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New Perspectives on Information

INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

OPCW ▶

Green Chemistry in Japan ▶

CHEMISTRY International

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From the Editor

As we are putting this issue to press, the IUPAC community is focusing on the prospect of gathering in Istanbul in early August for the IUPAC General Assembly and Congress. Hopefully, by that time, the tensions in that nation will have settled down and our attention can turn to chemistry. The anticipation of the General Assembly is palpable in our daily work. Various divisions, committees, and task groups are planning to meet and agendas and attendance lists are being generated and circulated actively among members.

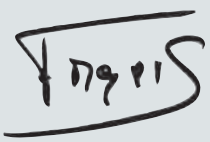
One unique aspect of this year's preparation, and which I am thrilled to observe, is the particular engagement of IUPAC National Adhering Organizations in attempting to include young chemists to come along under the Young Observers program. Already confirmed are young observers from the USA, UK, Japan, and Russia. Moreover, the Royal Society of Chemistry's Pan Africa Chemistry Network has also invited YOs from Ghana and from South Africa, while Germany reached out to YOs from Hungary, Slovakia, and Romania. A few more NAOs, including France, Italy, and India, are still working out plans that will hopefully allow for more YOs to participate.

The largest and oldest YO program is that of the USA, which has been in place for more than 30 years. As envisioned by former U.S. Bureau member Ed Przybylowicz, the YO program is a mechanism for getting new experts involved in IUPAC <www.iupac.org/publications/ci/2002/2401/forum-young.html>. The opportunity to be an observer at the GA, along with the mentorship by current members, provides a unique experience for YOs to learn first hand about IUPAC. In a 2002 presentation about the YO program, Przybylowicz noted that "Mechanisms need to be considered that will encourage involvement from all member countries of IUPAC, not just the larger countries."

The resurgence of interest in the YO program is welcome and timely, and well suited to the announcement that the traditional WCLM (World Chemistry Leadership Meeting) will this year focus on the "Future of Chemistry—IUPAC's Role."

The theme, as announced by the IUPAC Committee on Chemistry and Industry, which is organizing this year's meeting, is an opportunity for young leaders to voice their ideas about where chemistry will be in 25 years and how IUPAC should approach the future. Key topics will explore the future of chemistry in the context of the Millennium Development Goals, the scope of pure and applied research, the perceived role of IUPAC, and the career aspirations of the younger generation of chemists.

Whatever your interest, and whatever your age, please be sure to reach out to this year's young observers and stop by the General Assembly. Safe travels, and see you in Istanbul.



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Cover: "Map of Scientific Collaborations from 2005–2009," by Olivier H. Beauchesne, appears in "7th Iteration (2011): Science Maps as Visual Interfaces to Digital Libraries," Places & Spaces: Mapping Science, edited by Katy Börner and Michael J. Stamper. http://scimaps.org.

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**Back cover tear-off page : IUPAC periodic table of the elements, version 1 May 2013*

Vice President's Column

photo by Peter Cutts

by Mark Cesa

One of the most important tasks of the vice president is to carry out a critical assessment of the programs and projects of all IUPAC bodies. The Vice President's Critical Assessment is intended to provide a firm grounding in all of IUPAC's activities and set the basis for the direction IUPAC will take in the coming years.

IUPAC is an extraordinarily productive scientific organization. Thanks to more than 1400 dedicated and productive volunteers and the National Adhering Organizations, Associated Organizations, affiliates, fellows, and the Secretariat staff, IUPAC remains very strong and active in its core scientific areas of terminology, nomenclature, standards, and critical evaluation of data and new chemical subdisciplines. Within the divisions and operational standing committees, the Union has achieved a number of effective, focused collaborations with other scientific unions, national and regional chemical organizations, and industry.

The problems our global society faces—clean water and air, healthful food, sound resource management, safety and security, science education, to name a few—will require contributions from the chemical sciences in conjunction with other disciplines. It remains critically important to provide in-depth, focused research and scholarship in chemistry as part of holistic solutions for global, regional, and local problems.

The 2013 Vice President's Critical Assessment, presented to the Bureau at its meeting in April, explores some basic questions to evaluate IUPAC's contributions and provide a basis for the Union to continue to move forward productively:

- Is IUPAC's infrastructure adequate to enable the Union to achieve its goals?
- Are IUPAC's scientific priorities well suited to meeting the needs of the global chemical sciences for the benefit of humankind?
- What actions should IUPAC take to prepare it for an effective second century of relevant and valuable contributions to the chemical sciences?

Infrastructure

IUPAC derives its income from its National Adhering Organization subscriptions, publications, and earnings from its investment portfolio.

Income from national subscriptions has risen due both to increases in the national subscription charges and the growth in the number of National Adhering Organizations (NAOs). We are grateful to all our NAOs for their support.

IUPAC's publications are well respected. *Chemistry International* is admired for its content and presentation, and *Pure and Applied Chemistry* has a high impact factor. However, income from IUPAC's periodicals has been declining for several years. With the guidance of the Committee on Printed and Electronic Publications (CPEP), IUPAC is now exploring options for collaborating with a publishing partner to improve circulation of its publications, reduce costs, and increase income.

IUPAC's investment portfolio is strong due to the dedication and skill of the Finance Committee. Since the recent economic downturn, income from the investment portfolio has declined. In the short term, it may become necessary to modify IUPAC's operating budget to reflect current income until improvements can be realized. A task group should be formed with the goal of raising funds to help grow IUPAC's resource base.

The IUPAC Secretariat has traditionally been a great strength for the union, accomplishing an enormous amount of work despite its small size. However, recent high turnover among leadership and the divisions and standing committees has led to a loss of institutional memory. Staff and volunteers should take advantage of their contacts among prior officers and members whenever questions arise to assure the smooth operation of the Union.

The individual volunteers of IUPAC, scientists from all over the world that contribute to IUPAC projects, committees, and governance, are the lifeblood of the Union. In order for IUPAC to recruit the best scientists for its projects and programs, it must make it as easy as possible for the best scientists to become involved. The affiliate membership program can be an effective way to recruit new volunteers. IUPAC would be grateful for efforts by the National Adhering Organizations and scientific societies to encourage their members to become affiliates and to ensure that information on the benefits of affiliate membership is readily available.

Scientific Priorities

The projects in Divisions I–V are primarily focused on the traditional core activities of IUPAC (physical and biophysical, inorganic, organic and biomolecular, polymer, and analytical). Additionally, as would be expected, the projects in Division VIII concentrate on terminology, nomenclature, and references and standards. The operational standing committees (edu-

cation, industry, ChemRAWN or world needs) and Divisions VI and VII (environment and human health) focus largely on multidisciplinary projects in addition to core activities. These projects are more likely to span divisions, and they cover capacity building, issues of global need, teaching and training, and outreach to the public. Many of the divisions and standing committees have projects that incorporate scientists and engineers from other disciplines, reflecting their recognition of the evolving multidisciplinary nature of science and the responsibility of scientists to the scientific community as a whole and to the public welfare.

IUPAC is sponsoring about 30 conferences and workshops in 2013. This healthy and continuing program is a vital activity for the Union, and it is one of its major public faces to the chemistry community.

The International Year of Chemistry in 2011 is an outstanding example of the major influence IUPAC can have in the international community. The IYC generated worldwide interest and activity in chemistry and related sciences. New opportunities are arising that can provide mechanisms for IUPAC to carry forward the legacy of the IYC and to collaborate on multidisciplinary programs highlighting the value of chemistry to broader audiences.

A Strategic Review

The current activities in IUPAC include projects that address the traditional IUPAC goals along with activities targeting interdisciplinary collaborations, capacity building in the developing world, and provision of scientific data to assist in developing public policy.

Many potential new areas of active research in chemistry have emerged where such interdisciplinary collaborations are prerequisites for success. The challenge for IUPAC in the future will be to determine how, why, and when to incorporate new science into its activities.

IUPAC should define its unique role and value within the chemical enterprise so that its contributions are focused on areas where no other chemical society or organization can contribute meaningfully. A review of our strategy, building from the current statutory objectives of the Union and the current long-range goals, can serve this purpose and allow for clear and consistent communication of IUPAC's contributions and value to the broader chemistry community, other unions, and the public. A vision across the Union should be agreed upon that will help generate new projects in new areas and focus on issues of strategic importance to IUPAC. As we approach the centennial of IUPAC, now is a good time to review IUPAC strategy to assure that it continues to focus on relevant science.

The strategic review will concentrate on topics such as the following:

- How should IUPAC balance its emphasis on traditional areas in chemistry with new and emerging science?
- How should IUPAC distinguish itself from and cooperate with national and regional chemical societies?
- How can we make IUPAC's science knowledge usable to benefit the greater society, particularly the developing world?

Information will be gathered from sources throughout IUPAC, the academic and industrial chemistry enterprise, and other scientific communities. Each group will assess, from their point of view, the strengths, weaknesses, opportunities, and threats (known as SWOT analysis) that IUPAC faces. A framework for their assessment will include these questions:

- How can IUPAC be characterized today?
- What is their vision of a successful IUPAC in 2019 and beyond?
- How can IUPAC reach that goal?

The IUPAC Bureau, Executive Committee, and officers will be kept informed throughout the process and will be consulted frequently for their advice and comments. The strategy, to be developed over the next two years, will state the vision, mission, and overall goals of the Union, with recommended actions over the next three to six years.

The challenges for IUPAC are to strengthen its resources and to continue to identify how best to serve its constituencies, including chemists, national and regional organizations, the developing world, and the public at large. IUPAC should continue to evaluate its unique role within the chemical enterprise to facilitate the in-depth science that global chemistry needs in order to function, while at the same time organizing and providing scientific knowledge for the betterment of humankind.

It is indeed an honor and a privilege to serve IUPAC, and I look forward to working with all IUPAC members and volunteers to achieve these goals.

Mark Cesa <mark.cesa@ineos.com> has been vice president of IUPAC since January 2012. Previously in IUPAC he served on the Committee on Chemistry and Industry as secretary (2000–2003), vice chair (2004–2005), and chair (2006–2009). Cesa is a process chemistry consultant with INEOS Nitriles in Naperville, Illinois, USA.

IUPAC, OPCW, and the Chemical Weapons Convention

by Leiv K. Sydnes

IUPAC's ultimate goal is to serve humankind through chemistry. This is done in a number of ways that are not apparent to most people outside the Union. An important and visible service is the work done by IUPAC for the Organisation for the Prohibition of Chemical Weapons (OPCW).

The first formal contact between IUPAC and OPCW dates back to 2001. As part of OPCW's preparation for the First Review Conference of the Chemical Weapons Convention (CWC),[1] IUPAC received an invitation to produce a report evaluating the scientific and technological advances that had taken place in the chemical sciences since the convention entered into force in 1993. The reason for this request was that the Convention requires a review of the CWC every five years in recognition of the evolutionary nature of the agreement.

Within the treaty, there is an instrument that makes it possible to adjust and modify the Convention as deemed necessary, and the objective of the Review Conferences is to look into just that and recommend changes on the basis of a review of the implementation of the CWC and evaluation of relevant scientific and technological developments. Such advances may relate to the scope of the prohibitions set out in the CWC, they may affect the way the Convention is being implemented, or they may create opportunities for advancing international cooperation among States Parties[2] in areas such as protection against chemical weapons and the productive application of chemistry. Dialog between the OPCW and the scientific community in evaluating scientific and technological progress also creates opportunities to advance awareness of the CWC and its requirements in the scientific, technological, and industrial communities where the need for more knowledge about the Convention is apparent.

The decision to include IUPAC as a partner in the preparation of the conference was indeed a natural consequence of the fact that IUPAC was (and still is) the only independent, nongovernmental, international organization devoted to chemistry and the chemical sciences and their application in research, industry, and society. After a meeting between the OPCW leadership and an IUPAC delegation chaired by the then President Alan Hayes at the OPCW headquarters in The Hague, The Netherlands, there was no doubt that IUPAC should accept the offer with appreciation and start to do the work.

After thorough discussions, it was decided first to hold an international workshop with participants from all parts of the world and prepare a draft report, and then appoint a small team of authors to finalize the document. Following this plan, an international group of some 75 specialists from around 35 countries, covering the relevant fields of the chemical sciences, accepted the invitation to become involved in the work. During a workshop held in Bergen, Norway, in July 2002, the main parts of the report were drafted, and through subsequent electronic communication, the report was finalized. The document was widely distributed within OPCW, published in *Pure and Applied Chemistry* (*PAC*) as a technical report,[3] and finally presented at the Open Forum during the First Review Conference in May of 2003.[4]

Five years later, in April 2007, the process was repeated. This time Zagreb, Croatia, was the workshop venue. The meeting was organized and run following the same format as in Bergen since it had proved to work well. Participants came from all parts of the world, and like the first time, the final report was published in *PAC*.[5]

In 2011, the same process was repeated again, and IUPAC was asked to take the lead in the preparation of the report on chemistry and chemical technology required for the Third Review Conference scheduled for April 2013. Once more, IUPAC accepted the invitation with pleasure.

The 2012 Spiez Meeting

This time, the international workshop, run again using the same format as in Bergen, was held in February 2012 in Spiez, Switzerland, in the facilities of Spiez Laboratory, a Swiss defense establishment dealing with protection from nuclear, biological, and chemical threats. IUPAC assembled an international advisory committee and a program committee for the meeting; the latter consulted with the OPCW Technical Secretariat but had been given primary responsibility for the organization of the workshop. The workshop

consisted of eight topical plenary sessions, which focused on the following specific topics:

- Overview and Background
- Convergence of Chemistry and Biology
- New Synthesis and Toxicological Analysis Methods
- Developing New Materials and Delivery Mechanisms
- Advances in Industrial Production Methods
- Chemical Safety and Security: Possession, Transfer, and Acquisition
- Defense against Chemical Weapons Agents
- Chemical Safety and Security: Engaging the Chemical Community

In addition, there was one session dealing with technical discussions about new developments in technology and anticipated technological challenges.

In each plenary session, two or three speakers discussed the state of the art, presented current challenges, and predicted future developments within a given field or topic related to a category of advancement in the chemical sciences and chemical technology. After the presentations, there was time set aside for comments, discussions, and elaborations. Breakout sessions provided opportunities to further consider the information presented, and a facilitated, concluding discussion made it possible to look at issues in a larger perspective and draw conclusions based on extrapolations of trends and developments in recent years.

Conclusions were reached on a number of specific issues of importance in a chemical-weapons context, which was a significant development. However, just as important for the future standing and regulatory strength of the CWC is the assessment of how current trends in a number of scientific and technological disciplines are believed to have impact on the CWC. A report was published in *PAC*[6] in April 2013, just in advance of the Third Review Conference.* An understanding of the present situation is, therefore, important to "guesstimate" what the future holds; the following pages outline current trends and observations.

* Concurrent with the *PAC* article, Sydnes' commentary "Update the Chemical Weapons Convention," was published 4 April 2013 in *Nature* 496, 25–26; http://dx.doi.org/10.1038/496025a.

Pace and Nature of Advances

A major factor to consider is the pace of changes and advances in science and technology, which has quickened in recent years. In particular, a number of innovations in the medical and biological sciences, such as inexpensive and rapid DNA sequencing and synthesis, are driving advances forward very rapidly. Many of these innovations are chemistry based, and this is helping to expand chemistry to scientific disciplines where the knowledge of chemistry is limited and the consequences of dual use of chemicals is not acknowledged. In the long run, this might become an issue.

It is clear that the developments in the fields of science and technology continue to be evolutionary for the CWC rather than being disruptive with game-changing consequences. In the 10 years since the first workshop, such developments have not had a dramatic impact on how chemical weapons can be produced and used. It was noted that any application of new technologies to the production of traditional chemical weapons would depend on consideration of many factors, the outcome of which would depend on the country concerned. Many of the technologies discussed at the workshop may not yet be available to all developing countries or to all potential proliferators. The availability of crude chemical mixtures, containing chemicals that are highly toxic, remains a concern.

