

CHEMISTRY

International

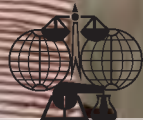
The News Magazine of IUPAC

November-December 2012

Volume 34 No. 6

**ALCHEMISTS
are US**

The Alchemica



INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

The European Chemicals Agency ►

ICSTI at Work ►



From the Editor

CHEMISTRY International

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

www.iupac.org/publications/ci

Managing Editor: Fabienne Meyers

Production Editor: Chris Brouwer

Design: pubsimple

All correspondence to be addressed to:

Fabienne Meyers

IUPAC, c/o Department of Chemistry

Boston University

Metcalfe Center for Science and Engineering

590 Commonwealth Ave.

Boston, MA 02215, USA

E-mail: edit.ci@iupac.org

Phone: +1 617 358 0410

Fax: +1 617 353 6466

Printed by:

Cadmus Communications, Easton, PA, USA

Subscriptions

Six issues of *Chemistry International* (ISSN 0193-6484) will be published bimonthly in 2012 (one volume per annum) in January, March, May, July, September, and November. The 2012 subscription rate is USD 110.00 for organizations and USD 50.00 for individuals. Subscription orders may be placed directly with the IUPAC Secretariat. Affiliate Members receive *CI* as part of their Membership subscription, and Members of IUPAC bodies receive *CI* free of charge.

Reproduction of Articles

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

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

ISSN 0193-6484

One way or another, we hope that you have already highlighted in your 2013 agenda the key dates of August 11 to 16. On behalf of the Turkish Chemical Society, you are invited to participate in the 44th IUPAC World Chemistry Congress, which will be held in Istanbul, Turkey. The abstract submission period is now open and the program, covering no less than 10 scientific topics, is presented in detail online at www.iupac2013.org. Please inform your colleagues, and thanks in advance for your help in disseminating the dates and venue of the event.

The IUPAC General Assembly and Council meeting take place at the same time and venue as the biennial Congress. For IUPAC members, the



joint meeting of the Congress and General Assembly is a unique opportunity to connect with the scientific community at large and at the same time to reconnect with IUPAC members and fellows who otherwise work remotely on ongoing projects and committee tasks. No doubt that in the coming issues of *CI*, we will hear about the coming events in

more detail and get updates on what to expect in Istanbul.

This issue includes a special call for the participation of younger chemists. The Congress organizers and IUPAC are joining efforts to encourage young chemists to participate in the Congress, and have established programs to offer travel assistance. See program details on page 16.

As in previous years, IUPAC will also reserve a special welcome at its Congress to a handful of outstanding young Ph.D. graduates who have received one of the IUPAC Prizes for Young Chemists, either for 2012 or 2013. The 2012 winners are presented on page 16. The prize was established in 2000 to encourage outstanding young research scientists at the beginning of their careers. It is awarded for the most outstanding Ph.D. thesis in the general area of chemical sciences. Please do look for them in Istanbul; aside from participating in the opening ceremony, they will also present their research as posters. All that said, if you are mentoring a graduate student who is about ready to complete his/her thesis before the end of the year, please bring to his/her attention that the call for nominations for the 2012 graduates is 1 February 2013. Besides the recognition and paid travel to the next Congress, the award also comes with a cash prize of USD 1000. What great motivation to wrap-up a thesis before 31 December strikes!

I hope to see you all—younger chemists and not so young—in Istanbul in early August 2013!

Fabienne Meyers

fabienne@iupac.org

www.iupac.org/publications/ci

Cover: *The Alchemical Quest* is the latest exhibit at the Chemical Heritage Foundation in Philadelphia; it's on display until 7 December 2012. See feature on page 4.

Contents

CHEMISTRY International November-December 2012 Volume 34 No. 6



Stamps International, 35

Vice President's Column

Our Roles, Responsibilities, and Legacy *by Mark Cesa* 2

Features

Alchemists Are Us: New Exhibit Shows the Influence of Alchemy on Modern Chemistry *by Neil Gussman and Michal Meyer* 4

Chemicals in the European Union: The European Chemicals Agency Experience *by Derek J Knight* 6

The Year of Chemistry at the Lycée Français d'Irlande
A Cross-Disciplinary, Multiclass Educational Project
by Johnny Marcelin and Sarah Magadoux 9

ICSTI at Work

An Interview with Brian Hilton *by Emma Thompson* 13

IUPAC Wire

Young Chemists to the 44th IUPAC Congress 16

John D. Petersen Appointed IUPAC Executive Director 16

Mozambique and Argentina Join IUPAC as Full Members 17

Winners of 2012 IUPAC Prizes for Young Chemists 17

Rachel O'Reilly Receives the 2012 IUPAC-Samsung
Young Polymer Scientist Award 18

Second CHEMRAWN VII Prize Awarded to Rashmi Sanghi 19

Ian Mills Awarded IUPAC SUNAMCO Prize 20

Mark Cesa and James Economy Named ACS Fellows 20

The Project Place

IUPAC Safety Training Program 21

Nomenclature Notes

InChIs and Registry Numbers *by Jeffery Leigh* 28

Making an impact

Guidelines for Reporting of Phase Equilibrium Measurements 24

Characterization of Photoluminescence Measuring Systems 24

IUPAC/CITAC Guide: Investigating Out of Specification Test
Results of Chemical Composition 25

A Brief Guide to Polymer Nomenclature 25

IUPAC-NIST Solubility Data Series—Recent Volumes 25

Conference Call

Going for Gold: The 44th International Chemistry Olympiad
by Mary Kirchhoff 26

On the Description of Nanomaterials
by Françoise Roure and John Rumble 28

What's in a Name? Possibly Death and Taxes!
by Richard M. Hartshorn and Hervé Schepers 29

IUPAC MACRO World Polymer Congress 2012
by Timothy Long 32

Where 2B & Y

34

Mark Your Calendar

37

Index for 2012

38

Our Roles, Responsibilities, and Legacy

by Mark Cesa



photo by Peter Cutts

It is a great honor to serve IUPAC as vice president. I have been privileged to work in IUPAC in several capacities, and as an industrial scientist I have a deep appreciation for the value of fundamental science in chemical innovation, the contributions of the chemical industry to improving the well-being of humankind, and the

role of IUPAC as the enabler of progress in global chemistry.

I began in IUPAC in 1997 as a Young Observer at the General Assembly and Congress in Geneva. I remember how impressive the meeting of the Committee on Chemistry and Industry was, especially the enthusiasm of the members and scope of activities of the committee. At the end of its meeting I approached the incoming chair, Nelson Wright, and offered to help with anything that was needed. Nelson offered me responsibility for the Safety Training Program (STP). I took on the STP and have never looked back. My work in IUPAC has given me an unparalleled exposure to the global chemistry community and a deep appreciation for the strength of commitment and contributions of all of the scientists who work as volunteers in IUPAC. No doubt all of us, from our National Adhering Organizations to our Associated Organizations to our many individual scientist volunteers working on IUPAC projects, share the satisfaction of contributing to the furtherance of worldwide chemistry.

This is an exciting and challenging time for IUPAC. As it approaches its second century, IUPAC must continue to make meaningful contributions and increase its influence. IUPAC needs to draw on the creativity and expertise of chemists around the world to discover and disseminate fundamental scientific knowledge and apply chemistry innovatively and safely to improve the quality of life. IUPAC must work at the interfaces between academia and industry and among the sciences to create valuable and exciting programs and initiatives.

As you know, the most important task for the vice president, as called for in the IUPAC Statutes, is the preparation of a "critical assessment of the programs and projects of all IUPAC bodies." At the IUPAC Bureau meeting last April I presented a summary of the areas that I intend to focus on.

I have begun examining in depth the projects and programs of IUPAC as they relate to our current long-range goals to provide the basis for reviewing the scope of IUPAC's activities, to illustrate the areas where IUPAC has particular strength, and to reveal areas deserving of greater emphasis. The rapid growth of scientific research and chemical production around the world illustrates the increasing globalization of chemistry. IUPAC must maintain and enhance its unique and traditional strengths in nomenclature, standardization, scientific conferences, and education to serve the global chemistry community.

We have seen how successful the International Year of Chemistry (IYC) was in energizing chemists all over the world, and now it is important for all of us in IUPAC to carry forward that momentum as we approach the 2019 Centennial of IUPAC. As one views this "legacy" for IUPAC in light of its mission and long-range goals, the following themes emerge as areas for focus:

1. the roles of chemists at the interfaces of the scientific disciplines
2. IUPAC's scientific contributions and the public good
3. the legacy of IYC as an integral part of IUPAC activities

IUPAC has made great strides toward building capabilities at the interfaces of the chemical disciplines and other sciences (e.g., through its interdivisional subcommittees in Green Chemistry and Materials Chemistry). We can explore possibilities as well for new interdivisional subcommittees and new interactions with other unions. The collaboration between IUPAC and the International Union of Pure and Applied Physics (IUPAP) on the validation of claims for new elements, the interactions between the Chemistry and the Environment Division (Division VI) and the Society for Environmental Toxicology and Chemistry (SETAC), and the cooperation between the Chemistry and Human Health Division (Division VII) and the International Union of Toxicology (IUTOX) can serve as models. All of the Divisions and Standing Committees are encouraged to explore new collaborations.


IUPAC should enhance its productive interactions with the chemical industries. As we often point out,

the chemical industry of the early 20th century took an active part in the establishment of IUPAC in 1919. The chemical industries, including the traditional commodity chemical and fine chemical manufacturers, the pharmaceutical and agrochemical industries, and the many new startup companies around the world focusing on areas such as medicinal chemistry and materials science, all have roles to play in expanding the scope of IUPAC activities. To this end, the Committee on Chemistry and Industry (COCI) is embarking on an effort to redesign and reinvigorate the Company Associates program. A task group to be headed by COCI will tackle this issue. COCI can also advise IUPAC leadership on how best to work at the academic/industrial interface to assist the chemical industry and to enable industry to assist IUPAC through collaborations with our divisions and standing committees through knowledge gained from its regional workshops in Western Europe, East Asia, the Middle East, and the North American Great Lakes region.

We chemists have a responsibility to the public to make our scientific knowledge available to decision makers so that sound regulations can be enacted that protect the public well-being and help the public appreciate the vital role of science, and chemistry in particular, in their lives. IUPAC can make its scientific intellectual property and knowledge bases available for the benefit of the greater society by exploring mechanisms for IUPAC, as an objective, non-political science-based organization, to offer its expertise to appropriate global parties interested in using this information for the benefit of the human condition.

In the past few years, IUPAC has explored collaborations of this type with the UNEP's Strategic Approach to International Chemicals Management (SAICM) and with the Organization for the Prohibition of Chemical Weapons (OPCW). In both cases, these organizations sought out IUPAC for its expertise in providing the scientific basis for action, and they have found our input of great importance to their success.

Recently I explored the IUPAC records, reports, and documents for information relating to IUPAC's contributions in several areas, including sustainable development, chemical safety and security, and toxicology. The contributions that IUPAC has made in these areas, and in fact all the areas where IUPAC works, are extraordinarily impressive. We need to convey this message clearly to all of IUPAC's stakeholders—NAOs, associated organizations, and the worldwide community of chemists—so that they can see how valuable IUPAC's work is for them. Examining IUPAC's current portfolio will also provide the basis for a review of IUPAC's strategy. The last strategic review was completed nearly 10 years ago, and with the rapid advances in the sciences and in the world at large, it will be beneficial to take a renewed look at our vision, mission, goals, and activities.

In recent issues of *CI*, we have heard from our officers about their hopes and concerns for IUPAC in the coming years. Clearly, all of our officers believe strongly in the capabilities and accomplishments of IUPAC, and so do I. I am eager to work with our officers and with all of our volunteers and staff to lead IUPAC toward its next biennium. 

I U P A C



Advancing Worldwide
Chemistry



IUPAC Prize for Young Chemists

Supporting the future of chemistry

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

Call for Nominations: Deadline is 1 February 2013.

For more information, visit www.IUPAC.org

or contact the Secretariat by e-mail at secretariat@iupac.org or by fax at +1 919 485 8706.

Alchemists Are Us

New Exhibit Shows the Influence of Alchemy on Modern Chemistry

by Neil Gussman and Michal Meyer

Try as we might to distance ourselves from alchemy and its centuries-old bad reputation, the truth is that these early empiricists laid the foundations of modern chemistry. Many experimental methods and lab practices started life with the alchemists and live on, with refinements, to this day. Distillation, purifying metals, isolating elements and compounds, and medical analysis were first practiced by alchemists, and then carried into the modern world as experimentalists began to call themselves chemists.



The Alchemical Quest, on display at Chemical Heritage Foundation in Philadelphia until 7 December, highlights the practical goals of alchemy. The exhibit features rare alchemical books of the 16th, 17th, and 18th centuries drawn from CHF's collections. The exhibit also highlights two fathers of modern science, Robert Boyle and Isaac Newton. Their avid involve-

ment in alchemy during their long and productive lives provided a bridge to modern chemistry.

In *Chemistry World* magazine (UK), December 2004, Vikki Allen writes, "The term alchemy originally referred to an ancient art of spiritual purification and transformation; a way for people to connect with the divine spirits. Although the origins of alchemy vary across the world, in the middle-ages the term became associated with man's desire to harness nature. Alchemists would strive to turn lead into gold and to produce the elusive 'elixir of youth.'

"The alchemist's profession was a mystery and the public viewed it with a mixture of fear and wonder. The alchemical symbols used at the time were unrecognizable to outsiders and the Church discredited the work. But the force of human nature meant the public still wanted what the alchemists were working towards; endless riches and eternal life." The public image of chemistry in the 21st century is hardly better than this image of alchemy. The public wants the clean water, abundant energy, and advanced materials chemistry can and does deliver, but is generally afraid of the word Chemical.

Obviously, some of the bad reputation of alchemy is deserved, but Allen reflects an outdated understanding of what alchemy was about. The best alchemists were not mystical dreamers, but skilled bench chemists. Painters would go to them for pigments, the ill for medicines, and mine owners for better acids to dissolve ores. The chemistry of today finds its origins in the alchemical labs of the Middle Ages and Early Modern periods.

Alchemy is a natural starting point for anyone interested in the history of science. Alchemy's goals were both practical (better medicine) and esoteric (creating the philosopher's stone that would transmute lesser metals into gold). Chemists have kept many of the practical goals, but abandoned the quest for the philosopher's stone in the 18th century.

Alchemy can be a dirty business—just ask Isaac Newton. He began one of his alchemical recipes with "Take of Urin one Barrel." He then instructs the owner of the newly acquired barrel to let the urine ferment for three months in the summer. Imagine being Isaac Newton's neighbor: The glory! The smell!

This story gets a laugh from people who've never encountered the history of science. Laughter is a good place to begin the story of chemistry; humor engages in a way that information and argument do not and provides a starting point for deeper exploration. Such as: Why did Newton want a barrel of urine? His recipe

was for making phosphorous, which had recently been discovered by a 17th-century ex-soldier and alchemist named Hennig Brandt, who had been trying to make the philosopher's stone. The glowing substance distilled from urine (white phosphorous) must at first have filled Brandt with hopes of success. Such stories take us into older understandings of matter, a time before elements as we know them.

Newton's alchemical work was rediscovered in the 19th century and the discoverers were horrified to find their scientific hero had feet of clay. By that time, alchemy was considered a historical dead end, a wrong turn along the highway of progress. At best, it could be considered a distraction from real science; at worst, it was pure charlatanry, certainly not worthy of practice by a scientific hero. Since then, historians have rediscovered the common heritage of alchemy and chemistry, which were inseparable in the 17th century. A new term, "chymistry," is now used to describe the chemical practices of that time.

If you're looking for a moral to this story, here's one: Progress is not a straight line from some moment in the past to now. Otherwise, enjoy the story. As to where Newton or his recipe followers got their barrel of urine, we have no idea. One colleague suggested that Newton would have parked his barrel outside a pub and waited. Modern chemists can breathe a sigh of relief: They can simply order their supplies.

The history of alchemy is the history of chemistry. The beautiful woodcuts and engravings found in the exhibit's books show visitors this strange, intriguing, and beautiful chapter in the history of chemistry. An accompanying digital book display interprets many of these evocative yet difficult to understand images. Dragons, roosters, flocks of birds, kings, queens, and hermaphrodites are translated into modern chemical processes. Alchemists didn't want to let just anybody into their secrets, so they hid them in plain sight, in complex word and picture allegories understandable only to other alchemists.


When alchemy faded into chemistry, the meaning behind these images was lost. But modern-day his-



torical sleuths have begun working out the chemistry behind these images. For example, an old alchemical book in our collection includes 12 images and accompanying text that are the steps or "keys" to making the philosopher's stone. The first three keys have been decoded by Lawrence Principe, a trained chemist and a historian of science at Johns Hopkins University. For example, the third key shows a dragon in the foreground and a rooster being eaten by a fox which is being eaten by another rooster.

It's a lovely image, but where's the chemistry? In this case, the dragon refers to a red crystal known as dragon's blood. Once you realize that sun indicates gold in the alchemical understanding, it doesn't take long to go from rooster to sunrise (crowing rooster) to sun to gold. The fox represents certain acids dissolving the gold and the rooster eating the fox shows a circular process. So gold is being dissolved and re-dissolved by certain acids (what we know as nitric and hydrochloric). Chlorine (only discovered as a gas in the 18th century) builds up and the gold volatilizes into gold chloride, which is a lovely ruby red color.

The chemistry that goes on in this gold chloride reaction was only worked out in the 19th century. Not bad for the shabby misunderstood alchemists of old. Perhaps one day historian chemists will unlock the rest of the keys. Only one thing is certain, there'll be no philosopher's stone at the end of it all. Though a little bit of recognition for the triumphs of alchemy would be appreciated.

CHF gratefully acknowledges the generous support provided by the National Endowment for the Humanities, Kathryn Hach-Darrow, and the ExxonMobil Chemical Company for *The Alchemical Quest*. 

Michal Meyer <mmeyer@chemheritage.org> is editor-in-chief of Chemical Heritage magazine. Neil Gussman <neilg@chemheritage.org> is strategic communications and media relations manager at Chemical Heritage Foundation.

Parts of the article were previously published on the CHF blog "Periodic Tabloid."



Chemicals in the European Union

The European Chemicals Agency Experience

by *Derek J Knight*

The European Chemicals Agency (ECHA) is the driving force for implementing the EU's groundbreaking chemicals legislation for the benefit of human health and the environment as well as for innovation and competitiveness. It helps companies to comply with the legislation, advance the safe use of chemicals, provide information on chemicals, and address chemicals of concern. Founded in 2007 and based in Helsinki, Finland, ECHA is a modern, science-driven organization that has rapidly grown to become one of the largest EU agencies.

ECHA is responsible for the main EU laws governing chemicals:

- Registration, Evaluation, Authorization, and Restriction of Chemicals (REACH) Regulation
- Classification, Labelling, and Packaging (CLP) Regulation.

