E-mail: pat@mail.bme.hu

8–12 October 2005 • Metallothionein • Beijing, China
5th International Conference on Metals and Metallothionein in Biology and Medicine
Prof. M. George Cherian, Department of Pathology, University of Western Ontario, London, Ontario N6A 5C1 Canada, Tel.: +1 519-661-2030, Fax: +1 519-661-3370, E-mail: mcherian@uwo.ca

17-20 October 2005 • Novel Materials • Shanghai, China
Fine Chemistry and Functional Polymers (FCFP-XV) & 1st International Symposium on Novel Materials and their Synthesis (NMS-I)
Prof. Yuping Wu, Department of Chemistry, Fudan University, Shanghai 200433, China, Tel.: +86 10 6255 9368, E-mail: wuyp@fudan.edu.cn

17–21 October 2005 • Radiochemistry • Beijing, China
Third Asia-Pacific Symposium on Radiochemistry (APSORC '05)
Prof. Z. F. Chai, Institute of High Energy Physics, Chinese Academy of Sciences, Yu Quan Rd. 19B, P.O. Box 918 Beijing 100039, China, Tel.: +86 10 8823 3191, Fax: +86 10 8823 3191, E-mail: apsorc2005@ihep.ac.cn

23–28 October 2005 • Ionic Polymerization • Goa, India
International Symposium on Ionic Polymerization
Prof. S. Sivaram, National Chemistry Laboratory, Polymer Chemistry Division, Dr. Homi Bhabha Road, Pune, Maharashtra, 411 008 India, Tel.: +91 20 2589 3030, Fax: +91 20 2586 3355, E-mail: sivaram@ems.ncl.res.in

6–9 December 2005 • Agriculture • Jesenik, Czech Republic
XXXIth International Conference—Chemistry for Agriculture
Dr. Adam Pawelczyk, Wroclaw University of Technology, Smoluchowskiego 25, 50-370 Wroclaw, Poland, Tel.: +48 (0) 71-3202930, Fax: +48 (0) 71-3203469, E-mail: adam.pawelczyk@pwr.wroc.pl

12–14 December 2005 • Arsenic Remediation • Dhaka, Bangladesh
Bangladesh Workshop on Origins and Remediation of Groundwater Contamination by Arsenic
Dr. Satinder Ahuja, Novartis Corporation (retired), 1061 Rutledge Court, Calabash, NC 28467 USA, Tel.: +1 910 287-2765, E-mail: sutahuja@xaranda.net

August 12 - 17, 2006

www.19icce.org / 19icce@19icce.org

"Chemistry and Chemical Education for Humanity"

19th International Conference on Chemical Education

KCS
Korean Chemical Society

IUPAC

Titles of Sessions : ◆ Public Understanding of Chemistry(•Chemistry in Societal Needs, Role of Chemists •Women and Chemistry •Environment and Chemistry •Green Chemistry) ◆The Challenges of Reforming Chemistry Education to Ensure Relevance and Quality(•Analytical Chemistry •Inorganic Chemistry •Organic Chemistry •Physical Chemistry •Industrial Chemistry •Network of Chemistry and Chemical Engineering Education •How Students Learn Chemistry) ◆New Ways of Teaching Chemistry(•Multimedia and Visualization for Chemistry Education •Microscale Laboratory Technique •Chemistry Demonstrations •Web-based Learning and Teaching •Use of Arts in Chemical Education •Peer-led Team Learning) ◆Preparing Teachers and College Faculty for Reform(•Chemistry Teacher Education •Science Education at Elementary Level •Chemistry in Secondary Schools • The Future of Chemistry Textbooks) ◆Introducing New Chemistry Contents (•Biochemistry and Biotechnology •Computational Chemistry •Forensic Chemistry •Materials Science •Polymer Chemistry)

Call for Symposiums and Workshops : We accept proposals for symposiums and workshops by December 5, 2005.

Call for Papers : Please submit your abstract(s) by May 31, 2006. Please visit our web site (www.19icce.org) or contact Prof. Choon H. Do (choondo@19icce.org) for further information.

Mark Your Calendar

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IUPAC poster prizes to be awarded

10–13 January 2006 • Green Chemistry • Delhi, India
Second International Symposium on Green/Sustainable Chemistry
Prof. M. Kidwai, Department of Chemistry, University of Delhi, Delhi-110007, India, Fax: +91 11 27666235, E-mail: kidwai_chemistry@yahoo.co.uk

12–15 March 2006 • Heterocyclic Chemistry • Gainesville, Florida, USA
7th Florida Heterocyclic Conference
Prof. Alan R. Katritzky, University of Florida, Dept. of Chemistry, Gainesville, FL 32611-7200, USA, Tel.: +1 352 392 0554, Fax: +1 352 392 9199, E-mail: katritzky@chem.ufl.edu

2–7 April 2006 • Photochemistry • Kyoto, Japan
XXIst IUPAC Symposium of Photochemistry
Prof. Masahiro Irie, Department of Chemistry and Biochemistry, Kyushu University, Graduate School of Engineering, Hakozaki 6-10-1, Fukuoka, Japan, Tel.: +81 92 642 3556, Fax: +81 92 642 3568, E-mail: irie@cstf.kyushu-u.ac.jp

11–15 June 2006 • Organic Synthesis • Merida, Yucatan, Mexico
16th International Conference on Organic Synthesis (ICOS 16)
Dr. Eusebio Juaristi, Instituto Politecnico Nacional, Departamento de Quimica, Avenida IPN #2508, Esquina Ticoman, Mexico City, DF, 07360, Mexico, Tel: +52 55 50613722, Fax: +52 55 57477113, E-mail: juaristi@relaq.mx