It was also acknowledged that advances in science and technology have numerous positive uses and are likely to be much more beneficial than harmful. The CWC seeks to strike an appropriate balance between preventing the use of toxic chemicals as weapons while not impeding the application of science and technology for beneficial purposes; achieving this balance will continue to be important in the future. As the pace of technological advances continues, the OPCW's role in providing developing countries with opportunities to receive equipment and training will continue to be important.

Continued Progress in Science and Technology

Science and technology continue to progress steadily in most areas of relevance to the CWC. Synthesis and production of chemicals may be improved through the use of flow microreactors, which provide safety

advantages for certain types of (exothermic) reactions or for reactions that involve toxic chemicals and by-products. However, significant research is required to optimize chemical processes in microreactor systems, and although the use of microreactors has become more and more widespread in recent years, dramatic advances have not been observed. It therefore remains unclear whether use of microreactors will have significant implications for the production of chemical weapons on a large scale.

Chemicals may also be produced through bio-mediated processes, an area that highlights increasing convergence between chemistry and other scientific disciplines, including biology. Developments in synthetic biology are also relevant to this trend. Toxins and bioregulatory molecules exemplify chemicals that are prohibited by both the Biological Weapons Convention[7] and Chemical Weapons Convention. As a result, the communities associated with both Conventions will need to continue considering how best to monitor relevant developments and address potential implications.

Boutros Boutros-Ghali, Secretary-General of the United Nations, at the presiding table of the United Nations Educational, Scientific and Cultural Organization (UNESCO) Headquarters in Paris, for the signing of Chemical Weapons Treaty. (1993)

Delivery technology in medicine is another field in which steady advances have occurred, driven largely by the development of improved medicines or chemotherapeutic agents. These advances include encapsulation in nano- or micro-scale carriers, improved targeting and uptake in biological tissues, and improved ability to deliver large molecular-weight molecules across biological barriers. The same techniques can potentially be employed for more effective delivery of toxic chemicals, although it was also emphasized during the workshop discussions that there is no evidence of this having taken place so far.

Analytical tools and opportunities exist to increase the technical convenience and applicability as part of the development of next generation analysis and detection systems. In particular, systems that are simple and robust to use and that combine multiple types of analysis would be extremely useful. Although such devices are not currently available, and the detection of toxins remains less reliable, participants suggested that it is only a matter of time before the technology meets necessary portability, robustness, and selectivity requirements. Miniaturization is also a key focus for future developments in field detection.

In the area of countermeasures, several continuing gaps were noted in the capacity to respond to incidents involving chemical weapons. Further research on absorbents for decontamination purposes will likely be needed, and strategies such as regional support systems to help provide capacity for the effective medical treatment of chemical weapon victims may be useful.

The ethical, legal, and operational concerns surrounding riot-control agents and incapacitating chemical agents[8] will also continue to be a topic considered by the OPCW. It remains a matter of consideration whether policy solutions such as new chemical schedules in the CWC or the creation of international norms surrounding the use of these types of chemicals will be needed in the context of the CWC.

Changing Context of the CWC

The gradually changing context of the CWC cannot be ignored. States Parties have traditionally been concerned with chemical weapons on a massive scale, and the Chemical Schedules[1c] and inspection regimes mainly focus on certain types and larger quantities of chemicals. However, it is quite conceivable that changes in production technology may make other types of chemicals and facilities more relevant in the not-too-distant future. Furthermore, scenarios involving the production of chemical weapons on a small scale by activists and terrorists are definitely different from those associated with large state-sponsored programs. These differences extend beyond the chemical agents and delivery systems and encompass signifi-

cantly different requirements when it comes to effective detection and monitoring.

A central aspect in this context is knowledge of synthetic chemistry and easy access to such competence. For example, scientific literature can now be accessed much more easily using search engines and readily available information technology. As advances continue to be made, a trend toward the democratization of science and technology is likely, and may have implications for the ongoing monitoring of relevant scientific progress and potential implications. There is also the fundamental issue of serendipity in scientific advances to keep in mind. As a result, it will continue to be important to consider how such events can be dealt with at the technological and institutional level.

Education, Outreach, and Partnerships

Finally, the 2012 Spiez workshop discussions emphasized the roles that may be played by many communities in promoting chemical safety and security. Education, outreach, and awareness-raising will be vital all over the world, and issues related to chemical weapons may be effectively embedded within a broader context of risk and messages about the responsible acquisition, use, and disposal of chemicals. It is therefore wise to promote, preach, and teach chemical safety and security in conjunction with other initiatives such as Responsible Care[9] and the Green Customs initiative.[10] The value of regional approaches should not be underestimated and national authorities dealing with CW issues, civil-society organizations, and scientific groups such as IUPAC and national chemical societies will clearly have complementary roles to play.

The need for increased awareness about chemicals in relation to chemical weapons in general and CWC in particular is also necessary among practicing chemists. Unfortunately, it is a fact that in most countries these topics are not even mentioned in the regular courses given at almost all universities. A welcome and very appropriate initiative, would be to develop relevant course material to cover these topics. Since the material needed for such an undertaking has to have a global perspective, the task is demanding and calls for contributions from focused task groups with international composition. This is a modus operandi which fits the IUPAC project system perfectly, and I am quite confident that IUPAC is looking forward to becoming involved in the generation and execution of relevant projects in this and related fields.

Code of Conduct

A way to increase the awareness in the chemical community could be to have each chemist draft a Code of Conduct adopted to each working situation and experiences. Within IUPAC, the idea of developing such a document has been aired, but until a few years back, the conclusion was always that the task was too difficult to handle well. The argument was that the dual use of many chemicals made it impossible to find the short, precise wording required in such an important document. Of course, the potential misuse would have to be properly described and spelled out, but the problem is that the same chemical principles and many of the same chemicals that are involved in abuse, misuse, and misconduct, contribute to the application of chemistry in the service of humankind when applied in a proper fashion. As a result, nothing happened for a long time.

What triggered a change was an initiative of the then OPCW Director-General, Ambassador Pfirter, who in a letter to the OPCW Scientific Advisory Board noted that "OPCW needs to clearly establish what it requires in the field of education, outreach, and international cooperation [.... and these] activities would benefit from increased cooperation with other international, regional, and national organizations." This led to a joint OPCW/IUPAC workshop in Oxford, England, in July 2005 (see www.iupac.org/project/2004-048-1-020) in which a range of topics were discussed: How to increase the awareness of the CWC in the scientific community, facilitate the integration of issues related to the Convention into chemistry teaching, and promote professional conduct of chemists and chemical engineers. Fruitful sessions and lively discussions generated significant ideas; one idea that was picked up swiftly was the push for a code of conduct.[11]

The need to develop a code of conduct for chemists was not a new idea in IUPAC.

The need to develop a code of conduct for chemists was not a new idea in IUPAC. A group under the leadership of Graham S. Pearson from the UK had in fact started to discuss just that before the Oxford meeting took place, but the acknowledgement of the need was further strengthened when several chemical-weapons issues, such as the general purpose criterion and the dual use of chemicals, were taken

into consideration. From an IUPAC point of view it was important to carry out the work as an inclusive process, which meant involving the whole organization and engaging the member countries before a proposal, in due course, could be presented. Such a process was carried through by Pearson's task group, and the resulting document was sent to the IUPAC Executive Committee, which decided not to move forward toward a formal recommendation, but to document the process and the discussion in an article in *Chemistry International*.[12] When studied carefully, it is clear that the basis for a Code of Conduct for chemists is in place. Is anyone ready to join such a cause?

Final Remarks

As chemists, we are fully aware of the blessings of our science, but almost on a daily basis we are reminded through news media about the problems chemicals may cause when used without proper consideration. However, we are probably never exposed to the dark side of chemistry more clearly than when we face the consequences of the use of chemical weapons. It is argued, correctly in my opinion, that chemistry cannot be blamed for chemical warfare, but since chemical reactions work even in the hands of those without knowledge of chemistry, the chemical community has the duty to be aware of the potential danger and act to prevent all misuse and abuse of chemicals. Collectively, the chemical community is not yet well prepared to do this job, but a good start would be to reflect on the trends and potential problems outlined in this piece and then act to improve the situation.

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2. In this context a State Party is a term used for a country/state that is a member of OPCW.
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7. The Biological Weapons Convention can be downloaded from The Biological and Toxin Weapons website at www.opbw.org.
8. Incapacitating chemical agents (ICA) are chemical compounds or mixtures of chemical compounds that are able to incapacitate human beings for some time. The topic is regularly dealt with at expert meetings like the ICRC Expert Meeting in Montreux, 24–26 March 2010. The report from the conference can be downloaded from www.icrc.org/eng/assets/files/publication/ICRC-002-045.
9. Responsible Care is a global initiative that works a) to improve the health, safety and environmental (HSE) performance in the chemical industry and b) to maintain an open and transparent communication with stakeholders. The initiative was launched in 1985 by the Canadian Chemical Producers' Association. For information, see for instance www.canadianchemistry.ca/ResponsibleCareHome.aspx.
10. Green Customs is an international initiative that is working to prevent illegal trade of environmentally-sensitive commodities. For information, go to its homepage at www.greencustoms.org.
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IUPAC project 2005-029-1-050 delivered a reliable, online resource to raise awareness about the Multiple Uses of Chemicals and the Chemical Weapons Convention—free online @ www.iupac.org/multiple-uses-of-chemicals

Green Chemistry in Japan

by Takashi Ushikubo

In Japan, Green and Sustainable Chemistry (GSC) is defined as innovations and advances in chemical technologies that can improve human and environmental health. The Green Chemistry Initiative, which was formed in September 1998 and comprised companies, universities, and the government, was intended to encourage technologies that could be used in sustainable development. Out of this initiative, the Green and Sustainable Chemistry Network (GSCN) was born in March 2000.

Although we did not have the term "GSC" in the 1960s, the research and development that form the foundation of industrial ecology were already taking place. For example, it was during this decade that mercury cell electrolysis was replaced by the ion exchange membrane method for the production of sodium hydroxide. The introduction of this environmentally benign process had been promoted by the Association for the Progress of New Chemistry, which was the forerunner to the Japan Association for Chemical Innovation (JACI). The GSCN, which is managed by JACI, is the center of a network that actively promotes collaboration in research and development through information exchange, communication, education, and international activities.

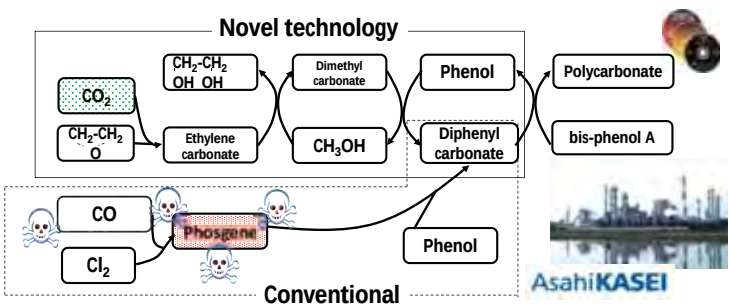
This article surveys recent progress in GSC technologies in Japan and the expectations for future innovation. In addition, it discusses the potential contribution of GSC toward reviving cities, towns, and the industries damaged by the Great East Japan Earthquake.

One of the activities of GSCN is the GSC Awards, started in 2001. GSC Awards are granted to individuals, groups, or companies that have greatly promoted GSC through their research, development, or commercialization.[1] These awards are given by Japan's Minister of Economy, Trade, and Industry; Minister of the Environment; or Minister of Education, Sports, Culture, Science, and Technology, depending on the particular achievement. By reviewing the winners of the GSC Awards, one gets a clear picture of the environmentally benign processes that have been commercialized in Japan in the past decade.

Novel Non-Phosgene Polycarbonate Production Process Using Byproduct CO_2 as Starting Material[2]

Polycarbonate is one of the most important and versatile engineering plastics. With superior transparency, impact resistance, and heat resistance, it is used in optical discs, home electronics, automobile parts, office equipment, and so on. About four million tons of polycarbonate is produced annually worldwide, with production expected to grow in future years. Almost all polycarbonate was manufactured through a process in which CO and chlorine are combined to form phosgene, a highly toxic gas, as an intermediate material. The phosgene process has a number of disadvantages, including the risk of environmental harm. Many attempts have been made to overcome the inherent risks in the phosgene process, but with little success until recently.

Asahi Kasei Corporation succeeded in commercializing the first non-phosgene polycarbonate production process in the world. The figure below compares this new method with the conventional phosgene process. This technology uses ethylene oxide and CO_2, that is the by-product of ethylene oxide synthesis. Ethylene carbonate is synthesized by the reaction between ethylene oxide and CO_2, and ethylene carbonate is converted to diphenyl carbonate via dimethyl carbonate. Furthermore, diphenyl carbonate reacts with bisphenol-A to produce high-quality polycarbonate. Also, high-purity monoethylene glycol is co-produced.



Novel non-phosgene polycarbonate production process using by-product CO_2 as a starting material.

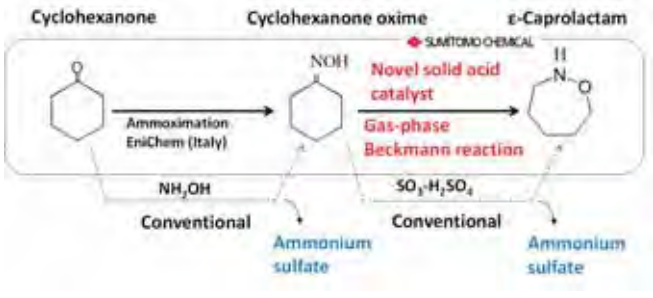
This technology successfully incorporated CO_2, which has a low chemical activity, into the polycarbonate main chain. In addition, this new process does not use methylene chloride as a solvent. This novel technology totally eliminates the problems of the phosgene process, while maintaining high production yields and conserving resources and energy. The new process reduces CO_2 emissions by 0.173kg per one kg of product polycarbonate.

Novel ε-caprolactam Production without Ammonium Sulfate Formation[3]

ε-Caprolactam is an important intermediate used in the production of Nylon 6 fibers and resins, the

worldwide production of which is estimated at about 3.8 million tons annually. Nylon 6 fibers and resins are used in a wide range of applications including clothes, automobiles, electric or electronic devices, as well as lapping films for foods. Almost all ε-caprolactam is produced through the Beckmann rearrangement of cyclohexanone oxime, and a large amounts of ammonium sulfate is co-produced, at least 1.6 times of caprolactam by weight, because highly concentrated sulfuric acid is used for the reaction promoter and the neutralization by ammonia is necessary in the process.

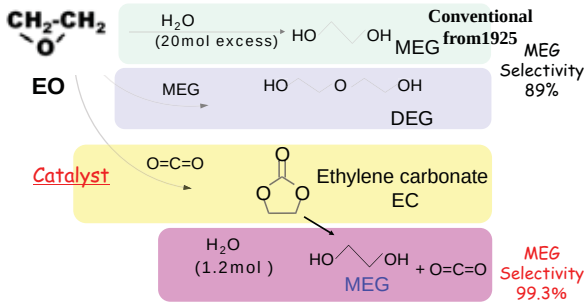
Sumitomo Chemical Company succeeded in commercializing the novel catalytic Beckmann rearrangement reaction proceeded under vapor phase conditions without ammonium sulfate co-formation. This process is conducted with a high-silica MFI zeolite catalyst instead of sulfuric acid. And an effective purification technology was developed to obtain a high-purity product with a reduction in the consumption of resources and energy. In order to carry out the production of ε-caprolactam without any ammonium sulfate production, Sumitomo Chemical commercialized a combined process in 2003, which involves an initial ammoximation step for obtaining cyclohexanone oxime, developed by EniChem (Italy), and a secondary step involving a vapor phase Beckmann rearrangement (see figure below).