These regulations ensure a high level of protection for human health and the environment by requiring that industry manufacture and use chemical substances safely. One of the main reasons for REACH is to fill information gaps for the large number of substances already in use in the EU. Under REACH, ECHA is responsible for obtaining, communicating, and using good-quality information on chemicals. Industry has to assess the hazards of substances for classification and risk assessment, and then adopt appropriate risk management measures to protect human health and the environment.

Another key strategic purpose of REACH is to address substances of concern that require regulatory intervention. The identification of such substances is facilitated by the process of compiling information on all chemical substances. The REACH and CLP processes and different actors involved are summarized in the figure on page 7.

REACH registrants have to provide information in the registration dossier on the intrinsic properties of all substances manufactured or imported at one tonne per annum or more. A key facet of REACH is to deal with old substances; these so called "phase-in" substances have to be registered by one of three dead-

lines according to their tonnage. The non-confidential information from registrations is disseminated by ECHA from the searchable database ECHA CHEM.

The standard information required for substances depends on the tonnage; the higher the tonnage, the more information needed. Substances are registered first with core data, with higher-tier studies applying at >100 tonnes and further studies at >1000 tonnes per annum. Registrants make testing proposals for such higher-tier studies and await approval to proceed with the testing following examination of the testing proposal by ECHA as part of the dossier evaluation work. ECHA also undertakes compliance checking of some of the registration dossiers to ensure that no mandatory information has been omitted.

The CLP Regulation requires chemical producers to use labelling and safety data sheets (SDSs) that communicate the hazardous properties of substances to end users. Some substances have mandatory classification and labelling that has been harmonized at the EU level. For other substances, self-classification applies, and industry has to use the available information, which for registered substances can be comprehensive. The classifications used by industry are disseminated by ECHA in the Classification and Labelling Inventory.

Addressing Substances of Concern

ECHA works with the European Commission and EU member states to regulate or restrict substances that pose a risk to human health or the environment. When necessary, the member states or ECHA (on a request from the commission) initiate the appropriate regulatory risk management process:

- Authorization is for "substances of very high concern" (SVHC), such as carcinogens; mutagens; or substances toxic for reproduction (CMRs); persistent, bioaccumulative, and toxic (PBT); very persistent and very bioaccumulative (vPvB); or of "equivalent concern." Substances with SVHC properties are first formally identified in the "Candidate List" then transferred, if appropriate, onto the "Authorization List." They can then only be marketed or used after the "sunset date" if they have been authorized based on a successful authorization application.
- Restriction is for when an unacceptable risk to humans or the environment has been identified.
- EU harmonized classification and labelling is for CMR substances or respiratory sensitizers (or for other hazards if justified for pesticide or biocide active substances).

REACH and CLP principles, processes and actors



Industry

Obtaining, using and communicating high-quality information on substances

- Pre-registration
- Data sharing
- Registration
- Self-classification
- Notification to the Classification and Labelling Inventory
- Industry obtains information on substances to assess hazards for classification and risk assessment to ensure safe use.
- Industry communicates to downstream users by labelling and by safety data sheets, including the exposure scenarios, i.e. operational conditions with associated risk management measures.
- ECHA disseminates registration and classification & labelling information.

Information on substances is of use in screening for potentially problematic substances



Member State
competent authorities

Dossier evaluation

- Testing proposal evaluation for decisions on conducting higher-tier studies
- Handling of compliance checks of some dossiers for compliance that no mandatory data are missing

Substance evaluation

- Community rolling action plan list of substances of potential risk
- Obtain any necessary information to clarify risk

Screening, prioritisation, risk management option analysis and selection of substances of concern for risk management



European Commission

Address substances of concern that warrant regulatory intervention

- Authorisation of substances of very high concern
 - Identification onto the candidate list
 - Transfer onto the authorisation list
 - Authorisation of use for successful applicants
- Restriction when unacceptable uncontrolled risks
- Harmonised classification and labelling of CMRs, respiratory sensitisers (and other hazards if justified)
- Member State competent authorities and European Commission initiate proposals, with the support of ECHA.
- European Commission applies the appropriate EU regulatory measure.

Substance evaluation is, in a sense, a link between registration and the risk management activities of REACH because it is the means of clarifying what to do regarding particular problematic substances. This is a separate process undertaken by Member States, coordinated by ECHA, to examine if more information, either on substance properties or their use and exposure, is needed to clarify whether there really is a risk. The substances to be evaluated are listed in the Community Rolling Action Plan (CoRAP). If the final outcome is that there is an uncontrolled risk, then a Member State can propose appropriate action under one of the REACH and CLP processes or refer to another EU regulatory instrument.

ECHA's Priorities and Strategic Aims

A key priority for ECHA is to ensure full readiness for the second registration deadline of 31 May 2013 for "phase-in" substances at >100 tonnes per annum. To meet this goal, the agency will continue to provide

support to lead registrants to assist them in preparing high-quality dossiers and chemical safety reports (CSRs), and to carry out targeted communication activities to reach out to new registrants.

Another major priority is the ongoing dossier evaluation work. ECHA has a deadline of 1 December 2012 for examining the testing proposals from the first registration deadline. It also has an ambitious target of completing compliance checks of 5% of the highest tonnage band by the end of 2013.

Authorization is the third driver for this year, because after the 1 December deadline for the first substances on the Authorization List, industry will submit applications for authorization to use those particular substances.

ECHA also has to prepare for two new regulatory schemes:

- When the EU Biocidal Products Regulation enters into effect on 1 September 2013, the EU biocides scheme will be transferred from the European Commission to ECHA. Therefore, ECHA has to

Chemicals in the European Union


prepare its IT systems to receive biocides dossiers, to create a biocidal products committee, and to recruit and train experts.

- Changes to the Prior Informed Consent Regulation will result in the transfer on 1 March 2014 of responsibility for tracking the export and import of hazardous chemicals from the European Commission to ECHA.

In its Multi-Annual Work Programme for 2013 to 2015, ECHA identifies strategic goals for achieving its ambitious vision. Although the following goals go beyond 2015, they provide direction to the agency about how to allocate resources and motivate staff:

- maximize the availability of high-quality data to enable safe manufacture and use of chemicals
- mobilize authorities to use data intelligently to identify and address chemicals of concern
- address scientific challenges by serving as a hub for the scientific and regulatory capacity-building

of member states, European institutions, and other actors

- embrace current and new legislative tasks efficiently and effectively, while adapting to upcoming resource constraints 

References

1. ECHA website: <http://echa.europa.eu/>
2. Regulation (EC) No 1907/2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH).
3. Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures.

Disclaimer: The views expressed in this paper are solely those of the author and the content of the paper does not represent an official position of the European Chemicals Agency.

Derek J Knight <Derek.KNIGHT@echa.europa.eu> is senior scientific advisor at the European Chemicals Agency in Helsinki, Finland.

IUPAC at the Helsinki Chemical Forum

by *Nicole J. Moreau*

As IUPAC past president, I had the opportunity to represent IUPAC at the 4th Helsinki Chemicals Forum organized 24–25 May 2012 at the ECHA headquarters. This important global forum brings together international and national authorities, politicians, industry leaders, NGOs, academics, and media representatives. The goal of the forum is to

Geert Dancet, executive director of the ECHA, welcomes attendees to the Helsinki Chemicals Forum.

allow dialog on key issues of global relevance related to chemical policy and chemical safety.

After the meeting, some delegates were invited to visit ECHA headquarters, where Derek Hansen, senior scientific advisor to the executive director, presented an “Introduction to ECHA, REACH, and CLP.” Furthermore, I had the great pleasure of having a discussion with some ECHA representatives and presenting some information about IUPAC.

I had the utmost interest in attending this very informative conference, which confirmed my feeling that IUPAC should collaborate with ECHA for the mutual benefit of the two organizations.

A simple look at the ECHA website and at the information it provides on chemicals legislation in Europe, reveals that ECHA shares with IUPAC several elements of vocabulary: terminology, data submission, name of the substances, and classification. It is evident that the IUPAC nomenclature is known by ECHA workforce, and that this

nomenclature should be used by the registrants. For instance, REACH regulation requires registrants of the same substance to share data in order to avoid duplication of tests. Therefore, for some tricky problems such as new compounds, nano or biological ones, IUPAC could be of help if needed. ECHA could also benefit from the InChI IUPAC system.

REACH and IUPAC share some common goals, such as ensuring the protection of human health and environment. So, how could we formally establish a fruitful collaboration? Could ECHA become a member of IUPAC? What would this necessitate from our respective organizations? These are questions I strongly think IUPAC officers and the Executive Committee should try to answer.

The fifth Helsinki Chemicals Forum will take place 18–19 June 2013 in Helsinki, Finland.

 www.helsinkiicf.eu/news/23052012.php



A Cross-Disciplinary, Multiclass Educational Project

by Johnny Marcelin and
Sarah Magadoux

During the 2011-2012 school year, and to commemorate the 2011 International Year of Chemistry, the Lycée Français d'Irlande in Dublin (LFI) launched an innovative educational experiment on the theme of chemistry that involved every level (20 classes from kindergarten to sixth year) and every subject (French, Spanish, music, history . . .).

The Lycée Français d'Irlande is a school recognized by the Agence pour l'enseignement français à l'étranger' (AEFE) with almost 500 pupils at two sites 7 km apart: a primary school (300 pupils) in Foxrock and a secondary school (190 pupils) in Clonskeagh. LFI is a partner with St Kilian's German School in the Eurocampus: a bi-lingual educational program for the first to third year of secondary school. The Eurocampus unites both schools, allowing for a bilingual teaching program that integrates these classes into the Irish educational system, thus offering pupils greater proficiency in English.

In 2011, the LFI, with the support of the scientific section of the French Embassy, decided to use the theme of the International Year of Chemistry to make pupils more aware of science, especially chemistry, in the context of a multidisciplinary teaching approach.

The IYC educational project undertaken by the Lycée Français d'Irlande gave rise to a model of scientific communication through which students made connections with places and subjects where they wouldn't expect to find chemistry. At the same time, the curriculum avoided reducing the chemistry to popular science. The goal was to develop a dialogue structured both horizontally with other disciplines and vertically with classes of all ages.

"The educational objective of the 'Chemistry and Sound' projects in second year and 'The Song of Nylon' project in fifth year was to foster the growth of knowledge of physics and of literary techniques.

During the 'Chemistry and Sound' project, the pupils carried out research on the great French chemists, wrote their biographies, and recorded their readings of them for an audiovisual presentation. Through this work they discovered the impact of chemical research on our daily life and became familiar with knowledge that can sometimes seem abstract. They also worked on writing their texts, and on reading aloud, which has to be perfect to be recorded.

The older children created a poetic documentary in the style of a documentary by Alain Resnais called 'The Song of Styrene' which they called 'The Song of Nylon'. They filmed the scientific procedure to explain the formation of nylon, and the pupils wrote a text in verse containing scientific explanations.

This work was focused on the following: disciplined work on oral expression, the pleasure of learning physics, and finally the acquisition of scientific knowledge through the history of science and experimentation. The pupils were actively involved in the project from setting up the experimental protocols to directing the scenario and the film. In this way, pupils from the different streams—literary, economic, and social and scientific—were able to see how they complement each other and the close link that can be created between art and science."

*Laurence Penny, French teacher
and Johnny Marcelin, physics teacher*



The Year of Chemistry at the Lycée Français d'Irlande

This dialogue between chemistry and other disciplines allowed the development of less traditional methods of acquiring skills.

"Chemistry, as a purely scientific discipline, seemed to offer few opportunities for a literary approach. However, the exotic character of the names of the elements and of some chemical reactions invited a playful and creative approach. 'L'Ouvroir de Littérature Potentielle' (OULIPO –the workshop of potential literature) beckoned, because it proposes an approach to literature which is at the same time poetic and systematic, even scientific: a question of writing while following the strict constraints inspired by the mathematical spirit. Olivier Salon, mathematician and writer, and an active member of OULIPO, therefore came to lead writing workshops on the theme of chemistry in the classes of third and fourth year. The plan: the collective writing of a text featuring all the letters of the periodic table in order, texts saturated with the sounds 'shi' and 'mi', with the sound of certain elements, Al, Cu, S, (parachesis) or even Alexandrine quatrains in an elogy to the elements. The educational interest of the project was to propose activities which were at the same time very demanding with regard to linguistic command and motivating because of their playful character. It also allowed the scientific and the literary to be brought together while casting a discreetly irreverent eye on matter, which was salutary in a project as vast and serious as the one we were engaged on."

Dorothee Potter-Daniau, French teacher



In 2010, "The Gastronomic Meal of the French" was inscribed on the UNESCO Representative List of the Intangible Cultural Heritage of Humanity. The International Year of Chemistry provided a perfect opportunity to publicize the link between chemistry and gastronomy. With that in mind, internationally renowned chemist and cook, Hervé This conducted workshops for students at LFI on 26 and 27 September 2011 in which he introduced them to the discipline of molecular gastronomy.

In the primary school, many projects during the year were based on a hands-on approach to "doing chemistry." The investigations carried out were enriched as soon as possible by work in the senior school's laboratory to show the continuity between science in primary school and in secondary school.

"In the context of the Year of Chemistry and of their own class project, 'Chemistry and Health,' which specifically dealt with food, the fourth class [was] brought to the senior school laboratory to carry out tests which revealed the presence of certain chemical products in everyday food. Just the word 'laboratory' was enough to motivate the pupils: the project went beyond the context of group work in class to take on a whole new significance in the official place for scientific experiments. One pupil even said that she was going to 'make her dream come true'...

They were welcomed by the headmistress, then walked along the corridors of the senior school with their eyes wide open, suddenly feeling small but honored. Then they were met by the biology and chemistry teachers, who taught some of their older brothers or sisters: the young chemists were able in one day to cross the years which separated them from adolescence. They were impressed by the teachers' white coats, the lab tables, and the proper chemistry equipment: test tubes, protective goggles, spatulas, [vials] of powder ... They were given instructions about the protocol of chemical experiments: handle powders carefully, note the characteristics of ... each food product before mixing it, observe the reaction (change of consistency, color) after mixing it. Concentrated and curious, they took up the challenge of finding the mystery food by comparing chemical reactions and went back to school and then home proud of having taken their place in the secondary school.

A human experiment, whether scientific or not, to be repeated to strengthen the link between primary and secondary school and focus our pupils on after fifth class ..."

Marie Audidier, fourth class teacher

A Cross-Disciplinary, Multiclass Educational Project

"Thanks to this project, the pupils of second/third class discovered that chemistry is all around us. In second class, the work on milk and eggs allowed the pupils to observe the chemical transformation of different substances. In third class, making recycled paper emphasized sustainable development while broaching the chemical aspect. The pupils were able to finish their project by making recyclable plastic in the chemistry laboratory in Clonskeagh with the secondary school science teachers. This project was all the more valuable to them as they were put in the real situation of 'little chemists'. They have great memories of this activity. The pupils' involvement and enthusiasm in preparing the exhibition were apparent, and it's obvious that this project was a great success."

Corinne Pieussergues, second/third class teacher

During the year, several different approaches to scientific communication were utilized: health café, conferences of experts, and a visit to a factory in which the pupils' involvement was as important in the preparation phase as in the actual visit and the circulation of information. Our aim was to show that there is no split between the science of laboratories and researchers and the science taught in school.



On 17 April 2012 Gérard Férey visited the Lycée Français d'Irlande as part of its year-long IYC project. Férey is a French chemist, academician, and inventor of hybrid new materials. In recognition of the international impact of his work, and his long and brilliant career (with more than 600 scientific papers), Férey was awarded the 2010 CNRS Gold Medal, France's highest distinction in scientific research.

"In the context of the Year of Chemistry and my teaching of economics and management, we decided to involve the fourth years in the overall project through a visit to the Servier pharmaceutical plant in Arklow. The pupils were divided into groups, with one group responsible for preparing questions and a more in-depth reflection on three chapters of our course with an economic dimension:

- How does the business create value? The added value of a medication
- How does the business launch itself on a new market? Innovation
- How does the business fix the price of a product? Patent protection, profitability of innovation, and competition from generic products.

A second group was to look at the social dimension by taking the chapter further:

- What is the place of the individual in the business? Recruitment, (qualified/non-qualified), continuing education, evaluation, promotion, and remuneration of employees.

The visit to the plant in Arklow and many interlocutors allowed us to give a more concrete turn to theoretical notions grasped in class like the discussion on the question of individual bonuses paid (or not) to employees who came up with innovative ideas."

*Allain Mikaël,
Economic and Social Sciences teacher.*

To communicate as widely as possible was at the heart of our project. Disseminating the pupils' work through modern media (www.chimie2011-2012.blogspot.ie) allowed it to come out of the classroom, creating a dynamic that brought the whole educational community together. The collective work of all the classes gave rise to an exhibition on 12 May 2012 of 30 or so class projects on 4 themes linking chemistry to water, health, cookery, and scientific innovation. The exhibit featured images of chemistry from the students' daily lives through panels that mixed drawings, texts, graphs, videos, and sounds.



The Outcome

The project had multiple objectives.

- The teaching of science: to make students aware of science by putting them in direct contact with practical applications in their daily lives. To develop an appetite for science starting in primary school.
- The pupils' career choices: to promote scientific careers to our students. While many students take the science stream in senior cycle, we've noticed a reduction in those going on to do science after leaving school, with more doing business studies or other subjects.

- Break the subject stereotypes: encourage and promote science careers for girls through example (conferences and meetings with numerous high-level scientists)
- Break down the barriers between subjects: introduce the theme of chemistry in all subjects in order to challenge the idea that the subjects are not connected.
- Introduce a team project and a practical exchange between the educational teams: this project was also the departure point for a rich educational exchange between the primary and secondary school teachers and between the different subjects around the scientific theme.
- Reinforce the sense of belonging and cohesion of the educational community in the school.

Most of these objectives were achieved. An analysis of the career choices of our current pupils will allow us to follow the pupils' and particularly the girls' choices in the years to come. 🧪

Johnny Marcelin is a chemistry teacher at the Lycée Français d'Irlande and was co-ordinator of the Year of Chemistry project. Sarah Magadoux <provisieur@lfi.ie> is headmistress of the LFI.

 www.lfi.ie/chimie.html
www.chimie2011-2012.blogspot.com

Meeting with IUPAC President Nicole Moreau

On 1 November 2012, Nicole Moreau, at the time president of IUPAC, visited the LFI and met with a group of 16-year-old girls to share her experiences as a female scientist. Speaking to the group, Moreau shared her enthusiasm and talked about how “chemistry is everywhere.” Over the course of the year, this group of girls interviewed several women scientists from varied backgrounds; the project culminated with the girls participation in the Women in Technology and Science's conference that took place on International Woman's Day (1 March 2012).

Later that evening, Moreau introduced *Effervescences*, a scientific one-man show specifically addressed to parents of students in LFI.



