# CHEMISTRY International

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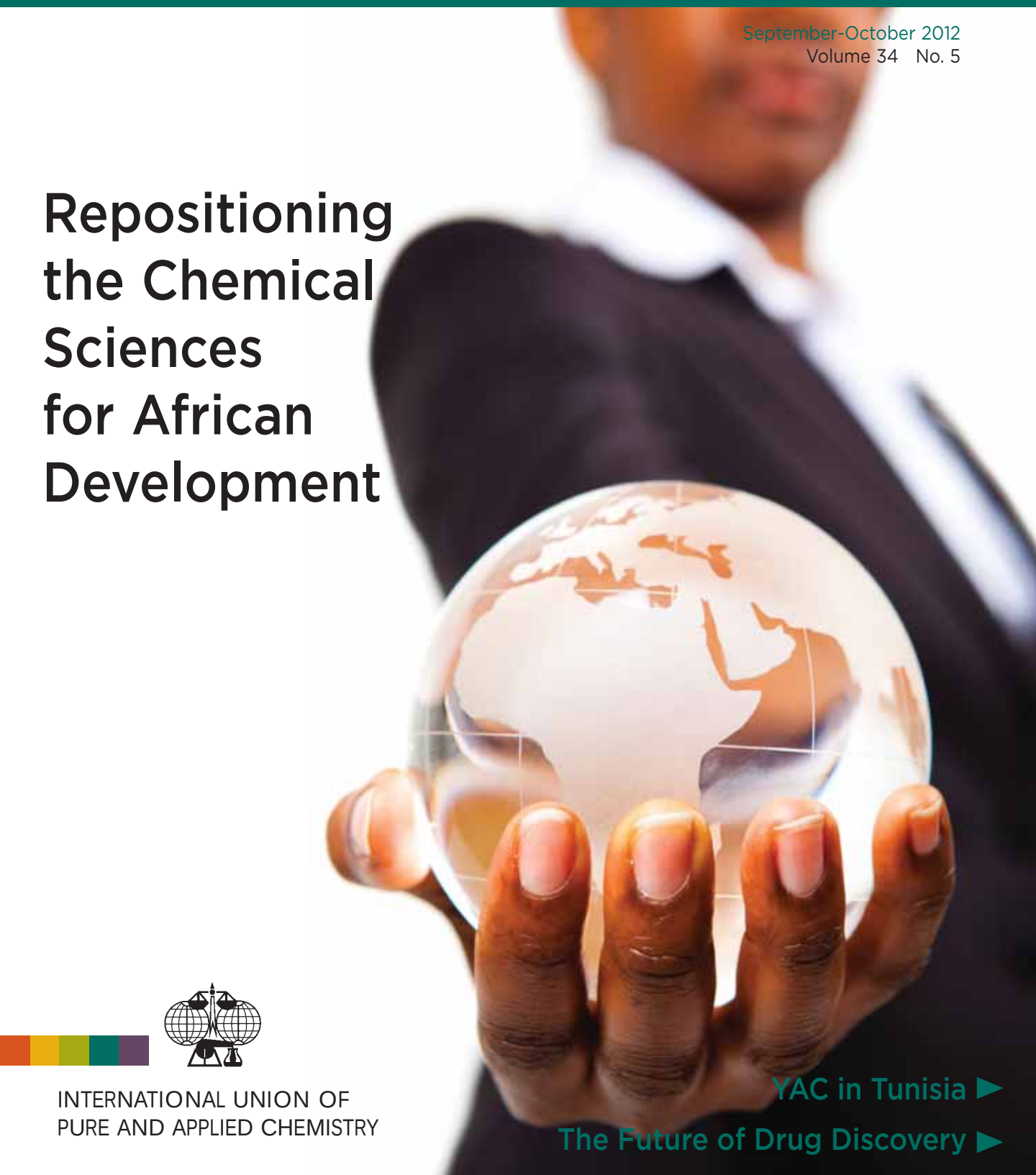
# Repositioning the Chemical Sciences for African Development



INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

YAC in Tunisia ►

The Future of Drug Discovery ►

**CHEMISTRY** International

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

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# From the Editor

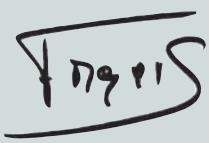
Africa—two features in this issue take us there. One, by Berhanu Abegaz offers a clear and hopeful vision of how Africa can become an active participant in the global scientific forum (p. 4). Abegaz presented these views just a year ago during the World Chemistry Leadership Meeting held at the IUPAC Congress in Puerto Rico in August 2011. The WCLM provided a prelude to the debate about chemistry's role in sustainable development. A report from that WCLM was presented in the Mar-Apr 2012 *CI*.

Abegaz states that "A challenge of Africa's strategic planning for development is how to unleash the power of this youth to bring about the continent's development." Without question, similar debates took place this year during the UN Rio+20 conference, which received abundant media coverage. Of relevance to chemists was the forum organized by ICSU, the International Council for Science (i.e., IUPAC's parent organization), on Science, Technology, and Innovation for Sustainable Development, which provided an opportunity to reflect on science's contribution to sustainable development since the first Earth Summit 20 years ago. Just as important, the forum explored how science can contribute most effectively in the future. Read more about the ICSU forum on page 12.

Three months after Rio+20, it may be somewhat easier to soak in the eloquently branded theme of the meeting: "The Future We Want." Download the pdf from www.un.org/en/sustainablefuture and there you have it: 49 pages containing 283 concise statements. It is impossible for chemists to ignore the call: Statements 213 to 223 are bundled in a section titled "Chemicals and Waste."

"We need to better explain what chemistry is all about," says Abegaz, recalling the story of a chemistry student who tried to explain to his mother what he was studying. That leads to the second feature of this issue that highlights Africa: a report on the Young Ambassadors for Chemistry—YAC—adventure in Tanzania (p. 7). YAC initiatives, supported by the IUPAC Committee on Chemistry Education, have been reported on several times in *CI*, but this latest experience in Tanzania shows a new level of engagement by the local community.

In these features, the role and importance of youth is prominent. This sentiment was expressed succinctly by Desmond Tutu, who began his video address to Rio+20 with a Keynan proverb: "The world was not given to you by your parents; it was lent to you by your children." These words said Tutu, ". . . tell you everything about the future I want—all the things people want for their own children, and for their children's children: A fair society. A healthy planet. Clean air. Safe drinking water. Good jobs. Energy security. Food security. The right to develop in a sustainable way . . ." (www.un.org/en/sustainablefuture/tutu.shtml).



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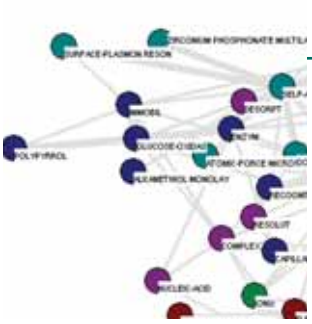


*Stamps International, 3*

# The Times They Are a Changing . . .

*by John Corish*

**Three years ago in this column I commented on the rapidity with which the global recession had descended upon us and on its severity. Unfortunately, it has not yet gone away but continues to influence, and in some cases control, almost every aspect of our lives.**

Despite the recessionary times, the International Year of Chemistry was a very significant success for us chemists, which we will better be able to quantify when the analyses that are underway have been completed. From a financial viewpoint, and as I indicated in an interim report on the IYC last year, we managed to live well within the monetary limit of half-a-million U.S. dollars of direct expenditure set by the Executive Committee. This was due principally to the generous sponsorship provided for the cornerstone events and general facilities, such as the website. The best estimate that is available for the direct cost to the Union is USD 146 000. There were, of course, also somewhat larger uptakes of some parts of our regular budgets, such as for printing and travel, because of the increased activity at the Secretariat and by the officers. Given the prevailing financial climate this is a very commendable outcome and we remain most grateful for the support given by our sponsors to the IYC, as well as to all who supported the year throughout the world.

*We remain most grateful for the support given by our sponsors to the IYC, as well as to all who supported the year throughout the world.*

The lingering recession has, however, adversely affected two of the Union's traditional income streams during the past year. The first and more severe of these and the one that will have the more immediate impact is the income from our publishing operations. Libraries all over the world have had their budgets reduced and have been scrutinizing their purchasing more closely. We have seen and reported over the past number of years a falloff in the sale of our journal *Pure and Applied Chemistry* and of our books. However, the indications are that decreases during this past year have been even more severe than had been anticipated. In addition, the challenge, not unique to us, of striking the correct balance in production between the printed and electronic versions of the journal remains. One idea that has been introduced for discussion, and which we are currently considering, is to seek new arrangements possibly entailing forming a relationship with an established publishing house that will result in reduced costs for us as well as gaining access for our publications to enhanced marketing capabilities. It is important to remember that the publication and dissemination of *Pure and Applied Chemistry* is an essential link in bringing the fruits of our nomenclature, terminology, and standardization work to the worldwide community of chemists. The Union has always been most generous in making the fruits of its work available as freely and widely as possible. It is becoming clear that the changed circumstances in which we now operate make it imperative that we seek to realize at least some of the value of the work undertaken by our members by putting in place mechanisms that will charge and produce income for us in return for the benefits of its usage.

The second change that has asserted itself, particularly during the past six months, is that the type of investment instrument–namely bonds—that was best suited to our needs is simply no longer available on the market to us or to anyone else. At its meeting in February 2012, the Finance Committee had decided to continue to place a part of our portfolio in bonds, but now the rates have declined to such an extent that the resulting returns would cause a substantial reduction in our ability to carry out the data collection and collation, research, and projects necessary to maintain the flow of information and services as we now do. While this is a less immediate problem for us it is nonetheless serious and we clearly need to find a solution to preserve or replace the income stream from our investments. This situation is of course being continuously monitored by those responsible and alternative solutions will in due course emerge.

This changed order of things has brought calls for action on the financial front to find a new foundation that will enable us to continue our work programs and to bring the outcomes of our divisions, standing committees, conferences, and workshops to the attention of the worldwide chemistry community. It is most important for us to stabilize and ensure the continued publication of *Pure and Applied Chemistry* as the main vehicle for the dissemination of the basic outputs for which IUPAC is universally known. The same is true for *Chemistry International*, which serves important func-

tions as a newsmagazine, highlighting and reporting on our activities and playing a unifying role between our various fields of endeavor. It is therefore essential that we maintain and hopefully increase our overall income so that we can support the project system from which our outputs emanate and also the other ways in which we promote our subject such as by assisting in the teaching of chemistry, by providing incentives through prizes for young chemists, and through assisting the Chemistry Olympiad. We also owe it to ourselves and to everyone who works pro bono for chemistry to become even more efficient in all of our operations so that we can do more with our funds. I am confident that we can achieve these objectives and will particularly welcome any suggestions that any of you may have as to ways in which you feel the work that you do for IUPAC can assist in our efforts to meet the challenges ahead.

**John Corish <jcorish@tcd.ie> has been treasurer of IUPAC since January 2008. He has served IUPAC at many levels since 1979, including chair of the Subcommittee on Materials Chemistry, president of the Inorganic Chemistry Division, and member of the Finance Committee.**

# Stamps International

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

## The Mother of All Molecules

The initial disclosure of the molecular structure of deoxyribonucleic acid (DNA) by James Watson and Francis Crick appeared as a short communication in the 25 April 1953 issue of the journal *Nature*. The authors concluded their seminal paper with the unassuming but far-sighted assertion that ". . . the specific pairing we have postulated immediately suggests a possible copying mechanism for the genetic material." It was indeed a breakthrough that transformed our understanding of cellular function and, in the ensuing decades, completely revolutionized fields as diverse as medicine, forensics, bioinformatics, and nanotechnology. In December 1962, almost exactly 50 years ago, Watson, Crick, and Maurice Wilkins, their collaborator at King's College, received the Nobel Prize in Physiology or Medicine for their momentous discovery. No account of those involved in the determination of the structure of DNA would be complete without mentioning the key role played by Rosalind Franklin, the British biophysicist and crystallographer (1920–1958) whose X-ray images provided crucial information that Watson and Crick used to build their original model of the iconic molecule.


The stamp from Gabon illustrated in this note, issued in 2000, commemorates the discovery of the structure of DNA as one of the most important scientific achievements of the 20th century. It is part of a set of three stamps that also feature the invention of the transistor and the development of controlled nuclear fission. In turn, the stamp from Tanzania (1990) celebrates the Nobel Prize awarded to Watson, Crick, and Wilkins and shows the famous DNA double helix in purple, with the linked light blue spheres presumably representing complementary hydrogen-bonded base pairs. It also belongs to an eclectic set of stamps that highlights some of the most important technological advances of the last century, including the breaking of the sound barrier by the Bell X-1 plane in 1947 and the descent of the bathyscaphe Trieste to the deepest part of the ocean in 1960. It has been less than 60 years since the structure of DNA was uncovered, so we ought to look forward to the many new exciting applications that are bound to emerge in the decades ahead.


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

# Repositioning the Chemical Sciences for African Development

*by Berhanu M. Abegaz*

**The beginnings of chemistry may be traced to ancient Egyptians nearly 4000 years ago. Evidence for this comes from the so-called *Ebers papyrus* found near Luxor, the old capital of Egypt in the Middle Nile area. This 110-page document, dating to 1550 BC offers much information, referring to up to 700 preparations of various substances. A lot of scientific knowledge that was developed in Egypt, the Middle East, and North Africa formed the basis for the development that emerged in Western Europe during the Renaissance.**

Despite these early beginnings, modern chemistry, as it relates to higher education and research, in Africa is no more than 100 years old. For example, the South African Chemical Institute is celebrating it's centennial this year. In Africa, much of the teaching of chemistry in the first half of the 20th century followed Western standards, with little done to adapt or modify it for relevance to African situations. What little serious research was conducted in Africa was aimed at attaining the quality of research conducted at parent institutions in Europe, Russia, and the USA. Not surprisingly, the pioneers who started this teaching and research in chemistry introduced what they knew best.

The chemical industry and applications of chemistry, which were created and developed in the West, provided so many useful products that to the rest of the world seemed to be just short of miracles. After all, it was the contributions of chemistry that allowed the USA to produce, for the first time, surplus agriculture in the 1950s and 1960s through the use of fertilizers, pesticides, and insecticides. Chemistry gave rise as well to drugs like antibiotics and other medicines and much, much more. Based on these experiences with chemistry, it was believed that economic development in Africa could be created through technology transfer or development assistance from the West. We know this didn't work; it's now clear that technology transfer alone is a faulty approach for bringing about lasting development anywhere, including Africa.

Whether it is in Africa or elsewhere, chemistry needs to redefine and reposition itself. I am not at all sure that we chemists have gone far enough to correct the love-hate relationship with chemistry that exists throughout much of the world. On the one hand, people tend to appreciate the contributions of chemistry, while on the other hate chemicals and the risks associated with them (and not without good reason).

*Young Ambassadors for Chemistry in Grahamstown, South Africa, in March 2007 (see July 2007 CI, p. 21).*

The International Year of Chemistry 2011, with its slogan "Chemistry—our life, our future," gave a huge boost to the image of chemistry among the general public. Chemistry must be relevant and understood by society. Some 25 years ago, an article entitled "The Chemist and His Mother" appeared in *Solutions* (the newsletter of the Chemical Society of Ethiopia), which was written by chemistry school teacher Yohannes Balcha. The article was a conversation between a chemistry student and his mother. The mother, sensing her son's stress as he prepared for exams, decided she should find out what chemistry was all about, thinking she might be able to alleviate some of his stress. The son tried very hard to explain what chemistry was all about, that it deals with understanding the composition and properties of matter . . ., but the mother, who listened with much patience and

eagerness, did not understand what her beloved son was talking about. In her unwavering determination to gain more insight, she decided to find out what this "chemistry of his" would eventually qualify him to be. So, she asks "Will the study of chemistry make you a builder?" "No!" he says to her, those who build roads study civil engineering and are called engineers. "Are you going to be a doctor?" "No! To be a doctor one studies medicine," he replys. The conversation continues in this way, with the son eloquently explaining what chemistry is not, but not succeeding in describing what it is, with the now distressed mother becoming increasingly frustrated. I think the conclusions from this little story are that we need to better explain what chemistry is all about to society.