Novel ε-caprolactam production without ammonium sulfate formation

Highly Selective Process for Mono-Ethylene Glycol Production from Ethylene Oxide[4]

Mono-ethylene glycol (MEG; $HOCH_2CH_2OH$) is used as an antifreeze and as a raw material for the production of polyester fibers and resins, mainly PET. A new process was developed by Mitsubishi Chemical Corporation for the production of mono-ethylene glycol to meet its growing demand in the world. While the MEG selectivity of the conventional non-catalyzed process is around 89 percent under typical conditions, the new process exceeds 99 percent. The key



Ethylene glycol synthesis process using novel homogeneous catalyst.

to the high selectivity is the two-step synthesis via ethylene carbonate, as in the figure above. The first step reaction is catalyzed by phosphonium salts and generates ethylene carbonate as an intermediate. This is followed by hydrolysis of ethylene carbonate in the second step. The hydrolysis is carried out under almost stoichiometric condition, although the conventional non-catalyzed hydrolysis is accomplished by the higher H_2O/ethylene oxide molar ratio. Several commercial plants utilizing the new process are already in operation throughout the world. This greener technology saves resources and the energy and reduces the amount of wastewater and CO_2 production.

In the early stages of Green and Sustainable Chemistry promotion in Japan, the GSCN focused on developing safer industrial technology, decreasing the environmental burden of industrial production (i.e., carbon dioxide, waste, and harmful byproducts), and on establishing a new philosophy and methodology for chemical research. Guidance from the Organization for Economic Cooperation and Development was helpful to Japan as it sought to improve the safety of chemicals and decrease pollution. A number of laws have been passed to reduce pollution and to promote recycling.

Expectations for Innovation in GSC Technology

Current GSC technologies contribute to sustainability, not only by decreasing the environmental impact of industrial processes, but also by increasing the prosperity of society. In order to expand GSC, the Ministry of Economy, Trade and Industry released the Technology Strategy Map on GSC in 2007. The 2010 issue of the map gave an overview of 153 GSC technologies that were related to the sustainability of energy, environment, natural resources, and a prosperous society. The Ministry is strongly promoting national research projects having to do with Green Innovation and Life Innovation.

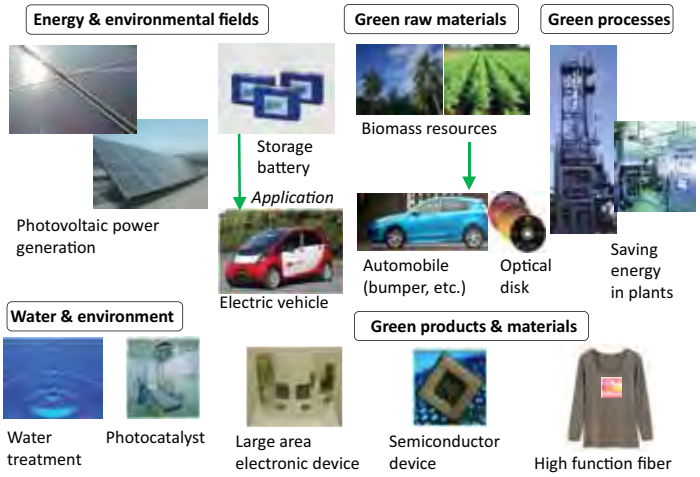
Universities and national laboratories have been collaborating with companies to develop fundamental science and technologies, such as catalysts, supercritical fluids, analysis, and computer chemistry. Also, the chemical industry has developed innovative sustainable materials for products such as photovoltaic power generation, hybrid/electric vehicles, water treatment, and high-function fiber, that accelerate the challenges in energy, the environment, and healthcare. In modern cars, for instance, innovative polymer materials reduce the weight and thereby increase the cars' energy efficiency.

The Great East Japan Earthquake of 11 March 2011 devastated certain areas of the country, especially the Tohoku district, and resulted in numerous long-term problems such as a diminished energy supply, extensive cleanup of land and water polluted by radioactive materials, and the need to rebuild industries and increase employment. Green and sustainable chemistry is expected to play an important role in the recovery effort. JACI has started the New Chemical Technology Research Encouragement Award, including an Award for Earthquake Disaster Recovery, to support the activities of young researchers engaged in researching new chemistry. In 2011, the following three researchers won the award for their unique ideas:

- Yoshitaka Takagai: Development of Speedy Radioactive Strontium Analysis Aystem and Its Application to Soil Monitoring Concerning Tokyo Electric Power Co.,Inc, Fukushima Daiichi Nuclear Power Plant Accident
- Shunsuke Kurosawa: Development of a Novel Scintillator for Radiation Monitor in the River
- Masami Hatayama: Phytoremediation of Heavy Metals and Metalloids Derived from Tsunami Sediments

In order to promote GSC for the future, JACI has been educating the public, especially younger students, about the broader benefits of chemistry for the planet and for society. JACI published the introductory textbook *Chemistry and Environment: An Introduction to Green Chemistry* for college and high school students. The first edition was published in April 2002 and has been used as a textbook at several colleges.

In addition, some aspects of GSC can be taught through micro-scale chemistry experiments, which are themselves environmentally benign. Kazuko Ogino of Tohoku University has been developing, promoting, and disseminating micro-scale chemistry experiments for some time. Ogino won the Foundation of Asian Chemical Society Distinguished Contribution to Chemical Education Award in 2011 and the GSC Award in 2007. Chemical companies and JACI are supporting such activities in Japan by helping the public to understand the features and benefits of micro-scale chemistry experiments.



The contribution of chemical technologies toward a sustainable society.

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International Training in Pesticide Ecological Risk Assessment

by Ronald Parker

Worldwide demand for food is growing due not only to increasing population, but also because higher percentages of the population in several large economies (e.g. BRICKS* and other rapidly growing countries) now have incomes that allow them to move beyond subsistence foods and demand fruits, vegetables and meats that were not possible in the recent past. As a result, the extent of land devoted to export-driven agriculture is also growing.

One side-effect of increasing agricultural production is a need for increased use of crop protection chemicals and with this, an awareness of the need to evaluate the impact of additional pesticide use. This need includes not only meeting maximum pesticide residue limits (MRLs) in export food commodities, but also protecting the natural environment in these newly agriculturalized regions.

Figure 1: Crops grown in subsistence agricultural systems are largely consumed locally.

The *eValuate* pesticide ecological risk assessment training materials respond to this need by providing a streamlined collection of methods, modeling tools, process descriptions, and terminology that can be used to evaluate the potential ecological risk of pesticide usage in an agricultural environment. This online module provides instruction in the risk assessment process and describes the process of evaluating pesticide environmental fate and transport information combined with laboratory toxicity data to provide an indication of potential ecological risk. The *eValuate* module is a medium to help risk assessors learn how to conduct and use the process of ecological risk assessment to help manage hazards and risks of pesticide use. It also includes valuable information, training materials, reference sources, and instructions on safe use and disposal of pesticides.

Background

All countries require pesticidal products, not only to sustain public health and well being, but also to protect crops from damage inflicted by insects and fungi and competition from weeds. Maintaining safe use of pesticides, however, necessitates that governments have a procedure to evaluate and approve (or disapprove) the pesticides that are used within their borders. Land-extensive agricultural systems present a different level of risk than subsistence agriculture in which most food is grown and consumed locally.

Newly developing countries experience a unique set of difficulties in performing risk assessments for pesticide registration. These difficulties often include: (1) too few experienced, professional staff, (2) high rates of personnel turnover and frequent need to train new staff, (3) inadequate laboratory facilities, (4) limited data on local species that most require official protection, (5) limited access to the chemical-specific environmental fate and toxicity data that are required to evaluate risk, and (6) lack of the data on local soils, water resources, and climatic zones that are needed to describe the areas that require protection. These difficulties have impeded all but a limited number of countries from regularly carrying out the detailed assessments that are needed to manage the risk of pesticide usage. Figure 1 and 2 depict the scale of the change that is occurring.

Recognizing these difficulties, the Organization for Economic Cooperation and Development (OECD), Working Group on Pesticides (WGP) initiated an International Pesticide Assessment Consultation held in Washington, D.C., in October 1998. Hosted jointly by

the U.S. Environmental Protection Agency's Office of Pesticide Programs (OPP) and the National Chemicals Inspectorate of Sweden, the consultation had several objectives.

1. To develop recommendations for how countries can work together better to share the work of pesticide risk assessments and, in doing so, consider how national or regional pesticide data review reports can be used most effectively.
2. To review the roles of national governments, intergovernmental organizations and non- governmental organizations in international cooperation on pesticide risk assessments and standard setting.
3. To discuss the most effective means of disseminating pesticide assessment information to countries, considering existing methods and availability of resources.

The WGP consultation also made recommendations that were relevant to deciding what to include in the *eValuate* module:

1. establish a list of websites containing useful information on pesticides, and distribute it widely
2. include a brief description of the most useful websites, along with some indication of the quality and currency of the information
3. encourage countries without access to the Internet to gain access by seeking assistance from developed countries
4. develop and disseminate a list of terminology definitions
5. look for opportunities to build regional networks, for information sharing or for developing coordinated regulatory systems
6. encourage national governments to coordinate pesticide reevaluations schedules to allow for timely work sharing
7. promote the idea of holding regional workshops on a regular basis in order to promote harmonization and to assist countries with less-developed pesticide risk management processes

In responding to the WGP proposal and to requests from developing countries, especially in Latin America, for assistance in ecological risk assessment of pesticides, the OPP provided funding for completion of a comprehensive risk assessment and training module based in large part on the methods used by OPP. The OPP module project was initiated in 2002 and developed through a contract with the Oak Ridge National Laboratory (ORNL) in Oak Ridge, Tennessee, in cooperation with OPP. Development of the the first draft versions of the *eValuate* module in English and in Spanish were completed by ORNL. The final version of *eValuate* went through final quality assurance/quality control review by the OPP Environmental Fate and Effects Division. The final versions include the extensive glossary, list of definitions, and process descriptions developed by IUPAC in both English and Spanish (see IUPAC project 2004-002-1-600; *PAC* 2006, Vol. 78, No. 11, pp. 2075-2154; http://dx.doi.org/10.1351/pac200678112075).

Figure 2: Much of the agricultural production in land-extensive agriculture enters into international trade.

Newly developing countries experience a unique set of difficulties in performing risk assessments for pesticide registration.

Other cooperators in this project have included the IUPAC Division VI –Chemistry and the Environment Division- Subcommittee on Crop Protection Chemistry, the Food and Agriculture Organization (FAO) Plant Production and Protection Division, the FAO/International Atomic Energy Agency Joint Division for Agriculture, and the OPP Field and External Affairs Division and Environmental Fate and Effects Division (see IUPAC projects 2004-011-1-600 and 2008-011-2-600).

The first drafts of this module recommended use of a relative (comparative) risk assessment paradigm

primarily for the advantages it would offer in aquatic exposure assessment. This paradigm offers the advantage that the results of the assessment are independent of the physical configuration assumptions for the assessment scenario (i.e., land to water ratios chosen, soil and weather selected, and timing of pesticide used in relation to important weather events). The relative risk methodology was eventually dropped due to difficulties in integrating the comparative risk results with those of other national and multinational assessment schemes.

Module Description

The module is designed to provide a step-by-step process for conducting an evaluation of ecological risks of pesticide use. The module includes guidance through the risk assessment/risk management process, OECD-compatible data handling, a glossary of pesticide terms and process descriptions, and links to exposure assessment computer models with use instructions, lists of international pesticide websites, and pesticide targeted risk management options. *eValuate* also provides access to a number of readily-available, easy-to-use assessment simulation tools for carrying out aquatic and terrestrial pesticide ecological exposure/risk assessments. These methodologies and tools can assist countries in making science-based decisions regarding the use and management of pesticides.

Module Field Testing

A workshop for field testing of EPA's Risk Assessment and Training Module was held at the headquarters of the Central American Commission for Environment and Development in San Salvador, El Salvador, 15–16 November 2004. The meeting was hosted and sponsored by the Commission and the U.S. Agency for International Development and was attended by 18 representatives of ministries of environment, agriculture, and health involved in the evaluation and registration of pesticides in Central America. Participants in the session represented the governments of El Salvador, Guatemala, Nicaragua, Costa Rica, Belize, Panama, and Honduras. A progress report on development of the module was made at the International Workshop on Crop Protection Chemistry in Latin America—Harmonized Approaches to Environmental Assessment and Regulation, held in San Jose, Costa Rica, in February 2005 (see July 2005 *CI*, www.iupac.org/publications/ci/2005/2704/cc1_140205.html).

Sections of the Module

The training module and tools are organized into the following seven sections:

Section 1: Introduction to Pesticide Ecological Risk Assessment

Section 2: Components of Pesticide Ecological Risk Assessment

Section 3: Pesticide Ecological Risk Assessment Models and Databases

Section 4: Ecological Risk Estimation and Characterization

Section 5: Pesticide Risk Management/Regulatory Activities

Section 6: Training Materials, Presentations, Example Training Class Schedule, Example Pesticide

Section 7: International Websites, Useful Historical References, Glossaries, Common Acronyms, and Units

Together, these seven sections of the module provide descriptions of methods, processes, procedures, and tools that can be used to carry out both aquatic (fish, amphibians, etc.) and terrestrial (birds, mammals, reptiles, etc.) ecological risk assessments. Methods and tools are designed to be, as much as possible, the same as, or compatible with those used in the USA and Canada.

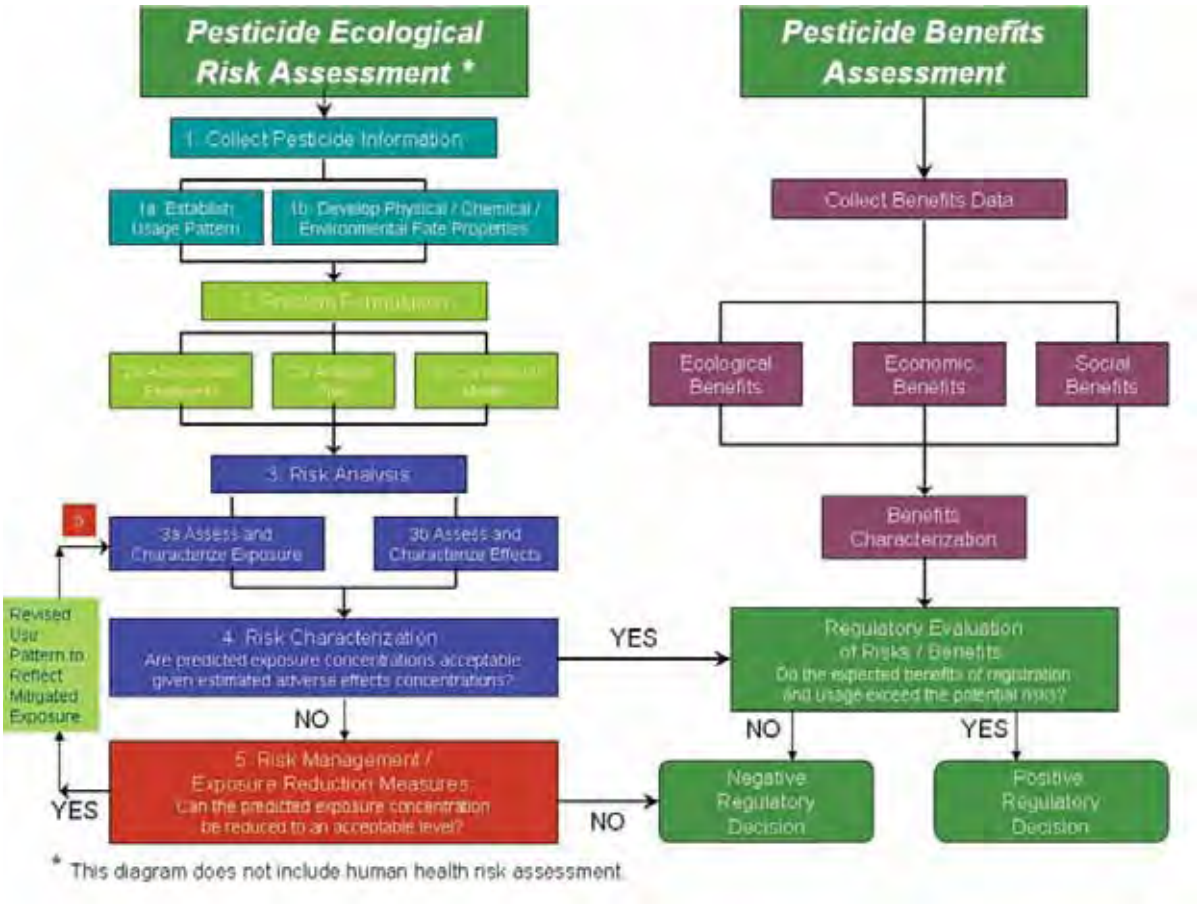

Figure 3. Overall Pesticide Evaluation Paradigm Used in eValuate.[1]

Overall Pesticide Evaluation Paradigm Used in *eValuate*

Figure 3, above, is a visual representation of the methodology used in *eValuate*. The diagram depicts the process of balancing potential risks with the estimated benefits derived from usage of a specific pesticide. The benefits section is included to provide a complete picture of the assessment process followed by the U.S. EPA. The *eValuate* module does not describe the process of evaluating benefits or of evaluating risk to human health.