Also during her visit in Dublin, Moreau delivered a lecture on “Madame Curie—More than the Scientist” to around 100 researchers and postgraduate students and professors from Trinity College Dublin. At the end of her stay in Ireland, she took part in the “Festival Robert Boyle” in the historic “Lismore Castle”.

The need to consolidate issues pertinent to a range of stakeholders within the scientific, technical and medical sectors is vital in the pursuit of interoperability and progress. Brian Hitson, chair of the International Council for Scientific and Technical Information's (ICSTI) U.S. Technical Activities Coordinating Committee, shares an insight into the organization's work.

interview by Emma Thompson

Emma Thompson (ET)—Firstly, could you give a brief history of ICSTI? How did you become involved with the organization?

Brian Hitson (BH)—ICSTI sits at a very busy intersection of stakeholders with common interests in scientific, technical, and medical communication. Like many of its members, whose histories date back 50, 100, or even 200+ years, the success of ICSTI, founded in 1985, has been its ability to adapt to change and stay relevant; it has been quick to detect and address both technical and strategic policy issues important to a broad swath of science, technology, and medical communities. Specifically, ICSTI brings together national libraries and STI/data centres, scientific unions, software and technology companies, standards organizations, and publisher groups in collaborative projects, workshops, and analytical studies. In terms of my involvement, the U.S. Department of Energy (DOE) is the largest funder of research in the physical sciences in the U.S. government, and clearly it is important to make the unclassified information emanating from this investment broadly and rapidly accessible. This role—providing access to DOE's STI—is the mission of my organization, the Office of Scientific and Technical Information (OSTI). OSTI has counterpart organizations in other federal science agencies—the National Library of Medicine at the National Institutes of Health, the Defense Technical Information Center at

the Department of Defense, the National Agricultural Library at the Department of Agriculture, and so on. In 2002, we worked together to provide transparent, one-stop access to practically all federal agencies' scientific databases and websites through the federated search engine Science.gov. Many of these challenges and opportunities we face as STI centers are addressed by ICSTI.

ET—What is the primary role of ICSTI's Technical Activities Coordinating Committee (TACC), of which you are chair?

BH—The Technical Activities Coordinating Committee (TACC) is ICSTI's forum for identifying technical interests that members have in common; for hearing and seeing very technical demonstrations of relevant products and technologies; and for developing and completing joint technical projects among subsets of members. To put this in context, ICSTI essentially brings global STI players together on two fronts:

policy issues and technical issues. The diversity of ICSTI membership naturally means that members will have diverse views of national and international information policy, but ICSTI provides a forum for sharing perspectives and broadening an understanding of individual members' interests. On the technical front, there are surprisingly fewer differences in members' interests. In fact, there are very common interests among members because information technology and information science are taking us all in similar directions; moreover, the needs of our respective customer bases are very similar.



Brian Hitson

ET—Can you give some examples of current or recent projects facilitated by the TACC?

BH—Yes, the beauty of TACC projects is that we can point to very tangible outcomes that would either not have been feasible, or would have been much more expensive for individual members to pursue independently. For example, TIB-Hannover—the German National Library of Science and Technology—worked with ICSTI members in proving the concept of data citation. This TACC project played a key role in the ulti-

* Article reprinted with permission, from *International Innovation: North America*, June 2012 (Research Media, UK, pp. 106-107).

mate establishment of DataCite, a consortium of organizations which issue digital object identifiers (DOIs) to make research data accessible on the Internet. In another project, Microsoft and OSTI partnered to adapt the Microsoft Audio Video Indexing System (MAVIS) to the complex scientific vocabularies used in DOE R&D videos. This project resulted in the multimedia search engine ScienceCinema, which searches on every spoken word in 2500 DOE and CERN videos. We are currently exploring projects in information trust and authority, data equivalence, and alternatives to traditional usage and value metrics.

ET—Who is ICSTI partnered with, and to what extent have such partnerships furthered your work?

BH—ICSTI has a long list of partner relationships. Generally, these are member-driven organizations similar in structure to ICSTI but which may focus on more specialized interests of a particular ICSTI sub-community. ICSTI has a “scientific associate” relationship with the International Council for Science (ICSU), which places us particularly close to information and data needs of specific scientific communities (e.g. pure and applied chemistry[†] and physics, biology, geology, mathematics). The ICSU relationship has included longstanding links with the Committee on Data for Science and Technology (CODATA), whose work has set the stage for many of today’s big data initiatives and ICSTI’s partnership with DataCite. Finally, the partnership with CENDI, the U.S.-based consortium of federal STI organizations, has resulted in an ICSTI agenda that is highly relevant to US science agencies. And, of course, ICSTI’s special support

[†] As a Scientific Associate of ICSU, ICSTI works closely with the scientific unions—including IUPAC—and CODATA (the Committee on Data for Science and Technology) to develop close working relationships with practising research scientists and science decision makers, and to position ICSTI at the forefront of changes in information seeking, sharing and usage behaviours of research scientists. With ICSU and CODATA, ICSTI develops joint projects and joint approaches to funding sources. ICSTI is represented on ICSU’s Strategic Coordinating Committee on Information and Data, which interim report was released in April 2011.

of WorldWideScience.org (WWS.org) and the role it plays in the WorldWideScience Alliance certainly enabled that global search engine to get off the ground and to ramp up its comprehensiveness much more quickly.

ET—Further to the above, your organization at the U.S. Department of Energy is the Operating Agent for WWS.org, for which ICSTI is the principal sponsor. How would you sum up the main purpose of WWS.org and the WorldWideScience Alliance (WWSA)?

BH—WWS.org provides a simultaneous search of 80+ national scientific databases containing some 400 million pages, most of which are not covered by the major commercial search

engines. WWS.org allows users to find the precise information they need without having to know the scope of any particular national scientific database nor having to search the databases individually. It also offers multilingual translations of both queries and search results in 10 different languages. The WWSA provides the multilateral governance structure for WWS.org, and Alliance membership consists of WWS.org source “owners” and sponsors, including ICSTI.

The Alliance provides strategic direction for WWS.org’s growth and development, establishes the criteria for adding databases to WWS.org searches, defines the funding model and annual budget, and actively markets WWS.org.

In 2011, WWS.org expanded its coverage to multimedia materials, and the next goal is to include coverage of scientific datasets. This milestone will be achieved in late 2012. DataCite, for example, will be added along with several other scientific data collections. Of course, WWS.org also continues to look for scientific and technical information from countries not currently covered, and for additional multimedia and data collections. These two areas, in particular, represent substantial opportunity for future expansion.

ET—How significant will the worldwide science gateway be in improving universal access to scientific knowledge? What do you believe will be its long-term benefits?

“With the exception of simply providing Internet access, I would suggest that WWS.org is probably the most tangible step forward in closing the digital divide—at least in the realm of science.”

BH—WWS.org has been at the forefront of deep web search over the past five years and has already made a significant impact on access to STI from the government and government-sanctioned organizations it represents. As the methods and practices for sharing and communicating scientific information rapidly evolve, WWS.org is likewise adopting new technologies and strategies to accelerate scientific discovery. Along with the integration of multimedia and the planned integration of datasets, WWS.org also released a mobile version of the site in 2011, thus enabling access for a user base where mobile phone usage has leapfrogged traditional technologies.

The “digital divide” has been widely noted by the World Summit on the Information Society and others. With the exception of simply providing Internet access, I would suggest that WWS.org is probably the most tangible step forward in closing the digital divide—at least in the realm of science.

ET—Building on the *Strategic Plan for 2011-2013*, where would you like to see ICSTI in the future?

BH—In these straitened financial times, ICSTI must continue to demonstrate that it delivers actual economic value to its members and to the scientific, technical, and medical (STM) community as a whole. A key element of ICSTI’s niche is that it does not have a political or commercial agenda. On the policy front, it is a forum that allows for frank and open discussion of diverse perspectives and needs, while on the technical front, it has proven its value as a seed bed for demonstrating and “market” testing particular technologies and for enabling project collaborations.

In the next three to five years, ICSTI will explore specific innovations in researcher workflow, semantic

search, deep mining and integration of text, data, multimedia, and social media—and the impact and potential of all of these technologies on science.

ET—How would you sum up your continued efforts to innovate?

BH—Just as a closing thought, on behalf of ICSTI, I would like to thank *International Innovation* for its efforts to highlight and disseminate information on leading-edge scientific and technological research. As it turns out, the individual members of ICSTI share this same purpose. Sir Isaac Newton’s oft-quoted “standing on the shoulders of giants” point essentially sums up the *raison d’être* of ICSTI and its individual members. In my own organisation at OSTI, we frame the spread of knowledge as a corollary, something like this: science advances only if knowledge is shared; therefore, accelerating the sharing of knowledge will accelerate scientific progress itself. 🏆

👉 www.icsti.org

Brian Hitson <hitsonb@osti.gov> is associate director of the U.S. Department of Energy’s Office of Scientific and Technical Information. He manages DOE’s repository of R&D results and OSTI’s classified, international, and administrative activities. Beyond his ICSTI and WorldWideScience roles, Hitson represents the U.S. in two information agreements under the International Energy Agency and the International Atomic Energy Agency.

Emma Thompson <emmat@researchmedia.eu> is at Research Media Ltd, which produces *International Innovation*—a leading global dissemination resource for the wider scientific, technology and research communities, dedicated to disseminating the latest science, research and technological innovations on a global level. Subscribe to the publication for free at www.research-europe.com.

Feature Articles Wanted

Contact the editor for
more information at
<edit.ci@iupac.org>.

Young Chemists to the 44th IUPAC Congress

The 44th IUPAC World Chemistry Congress, to be held 11–16 August 2013 in Istanbul, Turkey, will have as its theme “Clean Energy Through Chemistry.” To encourage young chemists to participate in this unique congress, the organizers have established two different programs, both offering travel assistance. The first program is especially targeted to young scientists from developing and economically disadvantaged countries; the second is open to chemists from any country. Awards of up to USD 1500 will be made available to qualified candidates as a contribution to the cost of their travel to attend the Congress and to meet Congress registration fees.

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

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

Young Observers at the IUPAC General Assembly

Concurrent with the Young Chemists initiative, IUPAC and individual National Adhering Organizations (NAOs) are offering a Young Observer program to provide young scientists with the opportunity to participate in sessions of the IUPAC General Assembly. Such sessions are generally reserved to IUPAC members of specific divisions and committees, but Young Observers can participate in these meetings—a unique opportunity to learn about IUPAC activities, establish international collaborations, and gain knowledge of global research activities.

IUPAC Young Observers will be invited from the pool of Young Chemists awards granted by the IUPAC Congress. Other NAOs, such as the USA, may have their own selection process. Those who are interested should inquire with the NAO from their country: www.iupac.org/nao.

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

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

The deadline for receipt of applications is 31 March 2013. Applications should be sent to Tahsin Kizilay <taum74@gmail.com>.

 www.iupac2013.org

John D. Petersen Appointed IUPAC Executive Director

Effective 1 August 2012, Dr. John D. Petersen is the new IUPAC Executive Director. Petersen succeeds Dr. Terrence A. Renner who has elected to retire at the end of this year.

Petersen comes to IUPAC from the neighboring Research Triangle Institute in North Carolina, where he was vice president of University Collaborations, Development, and Outreach. He obtained his Bachelor



of Science degree in Chemistry from California State University, Los Angeles. Thereafter, he completed his Ph.D. in inorganic chemistry at the University of California, Santa Barbara, as a student of Prof. Peter C. Ford.

Petersen's distinguished career includes positions as executive director of the RTP Solar Fuels Project, president of the University of Tennessee System, and academic appointments at the University of Connecticut, Wayne State University, Kansas State University, and Clemson University.

Petersen commented that "our world is facing some critical issues: developing renewable energy sources, maximizing sustainability, minimizing environmental issues such as global warming, as well as expanding the workforce of the future. The six long-range goals of IUPAC's strategic plan set the framework to meet these issues directly. It is exciting when one has the opportunity to interact with creative individuals and groups while assisting in the formulation of the strategies to implement goals. I believe that the breadth of my experience in all sectors of chemistry, my international connections, my ability to work with local and central governments, and my skill in assisting others in translating their visions into practice are assets for the job of executive director."



John Petersen (left), IUPAC Executive Director, Fabienne Meyers (center), IUPAC Associate Director, and Morton Hoffman, IUPAC member and U.S. representative on the Committee on Chemistry Education, at the ACS Northeastern Section event held on 11 October 2012 at Nova Biomedical Corp. in Waltham, Massachusetts, USA.

Mozambique and Argentina Join IUPAC as Full Members

In July 2012, the Academy of Sciences of Mozambique became the 59th National Adhering Organization to join IUPAC. The Academy was officially launched by the Head of State in February 2009. This event was followed by the First Plenary Session, which elected the Governing Body (Directive Council) and approved the internal regulations.

In September 2012, the Asociación Química Argentina also became a full NAO. Fittingly, AQA acquired full IUPAC membership and became the 60th NAO the same year that it celebrates its 100th anniversary.

Winners of 2012 IUPAC Prizes for Young Chemists

In early July 2012, IUPAC announced the winners of the 2012 IUPAC Prizes for Young Chemists, which are awarded for the best Ph.D. theses in the chemical sciences as described in 1000-word essays. The six winners are as follows:

- Khalid Albahily, University of Ottawa, Ottawa, Ontario, Canada
- Tzahi Cohen-Karni, Harvard University, Cambridge, MA, USA
- Alexander Spokoyny, Northwestern University, Chicago, IL, USA
- Judy I-Chia Wu, University of Georgia, Athens, GA, USA
- Lei Yang, Georgia Institute of Technology, Atlanta, GA, USA
- Charles Yeung, University of Toronto, Toronto, Ontario, Canada

The winners will each receive a cash prize of USD 1000 and travel expenses to the 44th IUPAC World Chemistry Congress, 11-16 August 2013, in Istanbul, Turkey, where they will present posters describing their award-winning works. They will also be invited to submit a short critical review on aspects of their research topic to be published in *Pure and Applied Chemistry*.

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

- Dr. Albahily: "Study of the Factors Affecting the Selectivity of Catalytic Ethylene Oligomerization"
- Dr. Cohen-Karni: "Nanowire Nanoelectronics: Building Interfaces with Tissue and Cells at the Natural Scale of Biology"
- Dr. Spokoyny: "Synthetic Investigations Featuring Boron-Rich and Multidentate Chalcoether-Containing Ligands"
- Dr. Wu: "Quantification of Virtual Chemical Properties: Strain, Hyperconjugation, Conjugation, and Aromaticity"
- Dr. Yang: "New Materials for Intermediate-Temperature Solid Oxide Fuel Cells to be Powered by Carbon- and Sulfur-Containing Fuels"
- Dr. Yeung: "Transition Metal Catalysis: Activation of CO₂, C-H, and C-O Bonds En Route to Carboxylic Acids, Biaryls, and N-Containing Heterocycles"

These young chemists completed their Ph.D.s in the USA or Canada, but they are well traveled and most have international experience, including bachelor or master's degrees from institution such as the King Saud University in Saudi Arabia, the Technion Institute of Technology and the Weizmann Institute of Science in Israel, Tung-Hai University in Taiwan, and Tsinghua University and Beihang University in China.

The Prize Selection Committee, which comprises members of the IUPAC Bureau with a wide range of expertise in chemistry, is chaired by IUPAC Past President Nicole Moreau. Moreau stated that "the Committee had a difficult task in selecting the winners, and exceptionally, we decided to award six winners instead of five as IUPAC did in former years. I can not wait to meet these young chemists at the IUPAC Congress next year in Istanbul and I wish them all great success in their future careers."

In view of the many high-quality applications, the committee also awarded five Honorable Mention awards:

- Hua Lu, University of Illinois, Urbana-Champaign, IL, USA
- Stephen Morin, University of Wisconsin, Madison, WI, USA
- David Scanlon, Trinity College Dublin, Dublin, Ireland
- Joerg Schrittwieser, University of Graz, Graz, Austria
- Sihai Yang, University of Nottingham, Nottingham, United Kingdom

There were 41 applications from 19 different countries. On the judging task, Javier Garcia-Martinez, Bureau member from Spain, commented that "this has been a really difficult task as the CV and the essays of some candidates are truly impressive."

Applications for the 2013 Prizes are now being solicited; application deadline is 1 February 2013.

 www.iupac.org

Rachel O'Reilly Receives the 2012 IUPAC-Samsung Young Polymer Scientist Award

Professor Rachel O'Reilly was presented with the 2012 IUPAC-Samsung Young Polymer Scientist Award at the recent IUPAC World Polymer Congress, held 24-29 June 2012 at Virginia Tech in Blacksburg, Virginia, USA. (see congress report p. 32). O'Reilly is the first UK winner of this award, which is presented every two years to the most promising young polymer scientist from any country under the age of 40.



photo by David Elmore

Rachel O'Reilly receiving the Samsung-IUPAC Young Polymer Scientist award from Minjae Lee, Samsung representative.

O'Reilly received an MA/MSc from Cambridge, UK, and a Ph.D. from Imperial College London. After a postdoc at IBM Research–Almaden in San Jose, California, and Washington University in Saint Louis, Missouri, she then began an independent position in 2005 at the University of Cambridge, UK. In 2009, she received a career-acceleration fellowship from the UK's Engineering and Physical Sciences Research Council, which allowed her to establish her independence and move her laboratory to the University of Warwick. In the past three years, she has published some 50 papers and has a research group of around 20 researchers. In June 2012, she became a professor at the University of Warwick, UK, at the age of 34.

Her research uses polymer synthesis to make novel nanomaterials, which can be utilized in a wide range of applications from materials science to medicine. Her interest is in trying to mimic some of the key features of natural functional nanomaterials such as viruses and cells, using polymer nanoparticles. Her group also works at the biological-materials interface to explore templating chemistries for polymer and oligomer synthesis. They utilize DNA as well as biopolymers for templating and are interested in the development of these techniques towards the preparation of sequence-controlled materials.

 www2.warwick.ac.uk/fac/sci/chemistry/research/oreilly

Second CHEMRAWN VII Prize Awarded to Rashmi Sanghi

The second CHEMRAWN VII Prize for Atmospheric and Green Chemistry was awarded to Dr. Rashmi Sanghi, Indian Institute of Technology in Kanpur, India, at the 4th International IUPAC Conference on Green Chemistry, held at Foz do Iguacu at the end of August 2012.

Sanghi received the award in recognition of her significant contributions in developing new methods and technologies that are being applied to minimize and eliminate hazardous substances in all compartments of the environment. In this context, her research has focused on the application of both microbes and nanoparticles, and her work on biomimetic synthesis of nanoparticles using fungi and polysaccharides as reactants, represents a novel approach, in addition to being simple to carry out and environmentally



Rashmi Sanghi (right) receives the CHEMRAWN VII Prize for Atmospheric and Green Chemistry from Leiv Sydnes, chair of CHEMRAWN.

friendly. She has also contributed to improved wastewater remediation using green technologies based on biopolymers. Sanghi's outreach activities are also very relevant in this context; through a large number of articles and lectures she has informed the chemical community as well as lay people about the needs to embrace green chemistry as the platform for a common future.