In 1969, a major conference was held in Kwame Nukrumah's capital, Accra, spearheaded by the Association of African Universities and under the auspices of the Organization of African Unity. The purpose was to establish the African University instead of simply a University in Africa. This debate and intellectual discourse led to recommendations to establish the African University, which was unfortunately derailed by the political and economic problems that Africa faced in the subsequent two decades. But the spirit and essence of that debate is as relevant today as it was 40 years ago. Nevertheless, the succeeding decades witnessed the expansion of higher education.

In the mid-1960s, Africa probably had fewer than 70 universities, now it has close to 700. This massive expansion of higher education resulted in the dilution of the quality of education. Universities focused more on teaching and less on research. Very little effort went into establishing endogenous world-class institutions that would generate new knowledge and undertake serious research to find solutions to the problems of African communities. For many African chemistry departments and research institutions, success is often measured against sets of external standards, such as how they compare to elite institutions outside the continent. As a result, they try to mimic European and North American institutions. This has led to two negative consequences: a lack of relevance and a failure to be innovative. As a result, with very few exceptions, chemistry research in Africa may have made small contributions to global science, but it has not delivered many products for use by the poor people on the ground.

In this regard, the rather slow-to-take-off initiative of the African Union—The Pan-African University—is an important step toward establishing a teaching and research institution more focused on African needs. The university is to be hosted by various countries in the five regions of the continent. Each institution will have a distinct focus area:

- basic sciences, technology, and innovation—Jomo Kenyatta University of Agriculture and Technology in Kenya
- earth sciences—Ibadan
- political science and governance—Yaounde
- water sciences—Algeria
- space sciences—Southern Africa

Pan-African bodies like the African Academy of Sciences and the Association of African Universities are expected to be intimately involved with these initiatives. The African Academy of Sciences participated in the curriculum development of the Pan-African University and argued for the inclusion of the Millennium Development Goals in the discussions. Signed by African heads of state in 2000, the target year for achieving these goals is 2015. Although many countries may be on course to achieve them, it is quite

**Benefits of Water Harvesting and Conservation** *by Joy Mwende Kioko, 15, Machakos Girls High School, Kenya, part of Our Children on Water International Art Exhibition. Organized by the Royal Society of Chemistry in celebration of the International Year of Chemistry, the exhibition featured works from European and African schoolchildren who were asked to express their feelings about water.*

www.chemistry2011.org/participate/featured-ideas/our-children-on-water

# Repositioning the Chemical Sciences for African Development

clear that many poor countries in Africa are unlikely to meet the goals. Therefore, they will remain as the key drivers for sustainable development for some years to come.

Of the eight Millennium Development Goals, six are clearly science driven and would involve chemistry. Scientists have a responsibility to respond appropriately to a world under stress from the effects of climate change. It is important to note that Africa is most vulnerable to these effects, although it may not have contributed as much as other regions to the causes of climate change. Scientists should adopt a broader science platform and engage in a more effective integration and collaboration with other disciplines and knowledge systems.

African scientists should highlight indigenous knowledge systems and strive for effective modernizations and inclusive innovations. There is a need for a new vision of science for sustainable development, which will demand a complete re-engineering of science education and research in Africa. Instead of teaching in fragmented disciplines, sustainable science would be unified and transdisciplinary. Sustainable science would include the epistemology of systems thinking and would encourage inclusive and responsible innovation.

*Young Ambassadors for Chemistry in Kasulu, Tanzania, in April 2012, moving tables to stage the public event held in the nearby football stadium—see feature p. 7.*

This new thinking and re-engineering has been a subject of much intellectual discourse in recent times. Many pan-African institutions (such as the African Academy of Sciences, Network of African Science Academies, African Technology Policy Studies Network, and the Pan African Chemistry Network) have been engaging in such debates. These discussions were stimulated during the Mandela era and the subsequent integration of South Africa into the African Union. The emergence of progressive African leaders at the turn of the 20th century (e.g., Thabo Mbeki of South Africa who proposed the Millennium Africa Recovery Plan, Abdoulaye Wade who came up with the Omega plan) paved the way for articulating a new vision for African development, popularly referred to as the New Partnership for African Development (NEPAD). This partnership resulted in the Consolidated Plan of Action, which includes several Flagship Programs, which are being implemented on regional and subregional levels.

Flagship Programs include such transdisciplinary fields as: biodiversity, biotechnology and indigenous knowledge; energy, water, and desertification; material sciences, manufacturing, laser, and post-harvest technologies; mathematical sciences; and information, communication, and space science technologies. African leaders have endorsed these programs and have established an African Ministerial Committee for Science and Technology, which meets regularly to monitor their progress. NEPAD has now been incorporated into the African Union under the name NEPAD Planning and Coordinating Agency.

Finally, a key issue for Africa's future is the need to encourage young people to become involved in science. Africa's population is now 1 billion, approximately 14 percent of the global population. Of importance, 71 percent of this population is below 25 years of age. This is both a challenge and an opportunity. A challenge for Africa's strategic planning is how to unleash the power of the youth to bring about the continent's development. The African Academy of Sciences has identified engaging the younger generation as a key strategic vision over the next decade. In this regard, it is important that they have role models in the scientific community for them to believe that they can help turn things around in Africa.

This commentary is based on the author's presentation at the World Chemistry Leadership Meeting held 2 August 2011 in San Juan during the IUPAC General Assembly (see Mar-Apr 2012 *CI*, p. 12).

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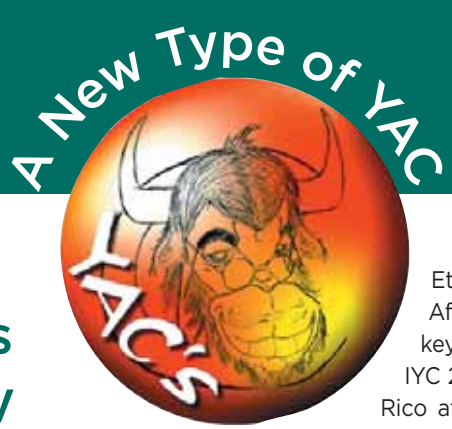
**www.aasciences.org**




# The Young Ambassadors for Chemistry Program Visits Tanzania

*by Lida Schoen, Erica Steenberg, and Mei-Hung Chíu*

**Regular readers of *Chemistry International* are likely familiar by now with the highly successful Young Ambassadors for Chemistry (YAC) program, which has been highlighted in these pages numerous times since its launch in 2004. However, the latest YAC event, which took place 25–27 April 2012 in Kasulu, Tanzania, stands out from the previous 12 iterations (see list on next page) since it was organized and sponsored in a completely different way.**

For those unfamiliar with YAC, it is a project of IUPAC's Committee on Chemistry Education (CCE) that has trained teachers around the globe to help students communicate the benefits of chemistry. A typical YAC event encompasses two to three days of teacher workshops, followed by a one-day public event where students—the Young Ambassadors for Chemistry—share their enthusiasm and interest with the public at large, either in a public square, like it happened in Cyprus (Jul-Aug 2010 *CI*), in a shopping mall as in Taipei (Mar-Apr 2005 *CI*), or as part of a science festival as in Grahamstown, South Africa (Jul-Aug 2007 *CI*). That last day of the YAC event is usually a festive time, with fun for everyone.

In February 2011, as part of the International Year of Chemistry celebrations, YAC events were held in Ethiopia to honor the Federation of African Societies of Chemistry that was key to securing the UN proclamation of IYC 2011. YAC staff also traveled to Puerto Rico at the time of the IUPAC Congress in July to meet with teachers and share ideas on how to further develop and best adapt the YAC program for the local community.

All previous YAC events have been top-down affairs in which international or government organizations have sponsored and organized the workshops and public events at the local level. The Tanzania event—held in the local football stadium with the attendance of 25 teachers from around Kasulu (up to 90 km away) and 50 students from the 14 participating secondary schools—was an entirely bottom-up affair. A group of 14 private schools hosted and facilitated the YAC course, which was locally organized and facilitated by headmaster Gideon Bunyaga of the Kasulu Secondary School.

The story of how this YAC event came to fruition begins with Thadeo Ntambala, who, along with 9 brothers and 2 sisters, grew up in rural Northwest Tanzania not far from the Jane Goodall chimps reserve. Although his parents were illiterate, Thadeo and his siblings went on to become highly educated. Thadeo obtained a Master's degree in telecommunications from Warsaw University of Technology, while his brothers all became engineers. While studying in Warsaw, Thadeo met his (Polish) wife Ewa, a chemist with her own consultancy business. Now based in the Netherlands for Thadeo's IT job, both have become dedicated to furthering education in Tanzania.

In 2010, Ewa approached long-time YAC director Lida Schoen about possibly organizing an event in Tanzania in 2011 to coincide with the International Year of Chemistry. Ewa, Thadeo, and Lida tried for

*Participants, organizers, and helpers of the Young Ambassadors for Chemistry in Kasulu, Tanzania.*

# A New Type of YAC

two years to obtain sponsorship for such an event, but, after many meetings and follow-up they were ultimately unsuccessful. Undaunted, Thadeo arranged a meeting in the Netherlands between his cousin (an engineer in Dar Es Salaam) and Schoen to discuss how they might handle the local organization and sponsorship. Somehow, he managed, getting a group of 14 private schools (including the headmaster of the Teacher Training College) to provide all local costs, including the expenses of the event and subsistence for the teachers, students, and the YAC team. Thadeo and Ewa paid all additional costs (flights, hotel, and local transportation). And, once Schoen and her colleague Erica Steenberg contributed a little as well, the whole effort got off the ground.

On 25 April 2012, the efforts of Thadeo and Ewa Ntambala finally paid off as the formal program of the Young Ambassadors for Chemistry project commenced in Kasulu, Tanzania.

After Schoen and Steenberg briefed the four representatives of the participating schools about the aims and history of the YAC project, participants were given course books and asked to start generating ideas for a chemistry-related Tanzanian "product" or phenomenon. Using an accessible "chemistry in our lives" theme, it was decided that the chemistry projects would involve the local production of soap and the preparation of cassava mash (a staple food) from scratch, providing an opportunity to talk about the dangers of the cyanide-containing variety.

From the beginning, the event attracted lots of attention from the public thanks to two well-amplified and natural leaders, chairman Julius Nzohumpa Ntidoga and science teacher Emmanuel Saguda Kingi of Kasulu Secondary School, who talked at length about the importance of chemistry for the region.

On the last day of the YAC program, the local football stadium was used to host the final public event. Similar to previous YAC events, the students prepared—with a little help from the trained teachers—DNA models and cosmetic products. As the crowd grew, the students acted in made-up TV commercials for their cosmetics and product lines. The students showed great creativity, incorporating little skits, raps, shouting, and dancing into their commercials. An international jury had the difficult job of declaring the winners of the student presentations.

At the end of the event, organizers presented certificates to all participating teachers and students.

Thadeo Ntambala recorded the entire YAC course and event. A four-minute summary of that footage is available on YouTube (with "subtitles"): search for it using "YAC Kasulu."

As is customary at YAC workshops, the teachers were asked to evaluate the program. Of the 18 who responded, 83 percent said they had learned much about the application of chemistry in their daily lives and that they regarded the activity as valuable. All the teachers said they would participate in YAC again. When asked if they would apply what they learned in their classrooms, only 22 percent said that they would not, primarily because of a lack of resources.

All of the organizers and organizations involved received letters of endorsement from Dr. Temechegn Engida, president of the Federation of African Societies of Chemistry. Although it was disappointing that funding from a larger organization could not be secured, this successful YAC course and event showed that CCE also supports bottom-up initiatives!

| YAC Travel Log |
|---|
| Kasulu, Tanzania, in April 2012 |
| Gorna Malina, Bulgaria, in November 2011 |
| San Juan, Puerto Rico , in July 2011 |
| Addis Ababa, Ethiopia, in February 2011 |
| Manila, Philippines, in April 2010 |
| Ipoh, Malaysia, in April 2010 |
| Nicosia, Cyprus, in April 2009 |
| Mauritius, in August 2008 |
| Grahamstown, South Africa, in March 2007 |
| Gwangju, South Korea, in February 2006 |
| Krasnoyarsk, Russia, in November 2005 |
| Buenos Aires, Argentina, in May 2005 |
| Taipei, Taiwan, November 2004 and again in December 2007 |


## Acknowledgments

- **Thadeo Ntambala** (Netherlands), initiator, organizer, and facilitator
- **Fabian Kagadye** (Dar Es Salaam), local organizer in Tanzania
- **Gideon Bunyaga**, headmaster Kasulu Secondary School, with his team of schools, local organizer in Kasulu
- The jury: **Ewa Delezuch Ntambala** (M.Sc., the Netherlands), **Joseph Mwangamila,** headmaster Teacher Training College (Kasulu), and **Gideon Bunyaga**
- **CCE** for facilitating travel and subsistence expenses for Lida Schoen (Netherlands)
- **IFF Netherlands** for donating concentrated oils for perfume
- **Annindriya, Netherlands** for donating small spray bottles for perfume
- **SASOL Germany** for donating detergent for shampoo
- **Seppic France** for donating emulsifier for the emulsion


**For more information, contact Lida Schoen <amschoen@xs4all.nl>.**

**www.iupac.org/project/2007-005-2-050**

# On the Future of Drug Discovery

*by Simon Campbell**

**The pharmaceutical industry has made important contributions to quality of life, longevity, economic growth, and education, and is a key component of the economic growth strategy for many countries. However, the industry is now under considerable pressure as the number of new chemical entities has not increased over the past decade, and there have been significant revenue losses as important drugs lost patent protection. Consequently, the sector has experienced major reductions in R&D budgets, closure of research sites, and the loss of thousands of skilled jobs. A new and sustainable funding model with public-sector participation is urgently required for world-class scientists to invent and develop innovative medicines that meet the medical needs of the 21st century and contribute to economic growth. This perspective considers how these objectives might be achieved, and aims to stimulate discussion.**

**First,** we should build consensus among a group of expert stakeholders with the common objective of informing and influencing future development of world-class healthcare innovation. Learned societies and professional bodies have obviously contributed to the government reviews of life sciences, but we now need to work together to ensure proper focus on drug discovery. Governments have stated a firm commitment to life sciences as a catalyst for growth, but emphasis appears to be on clinical trials, biologics, and


cell therapies rather than on cost-effective and orally delivered small molecules that are the bedrock of any healthcare system.

**Second,** future R&D should focus on therapeutic areas of significant medical need where transformative new drugs will improve quality of life, and bring economic benefit. For example, a recent survey showed that 38 percent of Europeans suffer from mental disorders, with depression being the single greatest burden of all human diseases. Brain disorders cost Europe almost 800 billion Euros per year, which is more than cancer, cardiovascular disease, and diabetes combined. Yet, Pharma is withdrawing from neuroscience research. To encourage investment in such challenging areas, it will be important to define efficacy/safety criteria early in drug discovery programs so that effective new agents can expect fair reimbursement and an acceptable return. This would minimize negative regulatory decisions—which often are made after a company has invested 10 years or more in discovery and development—and would help lower costs.