Characterizing Ecological Risk

Ecological risk is characterized in the natural field context within which the pesticide is used. Figure 4 on page 16 is a presentation of the context of a pesticide risk assessment. Characterizing the ecological risk is a process of comparing an estimated ecological concentration with a laboratory toxicity concentration. If the exposure concentration exceeds the concentration shown in the laboratory to be toxic, some level of risk may be assumed. See figure 5 on page 17.

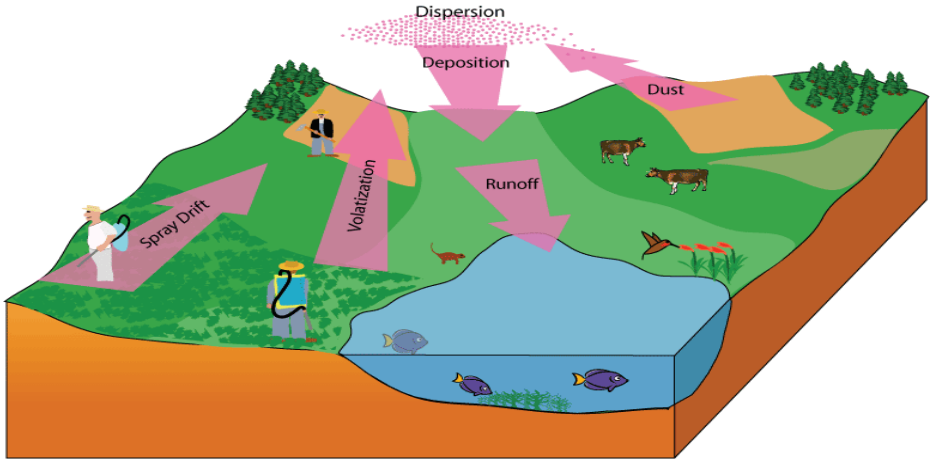

Figure 4. Physical diagram of ecological exposure assessment.

Ecological Exposure Assessment

Ecological exposure is estimated independently for aquatic animals and plants and for terrestrial animals and plants. Concentration values for each of these categories are estimated through a combination of field data collection and computer-simulation modeling. The two approaches used together have a synergy in which each compliments the other. With concentrations of more than 400 pesticides changing day-to-day and year-to-year, the cost of monitoring by itself is prohibitive. Computer simulation on the other hand, while it permits estimation of daily concentration values at many selected sites quickly and easily, has little value if the concentration values are not grounded in a known field reality. Monitored values, if collected with sufficient frequency and with contextual data, can be used to provide data points in time and in space that can be used directly in risk assessments, and possibly more important, may be used to develop, validate, and calibrate simulation models. Simulation models can be used to interpolate between and extrapolate beyond measured data points both in space and in time. Each method feeds the other in a way that enhances predictive ability far beyond the capacity of either one by itself.

Aquatic Ecological Exposure/Risk Assessment

Both Canada and the USA use the linked Pesticide Root Zone Model (PRZM) and Exposure Analysis Modeling System (EXAMS) developed by the EPA's Office of Research and Development. OPP is currently completing final quality control on a user-friendly method to perform PRZM/EXAMS assessments. This technology has the potential to enable regulators in developing countries to conduct complex aquatic pesticide assessments.

The PRZM model requires data on local crops, soils, topography, and weather. Collecting this data is labor intensive. Such data is typically available from national governments and through international organizations (FAO, UNEP, etc.). Data may be organized through work already completed on ecological regions.

Terrestrial Animal Ecological Exposure/Risk Assessment

Terrestrial wildlife exposure estimates conducted by the EPA/OPP are calculated for birds and mammals, emphasizing a dietary exposure route for uptake of pesticide active ingredients. These exposures are considered as surrogates for terrestrial-phase amphibians as well as reptiles. For exposure to terrestrial organisms, risk assessors primarily look at the residues of pesticides on food items and assume that organisms are exposed to a single pesticide residue in a given exposure scenario. Two approaches are used for estimating exposure to terrestrial wildlife, which are dependent on the application method: (1) spray applications and (2) granular, bait, and treated-seed applications. It should be noted that, although the screening-level, terrestrial-wildlife risk assessment focuses, in large part, on dietary exposure, risk assessors do consider the relative importance of other routes of exposure in situations where data indicate that pesticide exposures through routes other than dietary may be potentially significant contributors to wildlife risk.

Figure 5. Comparison of pesticide exposure to pesticide toxicity as a means of characterizing potential risk.[2]

For spray applications, estimation of pesticide concentrations in wildlife food items focuses on quantifying possible dietary ingestion of residues on vegetative matter and insects. The residue estimates are based on a nomogram that relates food-item residues to pesticide application rate. The nomogram is based on an EPA database called UTAB (Uptake, Translocation, Accumulation, and Biotransformation), a compilation of actual measured pesticide residue values on plants (see references 3 and 4).

www.iupac.org/project/2008-011-2-600

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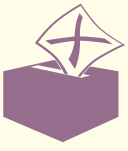
Election of IUPAC Officers and Bureau Members

According to IUPAC statutes, Council must elect officers of the Union and elected members of the Bureau. Nominations for the various positions that fall vacant at the end of 2013 had to be received by the Secretary General at the IUPAC Secretariat before 13 June 2013 (i.e., two months before the start of the Council meeting).

On 1 January 2014, Mark Cesa (USA), vice president and president elect, will become president. The vice president to be elected will be president elect on 1 January 2014 and will become president on 1 January 2016. Kazuyuki Tatsumi (Japan), current president, will become past president and remain an officer and a member of the Bureau for a period of two years. Meanwhile, Nicole Moreau (France), current past president, will retire while Secretary General René Deplanque (Germany) and Treasurer John Corish (Ireland) who were elected to four-year terms, 2012–2015, will continue their service for two more years.

Election Ballot



Vice President
- ❍ Gabriel A. Infante (Puerto Rico)
- ❍ Natalia Tarasova (Russia)
- ❍ Qi-Feng Zhou (China/Beijing)

Bureau
- ❍ Russell J. Boyd (Canada)
- ❍ Tavarekere K. Chandrashekar (India)
- ❍ Richard Hartshorn (New Zealand)
- ❍ Colin Humphris (UK)
- ❍ Christopher K. Ober (USA)
- ❍ Pietro Tundo (Italy)
- ❍ Jean-Pierre Vairon (France)
- ❍ Kaoru Yamanouchi (Japan)
- ❍ Qi-Feng Zhou (China/Beijing)

At its assembly in Istanbul, Turkey, on 14–15 August 2013, the Council will be asked to elect a vice president and members of the Bureau to fulfill the vacancies created by retiring members (see March-April 2013 *CI* for details; www.iupac.org/publications/ci/2013/3502/iw1_election.html).

Details on the election, including biographies of the nominees, are available online. To make your voice heard, contact your National Adhering Organization and get involved.

www.iupac.org/news/news-detail/article/nominees-for-election-of-iupac-officers-and-bureau-members.html

Winners of 2013 IUPAC Prizes for Young Chemists

The winners of the 2013 IUPAC Prizes for Young Chemists, awarded for the best Ph.D. theses in the chemical sciences as described in 1000-word essays, are as follows:

- Daishi Fujita, Japan, University of Tokyo, Tokyo, Japan
- Thomas Kempa, USA, Harvard University, Cambridge, MA, USA
- Huifeng Qian, China, Carnegie Mellon University, Pittsburgh, PA, USA
- Hailiang Wang, China, Stanford University, Stanford, CA, USA
- Qiao Zhang, China, University of California, Riverside, CA, USA

The winners will each receive a cash prize of USD 1000 and travel expenses to the 44th IUPAC World Chemistry Congress, 11–16 August 2013, in Istanbul, Turkey. They will be invited to submit a short critical review on aspects of their research topic to be published in *Pure and Applied Chemistry*. The awards will be presented to the winners of the 2012 and 2013 prizes during the Opening Ceremony of the Congress.

The essays describing the winners' theses can be found on the IUPAC website and cover a wide range of subject matter:

- Dr. Fujita: Protein Encapsulation within Synthetic Molecular Hosts
- Dr. Kempa: Nanowire Architectures for Next-Generation Solar Cells and Photonic Devices
- Dr. Qian: Controlling Gold Nanoparticles with Atomic Precision: Synthesis and Structure Determination
- Dr. Wang: Inorganic/Graphene Hybrid Nanomaterials for Electrochemical Energy Storage and Conversion
- Dr. Zhang: Nanomaterials Engineering and Applications in Catalysis

There were 43 applications from 15 different countries. The Prize Selection Committee awarded six Honorable Mentions:

- Sarah Bronner, USA, University of California, Los Angeles, CA, USA
- Paul Brown, UK, University of Bristol, Bristol, United Kingdom
- Gaston Corthey, Argentina, Universidad Nacional de La Plata, La Plata, Argentina
- Thierry Fouquet, France, Aix-Marseille University, Aix-en-Provence, France
- Sayantan Paria, India, Jadavpur University, Kolkata, India
- Joshua Robinson, USA, Stanford University, Stanford, CA, USA

www.iupac.org/news/news-detail/article/iupac-announces-winners-of-the-2013-iupac-prizes-for-young-chemists.html

Recipients of the IUPAC 2013 Distinguished Women in Chemistry or Chemical Engineering Awards

The awardees of the IUPAC 2013 Distinguished Women in Chemistry or Chemical Engineering are as follows:

- Irina P. Beletskaya, Moscow State University, Russia
- Annette Doherty, Senior VP Product Development, GlaxoSmithKline Plc, UK
- Mary Garson, University of Queensland, Australia
- Evamarie Hey-Hawkins, University of Leipzig, Germany
- Kazue Kurihara, Tohoku University, Japan
- Liliana Mammino, University of Venda, South Africa
- Elsa Reichmanis, Georgia Institute of Technology, USA
- Concepció Rovira, Institute of Materials Science of Barcelona, Spain
- Maria Vallet-Regi, Universidad Complutense, Spain
- Angela Wilson, University of North Texas, USA
- Yi Xie, University of Science & Technology of China, China

The awards program, initiated as part of the 2011 International Year of Chemistry celebrations, acknowledges and promotes the work of women chemists/chemical engineers worldwide (see Mar-Apr 2013 *CI*, www.iupac.org/publications/ci/2013/3502/iw2_call.html). The 11 awardees have been selected based on excellence in basic or applied research, distinguished accomplishments in teaching or education, or demonstrated leadership or managerial excellence in the chemical sciences. The awards committee was particularly interested in nominees with a history of leadership and/or community service during their careers.

In 2011, 23 women were honored during a ceremony held at the IUPAC Congress in San Juan, Puerto Rico, on 2 August 2011. The event was sponsored by a challenge grant from the American Chemical Society and by Dow Chemical. This year, a similar award ceremony will take place during the IUPAC Congress in Istanbul, Turkey, on 16 August 2013. The ceremony and reception in honor of the recipients will follow the symposium: *Women in Chemistry: Gaining Momentum*.

Green Chemistry for Life

On 29 March 2013, UNESCO Director-General Irina Bokova and the chief executive officer of the Russian company PhosAgro Maxim Volkov, signed a partnership agreement to promote "green chemistry." The agreement establishes the joint Green Chemistry for Life project, to be carried out in close cooperation with IUPAC, which will provide grants to support promising projects proposed by young scientists.

Established initially for five years, the project will provide grants worth a total of USD $1.4M to young scientists from developing countries who are working on the application of advanced chemistry technologies for issues like environmental protection, human health, food supplies and the use of natural resources.

Research projects will be chosen and monitored by an international scientific jury.

"Many countries, particularly developing countries, are badly in need of developing research capacities in green chemistry, and applying its fruits for the preservation of the environment and the introduction of environmentally sound technologies," said Irina Bokova. "This partnership reinforces UNESCO's longstanding efforts to foster this capacity, especially among the young generations of scientists, and address these challenges."

UNESCO Director-General Irina Bokova (left) and Maxim Volkov, chief executive officer of PhosAgro, signing a partnership agreement to establish the Green Chemistry for Life project.

"We view the Green Chemistry for Life project as an investment in the whole planet, and a successful example of how science and business can unite to create new knowledge aimed at protecting the environment," said Maxim Volkov. "I also believe this project will help to improve the prestige of chemistry and lead to more young scientists choosing to study the topic."

"This project inspired by the 2011 International Year of Chemistry, of which PhosAgro was a generous sponsor, represents a unique opportunity for IUPAC in providing high-standard expertise in green chemistry through its network for experts," said IUPAC Treasurer John Corish. "IUPAC will mobilize the help required for implementation of the young scientists' scientific activities and is committed to provide advice that may be needed from its divisions and standing committees."

The objective of the partnership between PhosAgro and UNESCO, to be implemented in close cooperation with IUPAC, is to enhance global international capacity to harness green chemistry to help address today's global sustainable development challenges.

PhosAgro is the largest phosphate-based fertilizer producer in Europe and the largest producer of high-grade phosphate rock worldwide. PhosAgro is also a leading producer of feed phosphates in Europe, and the only producer in Russia.

From Macro2012 to Macro2014

Virginia Tech, the host of Macro2012, recently pledged financial support of USD 10000 to the organizers of the Macro2014 Congress, to be held 6–11 July 2014, in Chaing Mai, Thailand.

"We were honored with the invitation to lead MACRO2012, and the Congress had profound and lasting effects for our university," said Tim Long, chemistry professor and associate director responsible for industry involvement and outreach for the Macromolecules and Interfaces Institutes at Virginia Tech. "We sincerely hope our pledge starts a new tradition for IUPAC when previous success can help catalyze success in the following Congress. "

Welcoming this gift, Michael Buback, president of the IUPAC Polymer Division, acknowledged Virginia Tech's lasting appreciation of the international com-

Timothy E. Long delivering his welcoming speech at Macro2012.

Photo by David Elmore.

munity and IUPAC and stated that the donation will be assigned to a specific activity at the Congress. Details about Macro2014 are online at www.macro2014.com.

Thieme–IUPAC Prize 2014 Call for Nominations

The Thieme–IUPAC Prize is presented every two years on the occasion of the IUPAC International Conference on Organic Synthesis (IUPAC–ICOS). The ICOS-20 will be held in Budapest, Hungary, on 29 June–4 July 2014.

Sponsored jointly by Georg Thieme Verlag, IUPAC, and the editors of *SYNLETT*, *SYNTHESIS*, *Science of Synthesis*, and Houben–Weyl, the prize is awarded to a scientist under 40 years of age whose research has had a major impact in synthetic organic chemistry.

The prize is given 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 1 January of the year in which the prize is awarded.

The Thieme–IUPAC Prize was 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, John F. Hartwig in 2004, David W. C. MacMillan in 2006, F. Dean Toste in 2008, Phil S. Baran in 2010, and Melanie S. Sanford in 2012.

The 2014 Call for Nominations is now open. The Nominations Deadline is 13 December 2013.

www.thieme-chemistry.com/en/our-service/conferences/thieme-iupac-prize/call-for-nominations.html

Polymer International–IUPAC Award—Call for Nominations

The call for nominations for the 4th *Polymer International*–IUPAC Award for Creativity in Applied Polymer Science or Polymer Technology is now open. The deadline for entries is 31 October 2013. Readers of *CI* are encouraged to recognize the achievements of their colleagues by nominating them for this award, which includes a cash prize of USD 5000.

The award will be presented at the IUPAC World Polymer Congress–MACRO 2014, 6–11 July 2014 in Chiang Mai, Thailand. The winner will be awarded USD 5000 plus travel and hotel accommodation expenses to attend MACRO 2014, where he/she will present an award lecture.