Rashmi Sanghi was born and raised in India where she also obtained all of her professional education, at the University of Allahabad in the Uttar Pradesh province, where she graduated with a Ph.D. in 1994. Her career so far has included positions at universities in India and abroad and at the Indian Institute of Technology in Kanpur where she currently is employed as a senior research scientist. Sanghi has had a significant number of publications in scientific journals in India and abroad and also several patents. Her wide interests have also developed significant competence in a range of chemical disciplines including organic synthesis, natural product chemistry, analytical chemistry, and nanochemistry, which she has applied to creating green solutions in her home country and abroad.

The CHEMRAWN VII Prize—conceived and established during 2008–2009 through cooperative efforts of the CHEMRAWN VII Future Actions Committee and the Organic and Biomolecular Chemistry Division of IUPAC (Division III)—was formally announced at the IUPAC General Assembly in Glasgow, UK, in 2009. The prize, made possible by a surplus from the CHEMRAWN VII conference on “Chemistry of

the Atmosphere: Its Impact on Global Change,” held in Baltimore in December 1991, is “to be awarded to a young scientist (under age 45) from a developing country, contributing in the field of green chemistry, emphasizing atmospheric chemistry.” The first prize was given in 2010 to Dr. N. Yassaa from Algeria for his research in atmospheric chemistry (see Sep-Oct 2010 CI, p. 19), so a shift to green chemistry on this occasion is really in the spirit of the prize. The award comprises a plaque and USD 5000 in cash.

The CHEMRAWN VII Prize is biennial and the next award will be announced in 2013 with a nomination deadline of early 2014. The winner of the 2014 CHEMRAWN VII Prize will be accommodated with a lecture at the 5th ICGC that will be in South Africa in 2014.

Ian Mills Awarded IUPAP SUNAMCO Prize

Long-time IUPAC member Ian Mills was awarded the International Union of Pure and Applied Physics SUNAMCO Senior Scientist Medal at the Conference on Precision Electromagnetic Measurements on Washington, held 1-6 July 2012 in Washington, D.C.

The IUPAP Commission on Symbols, Units, Nomenclature, Atomic Masses and Fundamental Constants recognized Mills with the award for “his outstanding contribution to the development of the International System of Units (SI) towards the adoption of a system based on fundamental physical constants.”

Mills was IUPAC ICTNS chair for 1998-1999 (known at the time as IDCNS) and is IUPAC representative on the International Bureau of Weights and Measures Consultative Committee for Units (BIPM CCU).

In his role as president of the CCU for the past 16 years, Mills has played a leadership role in the maintenance and development of the SI. This role includes being the senior author of the two latest editions of the *The International System of Units*. Mills has been active in developing a significant improvement in the SI that will eliminate the dependence on a material artifact for the kilogram and will also improve electrical, temperature, and amount of substance SI units. In the revised form, the SI will be based on the fact that certain fundamental constants of nature will have specified values when expressed in terms of the newly defined SI units.

Mark Cesa and James Economy Named ACS Fellows

The American Chemical Society (ACS) has named Mark Cesa, IUPAC vice president, and James Economy, president of the IUPAC Macromolecular Division from 1994-1997, to the 2012 class of ACS Fellows, a prestigious honor bestowed upon 96 distinguished scientists who have demonstrated outstanding accomplishments in chemistry and made important contributions to the ACS. The ACS Fellows Program was created by the ACS Board of Directors in December 2008 “to recognize members of ACS for outstanding achievements in and contributions to science, the profession, and the society.”



photo by Peter Cutts

James Economy with Nancy Jackson, immediate past president of ACS.

“These chemists hold the future to our country, to our way of life, and to the legacy we will leave for the next generation,” said ACS President Bassam Z. Shakhshiri. “Whether it’s producing renewable fuels, finding cures for afflictions such as diabetes, cancer, AIDS, and Alzheimer’s disease, or ensuring safe drinking water, these fellows are scientific leaders, improving our lives through the transforming power of chemistry.”

The 2012 fellows were recognized at an induction ceremony on 20 August 2012 during the society’s 244th National Meeting and Exposition in Philadelphia.

The Project Place

Information about new, current, and complete IUPAC projects and related initiatives.

See also www.iupac.org/home/projects.html

IUPAC Safety Training Program

Since 2000, the IUPAC Safety Training Program (STP) has trained 12 individuals from around the world on topics like chemical regulation and its impact upon industry and universities, hazards and operability analysis, process safety management, and emergency planning. Recently, the U.S. Department of State's Chemical Security Engagement Program (CSP) has developed an innovative partnership with IUPAC to fund chemical security and safety training through the STP. Qualified chemistry professionals are invited to apply for this program's one-to-three week individualized chemical security and safety training cycle at an IUPAC-affiliated chemical company. The time spent visiting and working at these IUPAC affiliated companies, known in the program as Company Associates, empowers trainees with the knowledge and skills to advance chemical security and safety best practices in their home institutions. After their training, participants are encouraged to apply these practices in their home country or facility. Then, IUPAC invites participants to present a talk at the next IUPAC Congress on the successes of their follow-up activities.

One of the first participants in the STP was Ali El-Emam from Mansoura University in Egypt who gained hands-on experience with safety practices during the two weeks in 2001 he spent at Bristol-Meyers Squibb research facilities in New Jersey, USA. Specifically, El-Emam's training covered the handling of hazardous chemicals, medical surveillance of employees, and crisis management. As a result of his participation, he took steps towards establishing a nationwide chemical safety program in Egypt. His program concept was so successful that it received funding from the United Nations Educational, Scientific, and Cultural Organization (UNESCO) and from Egypt's Ministry of Environmental Affairs.

Tersoo Charles Gwaza is another successful STP grantee. In 2002, he visited Sasol Research and Development in Sasolburg, Secunda, and Johannesburg, South Africa. While at Sasol, he deepened his knowledge about occupational hygiene, process safety management, hazard identification risk assessment, and accident investigation techniques. The practical knowledge thus acquired reaffirmed his commitment to chemical safety and shaped his ideas as to how such techniques and processes could be applied to Shell Nigeria, his home company. These ideas included serving on the Shell Nigeria accident investigation team, as well as working with his local government on safety and environmental issues.



STP Fellows Fabian Benzo (fourth from right) and Godfred Ansah Nyarko (second from right) visited Mitsui Chemicals in Japan in 2007.

Gwaza and El-Emam are just two examples of the positive imprint IUPAC STP grantees have on chemical safety in their countries. Over the years, STP has supported grantees to gain valuable insight into chemical safety practices and procedures and develop their own ideas and customized solutions applicable to their employers and home countries.

IUPAC's newly established partnership with CSP is an extension of this strong history and an exciting development since it will enlarge the scope of the project and enable a greater variety of participants. While the programs have somewhat different objectives, the IUPAC STP sits precisely at the nexus of the IUPAC and CSP mission spaces, thus offering each the ability to advance their missions and goals in fruitful collaboration, while improving chemical safety and security around the world.

While ideal STP candidates are mid-career professionals currently involved at supervisory or management levels in chemical companies, government institutions, or scientific laboratories, all chemical professionals are encouraged to apply. STP specifically seeks individuals who are involved in chemical safety and/or security in their day-to-day activities—such as chemical production or teaching—and who clearly demonstrate their willingness and potential to enact chemical safety and security best practices in their home country.

By providing financial support to STP, CSP seeks to reduce chemical threats by raising awareness of the dual-use nature of chemicals, providing training that fosters best practices for safe and secure chemical management, and facilitating international partnerships among chemical professionals in industry, academia, and government. CSP partners with chemical

The Project Place

industrial organizations like IUPAC to promote established best practices in chemical security. For more information about CSP, see www.csp-state.net

CSP supports the implementation of the STP under IUPAC through CRDF Global. CRDF Global is an independent, nonprofit organization that promotes international scientific and technical collaboration through grants, technical resources, training, and other services worldwide, including in Southeast Asia, the Middle East, and the North Africa region. As an implementer of CSP projects, CRDF Global recently partnered with the Indonesian Chemical Society to provide chemical safety and security training, administer research and development grants, and conduct professional development workshops.

CRDF Global, which operates in more than 40 countries worldwide through its U.S. headquarters and international offices, promotes peace and prosperity through collaboration in fields such as biology, chemistry, and physics. CRDF Global specializes in connecting scientific communities within countries that are transitioning to knowledge economies with specialized professional and academic resources. This work provides a critical entry point for members of the scientific community to advance economic development, solve societal challenges, promote security,

IUPAC is seeking **Host Companies** to host trainees for the IUPAC Safety Training Program (STP). The STP allows experts from developing countries to learn more about safety and security in chemical production by visiting and working at the company. Trainees are mid-level chemical professionals from around the world, who are engaged in aspects of safety and security in chemical production or teaching, and who are able to influence safety and security practices at their institution or elsewhere in their country. The program lasts one to three weeks and allows hosts to share their knowledge on chemical safety and security with trainees.

Trainee travel and living expenses are provided and compensation for host companies for the costs of conducting the training might be available. IUPAC hopes that you will consider support for the Safety Training Program by becoming a host company.

For more information, please contact Bernard West at bernard.west@sympatico.ca.

STP Fellows since 2000

June 2008 - Dr. Gursharn Singh Grover (National Chemical Laboratory, India) undertook a visit at Novozymes, Denmark.

Jan 2007 - Prof. Fabian Benzo (Universidad de la República, Montevideo, Uruguay) and Dr. Godfred Ansah Nyarko (Tema Lube Oil Company Ltd., Ghana) visited Mitsui Chemicals (Japan).

Nov 2005 - Prof. Said Mohamed Mahmoud Bayomi (Mansoura University, Egypt) received training at the facilities of the pharmaceutical company AstraZeneca in the UK.

Oct 2004 - Mr. Isiaka O. Bakare (Rubber Research Institute of Nigeria) visited Mitsui Chemicals Co. sites in Japan.

Oct 2003 - Ms. Jane B. Nyakang'o (UNIDO Kenya National Cleaner Production Centre) and Ms. Ana Luisa Arocena (CEMPRE Uruguay) visited the BP Chemicals Technology Center in Naperville, Illinois, USA and the acrylonitrile production plant in Lima, OH, USA.

Sep 2002 - Mr. Zhang GuoHong (Sinopec, China) received training at BP Chemicals Inc. USA research facilities in Naperville, IL and production facilities in Lima, OH.

Aug 2002 - Mr. Kelvin Khisa (UNIDO Kenya National Cleaner Production Centre) visited Sankyo Co., Ltd production and research facilities in Japan.

June 2002 - Mr. Tersoo Charles Gwaza (Shell Petrochemical Development Co, Nigeria) received training at Sasol Chemical Industries, South Africa.

Aug 2000 - Prof. Ali El-Emam (Mansoura University, Egypt) was hosted by Bristol-Myers Squibb in the USA.

encourage innovation, and improve human conditions. For more information about CRDF Global, visit www.crdfglobal.org/about-us.

Individuals interested in applying for the STP, should download an application form from the IUPAC STP website (see below) and send a completed application along with two letters of recommendation and résumé to Bernard West at bernard.west@sympatico.ca. Applications are accepted on a rolling basis. The IUPAC Committee on Chemistry and Industry (COCI) screens and selects applicants to the STP. CSP considers COCI selectees for funding with no additional application material required. Through CRDF Global, CSP-sponsored STP trainees receive travel and other implementation support that includes visa application assistance; airfare; transportation; lodging; medical insurance placement; training agenda development, and other related items.

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

Nomenclature Notes

InChIs and Registry Numbers

by Jeffery Leigh

Constructing a systematic name of a chemical compound of known structure means that it is necessary for the reader to know the detailed nomenclature rules required to do this. Such a person must work within a particular system, of which IUPAC and the Chemical Abstracts Service (CAS) provide possibly the two most complete. These are both designed in the English language, but a person whose mother tongue is not English may face a further barrier to developing a name if another language, such as Russian or Japanese, should be the language of primary use. However, all trained chemists should be able to recognize a chemical structure displayed using atomic symbols and bond connections, etc., as these are independent of language, even if the basic chemical symbols, recognizable by all chemists, use the roman alphabet. IUPAC has recently developed a computer methodology for recognizing and codifying chemical structures, and, the converse, for reproducing the chemical structure from such a code. This code is called an InChI (IUPAC International Chemical Identifier), and there is a related, more abbreviated, version called an InChIKey.

Principles provides a brief introductory guide to InChIs, and InChIKeys, along with CAS Registry Numbers. These are quite distinct from each other. Registry Numbers are unique numbers used to identify a spe-

cific compound in the CAS database. The numbers are assigned to a compound the first time that it appears in Chemical Abstracts (CA) and can be used thereafter to find all references to this compound when it appears again in CA. However, it has no further significance, and does not contain structural information. The user of CA must be familiar with CA nomenclature. In contrast, the recently developed InChI and its related InChIKey are strings of numbers, letters, and other symbols that provide a complete description of the structure of a compound (see www.iupac.org/inchi).

The strings are not comprehensible to a casual reader, though they are to a computer that is equipped with the necessary programs. The InChI system can now deal with many, but as yet not all, compounds that appear in the literature, but it is still under development. In theory, InChI software will eventually provide an InChI character string from structural data for any compound. InChIs are already being used by most of the major chemistry publishers and databases. The InChITrust website (www.inchi-trust.org) lists some of the many organizations now using it.

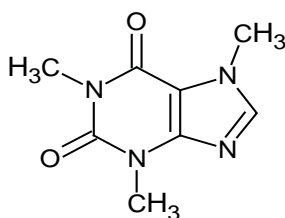
The InChI software represents features of the compound structure as a sequence of levels and in strict order, starting with the formula and then dealing with various features, such as atom connectivity and stereochemistry. Production of an InChI is reversible, in that with the appropriate computer program it can be derived from a drawing of the structure and it can then be used to regenerate the structure from which it is derived. This is not true of the InChIKey. An InChI may contain many tens of characters. An InChIKey is an abbreviated form which contains only 27 characters. It cannot be used to regenerate its parent structure, but it is still unique and is designed primarily for searching databases. In that sense it is like a Registry Number, but unlike the Number, it derives ultimately from a compound's structure.

Of course, a primary requirement for someone to use both InChIs and InChIKeys is that they possess the programs that can construct and interpret them. Like all IUPAC products, these are freely available to the chemistry community. *Principles* contains enough detail and references for a beginner to obtain the programs and to start to use them.

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

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

caffeine



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

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

Second block (8
letters), encodes
stereochemistry
and isotopes

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

InChIKey=RYYVLZVUVIJVGH-UHFFFAOYSA-N

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

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

Guidelines for Reporting of Phase Equilibrium Measurements (IUPAC Recommendations 2012)

Robert D. Chirico, et al.

Pure and Applied Chemistry, 2012

Vol. 84, No. 8, pp. 1785–1813

The critical importance of phase equilibrium properties in the development and optimization of numerous industrial processes is well established, particularly with regard to separation methods, such as distillation, extraction, and crystallization. This article includes recommendations for the reporting in the primary scientific literature of measurements involving phase equilibrium. The focus is on documentation issues, and many of the recommendations may also be applied to the more general fields of thermodynamic and transport properties.

This work builds upon earlier related efforts that span approximately 60 years. Especially in the last 20 years, several important and inter-related developments make imperative revision of the guidelines published previously [*Pure Appl. Chem.* 29, 395 (1972) and CODATA Bull. 21, 69 (1989)]. These developments include advances in the establishment of international standards for (1) evaluation and reporting of uncertainties (Guide for the Estimation of Uncertainty in Measurement, known as “GUM”); (2) terminology in physical chemistry (*Quantities, Units, and Symbols in Physical Chemistry*, also known as the “Green Book”); and (3) storage and exchange of experimental, predicted, and critically evaluated thermophysical and thermochemical property data (ThermoML). The present work is also motivated by major advances in electronic databases for thermophysical properties. In particular, procedures have been developed involving cooperation between the U.S. National Institute of Standards and Technology and journal editors and publishers to allow data reported in key journals to be easily incorporated into electronic databases and process simulation software without significant manual intervention. A further need for the present work stems from the rate of publication of phase equilibrium and property data that annually continues to increase, more than doubling in the last 10 years.

 <http://dx.doi.org/10.1351/PAC-REC-11-05-02>

Characterization of Photoluminescence Measuring Systems (IUPAC Technical Report)

Ute Resch-Genger and Paul C. DeRose

Pure and Applied Chemistry, 2012

Vol. 84, No. 8, pp. 1815–1835

Despite the widespread and increasing use of photoluminescence measuring techniques in materials science, (bio)analytical chemistry, medical diagnostics, and biotechnology, many method-inherent problems are often neglected, resulting in measurements that are unreliable and of poor quality. These problems include, e.g., the nonlinearity of the detection system, and spectral bandpass-, detector voltage- and polarization-dependent effects. Furthermore, the general need for correction of measured signals for unwanted contributions from instrument-dependent effects that are wavelength-, polarization-, and time-dependent is frequently underestimated despite the significant distortions in spectral shape and intensity that are often introduced. These luminescence-inherent drawbacks hamper the reliability of photoluminescence data, the comparability of measurements between instruments, and quantification from measured fluorescence intensities as well as the determination of relative fluorescence quantum yields.

These demands enhance the need for internationally accepted procedures for instrument calibration and instrument performance validation (IPV) in conjunction with suitable standards.

To improve the overall reliability and comparability of fluorescence measurements, the purpose of this document is to present and discuss procedures for the characterization and performance validation of photoluminescence measuring systems. Special emphasis is dedicated to steady-state measurements of photoluminescence in solution and monochromator-based systems such as are most commonly found in research-grade instrumentation. The aim of this report is also to increase the awareness for the importance of a reliable instrument characterization and to improve the reliability and comparability of measurements of photoluminescence.

 <http://dx.doi.org/10.1351/PAC-REP-10-07-07>

IUPAC/CITAC Guide: Investigating Out-of-Specification Test Results of Chemical Composition Based on Metrological Concepts (IUPAC Technical Report)

Ilya Kuselman et al.

Pure and Applied Chemistry, 2012
Vol. 84, No. 9, pp. 1939–1971

A metrological background for investigating out-of-specification (OOS) test results of chemical composition is discussed. When an OOS test result is identified, it is important to determine its root causes and to avoid reoccurrence of such results. An investigation of the causes based on metrological concepts is proposed. It includes assessment of validation data of the measurement process and its metrological traceability chains, evaluation of measurement uncertainty, and related producer's and consumer's risks. This approach allows distinguishing between OOS test results that indicate an actual change in chemical composition of an analyzed object, and OOS test results that are metrologically related with a certain confidence probability. Practical examples illustrating applications of the described approach in environmental and food analysis, as well in drug analysis and stability study of drug products, are described. Acceptance limits, warning and action lines for the test results, and corresponding producer's and consumer's risks are discussed.