*. . . the sector has experienced major reductions in R&D budgets, closure of research sites, and the loss of thousands of skilled jobs*

**Third,** we must address attrition as current failure rates during discovery and development are creating higher R&D costs that are simply unsustainable. One approach would be to expand precompetitive collaborations between industry/academia to focus on target selection/validation, predictive toxicology, and to identify patient subgroups that respond to agents with novel mechanisms of action. These initiatives would reduce risk, simplify clinical trials, and lower costs, which would make the sector more attractive for investment, and would also deter parallel and wasteful pursuit of nonvalidated targets. Companies would create intellectual property through innovative, but distinctive, medicinal chemistry programs.

**Fourth,** as Pharma contracts and Biotech struggles for new investment, we must consider alternative models of drug discovery that capitalize on our outstanding record of innovation and productivity. Networks of therapeutic centers of excellence should be established where expert medicinal chemists released by industry can work within multidisciplinary environments to exploit significant investments in biomedical research. Unused assets

from Pharma could be included, and a flow of spin-off companies would revitalize the biotech sector. Such an arrangement would help educate and train of the next generation of research scientists and help create new jobs.

**Fifth,** universities should be encouraged to appoint experienced industrial scientists as professors and researches in their world-class biomedical centers since chemists play a pivotal role in transforming biological discoveries into innovative new medicines. There is also a pressing need to invest in fundamental new chemistries to address challenging biological targets such as protein/protein and protein/nucleotide interactions that are currently beyond traditional drug templates. It is important to realize that the majority of medicinal chemistry "muscle" was located in Pharma and the significant expertise recently lost due to layoffs should be re-captured within therapeutic centers of excellence, or similar initiatives. If world-class Pharma/Biotech talent fades away, it will be difficult to rebuild it in the future.

Finally, any new funding model may require reallocation of current budgets rather than additional monies considering current deficit constraints. However, the European Union recently announced "Horizon 2020," which is investing 80 billion Euros in R&D to improve long-term competitiveness. Of this amount, 8 billion has been set aside for health care, which is considered to be a "major concern." (see http://ec.europa.eu/research/horizon2020) Public-private partnerships involving universities, research centers, and industry will play a key role, and therapeutic centers of excellence make a natural and synergistic fit. Governments, funding bodies, and charities should invest now for future growth, as economic benefits will largely depend on strong drug discovery capabilities that lead to new medicines for worldwide commercialization. Investment in medicinal chemistry will translate biological discoveries into commercial products, consistent with the EU's commitment to life sciences, and will provide economic gains.

The positive benefits of such exciting initiatives include the following:

- new biology would be translated by expert medicinal chemists into innovative new medicines to help meet the healthcare challenges of the 21st century
- quality of life would be improved within constrained healthcare budgets
- important disease areas abandoned by Pharma would receive proper attention, with consequent patient benefits
- assets not being pursued by Pharma would be revived and developed
- economic benefits would flow as innovative medicines enter world markets
- the science base would be strengthened with exciting career opportunities for the next generation of scientists
- the biotech sector would be revitalized as an additional source of innovation/discovery with a sustainable return on investment

**Simon Campbell <campbellsimon@btopenworld.com> is a synthetic organic chemist who spent most of his career at Pfizer where he was a key member of the research teams that discovered Cardura, Norvasc, and Viagra. He later became head of Worldwide Discovery. He has served as president of the Royal Society of Chemistry and now acts as a scientific consultant for biotechs, government agencies, and charities on an international basis.**

* This article is a follow-up to the WCLM held 2 August 2011 in San Juan during the IUPAC General Assembly (see Mar-Apr 2012 *CI*, p. 12). Although this article uses examples from the UK, the general principles presented by Campbell can apply to other regions worldwide.

## Linking Science and Policy at Rio+20

**In June 2012, ICSU organized a major five-day Forum on Science, Technology, and Innovation for Sustainable Development in the days just prior to the Rio+20 conference in Rio de Janeiro.**

According to the organizers, the forum was a great success and had a big impact on the outcomes for science at Rio+20 and beyond. Over 1000 people attended the event from 11–15 June, with another 1000 watching the live webcast and many more interacting via social media. The forum was organized by ICSU, in partnership with UNESCO, the World Federation of Engineering Organizations, the International Social Science Council, the Brazilian Ministry of Science, Technology and Innovation and the Brazilian Academy of Sciences.

The forum brought together leading international scientists, policy-makers, industry professionals, NGOs, journalists, and youth from more than 75 countries to explore the key role of interdisciplinary science and innovation in the transition to sustainable development, a green economy, and poverty eradication.

It was a very exciting and inspiring week for all. Alongside the main plenary sessions, the forum provided smaller spaces for learning, exchange, and networking via 25 side events which ran throughout the week.

"Ensuring a sustainable future in the face of inter-connected, human-induced challenges facing the Earth system urgently requires new knowledge and a new relationship between science and society," said the final communiqué from the forum. Scientists and policy-makers debated themes ranging from energy, food and water security to indigenous knowledge and the green economy. Two important conclusions stood out: the necessity for social and natural scientists to work closely together, and the need for integrated policy approaches.

*Professor Lidia Brito, director, Division of Science Policy and Capacity Building, Natural Sciences Sector, UNESCO, France, speaking at the forum.*

Future Earth, a new 10-year interdisciplinary initiative on research for global sustainability that will bring together natural and social scientists, was launched at the Forum <www.icsu.org/future-earth>.

The final outcome document adopted at Rio+20 on "The Future We Want" <www.un.org/en/sustainablefuture> contained several important references to science:

- need to strengthen the science-policy interface
- decision to develop a set of Sustainable Development Goals
- role and functions of a new High-Level Political Forum

Visit the ICSU forum page for access to all the sessions, summaries, blog and photos, and numerous links to blog and media highlights.

www.icsu.org/rio20/science-and-technology-forum

## ICSU Grants Programme 2013 Call for Applications

**The ICSU Committee on Scientific Planning and Review has issued a call for applications for the ICSU Grants Programme 2013, which supports collaborative scientific initiatives of relevance to science and society. It is a competitive, peer-reviewed program that is open to ICSU Scientific Unions, interdisciplinary bodies, and joint initiatives. It enables collaboration with ICSU Regional Offices and other members of the ICSU community.**

Proposals for 2013 grants must focus on ICSU's strategic priorities listed below and should be international and multidisciplinary. ICSU encourages submission of innovative proposals that (i) actively involve the ICSU Regional Offices, (ii) promote the involvement of young scientists, women scientists, and scientists from developing countries, and/or (iii) forge new partnerships between organisations that do not routinely collaborate.

### ICSU's Strategic Priorities

- Proposals should address, inter alia, issues such as water, energy, health, agriculture, and biodiversity and other issues that address the linked environmental, social, and economic dimensions of sustainable development.
- Proposals that address the need for dialogue between science and policy communities are encouraged. Proposals for review or assessment of scientific knowledge necessary for policy formulation are also welcome.
- Proposals should address, inter alia, issues such as data access, intellectual property rights, and the impact of recent developments in information technologies.
- Proposals for innovative endeavors to develop initiatives exploring new frontiers of science at the interface between different disciplines are encouraged.

The total funding available for the grants program in 2013 is Euro 280 000, with a ceiling of Euro 30 000 for each application.

The grants program is strictly reserved for ICSU members. Applications submitted by IUPAC shall be coordinated from the IUPAC Secretariat. IUPAC members with an interest in developing such a proposal should contact their division president or project committee chair as soon as possible. The ICSU deadline for receipt of applications is 1 December 2012.

icsu.org

## ICSU Issues Recommendations for Organizing International Scientific Meetings

**The universality of science, in its broadest sense, is about developing a truly global scientific community on the basis of equity and non-discrimination. Underpinning this broader concept of universality is the Principle of the Universality of Science (ICSU Statute 5), which deals with the free and responsible practice of science and also requires freedom of movement and of association. These rights and responsibilities extend to organizers and sponsors of international scientific meetings, as well as participants.**

In June 2012, the ICSU Committee on Freedom and Responsibility in the Conduct of Science issued recommendations to help avoid difficulties and improve the chances of a positive resolution where problems do occur. The recommendations are available on the Freedom and Responsibility portal.

www.icsu.org/freedom-responsibility/scientific_meetings_advice

## CHF Catalyst Series on Women in Chemistry

**Women have been central to the chemical and molecular sciences since antiquity, though their role has been—intentionally or not—obscured or missing in the annals of history. Now, the Chemical Heritage Foundations is setting the records straight with several initiatives.**

First, a new series of videos—the Catalyst Series—aims at encouraging young women to pursue careers in science. It tells the stories of fascinating women who dared to follow their drive for success and passion for chemistry—and changed the world for the better. The first three releases are Uma Chowdhry, retired senior vice president and chief science and technology officer of DuPont; Mary L. Good, former president of the American Chemical Society, undersecretary for technology in the U.S. Department of Commerce under President Clinton, and recipient of the Priestley Medal; and Kitty Hach-Darrow, cofounder of the Hach Chemical Company and the only woman to receive CHF's Pittcon Heritage Award.


The second project, Stories from the Field, captures scientific adventures and career insights in short, conversational audio interviews, conducted in part at the American Chemical Society's Fall 2012 National Meeting in Philadelphia.

A third initiative is the CHF oral history project that preserves the history of women's contributions to science, medicine, and technology in their own words. The oral histories in this collection focus on formative experiences, the importance of mentors and networks, as well as the changing roles of women in chemistry throughout the twentieth century.

www.chemheritage.org/discover/online-resources/women-in-chemistry

*For those who follow IUPAC history, Mary Good was very active and well respected in IUPAC in the 1980s. She was president of the Inorganic Chemistry Division from 1981 to 1985 and also served on the Executive Committee for eight years. She succeeded Ted Becker as chair of the U.S. National Committee for IUPAC, a position she held in 1987 when she was ACS president. Becker recalls that Good arranged major industry support for the IUPAC General Assembly in Boston in 1987 and remembers her as a major force on the Bureau and Executive Committee.*

*"You've got to take the opportunities as they appear," Mary Good.*

## The Global Young Academy Calls on Scientific Community to Promote Sustainability

**On 20 June 2012, the Global Young Academy issued a statement calling on the scientific community to do more to promote progress towards global sustainability. "The problem is not science, it is leadership," said GYA co-chair Rees Kassen.**

Members of the GYA feel a special urgency on sustainability, since many of them came of age in the period between the first "Earth Summit" on sustainability in Rio in 1992 and the United Nations Conference on Sustainability—the so-called Rio+20 meeting—held last June. "We are the inheritors of the decisions being made over the next three days," said GYA co-chair Bernard Slippers, "so we have a vested interest in charting the way forward."

According to GYA, the "Sandton Declaration" makes it clear that sometimes scientists are their own worst enemy. Reward structures in science often discourage or even punish public engagement and outreach. "This must change," Kassen says. The declaration calls on the scientific community to revise its reward structures to value knowledge mobilization by scientists themselves. It also encourages scientists to take a more active role in promoting the use of scientific evidence in decision making and encouraging inquiry-based science education in schools and universities.

The Global Young Academy, founded in 2010, describes itself as the voice of young scientists around the world. Members are chosen for their demonstrated excellence in scientific achievement and commitment to civil society. Currently there are 172 members from 54 countries in GYA.

**www.globalyoungacademy.net**

## In Memoriam

IUPAC was saddened to learn of the following deaths of Union colleagues. We shall remember them with respect and gratitude for their service to IUPAC.

**Prof. Rolf E. Bareiss** (Germany)—Rolf Eugen Bareiss, was almost 80, died on 24 April 2012. When he retired in 1997, he was editor in chief for *Hüthig & Wepf*. He was a titular member of the IUPAC Commission on Macromolecular Nomenclature (now Division IV, Polymer Division) from 1983 to 1993.

**Prof. H. Lawrence Clever** (United States)—Professor emeritus of chemistry at Emory University, Larry Clever died on 21 May 2012. He was an associate member on the Commission on Solubility Data in 2000–2001 and also a member on the Subcommittee on Gas Solubility Data, and again member on the Subcommittee on Solubility and Equilibrium Data in 2010–2011. He edited many volumes of the SDS series, and contributed to the volumes of other members of the commission.

**Prof. Toshio Masuda** (Japan)—Professor emeritus of material chemistry at Kyoto University, Japan, T. Masuda died 22 March 2012 at age 74. He was an associate member on the Commission on Polymer Characterization and Properties from 1988–1997 and titular member from 1998–1999.

**Prof. József Nyitrai** (Hungary)—Professor at the Budapest University of Technology and Economics, J. Nyitrai died earlier this year. His association to IUPAC started in 1991 when he became a National Representative on the Commission on Nomenclature of Organic Chemistry, and than an associate member from 1994–2001. From 2002–2003, he was a member of the Advisory Subcommittee of the newly established Chemical Nomenclature and Structure Representation Division (division VIII). He than continued as titular member on Division VIII from 2004 to 2007, associate member from 2008 to 2011. He was also Division VIII Representative on ICTNS from 2006 to 2009, and till this year, involved in several projects.

**Dr. Henrik Olesen** (Denmark)—Professor at the University Hospital of Copenhagen, Henrik Olesen died 15 April 2012. He is most notably the "founding father" of the NPU terminology (i.e., Nomenclature, Properties, and Units in Laboratory Medicine). He was an associate member on the Commission on Nomenclature, Properties, and Units (VII.C.1) from 1985 to 1997 and again in 2000–2001.

**Prof. Anders J. Thor** (Sweden)—Professor at the Swedish Standards Institute in Stockholm, Anders J. Thor died on 7 April 2012. He was ISO representative on ICTNS since 2000 and co-author on the IUPAC Green Book. He was a Associate Member on the Commission on Physicochemical Symbols, Terminology, and Units, from 1994 to 2001 and a National Representative from 2006 to this year.

**Remembrances prepared by IUPAC colleagues are available online at www.iupac.org/publications/ci/2012/3405/iw6_inmemoriam.html.**

## Impact of Nanotechnology on Chemistry: A Terminology Conundrum

The advent of nanoscience and nanotechnology has substantially influenced the vernacular of almost every scientific discipline leading to undiscovered realms of science and creating new research domains (e.g., nanochemistry, nanomedicine, nanomechanics, nanobiotechnology). The fact that nanotechnology does not belong to a single domain of science becomes obvious upon analyzing the publication and citation data. As scientists, standards organizations, and regulatory bodies struggle to agree on a universal terminology, the lack of descriptors and rules to systematize the naming system has led to a plethora of terms (nanoroses, nanobelts, nanoshells, nanocubes, etc.), which often refer to a subjective description of the nanoscopic structural attribute. The wide proliferation and acceptance of the "nanoterminology" in chemistry is reflected in the large and ever-increasing number of publications in all high-impact chemistry journals. In addition, the launch and success of a series of new journals (*ACS Nano*, *NanoLetters*, *Nanoscale*, *Small*, *NatureNanotechnology*) devoted to this area confirm the remarkable growth.

The scope of this IUPAC project (2007-040-2-200) entitled Analysis of the Usage of Nanoscience and Technology in Chemistry was to study the usage of nano-related terminology in chemistry and to analyze its penetration among the various chemical disciplines. Thus, this effort was mainly dedicated to mapping the nano-dominated publication domains by a detailed analysis of peer-reviewed papers, patents, and books. A global analysis of nano- in chemistry terminology should serve as a first step in delivering a guideline for IUPAC to propose some recommendations and suggested terminology in the future. This short summary is extracted from a longer report, available at iupac.org/project/2007-040-2-200, which helps clarify how the emergence of nanotechnology impacts the various fields of chemistry.