The winner will be selected by the Scientific Committee, representing *Polymer International* and the IUPAC Polymer Division. Nominees must be under age 40 on 31 December 2014 and must be available to present an award lecture at MACRO 2014. Please see website for specific details regarding the nomination process.

The *Polymer International*–IUPAC Award was awarded to Zhenan Bao in 2008, Molly Stevens in 2010, and Ali Khademhosseini in 2012.

http://onlinelibrary.wiley.com/journal/10.1002/(ISSN)1097-0126/homepage/polymer_internations_iupac_award.htm

Research Integrity—The Montreal Statement

The 3rd World Conference on Research Integrity, held 5–8 May 2013 in Montreal, focused international attention on research integrity, responsible conduct of research, and publication of research. Attendees had opportunities to learn the current state of worldwide progress on research integrity, discussed new challenges and emerging topics, and helped shape national and international responses.

The conference provided a forum for discussion and exchange of ideas, expertise, and experience among national and institutional leaders, policy makers, research funders, leaders of professional societies, journal editors, publishers, researchers, educators, administrators, and graduate and postdoctoral trainees.

Former IUPAC President Leiv Sydnes, chair of ChemRAWN and also chair of the ICSU Committee on Freedom and Responsibility in the Conduct of Science, attended the conference.

Areas of particular interest included:

- integrity in cross-national, cross-disciplinary and cross-sector partnerships
- trust in science, including political and media issues, responses to misconduct, and correction of the scientific record
- emerging challenges in research integrity associated with new technologies and scientific frontiers
- fostering research integrity through policies, codes, standards, and training

One outcome of the conference is the Montreal Statement, which offers guidance on integrity in cross-national, cross-disciplinary, and cross-sector research. At the conference, attendees had the opportunity to comment on a draft statement. The finalized version will be issued after a one-month comment period.

www.wcri2013.org

ICSU Consults on Open Access

Seeking to clarify its position on the related issues of open access publication of scientific literature and evaluation of research by metrics, ICSU has reached out to its membership organizations for their input. The results of this process may lead to corresponding resolutions being proposed to the General Assembly in September 2014.

The issues surrounding open access to scientific literature and data have become impossible for scientists to ignore, as national and supra-national funding agencies increasingly push the notion that the results of the research they fund must be freely available to all. Some new publication models require authors to pay a fee for the publication of their work, while many existing subscription-based journals and books have high subscription fees.

A new emphasis on open access to data, increasingly important in this data rich science era, is raising further issues regarding security, ethics, intellectual property rights, formal publication of data, incentives to scientists to provide their data, and more.

With research funders, universities and governments increasingly relying on quantitative metrics, in particular based on citation statistics, to evaluate universities, departments and individuals, there is also pressure on researchers to adopt practices that maximize these metrics.

ICSU asked its members, including IUPAC, to comment in general on these interrelated issues, and specifically to answer the following questions:

1. What requirements do funders of research in your country or subject area currently make, or plan to make, as regards open access publication, including open access to data? What advantages and disadvantages do you see in such open access requirements, whether in your country/subject area or elsewhere?
2. To what extent are metrics being used to evaluate universities, departments, and individuals in your country or subject area? What metrics are used? How are these influencing publication trends and incentives for researchers?
3. What useful role, if any, do you think ICSU can play in these matters?

Comments by 1 Sep 2013 are welcome. If you have any questions, please do not hesitate to contact webmaster@icsu.org.

www.icsu.org/news-centre/news/icsu-consults-membership-on-open-access

Description of Materials on the Nanoscale

Supported by an ICSU grant, CODATA (ICSU Committee on Data for Science and Technology) and VAMAS (the Versailles Project on Advanced Materials and Standards) have established an international working group to develop the requirements for a unified description system for materials on the nanoscale as well as the minimum information categories required to describe such nanomaterials.

The requirements are being developed with input from a broad range of scientific disciplines, as represented by ICSU unions and including IUPAC, and by diverse user communities. This work will enable standards developers, regulators, and researchers to describe nanomaterials uniquely, accurately, and unambiguously. This project represents one of the largest inter-union programs supported by ICSU. Experts from chemistry, physics, materials science, toxicology, pharmacology, materials science, biology, medicine, and the environmental sciences—representing over 20 countries—are working together for the first time to provide a consensus set of requirements that must be met for a nanomaterials description system to be effective and useful.

This project is an outgrowth of the 2012 ICSU/CODATA International Workshop on this subject. That workshop recommended that CODATA undertake a multidisciplinary approach to provide ISO and other standards and regulatory groups with science-based recommendations for a nanomaterial description system (see Nov-Dec 2012 *CI*, p. 28–29, www.iupac.org/publications/ci/2012/3406/cc2_230212.html).

The work is timely; the European Union has proposed a new definition for nanomaterials, and regulators through the world are actively considering how best to approach health, safety, and environmental issues associated with nanotechnology. While ISO and other groups are working on various aspects of a nanomaterial description system, no group is attempting to bring together the views of the many scientific disciplines and user communities who are concerned with nanotechnology.

IUPAC participation in this project, bringing its expertise in chemical nomenclature, is through Division VIII, the Chemical Nomenclature and Structure Representation Division.

For more information, contact John Rumble <jumbleusa@earthlink.net>, chair of the CODATA Nanomaterials Working Group, or Richard M. Hartshorn <richard.hartshorn@canterbury.ac.nz>, president of IUPAC Division VIII.

IUPAC Safety Training Program—Istanbul Workshop

A Workshop on the IUPAC Safety Training Program will take place 12 August 2013, during the IUPAC General Assembly in Istanbul. The workshop is an opportunity to share with the IUPAC community the recent activities by fellows of the program in their home countries; to evaluate the effectiveness of the Safety Training Program in terms of fellows' home country activities; to learn from invited speakers who are experts in health, safety, and environmental matters; and to solicit ideas for improvements in the program and for possible expansion to incorporate new host companies and new regional trainees. Similar workshops were held at the IUPAC GA/Congress in Ottawa in 2003, Beijing in 2005, Torino in 2007, Glasgow in 2009, and San Juan in 2011. This series has established itself as an important activity coordinated by the IUPAC Committee on Chemistry and Industry, COCI.

The Safety Training Program allows safety experts from developing countries to learn more about safety and environmental protective measures by visiting and working in plants of IUPAC Company Associates in the industrialized world. IUPAC administers the program to disseminate state-of-the-art knowledge on safety and environmental protection in chemical production. The beneficiaries are expected to use the training in their home countries to improve health, safety and environment.

Fellows of the IUPAC Safety Training Program who have been trained at host sites share written reports. A number of fellows will attend the workshop to present updates on actions taken since their training. In addition, the workshop will include lectures by regional speakers who are experts in chemical health, safety, and environmental protection issues particular to the pharmaceutical and biotechnology industries. The workshop will include a discussion to identify ideas for improvement and expansion of the scope of the Safety Training Program.

For more information, contact Task Group Chair Bernard West <Bernard.west@sympatico.ca>.

www.iupac.org/project/2013-011-2-022

www.iupac.org/committee/coci/safety-training-program.html

Fluorescence Correlation Spectroscopy (IUPAC Technical Report)

Jörg Enderlein
Pure and Applied Chemistry, 2013
Vol. 85, No. 5, pp. 999–1016

This report is an overview on the applicability of fluorescence correlation spectroscopy (FCS) for the accurate determination of translational diffusion coefficients and thus, via the Stokes–Einstein relation, of molecular size. Several of the most common sources of optical aberrations and their impact on the outcome of conventional FCS measurements were considered. A new variant of FCS, dual-focus FCS, which is robust against most of the considered aberrations is also described and reference values of diffusion coefficients for several fluorescent dyes across the visible spectrum are reported.

http://dx.doi.org/10.1351/PAC-REP-11-11-17

Atomic Weights of the Elements 2011 (IUPAC Technical Report)

Michael E. Wieser, et al.
Pure and Applied Chemistry, 2013
Vol. 85, No. 5, pp. 1047–1078

The latest tables of atomic weights (2011) are published in *Pure and Applied Chemistry*.[1] This biennial review of atomic-weight determinations and other cognate data has resulted in changes for the standard atomic weights of five elements: the atomic weight of bromine has changed from 79.904(1) to the interval [79.901, 79.907], germanium from 72.63(1) to 72.630(8), indium from 114.818(3) to 114.818(1), magnesium from 24.3050(6) to the interval [24.304, 24.307], and mercury from 200.59(2) to 200.592(3).

For bromine and magnesium, assignment of intervals for the new standard atomic weights reflects the common occurrence of variations in the atomic weights of those elements in normal terrestrial materials.[2] As such, bromine and magnesium have joined the earlier group of 10 elements—hydrogen, lithium, boron, carbon, nitrogen, oxygen, silicon, sulfur, chlorine, and thallium—which were expressed as intervals for the first time in the 2009 review to more accurately convey atomic weight variation.

The proper expression for an interval according to the latest *International Vocabulary of Metrology* is [a, b]. In this report therefore the notation of these atomic weights intervals has changed from [a; b], as they were first reporterd, to [a, b].

1. *PAC* 2013. For a collection of the reviews of the atomic weights of the elements, see www.iupac.org/publications/pac/series/atomicweights/
2. T.B. Coplen and N.E. Holden, "Atomic Weights—No Longer Constants of Nature" Mar-Apr 2011 *CI*, pp. 10–15; www.iupac.org/publications/ci/2011/3302/2_coplen.html

http://dx.doi.org/10.1351/PAC-REP-13-03-02

Glossary of Terms Relating to Thermal and Thermomechanical Properties of Polymers (IUPAC Recommendations 2013)

Michael Hess, et al.
Pure and Applied Chemistry, 2013
Vol. 85, No. 5, pp. 1017–1046

This document gives definitions of terms related to the thermal and thermomechanical properties of polymers prior to thermal decomposition. The terms are arranged in alphabetical order and cover definitions of relevant terms from physical chemistry, polymer science, and experimental techniques. The document considers to some extent earlier reports related to the terminology of thermal analysis (e.g., those published by the International Confederation for Thermal Analysis and Calorimetry, IUPAC Recommendations covered by the Compendium of Chemical Terminology, the so-called "Gold Book", and the second edition of the *Compendium of Polymer Nomenclature and Terminology*, the so-called "Purple Book").

Other publications consulted include ISO and ASTM Standards. In addition, the recently (*PAC* 2011, Vol. 83, No. 10, pp. 1831-1871) published document "Definition of terms relating to crystalline polymers," a revision of a superseded IUPAC recommendation published under the same title in 1989, has necessitated modifications of some older definitions. Thermal analysis is an extensive subject in its own right, and the reader is referred to specialized textbooks for further information.

http://dx.doi.org/10.1351/PAC-REC-12-03-02

Polymer Nomenclature

by Jeffery Leigh

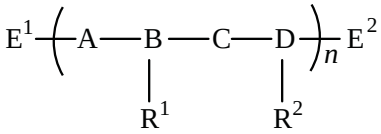
The aim of systematic IUPAC nomenclature is usually to introduce naming systems that define the structure of a molecule precisely, so that the reader can reproduce the exact structure of the molecule being discussed. The system works reasonably well for completely characterized small molecules, but cannot do so with the same level of precision for polymeric materials comprised of molecular chains (macromolecules), the structures of which are based on constitutional repeating units (CRUs). These repeat units may not be all of the same type and need not repeat in a regular fashion. A given polymer may consist of more than one chain and often of mixtures of different kinds of chain. In addition, there can be regular or irregular steric variations along the length of individual macromolecules and chains might be branched or linked to one another in diverse ways. For many polymers, the repetition may not be exactly regular, the material may consist of a mixture of chain macromolecules of different lengths, and the precise structure may not be known. Nevertheless, methods for naming such materials are necessary for general communication, and polymer chemists have been obliged to develop them. It is probably true that there is not yet a universal agreement among all polymer chemists as to how this should be done in every case, but there is a considerable consensus, and the new *Principles* presents its basic details.

A polymer is a substance composed of a collection of macromolecules of a range of molecular masses. As a consequence, it is characterized by an average molecular mass rather than a mass of a definite value, as typical of relatively small molecules. These macromolecules may consist of single strand, regular or irregular chains, or they may be double-stranded ladder-like structures or even sheets, the limit being a three-dimensional structure, which may be considered no longer to be within the province of polymers but better treated as a three-dimensional structure such as in a ceramic or glass. Finally, the polymers may be constituted of organic, organometallic, or even inorganic groups, including those of coordination type. Polymer nomenclature must attempt to describe all these types, and no satisfactory universal methodology has been developed.

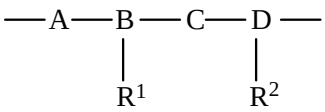
Two basic methods have been developed to give names which are comprehensible and broadly consistent with the apparent structure. Neither method conveys all the details of the polymer structure, but one capable of doing so would probably be too long and complicated to be easily comprehensible, even to the informed reader. A shorter form is often adequate for many purposes.

Most polymers consisting of regular, single macromolecular chains may be named using **structure-based nomenclature.** Example (a) shows a generalized structure of such a polymer. A, B, C, and D represent groups of atoms comprising the main chain while E and R denote the chain end-groups and pendant groups, respectively. The CRU for this generalized structure, and the CRU and name and of a real polymer are also shown. Precise rules are necessary to govern the selection of the CRU.

Example (a)



Representative single-strand polymer structure



Constitutional repeating unit (CRU)

CRU of a polymer named poly[oxy(1-methylene)]

Methods have also been developed to name irregular single-strand polymers and polymers of other structures, and these are also mentioned in *Principles*. Nevertheless, a precise structure-based name may be impossible to devise for a variety of reasons, such as lack of enough structural information. By far, the most widely used and easily implemented method of naming polymers is **source-based nomenclature** and example (b) shows three such names.

Example (b) polyacrylonitrile
polystyrene
poly(dimethylstannanediyl)

The first two names are based on the names of the reagents (which may be monomers) from which the polymers were synthesized, acrylonitrile and styrene in these cases, but they convey little information about structure. However, this use of a reagent name may not be always applicable. For example, the source reagent to synthesize the third polymer cannot be simply dimethylstannanediyl, even though

The next topic in this series will be the special case of boron hydrides.

the polymer name itself is easily comprehensible. All three source-based names are organic style, but for the third, which describes an inorganic single-strand polymer, an inorganic-style name is also available:

catena-poly[dimethyltin]

These are only very simple examples, but they hint at some of the complexities involved in naming polymers, which differ from some of the methods used for naming small molecules. *Principles* also describes how more complicated polymer structures can be named, and also abbreviations for names that are commonly used both in academe and in industry. As usual, a list of basic references is also provided.

The recommendations and advice of Professor Richard G. Jones (University of Kent, Canterbury, and chair of the IUPAC Subcommittee on Polymer Terminology) during the preparation of this note are gratefully acknowledged.

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

www.iupac.org/publications/ci/indexes/nomenclature-notes.html

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

Stamps International

Welcome Home, Flerovium!

The Joint Working Party (JWP), an ad hoc committee of experts drawn from the ranks of IUPAC and IUPAP, was created in 2005 and charged with the notoriously difficult task of assessing the claims and assigning priority to the discovery of new elements with atomic numbers greater than 111. This is not a trivial endeavor since the detection and unequivocal identification of isotopes of the so-called superheavy elements, having transient lifetimes and often being generated one atom at a time, is quite challenging. In 2011, after careful consideration of all the available data, the JWP adjudicated the discovery of elements 114 (flerovium) and 116 (livermorium) to the teams of nuclear scientists working collaboratively at the Joint Institute for Nuclear Research (JINR) in Dubna, Russia, and the Lawrence Livermore National Laboratory in California, USA. The names of the newest members of the periodic club and their symbols (Fl and Lv, respectively) were officially approved by IUPAC in May of 2012, with the former paying tribute to the Flerov Laboratory of Nuclear Reactions at the JINR, named in turn after the prominent Russian physicist Georgiy N. Flerov (1913–1990).