 <http://dx.doi.org/10.1351/PAC-REP-11-10-04>

A Brief Guide to Polymer Nomenclature

R. C. Hiorns, et al

Pure and Applied Chemistry, 2012
Vol. 84, No. 10, pp. 2167–2169

The “Brief Guide” gives a simple résumé of polymer nomenclature. It was prepared with the objective of disseminating throughout the international polymer community a short, easily assimilated, guide to the essentials of polymer nomenclature.

The two-page document is targeted at authors publishing in polymer-science journals, lecturers, students, indeed anyone who would like to know how

polymers are named in accordance with IUPAC recommendations.

The “Brief Guide” includes:

1. important terminology for polymer nomenclature;
2. concise explanations of source-based and structure-based nomenclature; and
3. hyperlinks to relevant primary publications.

Download from a pdf from *PAC* or for a quick printed version see the tear-off page of this issue.

 <http://dx.doi.org/10.1351/PAC-REP-12-03-05>

IUPAC-NIST Solubility Data Series—Recent Volumes

Volume 91. Phenols with Water.

Part 1. C₆ and C₇ Phenols with Water and Heavy Water
J. Phys. Chem. Ref. Data 40, 033102 (2011)
Part 2. C₈ to C₁₅ Alkane Phenols with Water
J. Phys. Chem. Ref. Data 40, 033103 (2011)

Volume 92. Metal Carbonates.

Part 1. Solubility and Related Thermodynamic Quantities of Cadmium(II) Carbonate in Aqueous Systems
J. Phys. Chem. Ref. Data 40, 043104 (2011)

Volume 93. Potassium Sulfate in Water

J. Phys. Chem. Ref. Data 41, 013103 (2012)

Volume 94. Rare Earth Metal Iodides and Bromides in Water and Aqueous Systems.

Part 1. Iodides
J. Phys. Chem. Ref. Data 41, 013104 (2012)

Volume 95. Alkaline Earth Carbonates in Aqueous Systems

Part 1. Introduction, Be and Mg
J. Phys. Chem. Ref. Data 41, 013105 (2012)
Part 2. Ca
J. Phys. Chem. Ref. Data 41, 023105 (2012)

All SDS volumes since Volume 66 (and published in *J. Phys. Chem. Ref. Data* since 1998) are available at <http://jpcrd.aip.org>; keyword search “IUPAC-NIST Solubility Data Series”



See back cover tear-off.

Conference Call

Going for Gold: The 44th International Chemistry Olympiad

by Mary Kirchoff

While the world's greatest athletes were competing in London for Olympic gold in July, an equally talented group of secondary school students was participating in the **44th International Chemistry Olympiad (IChO)**. The 2012 IChO engaged 283 students from 72 countries in practical and theoretical examinations at the University of Maryland, USA, from 21–30 July. The Dow Chemical Company was the sole sponsor of the competition and a major sponsor of the London Olympics, demonstrating its commitment to the Olympics of the body and mind in 2012.

The American Chemical Society (ACS) organized the 44th IChO, a significant undertaking as the host country is responsible for creating the preparatory, theoretical, and laboratory problems; arranging housing, transportation, meals, and excursions for more than 600 students, mentors, observers, and guests; and orchestrating the opening and closing ceremonies. Cecilia Hernandez, assistant director of Endowed Programs at ACS, coordinated all activities associated with the 44th IChO, with significant support provided by Kirsten Dobson and other colleagues across ACS.

Bryan Balazs served as chair of the 44th IChO Organizing Committee and was responsible for coordinating numerous committees and working with the International Steering Committee to ensure a successful program. Nobel Laureate Ahmed Zewail was the president of the 2012 Olympiad. IUPAC provided USD 10 000 to enable students from financially challenged countries to participate in the IChO.

The practical and theoretical examinations form the core of the International Chemistry Olympiad. The Scientific Committee, led by Michael Doyle and Andrei Vedernikov at the University of Maryland, crafted a set of written problems and laboratory exercises that challenged the brightest chemistry students in the world. Students took five hours to complete

each exam, which were administered on different days.

The results of the competition were announced during the closing ceremony at Georgetown University on 29 July. A total of 34 gold, 59 silver, and 87 bronze medals were awarded. Ten students received Honorable Mentions. The top gold medal was earned by Florian Berger of Germany, and all four members of the South Korean team were awarded gold medals. IUPAC presented certificates and books to Tzung-Hua Hsieh (Chinese Taipei), Diptarka Hait (India), and Takuya Yamakado (Japan), who were the top achievers on the theoretical and practical exams, respectively. Hait and Yamakado had identical scores on the laboratory practical. At the closing event, these students received a certificate signed by Prof. Kazuyuki Tatsumi, IUPAC President, and a copy of the two-volume History of IUPAC.

Let the Games Begin

The 44th IChO began with all of the pomp and circumstance of the London Olympics (minus the Queen, James Bond, and Paul McCartney). The opening ceremony was held on 22 July in the University of Maryland's DeKelboum Auditorium. William F. Carroll, chair of the ACS Board of Directors, presided over the opening ceremony. The ACS's executive director and CEO, Madeleine Jacobs, introduced each of the teams participating in the 2012 Olympiad. American culture was on display during the opening ceremony with performances by the Eagle Spirit Dancers and the University of Maryland Jazz Studies Combo.

A number of speakers, including Nobel Laureate Richard R. Schrock, congratulated the students on their selection as chemistry Olympians and encouraged them to pursue their interest in and study of chemistry. Maryland Governor Martin O'Malley and University of Maryland College Park President Wallace D. Loh welcomed the Olympians to the state of Maryland and the University of Maryland, respectively. Jerome Peribere, executive vice president of The Dow Chemical Company and president and CEO of Dow

Advanced Materials also gave welcoming remarks. Peter Wothers, chair of the IChO Steering Committee offered his perspectives on the competition as a for-



Olympiad students in front of the U.S. Capitol.

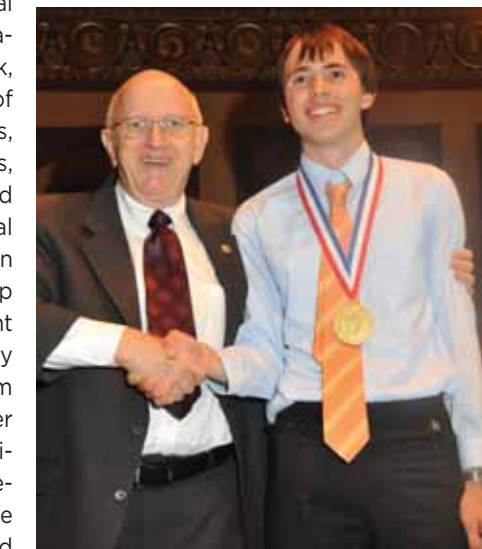
mer Olympian himself. Three students, Sona Guluzade of Azerbaijan, Yazan Ghannam of Syria, and Tomohiro Soejima of Japan, offered welcoming remarks to their peers.

The Competition

The chemistry knowledge and laboratory expertise of the students were tested during the five-hour laboratory practical and theoretical examinations. Between examinations and throughout the week, the students enjoyed many of Washington, D.C.'s attractions, including museums, monuments, and Capitol Hill. Students heard from a National Aeronautical and Space Administration (NASA) astronaut during a trip to NASA's Goddard Space Flight Center in Greenbelt, MD. They visited the National Aquarium and the Maryland Science Center in Baltimore, MD, and experienced America's pastime, baseball, during a game between the Baltimore Orioles and Oakland Athletics. ACS President Bassam Shakhshiri dazzled the students with a chemistry demonstration show at the University of Maryland. Students wrapped up their stay with a trip to King's Dominion, an amusement park in Doswell, Virginia.

Mentors had a heavy workload throughout the IChO. Following the opening ceremony, mentors inspected

IUPAC Vice President Mark Cesa addresses Olympiad participants.



Michael Doyle, chair of the Scientific Committee, with top gold medalist Florian Berger.

the laboratory set-up in preparation for the practical examination. They then translated the practical examination into the language of their students, with translation of the theoretical exam occurring later in the week. Translation is made more complicated if the students from a single country speak more than one language as their native tongue.

Mentors also spent time in jury meetings, discussing the questions on the practical and theoretical exams with members of the Scientific Committee. Once the exams were graded and distributed to the mentors, a full day of arbitration was held so that the mentors could meet with the authors of the problems to ensure that students received the maximum number of points they earned. The medal distribution was determined during the final jury meeting.

It would have been unfair to bring the mentors to Washington, D.C., and keep them in a hotel the entire week, so time was built into the schedule for visiting museums and monuments. The mentors also enjoyed a dinner cruise on the Potomac River and were reunited with their students upon completion of both exams at the reunion party, which was held at the French Embassy.

Recognizing Excellence

The highlight of the closing ceremony, which was held in Gaston Hall at Georgetown University, was the awarding of the medals. Bruce E. Bursten, 2008 ACS President, served as master of

ceremonies throughout the closing ceremony. YuYe Tong, chair of the Georgetown University Chemistry Department, welcomed everyone to historic Gaston Hall. Congratulations were extended to the students by Mark C. Cesa, vice president of IUPAC, and Marinda Li Wu, ACS president-elect. Everyone in the auditorium rose to their feet when the top gold medalist, Florian Berger, was announced. This show of support exemplified the spirit of the International Chemistry Olympiad as everyone—students, mentors, observers, and guests—recognized the extraordinary talent needed to achieve the top gold medal in the IChO.

The closing banquet of the Olympiad was held at the National Building Museum, a spectacular venue in which to celebrate the accomplishments of the extraordinary students who participated in the 44th International Chemistry Olympiad.

Preparations are well under way for the 45th International Chemistry Olympiad, which will be held in Moscow, Russia, in July 2013. Bryan Balazs transferred the IChO flag to Valery Lunin, president of the 45th IChO, during the closing ceremony. Next year's compe-

Conference Call

tition will continue the goal of the IChO in promoting the international exchange of pedagogical and scientific experiences in chemistry, while stimulating student interest in chemistry through independent and creative solving of chemical problems. It was truly an honor for the United States to host the 44th IChO, an experience that enhanced friendly interactions among young people with a passion and talent for chemistry and encouraged cooperation through international understanding.

Mary Kirchoff <M_Kirchoff@acs.org> is director of education for the American Chemical Society.

 www.icho2012.org

On the Description of Nanomaterials

by *Françoise Roure and John Rumble*

At the request of several groups involved in preparing standards for nanotechnology, the International Council for Science (ICSU) and CODATA organized a workshop addressing issues associated with developing systems for describing materials on the nanoscale (called nanomaterials for short).

The subject of describing nanomaterials is of great importance as nanotechnology progresses and becomes commercialized. Many recognized systems exist for naming and describing “traditional” materials—from chemicals to metals and alloys to polymers to biological species. The distinctive characteristics of nanomaterials and the broad interest in them, from researchers to regulators to the general public, makes it imperative to develop a robust system to describe them accurately—meaning a system that will allow complete specification of each unique nanomaterial as well as determination that two nanomaterials are the same (equivalency).

The **ICSU-CODATA workshop** was held on 23–24 February 2012 in Paris, with additional local support from the French government. Attendees included 51 representatives of 10 international scientific unions, the ISO Technical Committee 229 on Nanotechnology, industry, government, and academia, national standards development organizations, and the OECD.

Major Conclusions

1. The workshop reinforced the fact that materials with dimensions on the nanoscale (approx-

mately 1 nm to 100 nm) have structure, properties, and interactions that can be quite different from macroscopic materials.

2. Materials on the nanoscale are of interest to and involve many diverse scientific disciplines, with each discipline bringing many perspectives, some of which are unique to their discipline.
3. A wide variety of applications and technologies will take advantage of materials on the nanoscale in the future and these diverse uses will require different types and amounts of data.
4. Standards for describing materials on the nanoscale must be developed with the inclusion of perspectives from different scientific disciplines and different user communities.

The workshop acknowledged a shared interest across disciplines and user communities for accessing and using information about materials on the nanoscale. It strongly supported the position that a discipline-independent description system was necessary as an enabler for many purposes, including informed interactions and decisions among and by stakeholders communities that must be based on meaningful scientific knowledge. Such a system would allow responsible research and innovation in novel materials in many areas, including bio-nano engineered materials.

The workshop pointed out the negative consequences of a “business as usual” scenario, in which the development of a nanomaterials description system proceeds almost exclusively emphasizing only environmental, health, and safety (EHS) uses. In that scenario, the needs of other scientific disciplines and user communities would not be met in a timely fashion.

Consequently, the workshop defined some principles for guiding the development of a robust and high impact description system. Such a project should have:

- a well-defined governance for a project open to international cooperation researchers in many disciplines, perhaps through crowd sourcing
- consideration of multi-lingual needs
- early inclusion of general public and consumer needs
- early inclusion of engineering and technological needs
- early inclusion of public authority needs

The resulting system should possess the following characteristics:

Conference Call

- establishment of the uniqueness of a specific nanomaterial and equivalency of two nanomaterials
- accessibility and extensions to meet specific needs or those of interest groups
- open access of the core characterization set, generic ontologies, and data sets for use by all
- interoperable informatic formats
- strong curation and high scientific quality
- capability to respond to and include new knowledge and technology, that is, be dynamic
- provision of a level playing field by international cooperation in research on nanometrology

Recommendations

The workshop strongly endorsed a vigorous effort to facilitate the development of a robust description system for materials on the nanoscale. To this end, the workshop made the following recommendations:

1. A two-phase, pre-normative project should be started as soon as possible. The first phase is to determine the requirements for a description system for materials on the nanoscale that takes into account the needs of as many scientific and technical disciplines and user communities as possible.
2. The second phase would develop a potential list of minimum characteristics that meet as many of the requirements defined in 1 above as possible.
3. The International Scientific Unions, and similar bodies for disciplines without an union, provide an ideal mechanism for bringing together the scientific knowledge necessary to complete the projects in points 1 and 2 successfully.
4. The results of these projects should be presented to international standards development organizations such as ISO TC229 on Nanotechnology to facilitate the development of standards on description systems for materials on the nanoscale.
5. CODATA as an official ICSU committee is ideally placed to bring together different scientific knowledge through its access to International Scientific Unions.
6. VAMAS (Versailles Project on Advanced Materials and Standards), has ties to international standards development organizations such as ISO, and is ideally placed to provide strong leadership on pre-normalization research.
7. Consequently, CODATA and VAMAS should form a joint working group with the specific

goal of developing a pre-normative White Paper presenting the requirements for a robust description system for materials at the nanoscale based on the needs of all scientific and technical disciplines on an international and multi-lingual basis.

8. The joint CODATA-VAMAS working group should seek funding from a variety of international and national funding agencies, as well as consider partial funding from industry.
9. Work should commence as soon as approval from CODATA and VAMAS is obtained.

The agenda of the meeting is available at <www.codata.org/Nanomaterials/Index-agenda-Nanomaterial.html>.

The report is reproduced from the *CODATA Newsletter* 103, May 2012.

 www.codata.org

What's in a Name? Possibly Death and Taxes!

*by Richard M. Hartshorn
and Hervé Schepers*

"In this world nothing can be said to be certain, except death and taxes."

—Benjamin Franklin, 13 November 1789

It may appear something of a leap from this statement to nomenclature, but nomenclature can be tied to both of Benjamin Franklin's certainties . . . In the absence of nomenclature, the inability to identify a compound and consequently to find and examine material safety data sheets could lead to an accident, or perhaps prevent selection of appropriate treatment or clean-up procedures in the event of a mishap.

Alternatively, having an appropriate name for a compound can be vital to taxation and application of duties. Without a name it is impossible to decide whether a duty should be applied and at what level it might be appropriate (e.g., for a pharmaceutical or a commercial commodity). An extra complication in this case is one of language—different names are used in different languages, and means must be available for translation. This was developed in the article "Customs, Chemistry, and IUPAC: An Old Story" (March-April 2009 *CI*).

Conference Call

One might think it unlikely that Benjamin Franklin would have had nomenclature in mind when he wrote his well-known comment to Jean Baptiste Le Roy, a fellow scientist, known for his work on electricity, but perhaps it would be hasty to rule it out. After all, Franklin was something of a polymath, the strength of the relationship between the fledgling United States of America and France is well-known, and Franklin served as Ambassador to France for many years. It seems certain that Franklin followed Lavoisier's work closely and, in a 1788 letter to Lavoisier's wife and scientific collaborator, he expresses his thanks for Antoine Lavoisier's gift of his recent book on chemical nomenclature. Indeed, Benjamin Franklin and Antoine Lavoisier served together on a commission conducting a scientific inquiry into Dr. Mesmer's claims of medical cures and body control through the use of "animal magnetism" that was ordered by the King of France in 1784. The following quote expresses the importance that Lavoisier attached to nomenclature, so perhaps Benjamin Franklin would, indeed, have seen how nomenclature might be tied to his certainties in life:

"The impossibility of separating the nomenclature of a science from the science itself, is owing to this, that every branch of physical science must consist of three things; the series of facts which are the objects of the science, the ideas which represent these facts, and the words by which these ideas are expressed. Like three impressions of the same seal, the word ought to produce the idea, and the idea to be a picture of the fact. And, as ideas are preserved and communicated by means of words, it necessarily follows that we cannot improve the language of any science without at the same time improving the science itself; neither can we, on the other hand, improve a science, without improving the language or nomenclature which belongs to it."

—Antoine Lavoisier, *Elements of Chemistry*, 1790

These historical notes perhaps provide some context for the two-day nomenclature workshop **On Chemical Names and their Translation**, organized by the European Commission's Directorate General Taxation and Customs Union, Directorate General Translation and Belgium Customs and Excise Administration, that was held on 17-18 November 2011 within the frame of the International Year of Chemistry.

More than 80 delegates from EU taxation and customs authorities, translation departments, international organizations, and universities met for a workshop in Brussels, with a substantial portion of

the content being provided by IUPAC delegates from the Division of Chemical Nomenclature and Structure Representation. The venue, the Atomium, was highly appropriate to a workshop with a focus on a key aspect of chemistry (the Atomium was the main pavilion and icon of the 1958 World Fair of Brussels, it represents an elementary iron crystal enlarged 165 billion [thousand million] times).

As outlined above, there is a great need to establish common rules for nomenclature in order to facilitate trade and enforce regulations related to the import and export of commodities. For customs officials, different names mean different products; they cannot be blamed, they are not chemists. To take a very simple example, o-cresol, ortho-cresol, and 1,2-cresol might be considered three different products. It must be admitted also that nomenclatures are voluminous and almost unreadable for the common citizen (not to say even for most chemists).

A key role for IUPAC, therefore, is the development of clear nomenclature rules for naming compounds, and IUPAC has been doing this since it was first established. The much more recent work on the development of Preferred IUPAC Names (PINs) is a further refinement that will be very useful to organisations

The Atomium in Brussels.