To map and critically study the use of the prefix *nano* in various fields of chemistry, different search engines were used to compare the occurrence of nano-containing terms. This information was the input to understand the evolution and usage of nano-containing descriptive terms according to different criteria and to project their validity in scientific (chemical) language.

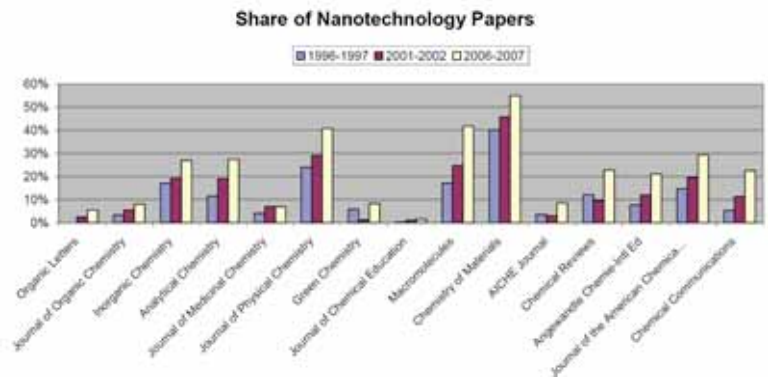
### Keyword-Based Search Strategy

The methodology for collecting key words was a two-step process: In a first step, widely popular chemistry search engines, such as Sci Finder, and the ones provided by the CAS and RSC were used. The hits on "nano*" were analyzed according to different criteria such as time, country, and source. In a second step, the process was repeated by restricting the search to some of the most highly cited journals of each chemistry discipline, to understand if nano- terminology has impacted all the areas of chemistry and if so, to what extent and at what rate. The detailed methodology is explained in the full report. The acquired dataset was based on records from 2000 to 2007 in the field of nano-enhanced publications.

### Findings and Observations

The share of nanotechnology papers in chemistry journals has more than doubled over the past 10 years from 12 percent in 1996–1997 to 26 percent in 2006-2007. While the share of nanotechnology papers has grown, there is considerable variation too:

- Nanotechnology papers accounted for more than 50 percent of all articles and reviews in the journal *Chemistry of Materials* and 40 percent or more in *Macromolecules* and the *Journal of Physical Chemistry*.
- General journals have a "balanced" number of nanotechnology-related papers, with an average of above 20 percent (in 2006).
- Journals in the inorganic and analytical chemistry cover nanotechnology to a similar extent.
- Organic, environmental, and medicinal chemistry journals have also experienced a growth in nano-papers; however, it is only around 10 percent.



- Chemical engineering (e.g., *AICHE Journal*) seems to be only incrementally influenced by the development of nano-terminology.
- Chemistry education is another area of low nanotechnology influence, which is not surprising, as the research-intensive phase generally precedes the transfer to educational concepts.

### A Closer Look at the Specialties

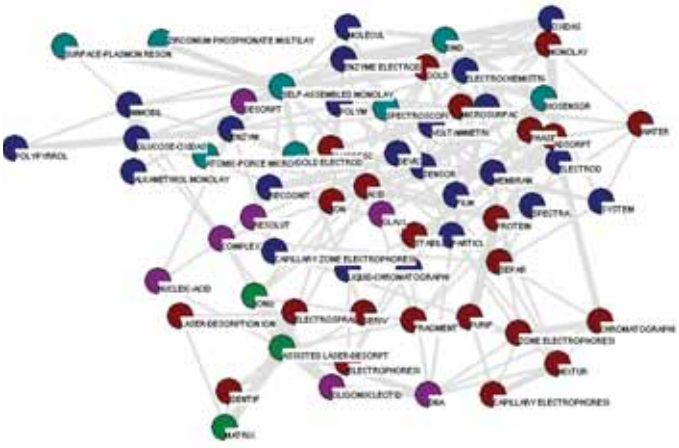
The data presented give an overview of the general impact of an emerging interdisciplinary research area, such as nanotechnology. However, no generalizations should be made at this stage. Another approach to explore the role of nanotechnology in chemistry is to explore the emerging intellectual structures associated with nanotechnology. To this end, the task group has carried out co-word analysis to see what kind of intellectual space nanotechnology occupies in certain chemistry journals. While it was not possible to cover all the journals, the findings and concepts have been applied on a selection of journals in different areas of chemistry and with different "nanotech intensity," including *Analytical Chemistry*, *Macromolecules*, *Chemistry of Materials*, and *Angewandte Chemie-International Edition.*

For each of these journals, all papers (articles and reviews) for 1996–1997, 2001–2002, and 2006–2007 were downloaded. The data were further processed using the Bibexcel bibliometric freeware developed by Prof O. Persson (Umeå University). Keywords were retrieved for each paper and a stemming algorithm was applied; co-word analysis was carried out on the basis of keywords associated with individual articles, meaning that the most frequent keywords in papers are related to each other on the basis of how often they co-occur.

Comparing the top keywords for the different time periods indicates how the journal has developed. Maps can also be a helpful way to visualize the changes over time. The maps were generated for all three periods of the four journals and can be found in the long report. As an example, the figure in the next column shows the keywords map for *Analytical Chemistry* for the period 2006–2007, which shows the main topics investigated during those years and the interconnections among them.

The closer two terms are on the map, the more closely related they tend to be. The different clusters resulting from the analysis of co-occurring terms are illustrated by varying colors.

In summary, the efforts made in this project confirm that nanotechnology crosses many fields, and has had



*Keywords map for Analytical Chemistry for the period 2006–2007.*

both a general and a discipline-specific impact on the development of chemistry-related terminology and publication. The citation distribution, change of key words, and analysis of nano-prefix terms and other co-word analysis suggests that terminology in nanotechnology has reached a relatively mature level at which convergence is an appropriate step.

**For more information contact Task Group Chairs Javier Garcia Martinez <j.garcia@ua.es> and Sanjay Mathur <sanjay.mathur@uni-koeln.de>.** **JGM is thankful to the University of Alicante and SM to the University of Cologne for providing financial support. The chairs would like to thank the contribution of Martin Meyer, Alan Porter, Ismael Rafols, and Jae Hwan Park for their help collecting, organizing, and discussing the data.**

**www.iupac.org/project/2007-040-2-200**

## Chemical Kinetic Data Evaluation for Atmospheric Chemistry and the IUPAC Kinetics Database

It is well established that emissions from human activities are leading to important changes in the composition of the global atmosphere. The impact of emissions on air quality on local and regional scales has been recognized for decades. The importance of intercontinental and global transport of air pollutants is now becoming apparent. More recently, it has become clear that anthropogenic emissions of greenhouse gases and aerosols are responsible for radiative forcing of climate change. To plan effective policy and actions to address these issues and plan a path to a

more sustainable future, it is critical that decision makers have the best available scientific understanding upon which to base their decisions.

Computational models are used extensively to understand the impacts of emissions on air quality on local, regional, and global scales and to understand the effects of human activities on the global climate system. An accurate representation of atmospheric chemistry is of critical importance in these models. In past models, the focus was on gas-phase chemistry. Modern models include the important effects of heterogeneous reactions and the formation and fate of atmospheric aerosols. The IUPAC Task Group on Chemical Kinetic Data Evaluation for Atmospheric Chemistry is engaged in a project to provide evaluated kinetic data available to the scientific community in an online database for use in the next generation of atmospheric models. This project is furthering the IUPAC strategic goals of (i) serving as a scientific, international, non-governmental body that objectively addresses global issues involving the chemical sciences and (ii) facilitating the development of effective channels of communication in the international chemistry community.

The Task Group is continuing to update and expand the evaluations, which have been published in a series of 10 peer-reviewed articles in *J. Phys. Chem. Ref. Data*, and five recent articles in *Atm. Chem. Phys.* The updated evaluations are available at <www.iupac-kinetic.ch.cam.ac.uk>, the website of the Centre for Atmospheric Science in the Department of Chemistry, University of Cambridge, UK. The group is updating data sheets and providing recommendations for rate constants for selected gas phase and heterogeneous processes for which new information has become available. In 2012, the panel will compile and submit for publication recommended data for heterogeneous reactions on liquid water and sulfuric acid surfaces and homogeneous reactions of halogenated organic compounds. These data are needed as inputs for the next generation of global and regional atmospheric models.

There is growing interest within the scientific community in the formation, fates, and environmental impacts of atmospheric aerosols. The chemistry and physics associated with atmospheric aerosols is very complex. With support from IUPAC, the project has put great effort into collecting and evaluating kinetic data for atmospherically relevant reactions and processes involving aerosols and has added several hundred data sheets containing evaluated data for heterogeneous reactions (e.g., reactions on ice surfaces, soot, mineral dust, sulfuric acid aerosol) over the past couple of years. This data facilitates more accurate representations of important heterogeneous processes in atmospheric models of climate and air pollution.

We take the completion of the migration of the kinetic and thermodynamic IUPAC database on atmospheric chemistry to its website as an opportunity to highlight several enhancements and capabilities recently implemented by the webmasters Glenn Carver and Hannah Barjat of Cambridge University. The website has been active since 1999. For details on the history of the website see Jan-Feb 2007 *CI*, p. 15.

The database is divided into summary tables for families of reactions, data sheets for individual reactions and supplementary information providing guides to the gas-phase and the heterogeneous data sheets and thermodynamic data used in the database. At the top of the home page there is a link to the five volumes published in *Atmospheric Chemistry and Physics* which are "snapshots" of the database at time of publication. Publication in *Atmospheric Chemistry and Physics* provides permanent documentation of the state of the database on a periodic basis in an easy to access and familiar format.

The **summary tables** provide kinetic data on (a) gas phase $O_x$, $NO_x$, $HO_x$, $SO_x$, organic compounds, inorganic and organic halogens; (b) heterogeneous reactions on ice substrates; (c) heterogeneous reactions on mineral dust substrates. Previous editions of the summary tables are available to facilitate the tracking of changes in the recommended kinetic information with time as new data or new aspects in evaluation become implemented.

The **data sheets** proper are brief summaries of available experimental data with notes giving details of the experimental procedures and are organized in

four broad groups, namely (i) gas phase reactions; (ii) photolysis reactions; (iii) heterogeneous reactions on solid substrates; (iv) heterogeneous reactions on liquid substrates. It is notable that the evaluation of heterogeneous reactions has been entirely refurbished from previous evaluations and also goes beyond what other evaluations have provided. It is based on an advanced framework of kinetic parameters to describe heterogeneous and multiphase processes in more detail. Particularly useful is the recently implemented search capability based on SMILES strings and IUPAC's InChI unique identifier of chemical compounds. It is planned to install an additional search capability based on functional group recognition to make it even more user-friendly given the more than 1000 data sheets now in the database. For each thermal reaction, a preferred value of the rate coefficient at 298K is given together with its temperature dependence, if available. The selection of the preferred value is discussed in some detail and estimates of the accuracies of the rate coefficients and temperature coefficients have been given for each reaction depending on the number of studies and their quality. For each photochemical reaction the data sheets list the preferred values of the photoabsorption cross sections and the quantum yields of the photochemical reactions together with comments on how these were selected.

The **supplementary information** at the bottom of the home page includes a brief guide to the data sheets explaining key definitions of kinetic parameters; a glossary of terms; an updated introduction to the heterogeneous data sheets; and a referenced list of thermodynamic data of relevant atoms, free radicals, and closed-shell molecules and the order of reactions within a family.

The **advantages** of the IUPAC kinetic database for atmospheric chemistry may be summarized as follows:

- extensive database accessible free of charge
- critical evaluation with justifying documentation as opposed to compilation of literature data
- frequent updates
- hard copy "snapshots" of the state of the database at a given point in time for easier traceability of recommendation changes

**For more information contact Tim Wallington <twalling@ford.com>.**

**www.iupac.org/project/2011-049-1-100**

## Global Chemical Safety and Sustainability

A regular project of the IUPAC Committee on Chemistry and Industry (COCI) is to coordinate a symposium and workshop on the Safety Training Program during the IUPAC Congress in order to accomplish the following:

- communicate to the public and IUPAC leadership on recent activities by Fellows of the program in their home countries
- evaluate the effectiveness of the program in terms of fellows' home country activities
- learn from invited speakers who are experts in health, safety, and environmental matters
- solicit ideas for improvement in the program and for possible expansion to incorporate new host companies and new regional trainees

The fifth in the series of IUPAC Safety Training Program workshops was held at the IUPAC Congress in San Juan, Puerto Rico, on 1 August 2011. The 2011 STP symposium and workshop, entitled, "IUPAC Safety Training Program: Global Chemical Safety and Sustainability," was a full-day event at the Congress. The Safety Training Program enables 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 environmental practices.

The symposium portion included several expert speakers from industry, academia, and government who covered a number of topics relevant to advancing the application of chemical safety practices in developed and developing countries: practices to improve chemical safety in schools and in industry, particularly in the pharmaceutical industry; chemical security; and Responsible Care.

Iwona Maciejowska of Jagiellonian University, Krakow, Poland, and EuCheMS vice chair for Eastern Europe spoke on an EU project, Project CHLASTS, that provides materials for chemical safety in educational laboratories. Maciejowska discussed the need for more chemical safety training for teachers and students in

European schools. She noted that there is often insufficient information on safety in textbooks and that students were often not prepared to work with toxic or dangerous substances. She described how Project CHLASTS was established to engage teachers and students in an ongoing safety dialogue. The project, which includes 15 partner institutions from 9 countries, involves legislation, safety procedures for labs, waste disposal procedures, and a practical guide for teachers entitled "Safety in the Chemical Laboratory." Produced in CD form in eight languages, the guide includes several appendices with guidelines for teachers, such as a list of incompatible chemicals. More information about the CHLASTS project is available at <www.chlasts.org>.

Maria I. Rivera, senior safety specialist with Pfizer Pharmaceuticals in Puerto Rico, spoke about laboratory safety in the quality-control facilities at Pfizer. Rivera described the company's approach to safety in the industrial workplace, emphasizing identifying hazards, assessing risks, and establishing corporate safety initiatives. She presented many detailed examples, including chemical inventory, storage, equipment maintenance, personnel training, and compliance with federal regulations. In all cases, Rivera noted, commitment to safety by all staff is critically important to achieving success.

COCI Member Bernard West of Westworks Consulting, Ltd. in Canada, spoke on "Responsible Care—a Process for Chemists," a global voluntary program designed to make the chemical enterprise safe and environmentally positive for the entire "life cycle" of a chemical, from research lab to manufacturing to the supply chain to the consumer to disposal of waste. Responsible Care, he said, is based on the ethic of "doing the right thing regardless of what the law says," creating inherently safe products and processes, collaborating with a variety of partners to implement, and taking all of these aspects into account in decision making.

West outlined the three components of Responsible Care: accountability to stakeholders, operations (over which chemical producers have direct control), and stewardship (a collaboration among suppliers, customers, and distributors). Corporations in 60 countries now adhere to Responsible Care, and there has been a 60 percent reduction in occupational health and safety incidents since 1991. In 2008, West noted, 33 percent of member companies reported zero incidents. He pointed out that Responsible Care is aligned with the strategic goals of IUPAC and with the Safety Training Program. West then described his COCI project on case studies in Responsible Care. The first case study was summarized in the May-June 2011 *CI*, p. 6. and a second is in progress.