The stamp illustrated in this note, issued on 21 January 2013, commemorates the birth centennial of Flerov (whose birthday was actually on 2 March 1913) and is the first ever showing the name and symbol of element 114. Flerov was born in Rostov-on-Dov, a port city in Southwestern Russia, not far from the Sea of Azov. He studied nuclear physics at the Leningrad Polytechnic Institute, worked for a while in the laboratory of the legendary nuclear physicist Igor Kurchatov (the "father of the Soviet atomic bomb") at the Russian Academy of Sciences and, together with Konstantin Petrzhak, discovered in 1940 the spontaneous fission of uranium. Following service in the Soviet Army during the Second World War and pioneering research in heavy-ion physics at the Institute of Atomic Energy in Moscow, he became the founding director of the Laboratory of Nuclear Reactions at the JINR, a position he held for more than 30 years (1957-1989). With due respect to the provisional systematic nomenclature devised by IUPAC for newly synthesized elements, flerovium is clearly an excellent choice for the element formerly known as ununquadium!

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

The ACS International Center: The New Way to Discover International Opportunities

by Steven R. Meyers and Julia M. Throop

Global organizations offer a burgeoning number of international opportunities to those seeking funding for scientific research and career advancement, but the individual chemist may find it increasingly difficult to identify the ideal fit among the dizzying quantity of those available. To overcome this difficulty, and to help opportunity-providers connect with opportunity seekers, the American Chemical Society (ACS) has collated a list of scientific research programs and opportunities on the newly established ACS International Center website (www.acs.org/ic). Sponsored by the ACS Committee on International Activities, the International Center is a curated, web-based repository connecting institutions and foundations worldwide with those seeking details about international opportunities by providing information on grants, scholarships, internships, professional training, and more.

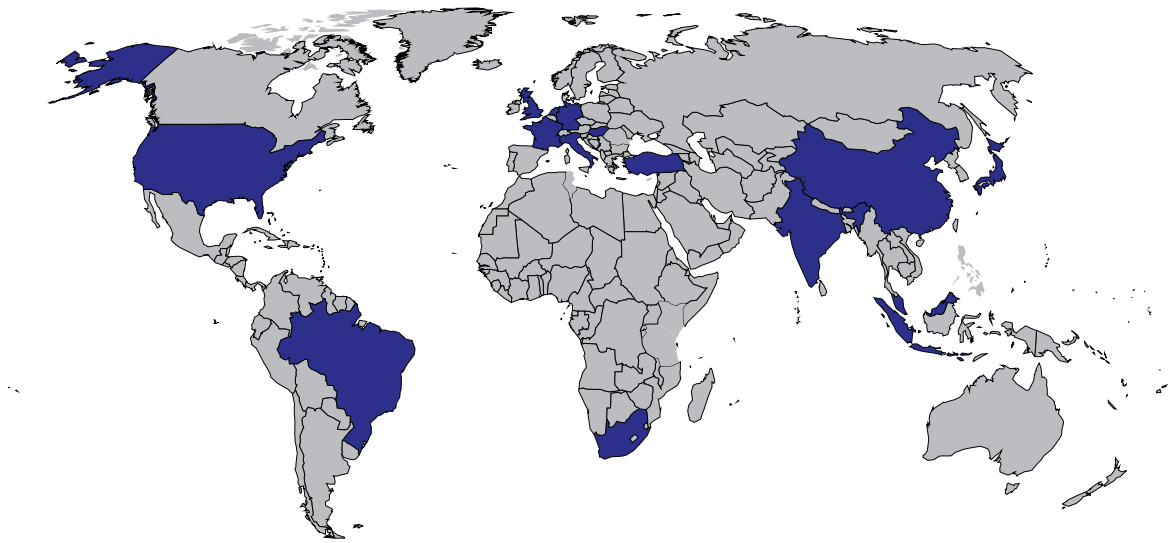
So far, the ACS International Center has assembled details on 350 searchable opportunities worldwide over 15 host geographies for scientists and engineers at 6 experience levels: high school teacher/student, undergraduate, graduate, postdoctoral fellow, academic faculty, and industrial professional.

To further its mission, the International Center has established a network of global affiliates, including government agencies, institutions, and non-profit organizations, who assist the International Center by contributing new and under-exposed opportunities to the site. So far, affiliations have been established with 10 global entities across 6 different geographies. In turn, the International Center provides a place for those affiliate entities to promote and vocalize new initiatives through web announcements, email newsletters, Twitter feeds, and promotional events, such as webinars and collaborative receptions, to a receptive audience of 163 000 ACS members worldwide.

Future plans for the project indicate a network of such affiliations with entities from all over the globe. Affiliates would be able to use the ACS International Center as a platform for their own initiatives, and to leverage the membership audience, subscription to the International Center newsletter, and website viewership to advance the global chemistry enterprise.

As the International Center builds toward this end goal, seekers and providers are welcome to visit www.acs.org/ic and to contribute missing international opportunities or testimonials on specific programs, or to participate as a personal reference. Contact ic@acs.org or follow the IC on Twitter @ACS_IC.

The ACS International Center's global affiliates.



Looking at Information from a New Perspective

by Bonnie Lawlor

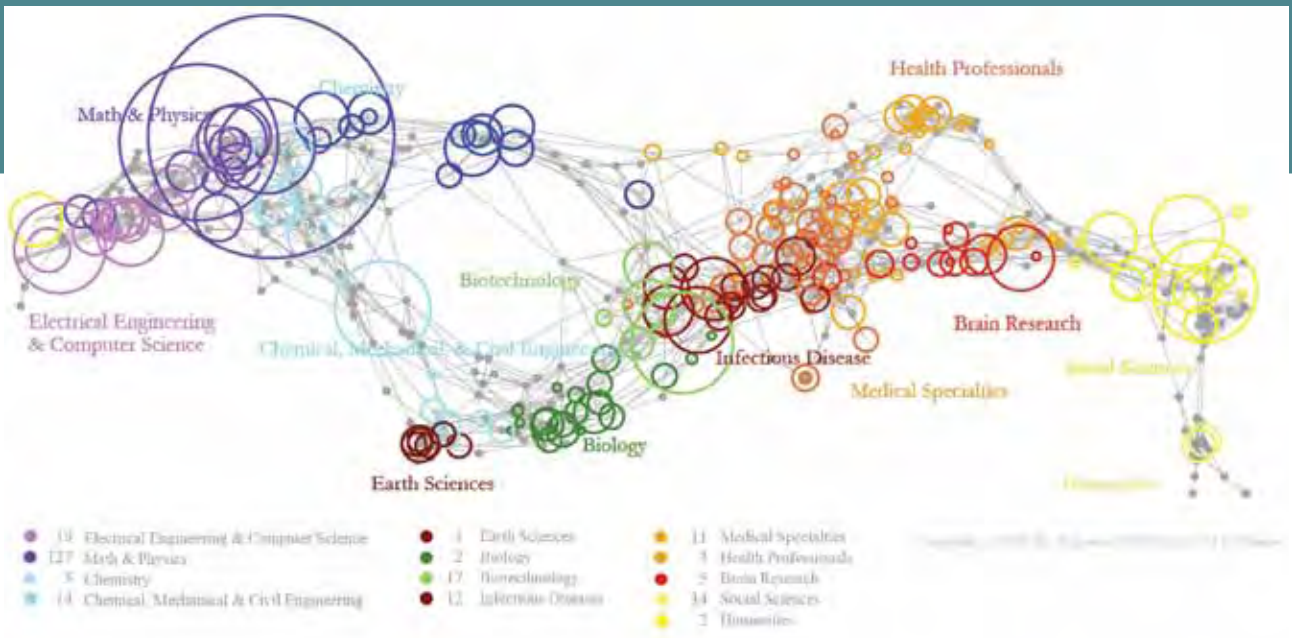
Since the launch of the first scientific and scholarly journals in 1665 (*Journal des Sçavans and Philosophical Transactions*), the amount of scientific information has continued to grow exponentially. It was estimated that 50 million scholarly articles had been published between 1665, when the *Journal des Sçavans* was first published, and the close of 2009, when the annual article output was estimated at 1504600.[1] How can these articles and the data they contain be mined to extract new information and advance scientific and scholarly research? To answer this question, a group of researchers, publishers, librarians, and technologists gathered for the National Federation of Advanced Information Services' conference **In Search of Answers: Unlocking New Value from Content**, held 24–26 February 2013 in Philadelphia, Pennsylvania, USA. The purpose was to highlight examples of how the application of technologies such as data mining, linking, analytics, and metrics can expose, enhance, and create new information and insights from data already at hand.

The opening keynote given by David Weinberger, senior researcher at the Berkman Center for Internet and Society and co-director of the Harvard Library Innovation Lab, set the stage for the meeting with a perspective on what it means to "know" in an era marked by an exponential growth of digital information and the emergence of multimedia data formats that are appearing with increasing frequency in e-journals. He stressed the importance of linked data and collaborative networks in the development of knowledge. Citing the difficulty in reaching scientific conclusions in the face of a constant stream of new data, he stressed the value of aggregating large, diverse datasets in order to unearth new "facts," both as an individual scientist, but better yet, in collaboration with other experts. Provocatively, he put forth the following question: If through data mining a new equation emerged that accurately predicted outcomes, but the "why" of the equation's accuracy was not understood, should that equation be considered invalid even if nothing exists to take its place? His point was that in some cases, predictable, actionable results can carry more weight than the "why" of the results, especially in an era of Big Data and the tools with which to dissect and analyze that data (this position is emphatically reinforced with examples in a new book entitled *Big Data: A Revolution that will Transform How We Live, Work and Think* by Viktor Mayer-Schönberger and Kenneth Cukier).

Weinberger was followed by the session "In Search of Answers: Scientists and Scholars Speak Out." In this session, researchers talked about their own initiatives, all of which were undertaken to create new knowledge and insights from existing content. Timothy Hitchcock, a professor at the University of Hertfordshire, UK, discussed his work in using text mining to uncover unexpected relationships and trends on a variety of topics in the humanities. Funded by JISC, a team downloaded and analyzed 127 million words of text that were extracted from the trials that form *The Proceedings of the Old Bailey* (1674–1913). Using the Mathematica 8 software, the full-run of 197000 recorded trials was examined. As a result, their work showed how accounts of trials evolved between the late seventeenth and early twentieth centuries. And an unexpected find of their study was that the accepted narrative of the evolution of the criminal trial was wrong, and that the rise of "plea bargaining" in the 19th century was a significant development in shaping the modern criminal justice system. Hitchcock stressed the importance of combining Big Data with statistical analyses and visualization as a means of simultaneously unearthing both macroscopic and microscopic patterns. He said that these tools will shape the future of scholarship and research across all disciplines.

Hitchcock's comments were reinforced by other speakers throughout the conference. John Coleman, director of the Phonetics Laboratory, Oxford University, UK, also focused on data mining, but the data was the spoken word–not text (about 9000 hours, 100 million words, or 2 Terabytes of speech)–the largest phonetics study ever undertaken. He pointed out that speech represents the largest electronic flow of information (4 billion Gigabytes/year) and that the goal of their project is to make large-scale audio files readily accessible and easily usable for researchers (e.g., relevant video clips and data describing taped experiments, speeches, etc.). Although the research is ongoing, the group has already developed and distributed tools for transcribing audio, for checking transcriptions, and for aligning the transcriptions with audio recordings. They are developing tools for interactive search and display of audio/transcript combinations and plan to

1. Jinha, Arif E., "Article 50 Million: an estimate of the number of scholarly articles in existence," *Learned Publishing*, Vol. 23, No. 3, July 2010.



An example of a Big Data visualization presented by Timothy Hitchcock. This UCSD Map of Science, created by information scientists Angela M. Zoss and Katy Börner, gives job information based on scientific discipline (Katy Börner, "Plug-and-Play Macroscopes," Communications of the ACM, Vol. 54 No. 3, Pages 60-6910.1145/1897852.1897871). Reproduced with permission.

create tools for indexing and searching phonetic transcriptions with interfaces to tools for visualization and statistical analyses.

Alberto Pepe, information scientist at the Center for Astrophysics, Harvard University, spoke on the ADS All-Sky-Survey, a major project with the objective of transforming the NASA Astrophysics Data System (ADS) from a literature resource to one that is also a data resource. ADS is the most accurate and complete record of published research in astrophysics, with papers ranging from the late 1700s through the present. All of the data (images, tables, object references) contained in these articles is being "astro-tagged" so that the data itself can be searched and analyzed while links to the original research, as well as to the relevant objects in the sky, are maintained. One outcome is a fascinating all-sky map in which published literature is overlaid on the sky. When viewed over time (pre–1900s to present) one can look at the "sky" and visualize what areas have been written about and when, link to the article to learn why, and ultimately identify what areas may be ripe for research. The map is expected to go live this year.

One of the most intriguing presentations was made by Larry Birnbaum, chief scientific advisor at Narrative Science, a company that grew out of work started in the computer science department at Northwestern University in Evanston Illinois. They have developed software and a set of statistical analytic tools that actually generate insightful text from raw data and charts. While many examples were based upon reams of financial data, they also are working with pharmaceutical companies to generate meaningful and timely actionable reports from clinical trial data. They are able to generate human-quality narratives from Big Data at machine speed and scale and provide companies with the ability to make better and faster decisions.

Christopher Burghardt, vice president of product and market strategy at Thomson Reuters IP & Science, spoke about data and nontraditional content from the perspective of current challenges to creating, finding, using, and citing such information. Many researchers do not want to publish data if they do not receive credit. His organization surveyed 417 researchers and found that only 16 percent believe they are receiving adequate recognition for publishing their data, 62 percent would publish more if they received credit, and 66 percent believe it is important/very important for them to get credit for publishing data independently from the credit they receive for their traditional journal articles. He noted that researchers deposit their data in a variety of locations: 51 percent on their personal websites, 47 percent in their department or institutional repository, 36 percent with third parties, 24 percent with publishers, and 17 percent with other sources. With more than 500 credible repositories around the globe (see http://databib.org/), it is not always easy to find data that is available. Burghardt discussed the *Data Citation Index* that was recently launched to facilitate data discovery, measure its use and re-use, provide standards for attribution, and promote new metrics for digital scholarship.

After hearing about new content generated as a result of applying text mining and statistical analysis to existing information, the discussion turned to new tools that have emerged for measuring the value of

scientific output. Andrea Michalek, co-founder of Plum Analytics, talked about metrics beyond the traditional bibliographic citation—a genre of metrics categorized as altmetrics. She noted that citation counts are not an immediate indicator of important research because it takes three to five years for research to receive a critical mass of citations. She also pointed out that informal forms of influence (e.g., blogs, news stories, downloads, etc.) are not cited and that as a result only 30 percent of items that demonstrate the value of research are actually used to highlight its impact. Her organization captures five different impact categories–usage (downloads, views), captures (saves, favorites), mentions (news, reviews), social media (shares, likes, tweets), and traditional citations (Web of Science, Scopus, Google Scholar, patents, etc.). They are able to merge the results from diverse sources and provide researchers and organizations with a snapshot of their research's impact. She emphasized that true value and relevance of research can only be measured by the combination of immediacy and citation impact.

Michalek's position was reinforced by Jason Priem, a doctoral student at the University of North Carolina, Chapel Hill. Priem stated that citations only tell a part of the story, quoting Thomas Kuhn, noted physicist turned historian, who said that spotting emerging research fronts will require tracking both "formal and informal communication." He mentioned the same types of informal "influencers" as did Michalek–discussions, saves, views, recommendations, shares, and citations. With the support of the Alfred P. Sloan Foundation, the National Science Foundation, Dryad, and others, Priem has co-founded another source of altmetrics, Impact Story. This is an open-source, web-based tool that helps researchers explore and share the diverse impacts of all their research products–traditional ones like journal articles, but also alternative products like blog posts, datasets, and software. It is also used by funding organizations who want to see what impacts they might be missing if they only consider citations to journal articles and patents.

IBM's Watson computer system competes against Jeopardy!'s two most successful and celebrated contestants —Ken Jennings (left) and Brad Rutter. *Source: IBM.*

At the end of the session on metrics the audience was asked if they agreed that new metrics are needed to measure the value of scholarly output due to the changes in scholarly communication that have resulted from collaborative research, open access, use of social media, and interactive communication. Using audience response devices, 53 percent strongly agreed and 42 percent agreed. When asked if the new metrics would replace or complement the traditional citations, the votes tallied with 91 percent saying that altmetrics will complement citations, 7 percent saying that they will replace citations, and the remainder having no opinion.