Conference Call

involved in trade. This work will identify one systematic or retained name for regulatory use – there are often several systematic and unambiguous names for a given compound that can be formed using different, but still acceptable nomenclature methods.

A nevertheless perturbing example for customs officials:

- copper(II) acetate monohydrate
- dicopper(II) tetraacetate dihydrate
- tetrakis(μ -acetato- κ^2O,O')bis[(aqua)copper(II)]

A second issue that is of great importance to the EU is that of translation of names. IUPAC nomenclature is developed and provided in English. Other languages mostly use IUPAC nomenclature as a basis, but numerous situations arise where the grammar and structure of a language is incompatible with a particular aspect of an IUPAC name. Typically the IUPAC recommendations for nomenclature in a particular area of chemistry are translated into other languages by national bodies such as chemical societies, but this is only done for a subset of languages, and nowhere near the number of languages that are used within the EU (currently 23 and regularly new Member States bring new languages to the list).

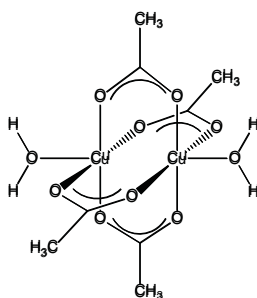
An example of a simple chemical name in all the current EU languages is:

EN	ethyl acetate	HU	etilacetát
BG	етил ацетат	IT	acetato di etile
CS	etyl-acetát	LT	etilacetatas
DA	ethylacetat	LV	etilacetāts
DE	Ethylacetat	NL	ethylacetaat
EL	οξικό αιθύλιο	PL	octan etylu
ES	acetato de etilo	PT	acetato de etilo
ET	etülatsetaat	RO	acetat de etil
FI	etyyliasettaatti	SK	etyl-acetát
FR	acetate d'éthyle	SL	etil acetat
GA	aicéatáit eitile	SV	etylacetat

That means that an organization such as the European Commission has to provide a mechanism to establish the equivalence of names that might be provided in different languages. A software package to achieve this task is currently under redevelopment (the first translation module was developed beginning of the 1980s), and part of the workshop was allocated

to presenting the challenges of translation of chemical names and outlining progress in this area.

The first day of the workshop contained an overview of general principles of nomenclature and other kinds of chemical names. More detailed sessions covered the nomenclature of organic chemistry (the Blue Book), inorganic chemistry (the Red Book), and polymer nomenclature (the Purple Book). These sessions were delivered by IUPAC specialists, mostly coauthors of the IUPAC books and from EU countries. The presentations were highly appreciated by the participants, many of them discovering or rediscovering the nomenclatures, and realizing also that IUPAC nomenclatures become rapidly a



matter for specialists or computers. In this sense, the IUPAC International Chemical Identifier (InChI) and the naming with software were also introduced.

Day two dealt with translation of names, the complexities that can arise in nomenclature when dealing with translation, and the software that is being developed to assist with this process. All of the presentations were illustrated with detailed examples of the ways that names are put together, and later talks examined the variations that can occur when the subtleties of other languages result in changes to either the detail or the structure of a name.

In particular, the study realized by the chemical software company ACD/Labs UK Ltd. to develop the translation rules and the dictionary in all the EU languages revealed some important difficulties in the chemical nomenclature itself. The main difficulty is certainly a concatenation of words in many EU languages like in German. If it is easy to recognize the two parts in the name “Ethylacetat”, but it becomes rapidly difficult to recognize the different parts in more complex cases. A development of general convention to distinguish name parts for such languages would be very important both for nomenclature and practical use of chemical names.

To an end, European Commission’s Directorate General Taxation and Customs Union is currently finalizing the development of the translation software with the results of the finished study and a new study will start soon to continue the work. Help is more than welcome. While this new study will obviously focus on European languages, IUPAC could consider the extension of this work to non-European languages as it would help to disseminate the “IUPAC color books”.

The proceedings of the workshop as well as more information on the European Customs Inventory

Conference Call



*Example of a confusing translation due to concatenation:
Ethylmethylpropandioat*

of Chemical Substances (ECICS) and its translation module can be obtained on http://ec.europa.eu/taxation_customs/customs/customs_controls/custom_laboratories/group_ecl/article_6754_en.htm or from Hervé Schepers <hervé.schepers@ec.europa.eu>.

Richard M. Hartshorn <richard.hartshorn@canterbury.ac.nz> is president of the IUPAC Division of Chemical Nomenclature and Structure Representation (Division VIII) and Hervé Schepers <Herve.Schepers@ec.europa.eu> is at the European Commission, DG Taxation and Customs Union.

IUPAC MACRO World Polymer Congress 2012

by Timothy Long

Virginia Tech and the Macromolecules and Interfaces Institute hosted the **44th IUPAC World Polymer Congress** in Blacksburg, USA, 24–29 June 2012. Timothy E. Long, S. Richard Turner, and Robert B. Moore organized the conference that attracted more than 1400 attendees from 52 countries with 60 percent international attendees. The Congress provided an international forum for scientific discovery, professional networking, research collaboration, interdisciplinary education, and dissemination of the most recent scientific advances. More than 1200 presentations (766 oral and 475 poster presentations) ensured a diverse technical program, and 12 plenary speakers provided some key focal points.

The themes of the conference focused on “Enabling Technologies for a Safe, Sustainable, Healthy World.” Polymers continue to enable many emerging technologies such as tissue regeneration, multilayer structures, processing, drug delivery, water purification, security,

biomedical technologies, alternate energy, sustainable resources, smart surfaces and interfaces, high-performance engineering, polymers, energy storage and generation, sensors, and electro-active devices. In most instances, these technologies require functional nanoscale polymers, and polymer design for intelligent response to external stimuli represents an exciting frontier. There is an over-arching need for these technological solutions of the future to also adhere to the principles of earth sustainability. Recent advances in ionic liquids and agricultural based feed stocks are extending performance and decreasing our dependence on petroleum-based monomers. The IUPAC MACRO World Polymer Congress 2012 assembled an international community for the presentation of recent advances in polymer synthesis, physical characterization, engineering, and performance in several complementary emerging technologies.

IUPAC MACRO World Polymer Congress 2012 comprised 11 parallel symposia and 145 technical sessions organized by leading scientists in the field of polymer science from across the globe. Participants stated that the lectures and topics presented in these symposia were very diverse and highlighted the up-to-date research in the polymer field. Moreover, the conference provided mechanisms for professional networking through evening poster sessions and the participation of industrial, national laboratory, government, and academic scientists and engineers. The program also ensured an integration of polymer design with recent advances in polymer characterization techniques with a focus on morphological structure and correlation of structure with properties and performance. Additionally, the conference was preceded by a short course, which allowed current and future scientific leaders in both academia and industry to network and gain appreciation for new directions prior to the conference.

Timothy E. Long delivering his welcoming speech.



Photo by David Elmore.

Conference Call



Virginia Tech Hokie Bird and President Jefferson Thomas.

IUPAC MACRO 2012 included the following symposia topics:

- Recent Developments in Synthesis
- Modern Methods of Characterizations
- Surfaces and Interfaces
- Macromolecules and Nanotechnology
- Macromolecules in Biotechnology and Medicine
- Complex Macromolecular Systems
- Energy, Optics, and Optoelectronics
- Polymer and Polymer-Based Membranes for Energy and Environmental Applications
- Commercial Frontiers
- Advances in Interdisciplinary Interactions
- Polymer Physics

In addition to the 11 parallel symposia, the conference also featured a total of 12 (5 U.S. and 7 international) plenary speakers who presented on a wide range of topics related to the themes of the conference. Plenary speakers were selected based on the diversity and impact of their research in the polymer science field. Plenary lectures highlighted the following topics:

- Polymers for Sustainable Optoelectronics
- Medical Innovation through Polymer Chemistry
- Controlled Synthesis of Functional Polymers
- Advancement of the Materials Sciences
- Nanostructured Materials
- Polymer Characterization
- Advances in Education
- Development in Aqueous Synthesis
- Purification and Separation Membrane Materials
- Synthesis of Complex Nanoparticles
- Polymer Physics
- Complementary Hydrogen Bonding

Among the awards presented during the conference were the following:

Plenary lectures at Burruss Auditorium.

Photo courtesy of Virginia Tech/Logan Wallace.

- DSM Performance Materials Award (Geoffrey Coates)
- Third *Polymer International*-IUPAC Award for Creativity in Applied Polymer Science or Polymer Technology (Ali Khademhosseini)
- Samsung-IUPAC Young Polymer Scientist (Rachel O'Reilly)
- Sigma-Aldrich Lectures (Luis Campos, Christine Luscombe, Anzar Khan)
- IUPAC-sponsored poster prizes (Sandra Tripp, Sarah N. Bronson, Brian T. Michal)

Apart from the technical program, the participants were welcomed by the Virginia Tech Hokie Bird and President Thomas Jefferson. They also enjoyed an evening at the welcoming reception, dinner receptions during poster sessions, a banquet reception with a presentation on origami by Robert J. Lang, several musical performances including the renowned Poly and the Mers (an "in-house" band of Virginia Tech faculty).

In an effort to reduce waste and remain a sustainable conference, the IUPAC MACRO 2012 organizers provided each attendee with a refillable water bottle, biodegradable bag, and a searchable flash drive for all submitted abstracts and conference proceedings. This is in an effort to reduce the amount of paper used in printing abstracts. As a result of IUPAC MACRO 2012, Virginia Tech has received two permanent water refill stations for future use.

IUPAC MACRO World Polymer Congress 2012 received generous financial supports from 39 sponsors. Additionally, some of these sponsors provided the conference materials and partially sponsored several events. Virginia Tech ensured the success of the conference with financial support and access to the university auditorium, lodging, lecture rooms, and poster ballroom.

MACRO 2014 will be held in Chiangmai, Thailand, from 6-11 July <<http://wildblueorganizer.com/macro2014>>.

Timothy Long <telong@vt.edu> is a professor at the Virginia Tech Macromolecules & Interfaces Institute. He was committee chair for the 2012 World Polymer Congress.

 www.macro2012.org



Where 2B & Y

Analytical Chemistry in Africa

7–9 May 2013, Marrakech, Morocco

The second international symposium on **Analytical Chemistry for a Sustainable Development** and the **4th Federation of African Societies of Chemistry Congress** will be held in Marrakech, Morocco 7–9 May 2013. It is the second meeting organized by the Moroccan Society of Analytical Chemistry for Sustainable Development; the first one was held in March 2010 at the Faculty of Sciences and Technologies of Mohammedia, University of Hassan II.

The symposium aims at bringing together researchers, scientists, engineers, and students to exchange and share their experiences, new ideas, and research results about all aspects of analytical chemistry and

green chemistry for sustainable development in Africa.

Symposium topics include

1. emerging techniques in analytical science
2. electroanalysis
3. pharmaceutical and biomedical analysis
4. food and environmental analysis
5. green chemistry for sustainable development in Africa

Abstracts for oral and poster presentation are invited. For full consideration, abstracts must be received by 20 December 2012. Brief abstracts (one page) should be submitted by e-mail to <amcaddassociation@yahoo.fr>.

 <http://amcadd.org/acsd13/>

Polymer

16–21 June 2013, Pisa, Italy

The **2013 Congress of the European Polymer Federation (EPF 2013)** will be held in Pisa, Italy, 16–21 June 2013. Hosted by the Italian Association of Polymer Science and Technology, the congress is being organized by Chairman Giancarlo Galli, University of Pisa.

The Congress will provide the polymer community with an international forum for scientific discovery and dissemination of most recent research advances, industrial innovation, interdisciplinary education, and professional networking. Major themes include:

- From monomers to polymers; New feedstocks and biotech resources; Novel synthetic routes.
- Advanced characterization and analysis of polymer structure, processability and final properties.
- Polymers at surfaces and interfaces across multiple length scales; Polymers and nanotechnology.

- Biobased and biorelated polymeric materials; Environmental applications.
- Polymers and sustainable development: Energy saving and recovery; Food applications; Recycling and life cycle assessment.
- Polymers for biomedicine, pharmaceuticals, and healthcare systems.
- Polymers for energy, optics, photonics, and electronics.

Participants are invited to submit abstracts by 1 February 2013. Early-bird registration is open until 1 April 2013.

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

 www.epf2013.org

Solution Chemistry

7–12 July 2013, Kyoto, Japan

The **33th International Conference on Solution Chemistry (33ICSC)** will be held 7–12 July 2013, Kyoto, Japan. This series of successful biennial conferences has been held in La Grande Motte (2011), Innsbruck (2009), and Perth (2007). The Kyoto conference will bring together scientists from all over the world to discuss up-to-date results in any of the many facets of solution chemistry. It will cover all aspects of solution chemistry: theoretical, experimental, simulations,

and practical applications. Sessions for the conference will include analytical chemistry, ionic liquids, extreme conditions, spectroscopy, coordination chemistry, biophysics, colloids and interfaces, theory and simulations, electrochemistry, and general sessions. Plenary lectures will be given by H.-J. Butt, F. Hirata, S.F. Lincoln, J.A. McCammon, and H. Ohno. The deadline for submission of abstracts is 30 March 2013.

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

 www.solnchem.jp/33ICSC

Polymer Spectroscopy

7-11 July 2013, Prague, Czech Republic

The **19th European Symposium on Polymer Spectroscopy** (ESOPS19), organized simultaneously as the 77th Prague Meeting on Macromolecules (PMM), will take place at the Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic in Prague on 7-11 July 2013.

Polymer spectroscopy represents an important part of polymer science. The ESOPS meetings are held every two to three years to review the latest research and development in the spectroscopic characterization and analysis of polymer systems. Contributions from all fields of spectroscopy are welcome. The scope

of the meeting ranges from theoretical and fundamental aspects to recent advances and novel developments in characterization and analysis of polymers. The symposium brings together scientists specialized in different spectroscopic techniques, giving them the opportunity to broaden their minds beyond their individual fields of work. The symposium is intended not only for those who are actively engaged in the field, from both academia and industry, but also for those wishing to become acquainted with the latest developments.

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

 www.imc.cas.cz/sympo/pmm2013

Stamps International

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

Grignard's Gift to Chemistry

More than a century after their inception, Grignard reagents are still among the most common and versatile reagents used in organic synthesis, and are a staple of every modern organic chemistry textbook. It was in 1900 that Victor Grignard (1871-1935), a young French chemist conducting his Ph.D. thesis research under the supervision of Philippe Barbier at the University of Lyon, discovered that alkyl- or aryl-magnesium halides could be readily used to prepare a variety of alcohols starting from simple aldehydes or ketones. This was a revolutionary yet straightforward method for the formation of carbon-carbon bonds and, within a decade, more than 700 papers on the application of the novel reagents were published worldwide. Almost exactly 100 years ago, Grignard shared the 1912 Nobel Prize in Chemistry with a fellow Frenchman, Paul Sabatier (1854-1941), who pioneered the application of finely divided metals as catalysts for the hydrogenation of organic compounds.

Although Grignard reagents are conventionally represented by the formula $RMgX$ (R = alkyl or aryl, X = halide), they exist in solution as a complex mixture

of species whose ratio depends on concentration, temperature, the steric and electronic properties of R and X , and the Lewis basicity of the solvent (i.e., the degree of solvation). The so called Schlenk equilibrium was extensively studied by the German chemist Wilhelm Schlenk (1879-1943), who also conducted groundbreaking studies with organolithium reagents and developed an array of elegant techniques and specialized glassware to handle air-sensitive compounds.

The French stamp illustrated in this note was issued in 1971 on the occasion of Grignard's birth centennial. It features a portrait of the famous chemist (not to mention his conspicuous mustache), some laboratory equipment, and the reverse side of his Nobel medal. Grignard has

been deservedly honored over time in multiple ways but perhaps the most unusual tribute is also one of the most recent: In 2009, the International Astronomical Union (one of IUPAC's sister organizations) approved the name Grignard for a 12.2-kilometer impact crater located near the northern pole on the Moon!

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



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

3–6 March 2013 • Heterocyclic Chemistry • Gainesville, Florida, USA

14th Florida Heterocyclic and Synthetic Conference (FloHet-2013)

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

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

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 Cátedra de Química Inorgánica 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

11–15 March 2013 • Polymer Characterization • Gwangju, 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, Istituto 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

16–21 June 2013 • European Polymer • Pisa, Italy

Congress of the European Polymer Federation (EPF-2013)

Prof. Giancarlo Galli Università di Pisa Dipartimento di Chimica e Chimica Industriale Via Risorgimento 35 I-56126 Pisa, Italy, Tel.: +39 050 221 9272, Fax: +39 050 221 9240, E-mail: gallig@dcci.unipi.it

7–10 July 2013 • Polymer Chemistry • Northern Territory, Australia

34th Australasian Polymer Symposium (34 APS)

Dr. Kevin Jack, University of Queensland, Centre for Microscopy & Microanalysis, Level 1, AIBN, Bldg. 75 St. Lucia, QLD 4072, Australia, Tel.: +61 7 3365 1143, Fax: +61 7 3346 3993, E-mail: k.jack@uq.edu.au

7–12 July 2013 • Solution Chemistry • Kyoto, Japan

33rd International Conference on Solution Chemistry (ICSC 2013)

Prof. Toshio Yamaguchi Fukuoka University Department of Chemistry Nanakuma, Jonan, Fukuoka 814-0180, Japan, Tel.: +81 092 871 6631 ext. 6224, Fax: +81 092 865 6030, E-mail: yamaguchi@fukuoka-u.ac.jp

8–11 July 2013 • Polymer Spectroscopy • Prague, Czech Republic

19th European Symposium on Polymer Spectroscopy (ESOPS 19)

Prof. Jiri Spevacek Academy of Sciences of the Czech Republic Institute of Macromolecular Chemistry Heyrovsky Square, 2 CZ-162 06 Prague Czech Republic

Tel.: +420 2 9680 9380, Fax: +420 2 9680 9410, E-mail: spevacek@imc.cas.cz

28 July–1 August 2013 • Organometallic Chemistry • Fort Collins, Colorado, USA

17th International IUPAC Conference on Organometallic Chemistry Directed Towards Organic Synthesis

Prof. E. Peter Kundig, Université de Genève, Département de Chimie Organique, CH-1211 Genève 4, Switzerland

Tel.: +41 22 379 6093, Fax: +41 22 328 7396, E-mail: peter.kundig@unige.ch

28 July–2 August 2013 • Novel Aromatic Compounds • Taipei, Taiwan

15th International Symposium on Novel Aromatic Compounds (ISNA-15)

Prof. Ken-Tsung Wong, Taiwan National University, Department of Chemistry No. 1, Sec. 4, Roosevelt Road, Taipei 10167 Taiwan, Tel.: +886 2 3366 1665, Fax: +886 2 3366 1667, E-mail: kenwong@ntu.edu.tw

4–9 August 2013 • Homogeneous and Heterogeneous Catalysis • Sapporo, Japan

16th International Symposium on Relations between Homogeneous and Heterogeneous Catalysis (ISHHC-16)