16-17 June 2006 • Neurotoxic Metals • Brescia, Italy
Workshop on Neurotoxic Metals: Lead, Manganese, and Mercury. From Research to Prevention
Dr. Roberto G. Lucchini, Institute of Occupational Health, University of Brescia, Italy, Brescia, Italy, Tel.: +39 0303996080, Fax: +39 0303996080, E-mail: lucchini@med.unibs.it

25–30 June 2006 • Analytical Sciences • Moscow, Russia
International Congress on Analytical Sciences
Prof. Vladimir P. Kolotov, Vernadsky Institute of Geochemistry, Russian Academy of Sciences, 19, Kosygin Str., Moscow B-334 119991 Russia, Tel.: +7 (095) 137 04 86, Fax: +7 (095) 938 20 54, E-mail: kolotov@geokhi.ru

2-7 July 2006 • Polymers and Organic Chemistry • Okasaki, Japan
12th International Conference on Polymers and Organic Chemistry 2006 (POC'06)
Prof. Shinichi Itsuno, Department of Materials Science, University of Technology, Toyohashi, 441-8580, Japan, Tel.: +81 532 44 6813, Fax: +81 532 44 6813, E-mail: itsuno@tutms.tut.ac.jp

16-21 July 2006 • Macromolecules • Rio de Janeiro, Brazil
41st International Symposium on Macromolecules—IUPAC World Polymer Congress MACRO 2006
Prof. Ailton de Souza Gomes, Caixa Postal 68525, Rio de Janeiro, 21945-970, Brazil, E-mail: asgomes@ima.ufrj.br or macro2006@linkway.com.br

23-28 July 2006 • Biodiversity and Natural Products • Kyoto, Japan
ICOB-5 & ISCNP-25 IUPAC International Conference on Biodiversity and Natural Products
Prof. Michio Murata, Department of Chemistry, Osaka University, Graduate School of Science, 1-16 Machikaneyama, Toyonaka, Osaka, 560-0043, Japan, Tel.: +81 6 6850 5437, Fax: +81 6-6850-5774, E-mail: iscnp25@ch.wani.osaka-u.ac.jp

6–11 August 2006 • Pesticide Chemistry • Kobe, Japan
11th International Congress of Pesticide Chemistry
Dr. Hisashi Miyagawa, Division Applied Life Sciences, Graduate School of Agriculture, Kyoto University, Kyoto 606-8502, Japan, Tel.: +81 75 753 6118, Fax: +81 75 753 6123, E-mail: miyagawa@kais.kyoto-u.ac.jp

12–17 August 2006 • Chemical Education • Seoul, Korea
19th International Conference on Chemical Education
Prof. Choon H. Do, Sunchon National University, Department of Polymer Science and Engineering, 315 Maegok-dong, Sunchon,, Chonnam 540-742, Korea, Tel.: +82 61 750 3565, Fax: +82 61 750 3565, E-mail: choondo@sunchon.ac.kr

Mark Your Calendar

13–18 August 2006 • Coordination Chemistry • Cape Town, South Africa
37th International Conference on Coordination Chemistry
Prof. K.R. Koch, Department of Chemistry, Univsersity of Stellenbosch, Private Bage X1 Matieland, Stellenbosch 7602, South Africa, Tel.: +27 21 808 3020, Fax: +27 21 808, E-mail: krk@sun.ac.za

10–15 September 2006 • Green Chemistry • Dresden, Germany
First International IUPAC Conference on Green-Sustainable Chemistry
Prof. Pietro Tundo, Dipartimento di Scienze Ambientali, Ca' Foscari, University of Venice, Calle Larga S. Marta, Dorsoduro 2137, I-30123 Venizia, Italy, Tel.: +39 41 2348642, Fax: +39 41 2348620, E-mail: tundop@unive.it

18–22 September 2006 • High Temperature Materials • Vienna, Austria
12th International Conference on High Temperature Materials Chemistry (HTMC XII)
Prof. Dr. Adolf Mikula, Wahringstr. 42, A-1090 Vienna, Austria, Tel.: +43 4277 52606, Fax: +43 4277 52679, E-mail: Adolf.Mikula@univie.ac.at

16–20 October 2006 • Chemistry for Life • Havana City, Cuba
27th Latin American Congress on Chemistry and 6th International Congress of Chemistry and Chemical Eng.
Prof. Alberto J. Núñez Sellés, Center of Pharmaceutical Chemistry, Sociedad Cubana de Quimica, Ave 21 & 200, Rpto. Atabey, Apdo. 16042 Havana, CP 11600, Cuba, Tel.: +53 7 218 178, Fax: +53 7 273 6471, E-mail: alberto@cgf.co.cu

2 0 0 7

IUPAC poster prizes to be awarded

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

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

2–6 August 2007 • Organometallic Chemistry • Nara, Japan
14th International Symposium on Organometallic Chemistry Directed Towards Organic Synthesis (OMCOS-14)
Prof. Kazuhiko Takai, Dept. of Applied Chemistry, Okayama University, Faculty of Engineering, Tsushimanaka 3-1-1, Okayama 700-8530, Japan, Tel.: +81 86 251 8097, Fax: +81 86 251 8094, E-mail: ktakai@cc.okayama-u.ac.jp

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

5–11 August 2007 • IUPAC 41st Congress • Torino, Italy
Chemistry Protecting Health, Natural Environment, and Cultural Heritage
E-mail: IUPAC.2007@unito.it

Visas

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