The conference closed with an attempt to answer the following question: Can the transformation of the world's cumulative content and data truly be transformed into knowledge? This was done taking a look at the role that artificial intelligence, specifically through IBM's Watson and its progeny, will play in the future. Frank Stein, director of the IBM Analytics Solution Center, noted that according to the International Data Corporation, the amount of information in the world is now doubling every two years and he questioned how we can ever turn that data into insights and knowledge. IBM took on the challenge to design a computing system that would rival a human's ability to answer questions posed in natural language, interpret meaning and context, and retrieve, analyze, and understand vast amounts of information in real time. Their first objective was to be able to answer questions in competition with humans on the popular TV show, *Jeopardy*. They started development in 2007 and by the fall of 2010 they believed that the new system, Watson, was ready. Key to their task was developing an algorithm that could not only parse a sentence, but also understand it. He used the following sentence as an example: "If leadership is an art then surely Jack Welch has proved himself a master painter during his tenure at General Electric (GE)." Could a computer deduce from this sentence that Jack Welch was the CEO at GE? Ultimately, it could. To get the results IBM acquired as much diverse information as possible and applied natural language processing, information

management, machine learning, and distributed computing with massively parallel processing. They used 90 high-powered servers and 10 refrigerator-sized racks for the machine. And they proved that Watson could win over the two previous biggest winners on *Jeopardy*. As a result, Watson captured the imagination of a wide audience.

Since then, IBM has made many enhancements to make the system practical in the real world. It is now 240 percent faster, only requires one rack of equipment, and can accept multi-dimensional input. Health care is their first area of interest. He pointed out that there are 95 new clinical trials launched every day and that medical information, much of which is unstructured, is doubling every five years. Yet, 81 percent of physicians report that they spend five hours or less per month reading medical journals! This is an area in which Watson can play a significant role. Their first product launch is in collaboration with the Sloan Kettering Clinic and will be focused on cancer treatments–specifically lung, breast, prostate, and colorectal cancers. They are also in discussions with organizations both in the financial and scientific arenas. Stein closed by saying that we are now in an era of being able to build knowledge through cognitive computing.

Everyone at the conference agreed that the combination of Big Data and technology is a major catalyst in the advancement of research and knowledge. To quote the authors of the book mentioned earlier in this report, ". . . the new techniques for collecting and analyzing huge bodies of data will help us make sense of our world in ways we are just starting to appreciate."

http://nfais.org/event?eventID=399

Science for Poverty Eradication and Sustainable Development

by Javier Garcia Martinez

Imagine having the opportunity to speak to the presidents of the national science academies of the entire world. What would you tell them? What brilliant idea might you share to solve our most urgent problems?

Trying to answer these critical questions is what a group of 134 leading scientists, some of them presidents of national science academies themselves, did from 25–27 February 2013 in Rio, Brazil (i.e., the same city where the Earth Summit (1992) and Rio+20 (2012) were held). Far from being an academic and formal meeting, the presidents of the science academies engaged in very vivid discussions using the Challenge Labs method, a format frequently used in the Davos meetings. In Challenge Labs, young scientists, many of them members of the Global Young Academy, moderate and provoke conversations on topics of great relevance, such as global heath, clean water access, universal science literacy, clean energy production, or food security. It was really refreshing seeing leading international scientists and academicians from prestigious organizations gather around flip boards to passionately discuss how science can provide specific solutions to real problems.

One of the goals of the science academies meeting was to identify and propose solutions to our new development goals. The original ones, the Millennium Development Goals (www.un.org/millenniumgoals), were signed by nearly all nations in 2000 and will expire in less than three years, in 2015. They are mainly related to poverty and its causes and consequences. For this reason, the Conference and General Assembly of the Global Network of Science Academies in Rio met under the theme: **"Grand Challenges and Integrated Innovations: Science for Poverty Eradication and Sustainable Development."**

The structure of the meeting was quite interesting. Instead of the typical large plenary sessions and reports from the different academies, the first day of the meeting was structured around Challenge Labs, a concept developed by the World Economic Forum to first present different topics, then discuss them in small groups, and finally report on them to the bigger group. Among the issues discussed in the were those that one would expect: health, energy, water, food security... although the one that attracted more interest was science literacy. There was a wide consensus on the importance of understanding the fundamentals of our global challenges as the first step toward solving them.

The first day of the meeting was led by members of the Global Young Academy, the new constituent of the InterAcademy Panel, formed from young scientists from all around the world, in clear contrast with the traditional national science academies. The second day was centered around the new Science Agenda and Future We Want. Several panels, based on the same format used in Davos, with very short presentations followed by questions from the public, were held to discuss critical topics, such as ethics, science

literacy, food security, and renewable energy sources. The result was a clear call to translate scientific results into improving the quality of life of those in need and inspiring the best minds to solve our common and urgent challenges.

Panel discussions were also part of a very full and diverse program that covered topics such as "The Role of Science in Coping with the Grand Challenges Facing Humanity," "Poverty Eradication and Sustainable Development," and "Grand Challenges and Integrated Innovation: Lessons from the Experience."

To make sure that all the ideas, proposals, and projects that come out of the discussions in Rio could see the light of reality, several funding agencies such as USAID, the Bill & Melinda Gates Foundation, and Grand Challenges Canada were present at the meeting and were actively involved in the discussions. In fact, during the lunches, several meetings were conducted between those who had just thought of a new project and potential funding agencies, which provided quick feedback on the possibilities of such a project.

One of the conclusions of the meeting was to create a website that will allow collecting ideas from people about priorities, best activities, and solutions regarding our most pressing challenges. This is your opportunity to tell the presidents of the national science academies about your brilliant idea to solve global problems. Think carefully, we all may rely on it.

The role of chemistry in providing very specific solutions to many of the challenges discussed was very clear during the deliberations held at the conference, from better materials for clean energy production to more effective drugs to treat wide-spread illnesses, such as malaria, AIDS, or tuberculosis. The positive role of chemistry in providing clean, safe water and the need to increase food security was also mentioned in several of the panels and challenge labs. Participants agreed that climate change, which was discussed on several occasions, was a main challenge for which better science in general, and chemistry in particular, is desperately needed.

What better inspiration for the new generation of scientists than to contribute to improving the lives of those in poverty? Following the footsteps of those great chemists who invented the solutions that make us healthier and able to enjoy life in so many ways, from penicillin to fertilizers, from clean water to vaccines, a new generation of chemists are critical to providing the solutions we need for a planet with 7-billion people. As President John F. Kennedy said at the American University in Washington, D.C., in 1963, "Our problems are man-made, therefore they may be solved by man. No problem of human destiny is beyond human beings." And science is the most (some would say the only) tool that men (and women) have to find the solutions to those problems.

Javier Garcia Martinez addresses representatives of the National Science Academies on the role of chemistry in a sustainable energy future.

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The ***Letter from Rio-2013***—the output of the IAP Conference—is available as one resource document online at www.interacademies.net/20197.aspx

Advanced Polymeric Materials

by Byung-Wook Jo and Michael Hess

The IUPAC-sponsored **World Forum on Advanced Polymeric Materials**, POLYCHAR 21, was held in March 2013 in Gwangju, South Korea. Founded in 1992, POLYCHAR had been held annually at the University of North Texas, Denton, until 2004 when it was held in Portugal, the first POLYCHAR held outside the USA. Since then, it has been held in Singapore (2005), Japan (2006), Brazil (2007), India (2008), France (2009), Germany (2010), Nepal (2011), and Croatia (2012).

Jean-Jacques Pireaux, Chair of the Prize Committee (left) and Holger Schoenherr (right)

Under the chairmanship of Byung-Wook Jo of Chosun University, Gwangju, 245 participants from 30 countries gathered from 11–15 March in the Kim Dae-Jung Convention Centre. There were 26 invited speakers and 71 oral contributions, 134 posters (in two sessions). The conference received strong support from the City of Gwangju, Chosun University, Korean Polymer Society, and numerous industry sponsors.

The name POLYCHAR is derived from polymer characterization, but the conference goes beyond that initial goal and now addresses the whole field of polymeric materials. The Short Course on Polymer Characterization, held usually on the first conference day, was established at the very beginning by the POLYCHAR founders: Witold Brostow, Michael Hess, and Kevin P. Menard. The Short Course serves as a tutorial for newcomers in the field of polymer science as well as an update by specialists in the field on recent developments in analysis and characterization of polymer systems. A full list of the topics covered in the Short Course can be found online at www.iupac.org/publications/ci/2013/3504/cc3_110313.html.

The focus of POLYCHAR 21 was "Promoting Green Chemistry," with sessions on Nano- and Smart Materials, Polymers in Electronics and Optoelectronics, Predictive Methods and Simulation, and Biomaterials and Natural and Biodegradable Polymers, among others.

The conference included three plenary speeches:

- Changhyun Choi (Samsung Total Petrochemicals, Chungnam, Korea): "Polymer Industry in Korea—Past, Present, and Future"
- Hiroyuki Ono (Tokyo University of Agriculture, Tokyo, Japan): "Ionic Liquids: Potential Partner for Biorafinery"
- Chris Ober (Cornell University, Ithaca, USA): "Lithography: A Tool in Accessing the Performance of Polymers and Other Materials Systems"

Nine keynote speakers introduced the individual sessions of the conference. A list of the topics covered in each session can be found at www.polychar21-korea.org.

Financial support from IUPAC allowed 12 students from emerging countries in Asia, Africa, and South America to attend.

The P.J. Flory Polymer Research prize was given to Betty L. Lopez, University of Antioquia, Medellin, Colombia, for her work on "Synthesis and Application of Meso-Nanoscopic Polymer Systems" and for fostering polymer science in Colombia.

The International Materials Science Prize was given to Holger Schoenherr, University of Siegen, Siegen, Germany, for his work on "Chemistry and Physics of Organic Biointerfaces" and for his successful international cooperation.

Three IUPAC Poster Prizes were awarded (full details online):

- Shuk Ping Wong (University of Hong Kong, China),
- Kwang-Ho Ko (Chosun University, Gwangju, South Korea)
- Jeremiah Millare (Mapua Institute of Technology, Manila, Philippines)

The Jűrgen Springer Prize for a Young Scientist was given to Jelena Ciric (University of Groningen, The Netherlands), "Size-Exclusion Chromatography with Multidetection in Combination with MALDI-TOF MS as a Tool for Unreavelling the Mechanism of the Enzymatic Polymerization of Polysaccharides"

The Bruce Hartman Prize for a Young Scientists went to Nicolas Delpove (Universite de Rouen, France), "Evidence of two Mobile Amorphous Phases in Semicrystalline Polylactide From Calorimetric Investigations"

The Carl Klason Prize for an Outstanding Student Presentation was awarded to the three ex aequo winners (full details online):

- Mathias Bechert (Friedrich-Alexander University, Erlangen, Germany)
- M. Elizabeth Welch (Cornell University, Ithaca, USA)
- Nowsheen Goonoo (University of Mauritius, Réduit, Mauritius)

The participants left Gwangju expressing their appreciation of a very effective conference with the familiar atmosphere they are used to from the earlier meetings. They were impressed by the kindness and great hospitality of the Korean people. POLYCHAR 22 will be held in Stellenbosch, South Africa, most likely in March 2014.

www.polychar21-korea.org

Biorefinery—Biobased Value Chains and Sustainable Development

8–12 September 2013, Olsztyn, Poland

The concept of a biorefinery generating a spectrum of biomass-based products arranged in a value chain is the biggest research challenge for the next decades. First, the development of this concept requires an interdisciplinary research approach. Second, applied research effects associated with biorefineries, new biorefinery processes, and products implemented in the future will integrate three fundamental areas of sustainable development: economy, environment, and society.

The **4th International Environmental Best Practices Conference "Biorefinery—Biobased Value Chains and Sustainable Development"** will summarize research achievements and new trends in many interrelated aspects associated with biorefinery processes and products. They will be discussed in the eight consecutive research panels of session presentations and posters:

1. Biorefinery—Research Progress and Opportunities
2. Feedstock
3. Genetics and Biotechnology
4. Biomass Pretreatment
5. Bioprocesses and Bioproducts
6. Valorization of Waste, Effluents and By-products by Microorganisms and Enzymes
7. Thermal, Chemical and Biochemical Conversion of Biomass to Useful Energy
8. Environmental Impact

www.ebp4.pl

See Mark Your Calendar for contact information.

Niger 2013

16–20 September 2013, Minna, Nigeria

The Chemical Society of Nigeria's 2013 international conference will be held under the theme "Global Sustainable Economic Development: Challenges and Opportunities for the Developing Nations." The event will take place 16–20 September 2013 in Justice Legbo Kutigi International Conference Centre, Minna, Niger State, Nigeria.

Participants who wish to present papers at the technical sessions are requested to submit their abstracts (200 words maximum) and full papers (A-4 typed double spaced, and 8 pages maximum) by email to loctechnical@chemsocnigeria.org.

All papers are to be peer-reviewed, and accepted papers will be published in the conference proceedings. The deadline for the submission of abstracts is 9 July 2013 and for the submission of full papers is 19 July 2013.

http://chemsocnigeria.org

Radiochemistry

22–27 September 2013, Kanazawa, Japan

The **5th Asia-Pacific Symposium on Radiochemistry '13** (APSORC13) will take place in Kanazawa, Japan, from 22–27 September, 2013. The symposium is dedicated to providing a platform for discussion and information exchange for current and emerging research in all fields of nuclear and radiochemistry as well as related disciplines and technologies. A special session on the issues caused by the Fukushima Daiichi Nuclear Power Plant accident in March 2011 will be also organized. The APSORC 13 is co-organized by The Japan Society of Nuclear and Radiochemical Sciences and Kanazawa University.

www.apsorc13.org

See Mark Your Calendar for contact information.

Planetary Systems

11–15 November 2013, Bangkok, Thailand

This symposium is the first of a new series of events initiated by COSPAR that aims to promote space research at a regional level in emerging countries. The symposia, to be held every two years in a different area of the world, will include multidisciplinary and training sessions.

This first symposium will address the theme "Planetary Systems of our Sun and other Stars, and the Future of Space Astronomy." It is open to participants from all regions, but scientists, young professionals, and students in Asia are encouraged to participate. The symposium will feature plenary lectures as well as parallel and poster sessions.

A capacity-building workshop on "Atmospheric Correction of Earth Observation Data for Environmental Monitoring: Theory and Best Practices" will also take place in Bangkok the week before the symposium, 4–8 November 2013. Participants from the Asian region will be selected by application.

www.cospar2013.gistda.or.th

Modern Physical Chemistry for Advanced Materials

26–30 June 2014, Kharkiv, Ukraine

The IUPAC-sponsored conference on **Modern Physical Chemistry for Advanced Materials** will take place 26–30 June 2014 in Kharkiv, Ukraine. The organizing committee has received agreements from V.N. Karazin Kharkiv National University and National Academy of Sciences of Ukraine to support the conference. This is the second conference organized by chemists of Kharkiv National University in collaboration with colleagues from other countries under the sponsorship of IUPAC and the National Academy of Science of Ukraine; the first one took place in Kharkiv in 2007 (see May-June 2008 *CI*).

The main goals of the conference are as follows:

- survey modern physical chemistry in Ukraine and compare it with the global discipline
- strengthen the international collaboration of Ukrainian physical chemists
- develop the physico-chemical foundations of modern material science, technology, and ecology

The conference will feature 20 plenary and invited lectures, which will be delivered by scientists from Brazil, France, Germany, Great Britain, Japan, Ukraine, and USA.

Abstracts for oral and poster presentations are invited. Brief abstracts (one page) should be submitted by email to <beketov2014@karazin.ua>.

See Mark Your Calendar for contact information.