Prof. Atsushi Fukuoka, Hokkaido University, Kita 21-10, Sapporo 001-0021, Japan

Tel.: +81 11 706 9140, Fax: +81 11 706 9140, E-mail: fukuoka@cat.hokudai.ac.jp

11–16 August 2013 • IUPAC 44th Congress • Istanbul, Turkey 

44th IUPAC Congress—Clean Energy Through Chemistry

Prof. Mehmet Mahramanlioglu, Turkish Chemical Society, Istanbul University, Department of Chemistry, TR-34320 Avcilar, Istanbul, Turkey

Tel.: +90 212 591 1996, Fax: +90 212 591 1997, E-mail: mehmah@istanbul.edu.tr, www.iupac2013.org

13–16 August 2013 • MacroMolecular Complexes • Clemson, South Carolina, USA 

15th International Symposium on MacroMolecular Complexes (MMC-15)

Prof. Anthony Guiseppi-Elie, Clemson University, Department of Chemical & Biomolecular Engineering, 132 Earle Hall, Clemson, SC 29634, USA, Tel.: +1 864 656 1712, Fax: +1 864 656 1713, E-mail: guiseppi@clemson.edu

18–23 August 2013 • Advanced Polymers via Macromolecular Engineering • Durham, UK

10th International Conference on Advanced Polymers via Macromolecular Engineering (APME-2013)

Prof. Neil R. Cameron, Department of Chemistry, Durham University, Durham, DH1 3LE, UK, Tel.: +44 191 334 2008, Fax: +44 191 384 4737, E-mail: n.r.cameron@durham.ac.uk

25–29 August 2013 • Analytical Chemistry • Warsaw, Poland

XVIIth European Conference on Analytical Chemistry (EuroAnalysis XVII)

Prof. Maciej Jarosz, Warsaw University of Technology, Department of Analytical Chemistry, Ul. Naokowskiego 3, PL-00 664 Warsaw, Poland, Tel.: +48 22 234 7408, Fax: +48 22 234 7408, E-mail: mj@ch.pw.edu.pl

28–29 September 2013 • Biorefineries • Brasília, Brazil

2nd Brazilian Symposium on Biorefineries (II SNBr)

Dr. Sílvia Vaz, Jr., EMBRAPA Agroenergy Parque Estação Biológica, Av. W3 Norte, Asa Norte Brasília, DF 70770-901 Brazil, Tel.: +55 61 3448 2315, Fax: +55 61 3448 1589, E-mail: silvio.vaz@embrapa.br

Visas

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

How to Apply for IUPAC Sponsorship

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

 www.iupac.org

Bookworm

- IUPAC and RSC Publishing, *obc*(3), 38(4)
 Macromolecular Symposia, 25(5)
 Principles of Chemical Nomenclature: A Guide to IUPAC Recommendations, 2011 Edition reviewed by G.J. Leigh, 26(1)
 The 2012 International Vocabulary of Metrology: "VIM" by Paul De Bièvre, 26(3)
 The Chemical Element: Chemistry's Contribution to Our Global Future reviewed by Julia Hasler, 22(2)

Conference Call

- Advanced Materials: Stories of Innovation by Neil Gussman, 30(5)
 Advanced Polymeric Materials by Vera Kovacevic and Michael Hess, 35(5)
 Agrochemicals by J.B. Unsworth, N.A. Shakil, J. Kumar, G.A. Kleter and J.B.H.J. Linders, 34(4)
 Challenges in Modern Analytical Chemistry by Slavica Ražić, 25(2)
 Chemical Safety and Security by Leiv K. Sydnes, 30(1)
 Chemistry of Natural Products and Biodiversity by Mary Garson, 32(1)
 Conducting Polymers by Majda Zigon, 28(1)
 Contemporary Chemistry for Sustainability and Economic Sufficiency by Supa Hannongbua, 30(3)
 Delivering Data in Science by John R. Helliwell and Brian McMahon, 32(4)
 Going for Gold: The 44th International Chemistry Olympiad by Mary Kirchhoff, 26(6)
 Halogen Bonding by David L. Bryce, 27(1)
 How Many Miles Have We Gone, InChI by InChI? by Alex Tropsha and Antony Williams, 33(5)
 IUPAC MACRO World Polymer Congress 2012 by Timothy Long, 32(6)
 Macromolecular Complexes by Heikki Tenhu, 26(2)
 Novel Materials and their Synthesis by Yuping Wu, 27(2)
 On the Description of Nanomaterials by Françoise Roure and John Rumble, 28(6)
 Physico-Chemical Methods in Drug Discovery and Development by Vladislav Tomišić and Zoran Mandić, 29(3)
 Recent Advances in Natural Products Chemistry by Minoru Isobe, 29(3)
 Trace Elements in Food by Eva M. Krupp and Jörg Feldmann, 33(1)
 Translating Food Chemistry into Health Benefits by Agnieszka Bartoszek and Mariusz Piskula, 27(2)
 What's in a Name? Possibly Death and Taxes! by Richard M. Hartshorn and Hervé Schepers, 29(6)

Features

- A Vision of Chemistry for 2050: The International Year of Chemistry Young Leaders Team, 4(3)
 Alan Alda on Radiance: The Passion of Marie Curie by Paul S. Weiss, 4(2)

- Alchemists Are Us by Neil Gussman and Michal Meyer, 4(6)
 An Artist's Hommage to the Elements by Santiago Alvarez, 5(4)
 Chemicals in the EU: the European Chemicals Agency Experience by Derek J Knight, XX(6)
 Chemistry's Role in Delivering Sustainable Development: A Report from the 2011 World Chemistry Leadership Meeting by Colin Humphris, 12(2)
 Icons of Boron Chemistry by Narayan S. Hosmane, 14(4)
 ICSTI at Work: An Interview with Brian Hitson by Emma Thompson, 13(6)
 Making Measurement Matter: How Do You Know Your Results Measure Up? by Gavin O'Connor and Louise Dean, 4(1)
 On the Future of Drug Discovery by Simon Campbell, 10(5)
 Reports from San Juan, Part I, 12(1)
 Reports from San Juan, Part II, 16(2)
 Repositioning the Chemical Sciences for African Development by Berhanu M. Abegaz, 4(5)
 Science for Haiti: A Call for a Response from the International Chemistry Community by Jorge Colón, 10(4)
 Size Matters: Measurement Helps Solve Nanoparticle Toxicity Challenges by Louise Dean, 6(4)
 The European Patent Office: Supporting Innovation in Chemistry by Guillaume Minnoye and Nataša Doslić, 10(3)
 The Formation of the International Association of Chemical Societies by Brigitte Van Tiggelen and Danielle Fauque, 9(1)
 The Global Experiment of the International Year of Chemistry: Water: A Chemical Solution by Javier Garcia Martinez and Rovani Sigamoney, 14(3)
 The Homo Sapiens Report by Michael Wadleigh and Birgit van Munster, 8(2)
 The IYC2011 at the Lycée Français d'Irlande - A cross-disciplinary, multiclass educational project, by Johnny Marcelin and Sarah Magadoux, 9(6)
 The Young Ambassadors of Chemistry Program Visits Tanzania by Lida Schoen, Erica Steenberg, and Mei-Hung Chiu, 7(5)

From the Editor

- See You in Istanbul (6)
 A Turning Point (1)
 Africa (5)
 IYC2011 + 1 and more (2)
 The Iconic Periodic Table (4)
 What Are You Waiting For? (3)

Internet Connection

- Periodic Tables on the World Wide Web by Leslie Glasser, 26(5)

IUPAC Wire

Winners of 2012 IUPAC Prizes for Young Chemists, 17(6)
2012 Thieme-IUPAC Prize Awarded to Melanie S. Sanford, 20(4)
2012-2013 IUPAC Bureau Membership, 21(1)
An IYC Periodic Table Project Unveiled, 21(4)
CHF Catalyst Series on Women in Chemistry, 14(5)
Flerovium and Livermorium Join the Periodic Table, 19(4)
Future Earth: Research for Global Sustainability, 19(4)
“G-Science” Statements Call for Action on Global Challenges, 21(4)
Gold Book PDF, 21(1)
ICSU Grants Programme 2013 Call for Applications, 13(5)
ICSU Issues Recommendations for Organizing International Scientific Meetings, 13(5)
Ian Mills Awarded IUPAC SUNAMCO Prize, 20(6)
In Memoriam—Professor Herbert D. Kaesz, 21(3)
In Memoriam, 15(5)
InChI 1.04, 18(1)
IUPAC Elections for the 2014-2015 Term, 20(3)
IUPAC General Assembly and World Congress – Expression of Intent, 31(3)
IUPAC Poster Prizes, 39(4)
IUPAC Prize for Young Chemists, 3(3), 4(4), 9(5)
John D. Petersen Appointed IUPAC Executive Director, 16(6)
Klavs F. Jensen Wins First IUPAC-ThalesNano Prize in Flow Chemistry, 18(3)
Linking Science and Policy at Rio+20, 12(5)
Lois Rossi to Receive the IUPAC International Award for Advances in Crop Protection Chemistry, 20(4)
Mark Cesa and James Economy Named ACS Fellow, 20(6)
Metrology for Safety, 20(3)
Michael Blackburn Awarded 2011 Arbuzovs Prize, 20(1)
Mozambique and Argentina Join IUPAC as Full Members, 17(6)
Possible Changes to The International System of Units, 20(1)
Rachel O'Reilly received the 2012 IUPAC-Samsung Young Polymer Scientist Award, 18(6)
Stephen Hanessian to Receive 2012 IUPAC-Richter Prize in Medicinal Chemistry, 19(3)
Sustainable Energy for All, 18(1)
The 2012 International Chemistry Olympiad (IChO) Comes to Washington, D.C., 18(1)
The Global Young Academy Calls on Scientific Community to Promote Sustainability, 14(5)
The second CHEMRAWN VII Prize awarded to Rashmi Sanghi, 19(6)
Third Polymer International-IUPAC Prize Awarded to Ali Khademhosseini, 19(3)
Young Chemists to the 44th IUPAC Congress, 16(6)

Making an impACT

A Brief Guide to Polymer Nomenclature, 25(6), supplement (6)
Analogue-Based Drug Discovery, 24(5)
Characterization of photoluminescence measuring systems, 24(6)
Chlorine-Free Synthesis for Green Chemistry, 24(4)
Guidelines for Reporting of Phase Equilibrium Measurements, 24(6)
IUPAC Glossary of Terms Used in Immunotoxicology, 24(5)
IUPAC-NIST Solubility Data Series, recent volumes, 25(6)
IUPAC/CITAC Guide: Investigating Out-of-Specification Test Results of Chemical Composition Based on Metrological Concepts, 25(6)
Liquid Intrusion and Alternative Methods for the Characterization of Macroporous Materials, 24(3)
Names and Symbols of the Elements with Atomic Numbers 114 and 116, 24(5)
PAC Does Conferences, 25(3)
Properties and Units in the Clinical Laboratory Sciences, 24(3)
Remote Sensing in Coastal Water Monitoring: Applications in the Eastern Mediterranean Sea, 24(3)
Terminology for Biorelated Polymers and Applications, 25(3)

Mark Your Calendar

Listing of IUPAC-Sponsored Conferences and Symposia, 39(1), 32(2), 34(3), 40(4), 40(5), 37(6)

Nomenclature Notes

InChIs and Registry numbers, 28(6)
Non-IUPAC Nomenclature Systems, 27(4)
On the Various Nomenclature Systems, 28(3)
Systematic and Trivial Nomenclature, 28(5)
What is IUPAC Nomenclature?, 24(2)

Officers' Columns

A System Comes of Age by Kip Powell, 2(4)
Our Roles, Responsibilities, and Legacy by Mark Cesa, 2(6)
For IUPAC, It's Now or Never by Nicole Moreau, 3(2)
Planning for the Future of IUPAC Based on the Success of IYC2011 by Kazuyuki Tatsumi, 2(1)
The Times They Are a Changing . . . by John Corish, 2(5)
What Is IUPAC's Place in an Ever-Changing World? by René Deplanque, 2(2)

The Project Place

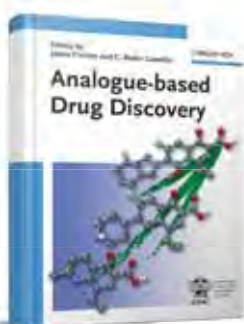
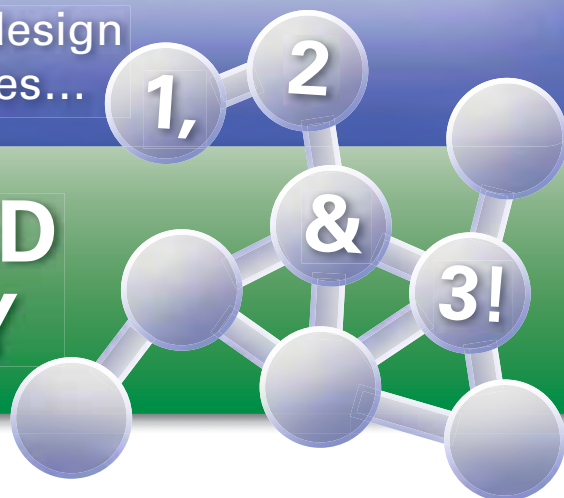
Chemical Kinetic Data Evaluation for Atmospheric Chemistry and the IUPAC Kinetics Database 17(5)
Definitions of Transfer Coefficient and of Partial Charge Transfer Coefficient in Electrode Kinetic, 21(2)
Engineered Nanoparticles and the Environment: Physicochemical Processes and Biotoxicity, 20(2)

Index for 2012

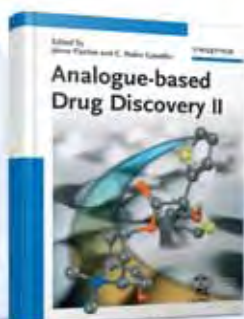
- Global Chemical Safety and Sustainability, 19(5)
Human Drug Metabolism Database, 22(1)
Impact of Nanotechnology on Chemistry: A Terminology Conundrum, 16(5)
Impact of Scientific Developments on the Chemical Weapons Convention, 23(1)
IUPAC Safety Training Program, 21(6)
Maintaining and Ensuring the Pesticides Properties Database, 22(4)
Management of Maritime Pollutants in European Ports, 23(1)
Metal-Binding Organic Ligands, 23(4)
Postgraduate Course in Polymer Science, 24(1)
Regional Water Quality Assessment and Regional Cooperation in the Middle East, 22(3)
Rules for Abbreviation of Protecting Group, 22(4)
Strategic Planning for a New Network for Heterocyclic Chemistry, 22(1)
Terminology and Nomenclature of Inorganic and Coordination Polymer, 20(2)
Terminology of Nanomaterials and Nanotechnology in Polymer Science, 22(4)
- Pull-Out/Tear-Off**
A Brief Guide to Polymer Nomenclature, supplement (6)
IUPAC Periodic Table of the Elements, version 1 June 2012, supplement (4)
- Provisional Recommendations**
Definition of the Halogen Bond, 23(5)
Glossary of Terms Relating to Thermal and Thermo-mechanical Properties of Polymers, 23(3)
Name and Symbol of the Element with Atomic Number 114 and 116, 25(1), 21(2)
Nomenclature of Thermal Analysis, 23(5)
Terminology and Nomenclature for Macromolecular Rotaxanes and Pseudorotaxanes, 25(1), 21(2)
Terminology for Self-Assembly and Aggregation of Polymers Polymer Division, 23(3)
Vocabulary for Nominal Properties and Nominal Examinations—Basic and General Concepts and Associated Terms, 23(5)
- Stamps International**
Grignard's Gift to Chemistry, 35(6)
2011: A Stamp Odyssey, 36(3)
Is the Future of Paper Money . . . Plastic? 28(2)
Russia's Leonardo, 24(1)
The Mother of All Molecules, 3(5)
To Sneeze or Not To Sneeze, 18(4)
- Where 2B & Y**
Advanced Polymers via Macromolecular Engineering, 18–22 August 2013, Durham, UK, 39(5)
Analytical Chemistry for the Environment, Health, and Water, 8–11 July 2012, Maputo, Mozambique, 31(2)
Analytical Chemistry in Africa, 7–9 May 2013, Marrakech, Morocco, 34(6)
Biorefineries, 28–29 September 2013, Brasília, Brazil, 39(5)
Biotechnology for GreenWorld, 16–21 September 2012, Daegu, Korea, 38(1)
Catalysis in Organic Synthesis, 15–20 September 2012, Moscow, Russia, 30(2)
Chemistry Education, ICCE-ECRICE 2012 PreConference Virtual Colloquium, May and June 2012, obc(1), 29(2)
Chemistry: The Key for Our Future, 2–6 July 2012, Mauritius, 38(1)
Coordination Chemistry, 9–13 September 2012, Valencia, Spain, 29(2)
Euromedlab, 19–23 May 2013, Milano, Italy, 29(5)
Green Chemistry, 25–29 August 2012, Iguacu, Brazil, 35(1)
Heteroatom Chemistry, 20–25 May 2012, Uji City, Kyoto, Japan, 29(2)
High-Temperature Materials Chemistry, 9–13 September 2012, Beijing, China, 32(3)
Inspiring Youth in Chemistry—An Exhibit, March–June 2012, Pennsylvania, USA, 32(3)
Internal Quality Control, 9–11 October 2012, Berlin, Germany, 33(3)
IUPAC2013 World Chemistry Congress, 9–16 August 2013, Istanbul, Turkey, ibc(4)
MacroMolecular Complexes, 13–16 August 2013, Clemson & Greenville, South Carolina, USA, 37(4)
Mycotoxins and Phycotoxins, 5–9 November 2012, Rotterdam, The Netherlands, 38(1)
Nano Systems and Applications, 21–25 November 2012, Coimbatore, India, 39(5)
Nanostructured and Biorelated Materials, 9–12 May 2012, Kathmandu, Nepal, 30(2)
Novel Aromatic Compounds, 28 July–2 August 2013, Taipei, Taiwan, 38(5)
Open Data and Information for a Changing Planet, 28–31 October 2012, Taipei, China, 37(4)
Pesticide Chemistry, 10–14 August 2014, San Francisco, CA, 30(2)
Philosophy of Chemistry, 7–10 August 2012, Leuven, Belgium, 33(3)
Physical Organic Chemistry, 9–13 September 2012, Durham, UK, 37(1)
Polymer Spectroscopy, 7–11 July 2013, Prague, Czech Republic, 35(6)
Polymer, 16–21 June 2013, Pisa, Italy, 34(6)
Solubility and Equilibria, 23–27 July 2012, Xining, China, 37(1)
Solution Chemistry, 7–12 July 2013, Kyoto, Japan, 34(6)
Space Research, 14–22 July 2012, Mysore, India, 36(1)
The Chemistry of Sustainable Supply Chains, 1 June 2012, Toronto, Ontario, Canada, 36(1)
The Periodic Table, 14–16 August 2012, Cusco, Peru, 33(3)
Toxicology, 16–19 October 2012, Lisbon, Portugal, 38(5)

A systematic OVERVIEW of drug design
by modification in 3 handy volumes...