Nancy Jackson, president of the American Chemical Society and manager of International Chemical Threat Reduction in the Global Security Center at Sandia National Labs (USA), spoke on the Chemical Security Engagement Program. Sandia National Laboratories assists the U.S. Department of State and other federal agencies in solving problems related to international chemical security. With the U.S. Department of State, Jackson has developed the Chemical Security Engagement Program, which raises awareness of chemical safety and security among chemical professionals and enables the practice of safety and security in the research, teaching, and commerce of chemicals. Explaining that chemical security threats exist across national boundaries, Jackson described how chemists and professional societies can become involved and active in the program. She noted that Chemical Security Engagement Program staff have run a number of training courses around the world in the past several years.

The afternoon workshop session focused on the activities of several recent Safety Training Program Fellows who work in industry and university settings in Africa, Latin America, and the Near East. All of the speakers were enthusiastic about their training experiences and follow-up, and all clearly have had an impact in their home countries.

Tersoo Charles Gwaza of Shell Petroleum Development Company, Port Harcourt, Nigeria, spoke on process-safety campaigns as a vital link in improving safety culture and performance at work. Gwaza received safety training at Sasol in South Africa. He stated that the increasing global dependence on energy has put more pressure on oil and gas production, so that the need for best safety practices cannot be overemphasized. Current projects and programs at Shell include sharing process safety best practices and knowledge from process-safety incidents, a website and chat forum aimed at reviewing process-safety initiatives, training modules on hazardous-area awareness for staff working in high-risk facilities, sharing of information about incidents with staff and contractors, and community-outreach programs aimed at creating awareness of domestic and road transport safety. These initiatives have proved valuable in creating a good safety culture in the workplace, Gwaza said, and some of the activities have positively impacted local communities as well.

Godfred A. Nyarko of Tema Lube Oil Company Ltd., Tema, Ghana, reported on "Building Health,

Safety, and Environmental Culture—Key to Excellent HSE Performance." Nyarko received training training at Mitsui Chemical Co. in Japan. He stated that visible leadership and workforce participation are the two pillars that drive workplace HSE excellence. Initiatives that have yielded excellent HSE performance in the workplace, communities, and with other stakeholders included annual chemical safety training for laboratory staff and HSE training for the company's contractors, a potential incident reporting award scheme, establishing a company Emergency Brigade responsible for all incidents, HSE operational and legal/regulation requirement documents, co-ordinating the company's ISO 14001 (EMS) Certification Program (2009–2010), and promoting an organization-wide weekly HSE Toolbox Talks Program. The HSE Toolbox materials are also being used at some churches for congregational education on HSE. Nyarko said he overcame an initial organizational view that "safety costs money and why bother," and he now has good support.

*Safety Training Program Fellows during the panel discussion: Fabián B. Benzo (left), Tersoo Charles Gwaza, Esma Toprak, and Godfred A. Nyarko.*

Fabián B. Benzo of the Facultad de Química, Universidad de la República, Montevideo, Uruguay, spoke on "Promoting HSE through the IUPAC Safety Training Program." Benzo received training at Mitsui Chemical Co. in Japan at the same time as Godfred Nyarko. He has disseminated the Globally Harmonized System of chemicals labelling through events in Uruguay and Paraguay and has started implementing the OHSAS 18000 standards in a local chemical company. Benzo has also recommended safety measures for static-electricity risk control in a plant producing powder products, and suggested the HAZOP method in the project phase of a production plant. At the university's school of chemistry, he has introduced safety containers designed to protect flammable liquids from static electricity, and he has taught courses on laboratory safety to undergraduates and graduate students. He is now developing a Uruguayan regional focal point for international chemical safety training.

Esma Toprak of the Department of Chemical Engineering at Bogazici University in Istanbul, Turkey, spoke on "The Pathway of Developing Occupational Health and Safety Management in Turkey." Toprak received safety training at BP Chemicals in the USA. Toprak stated that Turkey has an active chemical industry, but occupational safety and health problems exist. She described chemical safety training across Turkey, highlighting health and safety management. Universities can be the best place from which to disseminate HSE information to industry and academic institutions, she said. In safety education, occupational health and safety experts, university student volunteers, and others visit companies, schools, and homes, distributing printed materials such as case studies. These efforts build on the momentum of the International Year of Chemistry, Toprak noted. Although occupational safety and health practices are developing in Turkey, intensive efforts are devoted to improving OH&S management, including sanctions and penalties. In addition, to mitigate and reduce damage due to earthquakes, preventive measures are being taken such as strengthening buildings. Cooperation between Turkish government ministries is leading to projects for developing educational materials and integrating them into the curriculum to develop safety awareness. Occupational health examinations of workplaces are being carried out to reduce absenteeism and improve productivity.

The workshop closed with a panel discussion among the speakers and the workshop audience. This led to a number of ideas for the development of the Safety Training Program and its continuation. COCI members posed the following questions and topics to the program's fellows:

**Do you find that your role is more policeman or team player?**
Answers among the fellows varied across the spectrum, where some found that at the start of their efforts they had to take a "policeman" role, but there was clear agreement that over time they became regarded as team players.

**What did you find most useful in your training?**
Some examples included safety manuals in each lab with instructions, task reviews for new activities, and methods and tools generally in use at the host company facilities.

**What was the biggest obstacle you found in implementing improvements at home?**
Budgets and regulations, workforce skepticism, the "not invented here" factor, and overcoming established mindsets and cultures not conducive to safety improvements.

**What advice would you give to new trainees?**
Keep open eyes and ears, not just for yourself but for the benefit of your employer and your community, and keep an open mind to new ideas.

**What advice would you give to IUPAC? How can the Safety Training Program serve its trainees better?**
Find more host companies and arrange for them to take several trainees at a time; use the workplaces of current fellows as training sites for new trainees; and develop regional training around the areas where fellows live and work.

COCI is now actively developing options to increase the scope of the Safety Training Program. The next workshop is planned for the IUPAC General Assembly in Istanbul in 2013.

**This report was prepared Bernard West and Mark Cesa. For more information contact Mark Cesa <mark.cesa@ineos.com>.**

**www.iupac.org/project/2011-004-2-022**
**www.iupac.org/committee/coci/safety-training-program.html**

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

## Nomenclature of Thermal Analysis

The scope of this document is to provide scientists working in the field of thermal analysis with a consistent "definitions of terms" that are commonly used within the field to allow precise communication and understanding. In considering all the matters of nomenclature, the current Committee has followed the advice of the late Robert Mackenzie in that:

- terminology should be simple;
- abbreviations kept to a minimum;
- names based on particular instruments should be discouraged.

This document acknowledges that nomenclature develops—without regulated definition—as the field of thermal analysis develops. Some terms used by authors and scientists rapidly become accepted by the scientific community, even if the term is not consistent with past definitions, science or grammatically correct. However, if such a term is widely used and understood, it is reported here.

**Comments by 30 November 2012**
Dr. Jean Rouquerol
ICTAC Past-President
E-mail: jean.rouquerol@univ-provence.fr

media.iupac.org/reports/provisional/abstract12/rouquerol_prs.pdf

## Definition of the Halogen Bond

The task group recommends the definition given here for the halogen bond. The short definition is followed by a not exhaustive list of experimental and/or theoretical features, which can be used as evidence for the presence of a halogen bond. A comprehensive technical report is being prepared by the task group in order to relate the proposed definition with the past work on halogen bond and provide the rationale for the proposed definition.

**Comments by 30 November 2012**
Prof. Pierangelo Metrangolo
Politecnico di Milano, Milano, Italy
E-mail: pierangelo.metrangolo@polimi.it

media.iupac.org/reports/provisional/abstract12/metrangolo_prs.pdf

## Vocabulary for Nominal Properties and Nominal Examinations — Basic and General Concepts and Associated Terms

Scientists of disciplines in clinical laboratory sciences have long recognized the need of a common language for efficient and safe request of investigations, report of results, and communication of experience and scientific achievements. Widening the scope, most scientific disciplines, not only clinical laboratory sciences, rely to some extent on various nominal examinations in addition to measurements. The "International vocabulary of metrology—Basic and general concepts and associated terms" is designed for metrology, the science of measurement. The aim of the proposed vocabulary is to suggest definitions and explanations of concepts and terms related to nominal properties, i.e. properties that can be compared for identity with other properties of the same kind-of-property, but have no magnitude.

**Comments by 30 November 2012**
Françoise Pontet
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media.iupac.org/reports/provisional/abstract12/pontet_prs.pdf

## IUPAC Glossary of Terms Used in Immunotoxicology (IUPAC Recommendations 2012)

**D.M. Templeton, M. Schwenk, R. Klein, and J.H. Duffus**

*Pure and Applied Chemistry*, 2012
Vol. 84, No. 5, pp. 1113–1295

The primary objective of this "Glossary of Terms Used in Immunotoxicology" is to give clear definitions for those who contribute to studies relevant to immunotoxicology but are not themselves immunologists. This applies especially to chemists who need to understand the literature of immunology without recourse to a multiplicity of other glossaries or dictionaries. The glossary includes terms related to basic and clinical immunology, insofar as they are necessary for a self-contained document, and terms related to diagnosing, measuring, and understanding effects of substances on the immune system. The glossary consists of about 1200 terms as primary alphabetical entries, annexes of common abbreviations, examples of chemicals with known effects on the immune system, autoantibodies in autoimmune disease, and therapeutic agents used in autoimmune disease and cancer. The authors hope that among the groups that will find this glossary helpful, in addition to chemists, are toxicologists, pharmacologists, medical practitioners, risk assessors, and regulatory authorities. In particular, it should facilitate the worldwide use of chemistry in relation to occupational and environmental risk assessment.

http://dx.doi.org/10.1351/PAC-REC-11-06-03

## Names and Symbols of the Elements with Atomic Numbers 114 and 116 (IUPAC Recommendations 2012)

**Robert D. Loss and John Corish**

*Pure and Applied Chemistry*, 2012
Vol. 84, No. 7, pp. 1669–1672

A joint IUPAC/IUPAP Working Party (JWP) has confirmed the discovery of the elements with atomic numbers 114 and 116. In accordance with IUPAC procedures, the discoverers proposed names as follows: flerovium with the symbol Fl for the element with $Z$ = 114 and livermorium with the symbol Lv for the element with $Z$ = 116. The IUPAC Inorganic Chemistry Division recommended these proposals for acceptance, and they were adopted on 23 May 2012 by the IUPAC Bureau as delegated to act by the IUPAC Council meeting on 3–4 August 2011.

http://dx.doi.org/10.1351/PAC-REC-11-12-03

## Analogue-Based Drug Discovery: Contributions to Medicinal Chemistry Principles and Drug Design Strategies. Microtubule Stabilizers as a Case in Point (special topic article)

**Mohammad H. El-Dakdouki and Paul W. Erhardt**

*Pure and Applied Chemistry*, 2012
Vol. 84, No. 7, pp. 1479–1542

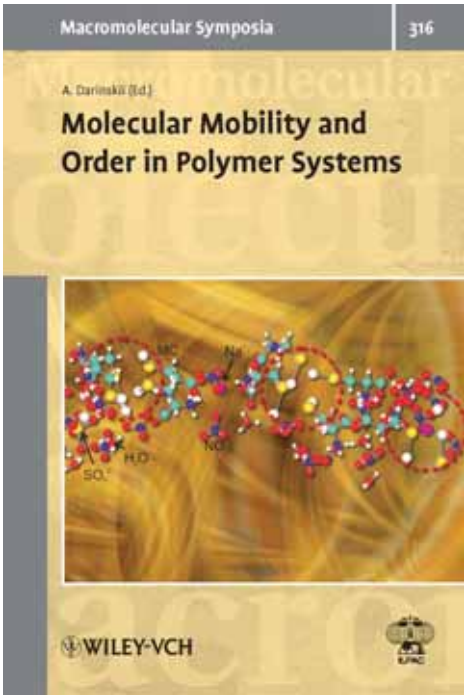
The benefits of utilizing marketed drugs as starting points to discover new therapeutic agents have been well documented within the IUPAC series of books that bear the title *Analogue-based Drug Discovery* (ABDD). Not as clearly demonstrated, however, is that ABDD also contributes to the elaboration of new basic principles and alternative drug design strategies that are useful to the field of medicinal chemistry in general. After reviewing the ABDD programs that have evolved around the area of microtubule-stabilizing chemo-therapeutic agents, the present article delineates the associated research activities that additionally contributed to general strategies that can be useful for prodrug design, identifying pharmacophores, circumventing multidrug resistance, and achieving targeted drug distribution.

http://dx.doi.org/10.1351/PAC-CON-12-02-13

## Macromolecular Symposia

Recent volumes of *Macromolecular Symposia* include contributions from recent IUPAC sponsored conferences.

**Molecular Mobility and Order in Polymer Systems**
**Vol 316, June 2012**
**doi:10.1002/masy.201290016**
*Issue edited by Anatoly Darinskii.*
The 7th International Symposium on Molecular Mobility and Order in Polymer Systems was held in St. Petersburg, Russia, from 6–10 June 2011.

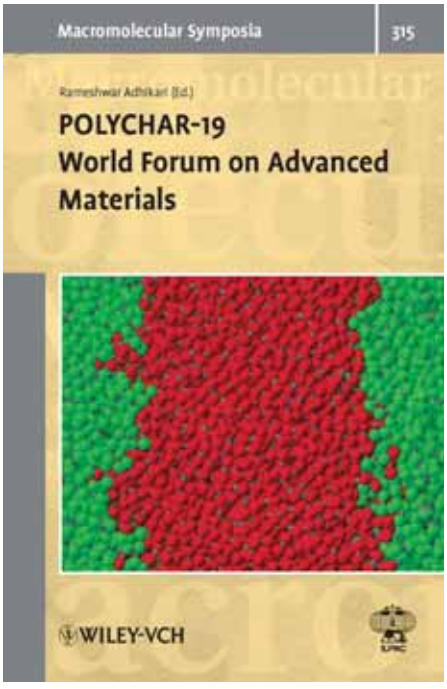



*This cover is selected from the article by P. Pakhomov et.al. and shows characteristic forms of filament-like aggregates.*

**POLYCHAR-19 World Forum on Advanced Materials**
**Vol 315, May 2012**
**doi:10.1002/masy.201290014**
*Issue edited by Rameshwar Adhikari.*
The 19th World Forum on Advanced Materials (POLYCHAR-19) was held at Kathmandu, Nepal, from 20–24 March 2011.

**Ionic Polymerization**
**Volume 308, October 2011**
**doi: 10.1002/masy.201190028**
*Issue edited by Stanislaw Penczek and Andrzej Duda.*
This issue includes contributions from the 19th IUPAC International Symposium on Ionic Polymerization (IP'09) held in Krakow, Poland, from 26–31 July 2009.

**Functional Polymeric Materials and Composites**
**Volume 313-314, March 2012**
**doi: 10.1002/masy.201290008**
*Issue edited by Bert Klumperman, Peter E. Mallon, Harald Pasch, and Albert J. van Reenen.*
This issue includes selected papers from the 11th Annual UNESCO/IUPAC Workshop and Conference on Functional Polymeric Materials and Composites was held in Stellenbosch, South Africa, from 27–29 April 2011.




*The cover is selected from the article by N. P. Adhikari and shows a typical snapshot of a system of flexible and semi-flexible polymer mixtures.*

http://onlinelibrary.wiley.com/journal/10.1002/(ISSN)1521-3900

## Periodic Tables on the World Wide Web

*by Leslie Glasser*

The Periodic Table of the Chemical Elements (to give it its full title) is the principal organizational feature of Chemistry. It initially found its rightful place through its brilliant use as a predictive tool by Dmitri Mendeleev (Дми́трий Ива́нович Менделе́ев) (1869) and was brought to its present scientific condition as a sequence in atomic number (rather than the earlier choice of atomic mass) through the spectroscopic investigations of Henry Moseley (1913). A currently developing (almost weekly) and entertaining blog of the Periodic Table can be found at the otherwise untitled http://scicommstudios.wordpress.com. Books about the Periodic Table abound. The Wikipedia article (http://en.wikipedia.org/wiki/Periodic_table) mentions a few of the more recent ones. But pride of place should go to Primo Levi's The Periodic Table (1984) which contains a series of short essays, each titled with the name of a chemical element, based on incidents in Levi's tragic life (briefly reviewed in http://dannyreviews.com/h/Periodic_Table.html).