Visas

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

How to Apply for IUPAC Sponsorship

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

www.iupac.org

Mark Your Calendar

Upcoming IUPAC-sponsored events
See also www.iupac.org/home/conferences.html for links to specific event websites

2013 (after 1 August)

28 July–1 August 2013 • Organometallic Chemistry • Fort Collins, Colorado, USA
17th International IUPAC Conference on Organometallic Chemistry Directed Towards Organic Synthesis
Prof. E. Peter Kündig, Université de Genève, Département de Chimie Organique, CH-1211 Genève 4, Switzerland
Tel.: +41 22 379 6093, Fax: +41 22 328 7396, E-mail: peter.kundig@unige.ch

28 July–2 August 2013 • Novel Aromatic Compounds • Taipei, Taiwan
15th International Symposium on Novel Aromatic Compounds (ISNA-15)
Prof. Ken-Tsung Wong, Taiwan National University, Department of Chemistry No. 1, Sec. 4, Roosevelt Road, Taipei 10167 Taiwan, Tel.: +886 2 3366 1665, Fax: +886 2 3366 1667, E-mail: kenwong@ntu.edu.tw

4–9 August 2013 • Homogeneous and Heterogeneous Catalysis • Sapporo, Japan
16th International Symposium on Relations between Homogeneous and Heterogeneous Catalysis (ISHHC-16)
Prof. Atsushi Fukuoka, Hokkaido University, Kita 21-10, Sapporo 001-0021, Japan
Tel.: +81 11 706 9140, Fax: +81 11 706 9140, E-mail: fukuoka@cat.hokudai.ac.jp

11–16 August 2013 • IUPAC 44th Congress • Istanbul, Turkey
44th IUPAC Congress—Clean Energy Through Chemistry
Prof. Mehmet Mahramanlioglu, Turkish Chemical Society, Istanbul University, Department of Chemistry, TR-34320 Avcilar, Istanbul, Turkey
Tel.: +90 212 591 1996, Fax: +90 212 591 1997, E-mail: mehmah@istanbul.edu.tr, www.iupac2013.org

13–16 August 2013 • MacroMolecular Complexes • Clemson, South Carolina, USA
15th International Symposium on MacroMolecular Complexes (MMC-15)
Prof. Anthony Guiseppi-Elie, Clemson University, Department of Chemical & Biomolecular Engineering, 132 Earle Hall, Clemson, SC 29634, USA, Tel.: +1 864 656 1712, Fax: +1 864 656 1713, E-mail: guiseppi@clemson.edu

18–23 August 2013 • Advanced Polymers via Macromolecular Engineering • Durham, UK
10th International Conference on Advanced Polymers via Macromolecular Engineering (APME-2013)
Prof. Neil R. Cameron, Department of Chemistry, Durham University, Durham, DH1 3LE, UK
Tel.: +44 191 334 2008, Fax: +44 191 384 4737, E-mail: n.r.cameron@durham.ac.uk

25–29 August 2013 • Analytical Chemistry • Warsaw, Poland
XVIIth European Conference on Analytical Chemistry (EuroAnalysis XVII)
Prof. Maciej Jarosz, Warsaw University of Technology, Department of Analytical Chemistry, Ul. Naokowskiego 3, PL-00 664 Warsaw, Poland, Tel.: +48 22 234 7408, Fax: +48 22 234 7408, E-mail: mj@ch.pw.edu.pl

8–12 September 2013 • Biorefineries • Olsztyn, Poland
4th International Environmental Best Practices Conferences: "Biorefineries: Biobased Value Chains for Sustainable Development"
Prof. Janusz Golaszewski, University of Warmia and Mazury, Centre for Renewable Energy Research, Oczapowskiego 8, PL-10 719 Olsztyn, Poland, Tel.: +48 89 523 4805, E-mail: janusz.golaszewski@uwm.edu.pl

22–27 September 2013 • Radiochemistry • Kanazawa, Japan
5th Asia-Pacific Symposium on Radiochemistry (APSORC '13)
Prof. Noriyuki Momoshima, Kyusyu University, Radioisotope Center, 6-10-1 Hakozaki, Fukuoka 812-8581, Japan
Tel.: +81 92 642 2703, Fax: +81 92 642 2706, E-mail: momoshima.noriyuki.551@m.kyushu-u.ac.jp

23–28 September 2013 • Ionic Polymerization • Awaji Island, Japan
21st International Symposium on Ionic Polymerization (IP2013)
Prof. Tatsuki Kitayama, Osaka University, Department of Chemistry, Toyonaka, Osaka 560-8531, Japan
Tel.: +81 6 6850 6230, Fax: +81 6 6841 0104, E-mail: kitayama@chem.es.osaka-u.ac.jp

24–26 September 2013 • Biorefineries • Brasília, Brazil
2nd Brazilian Symposium on Biorefineries (II SNBr)
Dr. Sílvio Vaz, Jr. , EMBRAPA Agroenergy Parque Estação Biológica, Av. W3 Norte, Asa Norte Brasília, DF 70770-901 Brazil, Tel.: +55 61 3448 2315, Fax: +55 61 3448 1589, E-mail: silvio.vaz@embrapa.br

17–22 October 2013 • Novel Materials • Shanghai, China

9th International Conference on Novel Materials and their Synthesis (NMS-IX)

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

8–13 December 2013 • Frontiers of Polymers • Auckland, New Zealand

12th International Conference on Frontiers of Polymers and Advanced Materials (ICFPAM 2013)

Prof. Paul Kilmartin, School of Chemical Sciences, University of Auckland, 23 Symonds Street, P.O. Box 92019, Auckland 1142 New Zealand

Tel.: +64 9 373 7599 x 88272, Fax: +64 9 373 7422, E-mail: p.kilmartin@auckland.ac.nz

2014

12–17 January 2014 • Carbohydrate • Bangalore, India

27th International Carbohydrate Symposium (ICS 2014)

Prof. N. Jayaraman, Indian Institute of Science, Department of Organic Chemistry, Bangalore 560 012, India

Tel.: +91 80 2293 2578, Fax: +91 80 2360 0529, E-mail: ics27@orgchem.iisc.ernet.in

27–28 February 2014 • Young Scientists • Blankenberge, Belgium

Chemistry Conference for Young Scientists 2014

Prof. Thomas Vranken, Universiteit Hasselt, Institute of Materials Research, Martelarenlaan 42, B-3500 Hasselt Belgium, Tel./Fax: +32 11 268 393, E-mail: thomas.vranken@chemcys.be

5–7 March 2014 • Applied Chemistry • Suva, Fiji

International Conference on Applied Chemistry 2014

Prof. S. Sotheeswaran, Institute of Chemistry Ceylon, Adamantane House, 341/22 Kotte Road, Rajagiriya, Sri Lanka, E-mail: sotheeswaran@hotmail.com

3–4 April 2014 • Chemistry Education • Colombo, Sri Lanka

Professional Chemical Education and Research for Industrial Development and Sustainable Economic Growth

Prof. Ramanee D. Wijesekera, University of Colombo, Department of Chemistry, P.O. Box 1490, Colombo 3, Sri Lanka, Tel.: +94 112 503 367, Fax: +94 112 503 367, E-mail: ramanee@chem.cmb.ac.lk

2–6 June 2014 • Polymer Systems • St. Petersburg, Russia

8th International Symposium on Molecular Mobility and Order in Polymer Systems

Prof. Tatiana Birshtein, Russian Academy of Sciences, Institute of Macromolecular Compounds, Bolshoi Pr. 31 RF-199004 Saint Petersburg, Russia

Tel.: +7 812 328 8542, Fax: +7 812 328 6869, E-mail: birshtein@imc.macro.ru

26–30 June 2014 • Physical Chemistry • Kharkiv, Ukraine

Modern Physical Chemistry-2014 (MPC '14)

Dr. Olexander Lebed, Department of Physical Chemistry, Karazin Kharkiv National University, Svoboda Square 4, UA-61022 Kharkiv, Ukraine, Tel.: +380 57 707 54 45, E-mail: beketov2014@karazin.ua

13–18 July 2014 • Chemistry Education • Toronto, Canada

23rd International Conference on Chemistry Education (ICCE-23)

Prof. Judith C. Poë, University of Toronto, Mississauga, Department of Chemical & Physical Sciences, 3359 Mississauga Road, Mississauga, ON L5L 1C6, Canada

Tel.: +1 905 828 3803, Fax: +1 905 828 5425, E-mail: judith.poe@utoronto.ca

13–18 July 2014 • Photochemistry • Bordeaux, France

XXVth IUPAC Symposium on Photochemistry

Dr. Dario M. Bassani, Université de Bordeaux, ISM, UMR 5255, 351, Cours de la Libération, F-33400 Talence, France, Tel.: +33 540 002 827, Fax: +33 674 035 055, E-mail: d.bassani@ism.u-bordeaux1.fr

10–14 August 2014 • Pesticide Chemistry • San Francisco, California, USA

13th International Congress on Pesticide Chemistry

Dr. Kenneth D. Racke, Dow Agrosciences, 9330 Zionsville Road Building 308/2E, Indianapolis, IN 46268, USA

Tel.: +1 317 337 4654, Fax: +1 317 337 4649, E-mail: kracke@dow.com

17–22 October 2013 • Novel Materials • Shanghai, China

9th International Conference on Novel Materials and their Synthesis (NMS-IX)

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

8–13 December 2013 • Frontiers of Polymers • Auckland, New Zealand

12th International Conference on Frontiers of Polymers and Advanced Materials (ICFPAM 2013)

Prof. Paul Kilmartin, School of Chemical Sciences, University of Auckland, 23 Symonds Street, P.O. Box 92019, Auckland 1142 New Zealand

Tel.: +64 9 373 7599 x 88272, Fax: +64 9 373 7422, E-mail: p.kilmartin@auckland.ac.nz

2014

12–17 January 2014 • Carbohydrate • Bangalore, India

27th International Carbohydrate Symposium (ICS 2014)

Prof. N. Jayaraman, Indian Institute of Science, Department of Organic Chemistry, Bangalore 560 012, India

Tel.: +91 80 2293 2578, Fax: +91 80 2360 0529, E-mail: ics27@orgchem.iisc.ernet.in

27–28 February 2014 • Young Scientists • Blankenberge, Belgium

Chemistry Conference for Young Scientists 2014

Prof. Thomas Vranken, Universiteit Hasselt, Institute of Materials Research, Martelarenlaan 42, B-3500 Hasselt Belgium, Tel./Fax: +32 11 268 393, E-mail: thomas.vranken@chemcys.be

5–7 March 2014 • Applied Chemistry • Suva, Fiji

International Conference on Applied Chemistry 2014

Prof. S. Sotheeswaran, Institute of Chemistry Ceylon, Adamantane House, 341/22 Kotte Road, Rajagiriya, Sri Lanka, E-mail: sotheeswaran@hotmail.com

3–4 April 2014 • Chemistry Education • Colombo, Sri Lanka

Professional Chemical Education and Research for Industrial Development and Sustainable Economic Growth

Prof. Ramanee D. Wijesekera, University of Colombo, Department of Chemistry, P.O. Box 1490, Colombo 3, Sri Lanka, Tel.: +94 112 503 367, Fax: +94 112 503 367, E-mail: ramanee@chem.cmb.ac.lk

2–6 June 2014 • Polymer Systems • St. Petersburg, Russia

8th International Symposium on Molecular Mobility and Order in Polymer Systems

Prof. Tatiana Birshtein, Russian Academy of Sciences, Institute of Macromolecular Compounds, Bolshoi Pr. 31 RF-199004 Saint Petersburg, Russia

Tel.: +7 812 328 8542, Fax: +7 812 328 6869, E-mail: birshtein@imc.macro.ru

26–30 June 2014 • Physical Chemistry • Kharkiv, Ukraine

Modern Physical Chemistry-2014 (MPC '14)

Dr. Olexander Lebed, Department of Physical Chemistry, Karazin Kharkiv National University, Svoboda Square 4, UA-61022 Kharkiv, Ukraine, Tel.: +380 57 707 54 45, E-mail: beketov2014@karazin.ua

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IUPAC Periodic Table of the Elements

1																	18
1 **H** hydrogen [1.007, 1.009]	2		Key: atomic number **Symbol** name standard atomic weight									13	14	15	16	17	2 **He** helium 4.003
3 **Li** lithium [6.938, 6.997]	4 **Be** beryllium 9.012											5 **B** boron [10.80, 10.83]	6 **C** carbon [12.00, 12.02]	7 **N** nitrogen [14.00, 14.01]	8 **O** oxygen [15.99, 16.00]	9 **F** fluorine 19.00	10 **Ne** neon 20.18
11 **Na** sodium 22.99	12 **Mg** magnesium [24.30, 24.31]	3	4	5	6	7	8	9	10	11	12	13 **Al** aluminium 26.98	14 **Si** silicon [28.08, 28.09]	15 **P** phosphorus 30.97	16 **S** sulfur [32.05, 32.08]	17 **Cl** chlorine [35.44, 35.46]	18 **Ar** argon 39.95
19 **K** potassium 39.10	20 **Ca** calcium 40.08	21 **Sc** scandium 44.96	22 **Ti** titanium 47.87	23 **V** vanadium 50.94	24 **Cr** chromium 52.00	25 **Mn** manganese 54.94	26 **Fe** iron 55.85	27 **Co** cobalt 58.93	28 **Ni** nickel 58.69	29 **Cu** copper 63.55	30 **Zn** zinc 65.38(2)	31 **Ga** gallium 69.72	32 **Ge** germanium 72.63	33 **As** arsenic 74.92	34 **Se** selenium 78.96(3)	35 **Br** bromine [79.90, 79.91]	36 **Kr** krypton 83.80
37 **Rb** rubidium 85.47	38 **Sr** strontium 87.62	39 **Y** yttrium 88.91	40 **Zr** zirconium 91.22	41 **Nb** niobium 92.91	42 **Mo** molybdenum 95.96(2)	43 **Tc** technetium	44 **Ru** ruthenium 101.1	45 **Rh** rhodium 102.9	46 **Pd** palladium 106.4	47 **Ag** silver 107.9	48 **Cd** cadmium 112.4	49 **In** indium 114.8	50 **Sn** tin 118.7	51 **Sb** antimony 121.8	52 **Te** tellurium 127.6	53 **I** iodine 126.9	54 **Xe** xenon 131.3
55 **Cs** caesium 132.9	56 **Ba** barium 137.3	57-71 lanthanoids	72 **Hf** hafnium 178.5	73 **Ta** tantalum 180.9	74 **W** tungsten 183.8	75 **Re** rhenium 186.2	76 **Os** osmium 190.2	77 **Ir** iridium 192.2	78 **Pt** platinum 195.1	79 **Au** gold 197.0	80 **Hg** mercury 200.6	81 **Tl** thallium [204.3, 204.4]	82 **Pb** lead 207.2	83 **Bi** bismuth 209.0	84 **Po** polonium	85 **At** astatine	86 **Rn** radon
87 **Fr** francium	88 **Ra** radium	89-103 actinoids	104 **Rf** rutherfordium	105 **Db** dubnium	106 **Sg** seaborgium	107 **Bh** bohrium	108 **Hs** hassium	109 **Mt** meitnerium	110 **Ds** darmstadtium	111 **Rg** roentgenium	112 **Cn** copernicium		114 **Fl** flerovium		116 **Lv** livermorium		

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

Notes

- IUPAC 2011 Standard atomic weights abridged to four significant digits (Table 4 published in *Pure Appl. Chem.* 85, 1047-1078 (2013); http://dx.doi.org/10.1351/PAC-REP-13-03-02. The uncertainty in the last digit of the standard atomic weight value is listed in parentheses following the value. In the absence of parentheses, the uncertainty is one in that last digit. An interval in square brackets provides the lower and upper bounds of the standard atomic weight for that element. No values are listed for elements which lack isotopes with a characteristic isotopic abundance in natural terrestrial samples. See PAC for more details.
- "Aluminum" and "cesium" are commonly used alternative spellings for "aluminium" and "caesium."
- Claims for the discovery of all the remaining elements in the last row of the Table, namely elements with atomic numbers 113, 115, 117 and 118, and for which no assignments have yet been made, are being considered by a IUPAC and IUPAP Joint Working Party.

For updates to this table, see iupac.org/reports/periodic_table/. This version is dated 1 May 2013.

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