However, the main concern in this brief review is to present a number of the more interesting interactive or unusual periodic tables that are available for inspection on the web. A very informative example of a straight-forward presentation that was early in the field and yet remains current, with much additional information, such as the Chemdex "directory of chemistry" which links to chemical sites around the world, is Web Elements <www.webelements.com> from the University of Sheffield and Mark Winter. The major chemical societies have their own sites, of course. The American Chemical Society has a table in a half-dozen or so languages (http://acswebcontent.acs.org/games/pt.html) while the UK Royal Society of Chemistry features the interactive Visual Elements Periodic Table <www.rsc.org/periodic-table> with an artistic representation of each element. For the 2011 International Year of Chemistry, the Royal Australian Chemical Institute produced an artistic "Periodic Table on Show" <www.raci.org.au/periodic-table-on-show> developed by a number of local printmakers. The authoritative IUPAC version includes current values of atomic masses <www.iupac.org/reports/peri-


*Daniel Radcliffe sings "The Elements" on The Graham Norton Show, series 8, episode 4, BBC One.*

*Periodic Table on Show, produced by the Royal Australian Chemical Institute for the 2011 International Year of Chemistry <www.raci.org.au/periodic-table-on-show>.*

odic_table>. A beautiful version is the "Photographic Periodic Table of the Elements" <periodictable.com> which displays photographs of samples of the elements. An unusual Periodic Table <www.colorado.edu/physics/2000/applets/a2.html> shows the atomic emission spectra of many of the elements together with the associated filling of the energy levels (but don't read too much into the pictures of the "whizzing" electrons and nuclei!)

Among the more entertaining versions is the song by Tom Lehrer listing the chemical elements set to music, with a clever cartoon version <www.youtube.com/watch?v=SmwlzwGMMwc&feature=related> and a very creditable version by Daniel Radcliffe (the "Harry Potter" star) <www.youtube.com/watch?v=rSAaiYKF0cs&feature=related>. Every chemist should be familiar with the quite exceptional Periodic Table of Videos <www.periodicvideos.com> from the University of Nottingham, which has short videos related to each of the chemical elements—and much, much more. The videos are often narrated by the engaging Prof. Martyn Poliakoff, FRS. See also an essay in <www.sciencemag.org/content/332/6033/1046.full>.

*Martyn Poliakoff, the University of Nottingham, in his video discussion of flerovium, one of two new elements.*

The Periodic Table is a living entity, and two elements have just (30 May 2012) been accepted for inclusion: flerovium, $^{114}$Fl, and livermorium, $^{116}$Lv <www.iupac.org/news>.

Many have recognized that the Periodic Table provides an excellent organizing principle which can be applied well beyond chemistry. For instance, the website <web.mit.edu/dryfoo/www/Info/condiments.html> lists a "Table of Condiments That Periodically Go Bad" (which includes the "useful fact" that Vegemite—number 34—lasts two months after opening!). Mathematicians are reported to be in the process of creating a periodic table of shapes <www.newscientist.com/article/dn20134-atoms-ripple-in-the-periodic-table-of-shapes.html> and <www.cosmosmagazine.com/news/4061/mathematicians-create-periodic-table-shapes>. In order to deal with the complication of these multiple types of periodic tables, there is a "Periodic Table of Periodic Tables" <www.keaggy.com/periodictable> which links to an extensive, and eclectic, set of Periodic Tables.

A striking resource is the Periodic Table in nearly 400 languages, including some that are extinct or have been constructed (In Czech, but quite clear <www.jergym.hiedu.cz/~canovm/vyhledav/chemici2.html>; note that two screens are viewable, with the second providing access to historical information).

Finally, there is Mark Leach's "Internet Database of Periodic Tables" <www.meta-synthesis.com/webbook/35_pt/pt_database.php?PT_id=286> which currently has more than 450 links to Periodic Tables of various kinds, both chemical and others.

**Leslie Glasser <leslieglasser@yahoo.co.uk> is at the Nanochemistry Research Institute of Curtin University in Perth, Australia. He is the former chair of the IUPAC Committee on Printed and Electronic Publications.**

An earlier version of this review was published as an editorial in the *Australian Journal of Education in Chemistry*, issue 71, pp. 3–4, 2011; reproduced with permission; www.raci.org.au/divisions/further-information-2/ausjec.

**www.iupac.org/publications/ci/2012/3405/ic.html**

## Systematic and Trivial Nomenclature

*by Jeffery Leigh*

**Nomenclaturists recognize two general classes of nomenclature, systematic and trivial. Perhaps the use of the word trivial is unfortunate, because its usual meaning in every-day English according to the *Oxford English Dictionary* (OED) is "of small account, little esteemed, paltry, poor, trifling, inconsiderable, unimportant, slight." However, the OED lists several other meanings, some derived from a Latin word implying "three." A more general common meaning listed in the OED is "such as met with anywhere, common, commonplace, ordinary, trite." The word trivial was adopted when nomenclature was in its infancy and when its use in the latter sense was more usual, and that is why it is still used in that sense today. It is not intended to be dismissive.**

The traditional names of the elements are trivial in this sense. They are non-systematic and many have been adopted from alchemy and early chemistry. For example, the term mercury was applied to many plants, persons, and things as well as the metal itself, which was also called quicksilver, for obvious reasons. An alternative name, hydrargyrum, from which the symbol Hg was derived, is a compound word from Latin and Greek meaning liquid silver. The reason for such names is very evident, but that can hardly form the basis of a systematic nomenclature for all elements. However, most element names are so deeply embedded in many languages that even IUPAC has refrained from generally systematizing them. Nevertheless, during the 1990s it became clear that many scientists needed to write and speak about elements that had yet to be prepared, and that names and symbols were required. Hence, IUPAC developed names and symbols for such elements that are immediately recognizable and based upon their atomic numbers. These names are provisional and are replaced as soon as a given element is prepared and unequivocally characterized. Perhaps unfortunately, the unambiguous systematic name is then replaced by a trivial name suggested by the scientists who first prepared the element.

Trivial names for compounds are used by chemists everywhere, and such names are clearly useful for much exchange of information, especially within a given lab. However, IUPAC attempts to devise a fully systematic approach to the names of substances, which imply unequivocally their chemical constitutions. Such names should be used when an unambiguous identification of compounds is required, as in scientific documents, international treaties, patents, and legal definitions. This is why IUPAC nomenclature can sometimes appear to be so complicated.

There are other kinds of systematic nomenclature. The Chemical Abstracts Service of the American Chemical Society has its own systematic system, similar to IUPAC's, and with similar aims, but not identical. Other nomenclatures may be systematic, but in a manner differing from IUPAC's. For example, ISO lists approved names for pesticides, such as afidopyropen, which should be recognizable by professionally qualified users rather than solely by chemists. Such names should be translatable into other scripts and into languages other than English. The entry for the pesticide afidopyropen (for details see <www.alanwood.net/pesticides>) also lists French and Russian versions of the name, a guide to (British) English pronunciation of the English name, the chemical structure, and full IUPAC and CAS names. The short ISO name is clearly preferable to the IUPAC systematic name for everyday commercial use, though the ISO listing also provides citations of relevant InChIKeys and InChIs.

Similarly, the World Health Organization issues a list of international nonproprietary names for drugs (INNs), which are names devised and classified according to the pharmacological activity of the substance cited. This is also systematic, but is only loosely derived from IUPAC nomenclature. WHO lists proposed INN names together with a structural formula. Details of the listings can be found, for example, in WHO *Drug Information*, 23(2), 2009, which may be accessed online. The names are given in a form of Latin, and then in English, French, and Spanish, with an indication in each language of its claimed activity, its molecular formula, and its CAS registry number. The names listed here are proposed names, and recommended names are listed elsewhere.

These systems are a selection of those available. Many refer back to systematic IUPAC names, but are adapted to specific purposes. *Principles* offers a brief guide to some of these, together with suitable references for wider consultation.

**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/project/2006-029-1-800**



**Next in this series will be a review of InChIs and Registry numbers.**

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*Under the auspice of*

# Advanced Materials: Stories of Innovation

*by Neil Gussman*

On a clear, unseasonably warm evening in late February 2012, nearly 200 people gathered at the Chemical Heritage Foundation, in Philadelphia, Pennsylvania, to hear experts discuss the past, present, and future of materials science. The on-stage discussion brought together six research leaders from the chemical industry to talk with Ivan Amato, author of the book *Stuff: The Materials the World is Made of.*

Titled **Advanced Materials: Stories of Innovation**, the event was a partnership between *Discover* magazine and the Chemical Heritage Foundation. Michal Meyer, editor in chief of *Chemical Heritage* magazine, opened the event by connecting materials science with the long history of chemistry and alchemy. She quoted a recipe from the noted alchemist Sir Isaac Newton "Take of urine one barrel and let it ferment three months in summer . . ." showing the strong commitment and limited resources of the first chemical experimenters.

Following Meyer, Corey Powell, editor in chief of *Discover*, linked the event to the magazine's annual issue "Visible Planet" that shows readers "the marvelous hidden in the mundane" through stories of how scientists see common objects. "There is no better example of that than the chemical perspective," Powell said. "We live and breathe chemical processes, but we don't think about them."

Amato introduced the event and the panel. He said, "The periodic table of elements amazes me. It is the "Mother of All Pantries." Every material thing that ever was, is, or will be resides in that discovery. We should all have a copy in a shrine-like environment between two candles."

*Panelist (from left) Christopher D. Pappas, Mark Doriski, and Gregory Nelson.*

Materials science is more than the elements, it's how they are combined," Amato said. "The history of technology innovation is closely tied to innovation in materials." Amato introduced the six panelists, who he said were in the business of bringing new materials into existence:

- **Thomas M. Connelly, Jr.**
  Executive Vice President and Chief Innovation Officer, DuPont
- **Ryan Dirkx**
  Vice President, Research and Development, Arkema Inc.
- **Mark Doriski**
  Global Intermediates Technology Manager, ExxonMobil Chemical Company
- **Gregory Nelson**
  Senior Vice President and Chief Technology Officer, Eastman Chemical Company
- **Christopher D. Pappas**
  President and CEO, Styron
- **A.N. Sreeram**
  Vice President, Research and Development, Advanced Materials Division, The Dow Chemical Company

Amato then introduced the first of three questions he would ask the panelists to discuss before opening up the event to audience questions:

**What roles have materials innovations played in the recent history of technology?**

First to answer the question was Sreeram who pointed out that "48 percent of the energy consumed in America is used to heat, cool, and light our living spaces." He talked about Dow insulation products as an example of an advance in materials leading to better quality of life for everyone through reduced energy consumption. He also contrasted the obvious advanced materials that surround us in personal electronic devices with the invisible advanced materials such as the reverse osmosis filters that turn sea water into drinking water.

Connelly said, "The world has enough stuff by and large. It needs smarter stuff, higher performing stuff, greener stuff. We need to look at the value side of the equation, not just the volume side." He talked about

the recent rapid advances in photovoltaic technology. "From the discovery of the photoelectric effect in 1880 until 2000, the world installed one gigawatt of photovoltaics. Last year we added more than 10 gigawatts, enabled by advanced materials."

Pappas explained that materials innovation can also take the form of refining and enhancing the properties of existing compounds. He said Styron adds new functional groups to styrene-butadiene to give tire makers rubber that can maintain wet grip while reducing rolling resistance. "You can innovate around basic technology, not just brand new things," Pappas said.

Following the point Pappas made, Doriski said synthetic lubricants were invented in the 1930s but have been growing in the automotive market with research and innovation in the last two decades. He said the USA could reduce gas consumption by a billion gallons per year by switching to synthetic lubricants.

Nelson talked about interacting with consumers, explaining how Eastman's TRITAN lets consumers choose BPA-free plastics in food containers. "Consumers are becoming part of the product development equation," said Nelson. "They care how you have made this product, what you have made it from. They are telling us, 'We care what happens to us when we interact with this product.'"

"Materials innovation is going to be about the creativity of our scientists and about interacting with informed consumers," said Nelson.

Dirkx said he entered an undergraduate materials science program focused on ceramics since he wanted to study advanced ceramics for nose cones on spacecraft. When he went to his first lab he saw a row of coffee cups on the lab bench—confirming his worst fear about studying ceramics. "Then the professor picked up one of those cups and hammered a nail into a board with the side of the cup," Dirkx said. "Materials had me at that point."

Dirkx talked about his company's long history in biopolymers. Arkema has made nylon from castor oil for almost 60 years, a slightly different nylon that resists cold very well and is used as brake lines on all trucks in the Yukon and Siberia. Dirkx said, "We have sold biopolymers for decades because they work, not because they are plant based."

As a follow up to the opening question, Amato asked Pappas about the balance between characteristics of the rubber his company develops. "Is it a trade-off between rolling resistance and wet weather performance?" Amato asked. "Those seem to be pulling in opposite directions."

"Our scientists have been able to reduced rolling resistance without compromising wear and wet grip," Pappas said. "That kind of innovation tends to rapidly take over a market."

Sreeram added, "Another example is high-temperature elastomers." He said that in normal plastics, increasing temperature resistance means lowering elasticity. High-temperature elastomers went from scientific publication to the market in less than a year because the demand was great.

*Host Ivan Amato (left), with Thomas M. Connelly and A.N. Sreeram.*

Amato then introduced question two:

**It takes a lot of science, a lot of engineering, and a lot of good management to nurture a good idea and translate it into a consequential new material. How do your companies create cultures in which all of that can happen?**

Doriski said, "Commitment and collaboration are the keys to a culture of innovation. We have 18 000 scientists and a billion-dollar research budget and collaborate with many universities."

Connelly stressed the need for a culture that can foster innovation. Leaders need "a tolerance for uncertainty," he said. "You can't be too quick to make a decision and close off optionality." But when the decision is made "You have to be ruthless," Connelly said. "You can't have pet projects. Most things we work on will fail." Research leaders need market insight and judgment to pick the right projects.

Nelson said he was asked by an Eastman board member what he would do if he got a 10 percent increase in his R&D budget. His answer: "I would give a third of the money to our marketing department to

hire market insights people. I do not want to develop products no one wants." He continued, "Innovation is different than invention. Innovation serves the needs of people."

Amato posed the third question to the panel:

**What are the grand materials-related challenges that face society now?**

Amato asked them to go beyond the context of their own businesses and the chemical industry. "Think about problems that may not have solutions now."

"Cars need to get smaller. The cars of the future aren't going to look like the cars we have today," Connelly said. "With all respect to ExxonMobil, there is a future for the electric vehicle. We need new materials for inverters, new materials for energy storage, we need new materials to take weight out of vehicles."

*A.N. Sreeram (left) and Ryan Dirkx.*

Doriski responded recommending ExxonMobil's report on the future of energy to Connelly and the panel. He then explained how synthetic lubricants reduce waste by reducing maintenance. He talked about industrial gearboxes and automatic transmissions in cars. With synthetics, industrial gearboxes, such as those on wind turbines, run many times longer between oil changes, increasing efficiency and reducing waste. He said automatic transmission fluid now lasts as long as the car.

Nelson said he read ExxonMobil's report and noted that over the next 30 years the projected greatest source of new energy will be saved energy. He said every process uses energy and that small savings in many processes add up to the energy that will allow more people around the world to move into the middle class.

Pappas returned to the automotive theme saying Styron developed molded polymer seats that replace metal seat frames, reducing overall weight of the vehicle. He said LED lighting and all the materials innovations that make it possible will be another source of significant energy savings in the future.

Amato said new materials change the landscape of our world. The first time he encountered LED lighting on a vehicle was in the 1990s and now LED lights are common.

The first questioner from the audience asked if fracking and the availability of cheap natural gas would change the chemical landscape in the way coal tar became the raw material for so many chemical innovations of the 19th century. Pappas said the chemical industry has already changed. Cheap natural gas has already led to billions in investment and thousands of jobs on the Gulf Coast as well as in Pennsylvania and surrounding states.

Sreeram said he read an article titled "RIP American Chemical Industry" in 2008, but with falling natural gas prices "We got our swagger back."

Thomas R. Tritton, president and CEO of CHF, asked about self-healing polymers. Dirkx said he had examples with him on a display table on the third floor, and that more innovations were on the way.

Another questioner asked what the world would be like 200 years in the future. Sreeram said "Whatever we say will be wrong. The amount of change we will see in 200 years makes it impossible to predict."

Janice Shaw, a chemistry and physics teacher from West Philadelphia Catholic High School, said "I love to come to events like this because this is how I get a jump start to give enthusiasm to the kids I meet every day."

Paul McGibney, a chemistry teacher at Ridley High School, Philadelphia, said "I get my kids involved in materials science by using organic LEDs and carbon nanotubes for classroom projects. Where do you see nanotechnology being incorporated in materials in the future?"

Pappas said practical large-scale use was still in the future. Sreeram gave examples of current uses of nanotechnology in catalysts and microelectronics. "In the case of carbon nanotubes, we need to separate out is it a technology looking for an application or the other way around."

Following Sreeram, Dirkx said, "There is fundamental difference between bulk material properties and

what happens when you downscale it." He described the change in properties from bulk, to thin coating to nanoscale as discontinuous. "There is a lot for us to do in this nanospace to develop new materials."

The final question of the event went to Steven Freeman, who teaches innovation at the University of Pennsylvania. He asked for an example of radical change versus the incremental changes described in much of the discussion.

Connelly answered first. "I think there is a basic change in the way biology is going to impact the materials sciences. We engineer biological process and produce very specific products at room temperature, atmospheric pressure and in aqueous media with no exotic metals."

Pappas said the incremental advances in materials over the past 20 to 30 years add up a major change. "Breakthroughs are the sum of incremental changes over time," he said.

**See videos of the event at http://discovermagazine.com/events/chf/chf-advanced-materials-stories-of-innovation.**

**Neil Gussman <NeilG@chemheritage.org> works at the Chemical Heritage Foundation. CHF shares common goals with, and is an Associated Organization of, IUPAC.**

# How Many Miles Have We Gone, InChI by InChI?*

## *by Alex Tropsha and Antony Williams*

How simple the communications between people of different nations would have been had we all shared the same language! The attempts to develop such a universal language adopted by the entire human population have not been tremendously successful (e.g., Esperanto), but chemists, on the other hand, have succeeded in developing a language they all understand, that of chemical structure. Chemists of all nations could easily communicate their thoughts using traditional chemical structure drawings, but this way of information exchange becomes increasingly prohibitive with the growth of chemical databases. This is when special means for compact encoding of chemical structures such as SMILES and InChI become critical, making it feasible to store and transmit huge amounts of chemical information (many current chemical databases such as PubChem or ChemSpider include many tens of millions of records).

At the ACS meeting in San Diego in March 2012, we had an opportunity to celebrate the impact of the **InChI (the IUPAC International Chemical Identifier)** on the ability to communicate, link, and enhance the integration of chemistry across databases, across the Internet and in publications. Unlike the proprietary SMILES format, InChI was designed to be "a freely available, nonproprietary identifier for chemical substances that can be used in printed and electronic data sources, thus enabling easier linking of diverse data compilations and unambiguous identification of chemical substances." Over the past decade, InChI has become widely recognized and used by the chemical community to search, connect, and exchange chemical structures. The first InChI symposium to be held at an ACS meeting was organized to highlight the history, recent developments, interesting applications, and current trends in InChI. The unique gist of this full-day symposium in the San Diego 2012 program could probably be best summarized by the presentation title of one of the speakers, who had the title "InChIs here, InChIs there, InChIs everywhere!" (see page 34).

*Alan McNaught (left) chaired the original IUPAC activity that lead to the development of InChI in 2000 and has followed the project since. Jason Wilde is from the Nature Publishing group, represented on the InChi-Trust.*

The morning session opened with Steve Heller presenting a brief history on how the InChI project started and an update on the present status. He emphasized that InChI was meant primarily to provide a way to link information, to be an addition to what is available today, not a replacement, and is an algorithm to produce a unique label. He commented on the success of InChI, with one measure being the uncoerced adoption that has been shown by publishers, database providers, and software developers.

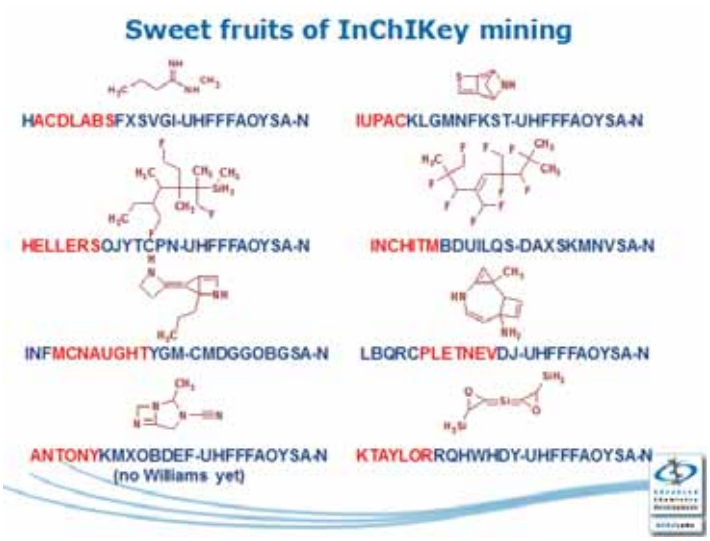
Antony Williams from the Royal Society of Chemistry Cheminformatics team, and member of the ChemSpider project, discussed the "Great promise of navigating the internet using InChIs" and reflected on what the original purpose of InChI was and how far we had come in a relatively short period of time in terms of meeting the goals. In contrast to his usual focus on data quality issues, he started by commenting that the talk was about quantity—how much data was now being linked together and could be discovered using InChI as the linker. He asked "What would be the situation if InChI never existed?" and answered with the fact that ChemSpider would never have been built without it.

*Jignesh Bhate (left), Molecular Connections, and Antony Williams, symposium chair (RSC & ChemSpider).*

Keith Taylor from Accelrys provided an overview of why Accelrys supports InChIs in its cheminformatics toolkit despite having its own unique identifiers already. He emphasized it was because the community asked for InChIs and found them to be valuable. He provided examples of how different online systems used InChI and what the results were when Accelrys tools were used to perform searches against the online databases.

Martin Walker from the State University of New York at Potsdam discussed the use of InChIs in Wikipedia and their use in ChemBoxes and DrugBoxes. He also discussed how InChIs became an important part of the RSC Learn Chemistry wiki, an open website hosting educational content and encouraging educators to contribute their own data. The site hosts chemical data for over 2100 common chemicals and uses InChI and InChIKeys to facilitate structure searching across the site and as the basis of interactive quizzes.

Andrey Yerin from ACD/Labs gave a fascinating presentation regarding InChIKey collisions and how to experimentally estimate the rate of their occurrence using algorithmically-generated structure libraries. His conclusion was that InChIKeys do have a very low rate of collision as the degree of randomness, as expected by the design of the InChIKey, is very high. He did provide some very amusing examples of InChIKeys that contained "hidden words" and examples are shown in the figure below.




As a final talk in the morning session Juergen Swienty-Busch talked about where InChIs are (i.e., "here, there and everywhere"). He showed how InChIs continue to proliferate in popularity across chemistry databases on the web and how Elsevier now includes them in its Reaxys database as well as in its publications associated with data. Reed-Elsevier looks forward to further advances in InChI. Elsevier Properties SA is a board member on the InChI Trust and Elsevier is involved as members of three of the working groups. This indicates their belief in the standard.

The discussion of InChI continued in the afternoon. Yulia Borodina (U.S. FDA) discussed the challenges facing the FDA Substance Registration System when dealing with complex compounds such as biopolymers or synthetic polymers. Standard InChI is not designed to handle such structures, but it could be used to describe monomers and other building blocks of these complex structures.

Marcus Sitzmann from NCI discussed how InChI/InChIKeys are used within the NCI Chemical Identifier Resolver to annotate more than 80M unique chemical structures.

Daniel Lowe from NextMove Software addressed features in IUPAC nomenclature that cannot be addressed by standard InChI such as accurate representation of tautomers and mixtures of stereoisomers. These cases require special treatment.

In a flash talk, Richard Kidd discussed the use of InChI within the Royal Society of Chemistry and RSC's contribution to the development of InChI standards.

Feranc Szalai from Mcule (Budapest, Hungary) highlighted the importance of InChI for unified annotation of chemical structures in aggregated databases that is independent of drawing conventions, tautomeric states, and other features such that each unique chemical structure is annotated only once. He stated that InChI provides the best solution for this problem.

Jon Chambers from EBI (Cambridge) made similar observations based on their group experience in assembling data in the ChEMBL database from different sources. He described their UniChem system that uses the standard InChI as a means of normalizing between different sources of chemical structures.

Bill Armstrong from Louisiana State University shared his experience in creating a teaching methodology to help researchers understand InChI as a unique, non-proprietary tool for identifying chemical structures.

Jason Wilde from the Nature Publishing Group (London) described the efforts of the InChI Trust to support the development of a nonproprietary InChI standard and discussed the ongoing efforts to provide technical solutions to develop standard InChI for difficult cases of complex structures such as polymers and mixtures.

Steve Boyer from IBM (San Jose, CA) described recent efforts of their group to employ InChI for annotating chemical structures in patents as part of chemical name to structure conversion. Their approach replaces chemical names in patent documents by InChI, enabling the search for chemical structures within certain textual content in the patents and patent literature.

In the final talk of the symposium, Laura Croft from Nature Publishing Group (London) described the launch of *Nature Chemistry* as part of nature.com and emphasized the utility of InChI to increase the discoverability of chemical structures and related information on nature.com and on the web in general.

This brief summary of presentations at the InChI symposium underscores the importance of InChI as universal identifier of chemical structures. InChI continues to proliferate in various areas of chemical research and to serve as a critical means of chemical information dissemination and exchange. The anticipated new developments will likely warrant a new InChI symposium within the next couple of years.

**Alex Tropsha and Antony Williams were the symposium organizers. Alex Tropsha <alex_tropsha@unc.edu> is an adjunct professor of biomedical engineering and of computer science at the University of North Carolina in Chapel Hill, North Carolina, USA. Antony Williams <WilliamsA@rsc.org> is with the Cheminformatics Department of the Royal Society of Chemistry and is a member of the ChemSpider project.**

* Reproduced with permission from the *Chemical Information Bulletin* of the ACS Division of Chemical Information Vol. 64, No. 2: Summer 2012; http://bulletin.acscinf.org/node/325.

### Additional Online Resources

- Symposium presentations are available at **http://edmc.acs.org/Common/presentation.aspx/Spring2012/CINF/CINF007** and **http://edmc.acs.org/Common/presentation.aspx/Spring2012/CINF/CINF007PM**
- InChI FAQs: **http://www.inchi-trust.org/faq**
- Antony Williams online talk "Navigating an Internet of Chemistry via ChemSpider" (20 October 2011): **www.ccce.divched.org/blog/521**

## Advanced Polymeric Materials

### *by Vera Kovacevic and Michael Hess*

**POLYCHAR, The World Forum on Advanced Polymeric Materials,** belongs to a series of annual conferences taking place in different countries starting in USA (from 1992 until 2003), then moving on to Portugal (2004), Singapore (2005), Japan (2006), Brazil (2007), India (2008), France (2009), Germany (2010) and Nepal (2011). The conference enjoys a high international reputation and has been sponsored by IUPAC for more than 10 years.

The **20th World Forum on Advanced Polymeric Materials—POLYCHAR 20**—was held from 26–30 March 2012 in Dubrovnik (Croatia), a medieval city, included in UNESCO's World Heritage List. The POLYCHAR Scientific Committee, with 53 countries represented, nominated the University of Zagreb, Faculty of Chemical Engineering and Technology as the organizer of POLYCHAR 20 conference, with Vera Kovacevic as the conference convener and Stanislav Kurajica as the conference chair.

The name POLYCHAR is derived from polymer characterization but goes beyond the 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 idea was to provide basic and up-to-date information on the popular characterization techniques by well-known specialists in a condensed presentation (covered by reference material) to students and newcomers in this field.

The Short Course on Polymer Characterization was held 26 March 2012, the first day of the POLYCHAR 20:

- Polymer Tribology and its Relation to Mechanics, Witold Brostow, University of North Texas, Denton, Texas
- Dynamic Mechanical and Thermophysical Analysis, Michael Hess, Chosun University, South Korea
- Polymer Molecular Dynamics around Glass Transition, Jean Marc Saiter, University of Rouen, France
- Electron Microscopy of Polymers: Techniques and Examples, Goerg H. Michler and Sven Henning, Martin-Luther-University Halle-Wittenberg, Institute of Physics, Halle (Saale), Germany
- Modern Microscopic Techniques, Holger Schönherr, University of Siegen, Germany
- Positron Annihilation of Polymers, Frans Maurer, Lund University, Sweden
- X-ray Diffraction of Polymers, Ivan Šmit, Ruđer Bošković Institute, Zagreb, Croatia
- Electrical Properties of Polymers and Polymer Composites, Traian Zaharescu, National Institute of Electrical Engineering, Bucharest, Romania
- Molecular Characterization of Synthetic Polymers by Liquid Chromatography, Dusan Berek, Slovak Academy of Sciences, Bratislava, Slovakia

About 300 registered participants from academia and industry, from 43 countries and 5 continents attended POLYCHAR 20 that offered 110 oral presentations and 156 posters in three parallel sessions covering the following topics:

- Predictive Methods and Simulations
- Structure-Property Relationships
- Surfaces, Interfaces, Adhesion and Tribology
- Materials Synthesis
- Rheology and Processing
- Mechanical Properties and Performance
- Electrical and Dielectric Properties
- Nanomaterials and Smart Materials
- Biomaterials, Green Materials and Composites
- Materials for Energy and Recycling
- Natural and Biodegradable Polymers

Following is a sampling of the 15 invited lectures that covered a broad range of subjects:

- Jung-Il Jin, Korea University, "First organic high temperature ferromagnetic compositions—a scientific lesson learned from DNA"
- Giovanni Camino, Polytechnic University of Turin, "Surface and bulk contribution to polymers and nanocomposites ignition"
- Marianne Gilbert, Loughborough University, "Hydrotalcite as secondary stabilizer for PVC"
- Masaru Matsuo, Department of Polymer Science and Materials, Dalian University of Technology, "Structures of high modulus and high strength polymer materials evaluated by X-ray, positron annihilation, $^{13}$C NMR"
- José Miguel Martin Martínez, University of Alicante, "Degradable polyurethane adhesives based on rosin and tung oil diols"

Being an IUPAC-sponsored international conference, POLYCHAR 20 attracts scientists from all over the world reflecting the philosophy of the POLYCHAR conferences that is to provide an international forum, especially for students and young scientists. The principal aim is to give them opportunity to meet with their peers and with well-known scientists and to exchange experiences, make contacts and present their results to the scientific community. IUPAC's financial support enabled the attendance of 12 students and young researchers from scientifically emerging countries.

The broad span of contributions to POLYCHAR 20 is probably best represented by the awardees of the conference and their contributions. The P.J. Flory Polymer Research prize was awarded to Robert F.S. Stepto, Manchester Materials Science Centre, for his work on thermoplastics including thermoplastic starch materials. The International Materials Science Prize was given to Hyoung Jin Choi, Inha University, Incheon, for his work on rheology and electro-rheology.

Three IUPAC Poster Prizes were awarded:

- Zuzana Morávková Rozlivková, Institute of Macromolecular Chemistry, Academy of sciences of the Czech Republic for her poster "Polyaniline prepared in water-ethanol mixture"
- Sven-Christian Sidenstein, University of Siegen, Germany (advisor Holger Schoenherr), for his poster "Internal organization does matter: tracerdiffusion in poly(methyl acrylate) brushes and spin-coated films"
- Mirna Petkovic Didovic, University of Rijeka, School of Medicine, Croatia (advisor Srecko

Valic), for her poster "Correlation between orientations of nanoclay and natural rubber crystallites in natural rubber/clay nanocomposites"

The Jűrgen Springer Prize for a Young Scientist was given to Marianna Pannico, Institute of Chemistry and Technology of Polymers, Pozzuoli, for the presentation "Stabilization Effects of Functional POSS in Epoxy Resins: Spectroscopic and Dynamic-Mechanical Studies."

The Bruce Hartman Prize for a Young Scientists was awarded to Malgorzata Walczak, Centre of Molecular and Macromolecular Studies, Lodz, for the poster "Characterization of PC/PS Multilayered Films."

The Carl Klason Prize for an Outstanding Student Presentation was awarded to three ex aequo winners:

- Michael Härth, Friedrich-Alexander University, Erlangen, for the poster "Simple Approximate Solution for Modeling the Spreading of a Drop in Partial Wetting Case"
- Zhansaya K. Sadakbayeva, Institute of Macromolecular Chemistry, Prague, for the poster "Interpenetrating Networks Based Hydrogels"
- Zrinka Buhin, University of Zagreb, Zagreb, for the oral presentation "In Situ Emulsion Polymerization and Characterization of Poly (Butyl Acrylate-co-Methyl Methacrylate)/Silica Nanosystems"

Because of the great number of very good student presentations, five Diplomas of Distinction for a Student Presentation were given:

- Aline Bassi Denis, Instituto de Quimica de São Carlos, São Carlos, for the poster "Residual Monomer Determination of Dental Resins with Different Photoinitiators"
- Rajesh Pandit, Tribhuvan University, Kathmandu, for the poster "Epoxidation Effect of Butadiene Block on Morphology and mechanical Properties of SBS Block Copolymer"
- Ricarda Schröder, Aachen University, Aachen, for the poster "Zwitterionic Microgels Based on N-Vinylcaprolactam and Sulfo-, Carboxy-, and Phosphobetaine"
- Selda Sen, Istambul Technical University, Istanbul, for the poster "A Study on Electrospinning of Acrylonitrile and Itaconic Acid Copolymers"
- Ângela Dias, Universidade do Porto, Porto, for the presentation "Effect of Added Amines on the Morphology of Vesiculated Polyester Particles"

Special acknowledgements were given to the retired Croatian professors from the Zagreb University, Faculty of Chemical Engineering and Technology:

- Zvonimir Janovic, for his selfless scientific and educational work in the area of polymer science and materials;
- Mladen Bravar, for his important contributions to supervising and education of young scientists in the area of advanced materials;
- Branko Kunst, for his pioneering work in physical chemistry of polymers and successful mentoring of young scientists and students.

Manuscripts of the POLYCHAR 20 participants will be published in *Macromolecular Symposia*, *Polymer Engineering & Science*, *Materials Research Innovations,* and *Chemistry & Chemical Technology*.

POLYCHAR 21, 18–22 March 2013, will be held in Daegu, South Korea.

**www.polychar20-croatia.com**

*Group photo of participants at POLYCHAR 20.*

## Toxicology

### 16–19 October 2012, Lisbon, Portugal

The Portuguese Toxicology Association will host the **European Society of Toxicology in Vitro 2012 International Congress**, ESTIV2012, in Lisbon, Portugal, 16–19 October 2012.

As in previous ESTIV events, this conference will bring together researchers and students from academia and industry involved in the development and use of in vitro methods in toxicology. The scientific program includes state-of-the-art lectures, workshops, and original communications and poster sessions. ESTIV 2012 will cover a broad range of topics addressing systemic toxicity, local toxicity, developmental toxicity with emphasis on physiologically relevant markers, marker profiles, and molecular mechanisms and pathways.

ESTIV2012 will explore challenges and successes of non-animal approaches for toxicity testing. As with previous ESTIV Conferences, a special student session will also be organized, where young researchers will be invited to briefly present their work, with an award for the best presentation. For the first time and in addition to the cutting-edge topics that will be covered in the conference, a practical workshop will be organized on 20 October. Participants will gain hands-on experience with computerized in vitro—in vivo extraplotation strategies.

In addition to the scientific program, attendees will experience the warm hospitality, excellent climate, rich culture, and great food that Lisbon has to offer. The conference venue is located in the new part of the city, close to the airport and the Expo waterfront.

ESTIV2012 will focus on new developments in toxicity testing and the mechanism of action of chemicals and nanomaterials, with a special emphasis on the following themes:

- Dermal Toxicity
- Ocular Toxicity
- Dermal Sensitization
- Innate Immune Responses in Toxicity
- Carcinogenicity Testing
- Reproductive and Developmental Testing
- Systemic Toxicity
- Computational Toxicity and Toxicokinetics

**www.estiv2012.com**

## Novel Aromatic Compounds

### 28 July–2 August 2013, Taipei, Taiwan

The International Symposium on Novel Aromatic Compounds was founded in 1970 by T. Nozoe, who discovered the first nonbenzenoid aromatic compound, hinokitiol, in Taipei. The name and the goal of this symposium series have evolved as the research and applications of aromatic compounds thriving in diverse range of disciplines. The **15th International Symposium on Novel Aromatic Compounds** (ISNA-15), to take place 28 July–2 August 2013 in Taipei, will be a historic occassion. To continue the blossoming tradition of previous ISNA symposia, ISNA-15 will provide an interactive platform for researchers worldwide to present new findings and exchange innovative ideas on advanced synthesis, structure-property relationship, and applications of novel aromatic compounds.

The scientific program of this symposium includes the Nozoe memorial lecture, plenary lectures, invited lectures, oral communications, and poster presentations. Attendees will find Taipei to be a vibrant city where East meets West.

**Symposium Topics**

- Aromaticity and Novel Aromatic Systems—Theory, Synthesis, and Experiment
- Aromatic Polymers and Oligomers—Synthesis, Properties, and Applications
- Molecular and Supramolecular Aromatic Devices, Switches, Machines
- Fullerenes and Concave Aromatics, Graphene, Carbon Nanotube Related Aromatics
- Macrocyclic Aromatic Compounds
- Aromatics for Conducting, Magnetic, and Optoelectronics

Confirmed plenary lecturers include Jean-Luc Brédas, Klaus Müllen, Eiichi Nakamura, Shie-Ming Peng, Timothy M. Swager, Yoshito Tobe, and Daoben Zhu. The Nozoe Lecturer will be Andrew B Holmes.

**See Mark Your Calendar for contact information.**

**www.isna15.org**

## Nano Systems and Applications

21–25 November 2012, Coimbatore, India

The **6th International Symposium on Macro- and Supramolecular Architectures and Materials (MAM-12): Nano Systems and Applications** will take place 21–25 November 2012 in Coimbatore, India. The conference is jointly organized by the Centre for Nano Science and Technology, K S R College of Technology, Tiruchengode, Namakkal, Tamil Nadu, India, and the World Class University, Gwanju Institute of Science and Technology, South Korea.

The conference will cover a wide range of topics in nanotechnology and its applications. Keynote and plenary lectures will be delivered by eminent , scientists such as Nobel Laureates Peter Grunenberg (Germany) and Aaron Ciechanover (Israel).

**See Mark Your Calendar for contact information.**

**www.mam12.ksrct.ac.in**

## Advanced Polymers via Macromolecular Engineering

18–22 August 2013, Durham, UK

The **10th International Conference on Advanced Polymers via Macromolecular Engineering** (APME 2013) will be held at Durham University in the UK from 18–22 August 2013. Organized and hosted by the Durham Centre for Soft Matter, APME 2013 will be the latest in a series of successful meetings, the most recent of which were held in Cappadocia (Turkey) (2011), Dresden (2009), and Miami (2007).

The focus of the meeting will be on recent advances in polymer chemistry, polymer synthesis, and polymer characterization. Topics to be covered include the following:

- Radical Polymerization
- Step Growth Polymers
- Functional Polymers
- Supramolecular Polymers
- Polymer Colloids
- Polymers at Surfaces and Interfaces
- Polymer Characterization
- Biomaterials and Polymers for Medical Applications
- Renewable/Sustainable Polymers
- Plastic Electronics
- Polymers for Energy Applications
- Complex Macromolecular Architectures
- Polymers and Industry

Seven plenary speakers will present their latest research along with 32 invited speakers. The program will also include some 48 contributed presentations, 16 contributed short talks for younger researchers, and a poster session, which will provide participants the opportunity to highlight their recent work.

**See Mark Your Calendar for contact information.**

**www.dur.ac.uk/soft.matter/apme2013**

## Biorefineries

28–29 September 2013, Brasília, Brazil

The **2nd Brazilian Symposium on Biorefineries**, to be held 28–29 September 2013 in Brasília, Brazil, is aimed at promoting dialogue about the possibilities and challenges related to biorefineries and the development of a Green Economy. Its topics are as follows:

- raw materials
- advances in chemical, biochemical, and thermochemical processes
- advances in analytical techniques and methodology
- economic potential of new products and their sustainability

The symposium is limited to 300 attendees from industry, government, and research institutions in Brazil and throughout the world. An opening lecture will be delivered by a leading biorefinery researcher on the evening of 27 September, followed by a reception with the press.

The event has a strong international profile (speakers and audience), and will have simultaneous English-Portuguese translation.

**See Mark Your Calendar for contact information.**

**www.siadeb.org/snbr**

# Mark Your Calendar

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

## 2012 (after 15 September)

*IUPAC poster prizes to be awarded*

**15–20 September 2012 • Catalysis in Organic Synthesis • Moscow, Russia**
*International Conference on Catalysis in Organic Synthesis*
Prof. Mikhail P. Egorov, Russian Academy of Sciences, Zelinsky Institute of Organic Chemistry, 47 Leninsky Prospekt, B-334, RF-119991 Moscow, Russia, Tel.: +7 095 135 5309, Fax: +7 095 135 5328, E-mail: mpe@ioc.ac.ru

**16–21 September 2012 • Biotechnology • Daegu, Korea**
*15th International Biotechnology Symposium and Exhibition*
IBS 2012 Secretariat, 6F, Sunghwa B/D, 1356-51 Manchon, 1-Dong, Suseong-Gu, Daegu 706-803, Korea
Tel.: +82 53 742 5557, Fax: +82 53 742 9007, E-mail: info@ibs2012.org

**14–19 October 2012 • Novel Materials • Xian, China**
*8th International Conference on Novel Materials and their Synthesis*
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

**23–26 October 2012 • Green Chemistry • Moscow, Russia**
*4th International Chemical Assembly on Green Chemistry*
Prof. Ekaterina S. Lokteva,Moscow State University, Department of Chemistry, Leninsky Gory, 1, RF-119991 Moscow, Russia, Tel: +7 495 939 3337, Fax: +7 495 939 4575, E-mail: les@kge.msu.ru

**5–9 November 2012 • Mycotoxin • Rotterdam, Netherlands**
*7th World Mycotoxin Forum and XIIIth International IUPAC Symposium on Mycotoxins & Phycotoxins*
Ms. Helena B. Bastiaanse (Program Coordinator), Bastiaanse Communication, P.O. Box 179, NL-3720 AD Bilthoven, Netherlands, Tel.: +31 302 294 247, Fax: +31 302 252 910, E-mail: helena@bastiaanse-communication.com

**21–25 November 2012 • Supramolecular Architectures and Materials • Coimbatore, Tamil Nadu, India**
*6th International Conference on Macro- and Supramolecular Architectures & Materials (MAM-2012)*
Dr. Venkatchatalam Rajendran Director, Center for NanoScience & Technology, K.S. Rangasamy College of Technology, K.S.R. Kalvinagar, Tiruchengode, Namakkal, Tamil Nadu 637 215, India
Tel.: +91 428 827 4880, Fax: +91 428 827 4880, E-mail: veerajendran@gmail.com

## 2013

*IUPAC poster prizes to be awarded*

**22–23 January 2013 • Test Results in Analytical Chemistry • Tel Aviv, Israel**
*Workshop on Human Errors and Out-of-Specification Test Results in Analytical Chemistry*
Prof. Ilya Kuselman National Physical Laboratory of Israel Givat Ram IL-91904 Jerusalem Israel
Tel.: +972 2 630 3501, Fax: +972 2 630 3516, E-mail: reut@bioforum.co.il

**17–22 February 2013 • Scanning Electrochemical Microscopy • Ein Gedi, Israel**
*7th Workshop on Scanning Electrochemical Microscopy*
Prof. Daniel Mandler, The Hebrew University of Jerusalem, Department of Inorganic and Analytical Chemistry, Safra Campus, IL-91904 Jerusalem, Israel,
Tel.: +972 2 658 5831, Fax: +972 2 658 5319, E-mail: mandler@vms.huji.ac.il

**11–13 March 2013 • Metal Ions in Biology • Punta del Este, Uruguay**
*12th International Symposium on Metal Ions in Biology and Medicine*
Dr. Dinorah Gambino Universidad de la República Cáterdra de Química Inorganíca Facultad de Química 2124 Avenida General Flores Montevideo 11700 Uruguay
Tel.: +598 2 924 9739, Fax: +598 2 924 1906, E-mail: dgambino@fq.edu.uy

**18–22 March 2013 • Polymer Characterization • Daegu, Korea**
*21st International Conference on Polymer Characterization—World Forum on Advanced Materials (PolyChar-21)*
Prof. Witold Brostow, University of North Texas, Department of Materials Science & Engineering, P.O. Box 305310, Denton, TX 76203-5310, USA, Tel.: +1 940 565-4358, Fax: +1 940 565-4824, E-mail: brostow@unt.edu

**19-23 May 2013 • Clinical Chemistry & Laboratory Medicine • Milan, Italy**
*20th IFCC-EFLM European Congress on Clinical Chemistry & Laboratory Medicine; 45th Congress of the Italian Society of Clinical Biochemistry & Clinical Molecular Biology*
Dr. Ferruccio Ceriotti, Instituto Scientifico Ospedale San Raffaele, Servizio di Medicina di Laboratorio, Via Olgettina 60, I-20132 Milano, Italy, Tel.: +39 10 226 432 282, E-mail: ceriotti.ferruccio@hsr.it

# I U P A C

ADVANCING THE WORLDWIDE ROLE OF CHEMISTRY FOR THE BENEFIT OF MANKIND

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Österreichische Akademie der Wissenschaften *(Austria)*
Bangladesh Chemical Society *(Bangladesh)*
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