ANALOGUE-BASED DRUG DISCOVERY



EDITORS:
JANOS FISCHER,
C. ROBIN GANELLIN
Hardback | 606 Pages
February 2006
ISBN: 978-3-527-31257-3



EDITORS:
JANOS FISCHER,
C. ROBIN GANELLIN
Hardback | 600 Pages
August 2010
ISBN: 978-3-527-32549-8



EDITORS:
JANOS FISCHER,
C. ROBIN GANELLIN,
DAVID P. ROTELLA
Hardback | 386 Pages
December 2012
ISBN 978-3-527-33073-7

Featuring a combined total of 36 analogue drug classes and 24 case studies, these three volumes provide a unique systematic overview of drug design by modification.

Originating from a project of the IUPAC sub-committee on Medicinal Chemistry and Drug Development, the three volumes summarise past and present strategies for successful drug analogue development across all therapeutic fields.

Each volume is available to purchase separately in print and electronically.



How to order:

EUROPE, MIDDLE EAST, ASIA & AFRICA
John Wiley & Sons Ltd
Tel: +44 (0)1243 843294 Fax: +44 (0)1243 843296
E-mail: cs-books@wiley.co.uk
www.wiley.com

NORTH, CENTRAL & SOUTH AMERICA
John Wiley & Sons Inc
Tel: 877 762 2974 Fax: 800 597 3299
E-mail: custserv@wiley.com
www.wiley.com

GERMANY, SWITZERLAND & AUSTRIA
Wiley-VCH Verlag GmbH
Tel: +49 6201 606 400 Fax: +49 6201 606 184
E-mail: service@wiley-vch.de
www.wiley-vch.de

www.wiley.com

 **WILEY-VCH**

IUPAC

ADVANCING THE WORLDWIDE ROLE OF CHEMISTRY FOR THE BENEFIT OF MANKIND

MISSION

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

President:
Kazuyuki Tatsumi (Japan)

Vice President:
Mark C. Cesa (USA)

Past President:
Nicole J. Moreau (France)

Secretary General:
René Deplanque (Germany)

Treasurer:
John Corish (Ireland)

NATIONAL ADHERING ORGANIZATIONS

- Asociación Química Argentina (*Argentina*)
Australian Academy of Science (*Australia*)
Österreichische Akademie der Wissenschaften (*Austria*)
Bangladesh Chemical Society (*Bangladesh*)
The Royal Academies for the Sciences and Arts of Belgium (*Belgium*)
Brazilian Chemical Society (*Brazil*)
Bulgarian Academy of Sciences (*Bulgaria*)
National Research Council of Canada (*Canada*)
Sociedad Chilena de Química (*Chile*)
Chinese Chemical Society (*China*)
Chemical Society located in Taipei (*China*)
Croatian Chemical Society (*Croatia*)
Sociedad Cubana de Química (*Cuba*)
Pancyprrian Union of Chemists (*Cyprus*)
Czech National Committee for Chemistry (*Czech Republic*)
Det Kongelige Danske Videnskaberne Selskab (*Denmark*)
National Committee for IUPAC (*Egypt*)
Chemical Society of Ethiopia (*Ethiopia*)
Suomen Kemian Seura—Kemiska Sällskapet i Finland (*Finland*)
Comité National Français de la Chimie (*France*)
Deutscher Zentralausschuss für Chemie (*Germany*)
Association of Greek Chemists (*Greece*)
Hungarian Academy of Sciences (*Hungary*)
Indian National Science Academy (*India*)
Royal Irish Academy (*Ireland*)
Israel Academy of Sciences and Humanities (*Israel*)
Consiglio Nazionale delle Ricerche (*Italy*)
Caribbean Academy of Sciences—Jamaica Chapter (*Jamaica*)
Science Council of Japan (*Japan*)
Jordanian Chemical Society (*Jordan*)
Korean Chemical Society (*Korea*)
Kuwait Chemical Society (*Kuwait*)
Fonds National de la Recherche (*Luxembourg*)
Institut Kimia Malaysia (*Malaysia*)
Academy of Sciences of Mozambique (*Mozambique*)
Koninklijke Nederlandse Chemische Vereniging (*Netherlands*)
Royal Society of New Zealand (*New Zealand*)
Chemical Society of Nigeria (*Nigeria*)
Norsk Kjemisk Selskap (*Norway*)
Chemical Society of Pakistan (*Pakistan*)
Polska Akademia Nauk (*Poland*)
Sociedade Portuguesa de Química (*Portugal*)
Colegio de Químicos de Puerto Rico (*Puerto Rico*)
Russian Academy of Sciences (*Russia*)
Serbian Chemical Society (*Serbia*)
Slovak Chemical Society (*Slovakia*)
Slovenian Chemical Society (*Slovenia*)
National Research Foundation (*South Africa*)
Ministerio de Educación y Ciencia (*Spain*)
Institute of Chemistry, Ceylon (*Sri Lanka*)
Svenska Nationalkommittén för Kemi (*Sweden*)
Swiss Chemical Society (*Switzerland*)
Tanzania Chemical Society (*Tanzania*)
Chemical Society of Thailand (*Thailand*)
Société Chimique de Tunisie (*Tunisia*)
Türkiye Kimya Derneği (*Turkey*)
National Academy of Sciences of Ukraine (*Ukraine*)
Royal Society of Chemistry (*United Kingdom*)
National Academy of Sciences (*USA*)
Programa de Desarrollo de Ciencias Básicas (*Uruguay*)



INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY



A Brief Guide to Polymer Nomenclature

Version 1.1 (2012)

R. C. Hiorns (France),* R. J. Boucher (UK), R. Duhlev (UK), K.-H. Hellwich (Germany), P. Hodge (UK), A. D. Jenkins (UK), R. G. Jones (UK), J. Kahovec (Czech Republic), G. Moad (Australia), C. K. Ober (USA), D. W. Smith (USA), R. F. T. Stepto (UK), J.-P. Vairon (France), and J. Vohlidal (Czech Republic). *E-mail: polymer.nomenclature@iupac.org; Sponsoring body: IUPAC Polymer Division, Subcommittee on Polymer Terminology.

1) Introduction

The universal adoption of an agreed nomenclature has never been more important for the description of chemical structures in publishing and on-line searching. The International Union of Pure and Applied Chemistry (IUPAC)^{1a,b} and Chemical Abstracts Service (CAS)² make similar recommendations. The main points are shown here with hyperlinks to original documents. Further details can be found in the IUPAC Purple Book.³

2) Basic Concepts

The terms polymer and macromolecule do not mean the same thing. A polymer is a substance composed of macromolecules. The latter usually have a range of molar masses (unit g mol⁻¹), the distributions of which are indicated by dispersity (*D*). It is defined as the ratio of the mass-average molar mass (*M_m*) to the number-average molar mass (*M_n*) i.e. *D* = *M_m*/*M_n*.⁴ Symbols for physical quantities or variables are in italic font but those representing units or labels are in roman font.

Polymer nomenclature usually applies to idealised representations; minor structural irregularities are ignored. A polymer can be named in one of two ways. Source-based nomenclature can be used when the monomer can be identified. Alternatively, more explicit structure-based nomenclature can be used when the polymer structure is proven. Where there is no confusion, some traditional names are also acceptable.

Whatever method is used, all polymer names have the prefix poly, followed by enclosing marks around the rest of the name. The marks are used in the order: {{()}}. Locants indicate the position of structural features, e.g., poly(4-chlorostyrene). If a source-based name is one word and has no locants, then the enclosing marks are not essential, but they should be used when there might be confusion, e.g., poly(chlorostyrene) is a polymer whereas polychlorostyrene might be a small, multi-substituted molecule. End-groups are described with α - and ω -, e.g., α -chloro- ω -hydroxy-polystyrene.³

3) Source-Based Nomenclature⁵

3.1 Homopolymers

A homopolymer is named using the name of the real or assumed monomer (the 'source') from which it is derived, e.g., poly(methyl methacrylate). Monomers can be named using IUPAC recommendations, or well-established traditional names. Should ambiguity arise, class names can be added.⁶ For example, the source-based name poly(vinylloxirane) could correspond to either of the structures shown below. To clarify, the polymer is named using the monomer, i.e., class name:monomer name. Thus on the left and right, respectively, are polyalkylene:vinylloxirane and polyether:vinylloxirane.

3.2 Copolymers⁷

The structure of a copolymer can be described using the most appropriate of the connectives shown in Table 1. These are written in italic font.

3.3 Non-linear polymers⁵

Non-linear polymers and copolymers, and polymer assemblies are named using the italicized qualifiers in Table 2. The qualifier, such as *branch*, is used as a prefix (P) when naming a (co)polymer, or as a connective (C), e.g., *comb*, between two polymer names.

Table 1 – Qualifiers for copolymers.⁷

Copolymer	Qualifier	Example
unspecified	<i>co</i> (C)	poly(styrene- <i>co</i> -isoprene)
statistical	<i>stat</i> (C)	poly[isoprene- <i>stat</i> -(methyl methacrylate)]
random	<i>ran</i> (C)	poly[(methyl methacrylate)- <i>ran</i> -(butyl acrylate)]
alternating	<i>alt</i> (C)	poly[styrene- <i>alt</i> -(maleic anhydride)]
periodic	<i>per</i> (C)	poly[styrene- <i>per</i> -isoprene- <i>per</i> -(4-vinylpyridine)]
block	<i>block</i> (C)	poly(buta-1,3-diene)- <i>block</i> -poly(ethene- <i>co</i> -propene)
graft ^a	<i>graft</i> (C)	polystyrene- <i>graft</i> -poly(ethylene oxide)

^a The first name is that of the main chain.

Table 2 – Qualifiers for non-linear (co)polymers and polymer assemblies.⁵

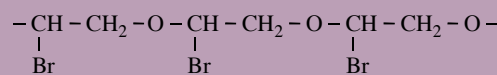
(Co)polymer	Qualifier	Example
blend	<i>blend</i> (C)	poly(3-hexylthiophene)- <i>blend</i> -polystyrene
comb	<i>comb</i> (C)	polystyrene- <i>comb</i> -polyisoprene
complex	<i>compl</i> (C)	poly(2,3-dihydrothieno[3,4- <i>b</i>][1,4]dioxine)- <i>compl</i> -poly(vinylbenzenesulfonic acid) ^a
cyclic	<i>cyclo</i> (P)	<i>cyclo</i> -polystyrene- <i>graft</i> -polyethylene
branch	<i>branch</i> (P)	<i>branch</i> -poly[(1,4-divinylbenzene)- <i>stat</i> -styrene]
network	<i>net</i> (C or P)	<i>net</i> -poly(phenol- <i>co</i> -formaldehyde)
interpenetrating network	<i>ipn</i> (C)	(<i>net</i> -polystyrene)- <i>ipn</i> -[<i>net</i> -poly(methyl acrylate)]
semi-interpenetrating network	<i>sipn</i> (C)	(<i>net</i> -polystyrene)- <i>sipn</i> -polyisoprene
star	<i>star</i> (P)	<i>star</i> -polyisoprene

^a In accordance with IUPAC organic nomenclature, square brackets enclose locants that refer to the numbering of the components of the fused ring.

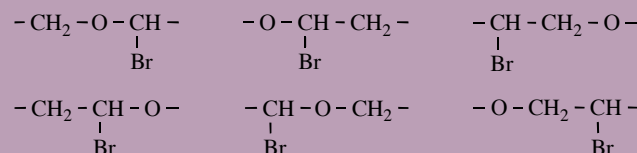
4) Structure-Based Nomenclature

4.1 Regular single-strand organic polymers⁸

In place of the monomer name used in source-based nomenclature, structure-based nomenclature uses that of the **preferred** constitutional repeating unit (CRU). It can be determined as follows: (i) a large enough part of the polymer chain is drawn to show the structural repetition, e.g.,



(ii) the smallest repeating portion is a CRU, so all such possibilities are identified. In this case:



(iii) the next step is to identify the subunits that make up each of these structures, i.e., the largest divalent groups that can be named using IUPAC nomenclature of organic compounds such as the examples that are listed in Table 3; (iv) using the shortest path from the most senior subunit to the next senior, the correct order of the subunits is determined using Figure 1; (v) the preferred CRU is chosen as that with the lowest possible locant(s) for substituents.

In the above example, the oxy subunits in the CRUs are heteroatom chains. From Figure 1, oxy subunits are senior to the acyclic carbon chain subunits, the largest of which are bromo-substituted -CH₂-CH₂- subunits. 1-Bromoethane-1,2-diyl is chosen in preference to 2-bromoethane-1,2-diyl as the former has a lower locant for the bromo-substituent. The preferred CRU is therefore oxy(1-bromoethane-1,2-diyl) and the polymer is thus named poly[oxy(1-bromoethane-1,2-diyl)]. Please note the enclosing marks around the subunit carrying the substituent.

Polymers that are not made up of regular repetitions of a single CRU are called irregular polymers. For these, each constitutional unit (CU) is separated by a slash, e.g., poly(but-1-ene-1,4-diyl/1-vinylethane-1,2-diyl).⁹

¹ Freely available on: (a) <http://www.iupac.org/publications/pac/>;

(b) <http://www.chem.qmul.ac.uk/iupac/>

² <http://www.cas.org/>.

³ IUPAC. "The Purple Book", RSC Publishing, (2008).

⁴ IUPAC. *Pure Appl. Chem.* **81**, 351–352 (2009).

⁵ IUPAC. *Pure Appl. Chem.* **69**, 2511–2521 (1997).

⁶ IUPAC. *Pure Appl. Chem.* **73**, 1511–1519 (2001).

⁷ IUPAC. *Pure Appl. Chem.* **57**, 1427–1440 (1985).

⁸ IUPAC. *Pure Appl. Chem.* **74**, 1921–1956 (2002).

⁹ IUPAC. *Pure Appl. Chem.* **66**, 873–889 (1994).



A Brief Guide to Polymer Nomenclature

Version 1.1 (2012)

Table 3 – Representations of divalent groups in polymers.⁸

Name	Group ^a	Name	Group ^a
oxy	- O -	propylimino	$\begin{array}{c} \text{-N-} \\ \\ \text{CH}_2\text{CH}_2\text{CH}_3 \end{array}$
sulfanediyl	- S -	hydrazine-1,2-diyl	$\text{-NH-}\overset{1}{\text{N}}\text{-}\overset{2}{\text{NH}}\text{-}$
sulfonyl	- SO ₂ -	phthaloyl	
diazenediyl	- N = N -	1,4-phenylene	
imino	- NH -	cyclohexane-1,2-diyl	
carbonyl	$\begin{array}{c} \text{O} \\ \\ \text{-C-} \end{array}$	butane-1,4-diyl	$\overset{1}{\text{-CH}_2}\overset{2}{\text{CH}_2}\overset{3}{\text{CH}_2}\overset{4}{\text{CH}_2}\text{-}$
oxalyl	$\begin{array}{c} \text{O} \quad \text{O} \\ \quad \\ \text{-C-} \quad \text{C-} \end{array}$	1-bromoethane-1,2-diyl	$\overset{1}{\text{-CH}}\overset{2}{\text{-CH}_2}\text{-}$ Br
silanediyl	- SiH ₂ -	1-oxopropane-1,3-diyl	$\begin{array}{c} \text{O} \\ \\ \text{-C-}\overset{2}{\text{CH}_2}\overset{3}{\text{CH}_2}\text{-} \\ \\ \text{O} \end{array}$
ethane-1,2-diyl	$\overset{1}{\text{-CH}_2}\overset{2}{\text{-CH}_2}\text{-}$	ethene-1,2-diyl	$\overset{1}{\text{-CH}}\overset{2}{\text{=CH}}\text{-}$
methylene	- CH ₂ -	methylmethylene	$\begin{array}{c} \text{-CH-} \\ \\ \text{CH}_3 \end{array}$

^a To avoid ambiguity, wavy lines drawn perpendicular to the free bond, which are conventionally used to indicate free valences,¹³ are usually omitted from graphical representations in a polymer context.

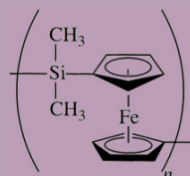
4.2 Regular double-strand organic polymers¹⁰

Double-strand polymers consist of uninterrupted chains of rings. In a spiro polymer, each ring has one atom in common with adjacent rings. In a ladder polymer, adjacent rings have two or more atoms in common. To identify the preferred CRU, the chain is broken so that the senior ring is retained with the maximum number of heteroatoms and the minimum number of free valences.

An example is The preferred CRU is an acyclic subunit of 4 carbon atoms with 4 free valences, one at each atom, as shown below. It is oriented so that the lower left atom has the lowest number. The free-valence locants are written before the suffix, and they are cited clockwise from the lower left position as: lower-left, upper-left:upper-right, lower-right. This example is thus named poly(butane-1,4:3,2-tetrayl). For more complex structures, the order of seniority again follows Figure 1.

5) Nomenclature of Inorganic and Inorganic-Organic Polymers¹¹

Some regular single-strand inorganic polymers can be named like organic polymers using the rules given above, e.g., $\{\text{O-Si}(\text{CH}_3)_2\}_n$ and $\{\text{Sn}(\text{CH}_3)_2\}_n$ are named poly[oxy(dimethylsilanediyl)] and poly(dimethylstannanediyl), respectively. Inorganic polymers can also be named in accordance with inorganic nomenclature, but it should be noted that the seniority of the elements is different to that in organic nomenclature. However, certain inorganic-organic polymers, for example those containing metallocene derivatives, are at present best named using organic nomenclature, e.g., the polymer on the left can be named poly[(dimethylsilanediyl)ferrocene-1,1'-diyl].

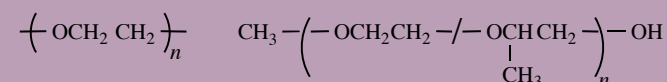


6) Traditional Names

When they fit into the general pattern of systematic nomenclature, some traditional and trivial names for polymers in common usage, such as polyethylene, polypropylene, and polystyrene, are retained.

7) Graphical Representations^{12,13}

The bonds between atoms can be omitted, but dashes should be drawn for chain-ends. The seniority of the subunits does not need to be followed. For single-strand (co)polymers, a dash is drawn through the enclosing marks, e.g., poly[oxy(ethane-1,2-diyl)] shown below left. For irregular polymers, the CUs are separated by slashes, and the dashes are drawn inside the enclosing marks. End-groups are connected using additional dashes outside of the enclosing marks, e.g., α -methyl- ω -hydroxy-poly[oixirane-co-(methyloxirane)], shown below right.



8) CA Index Names²

CAS maintains a registry of substances. In the CAS system, the CRU is called a structural repeating unit (SRU). There are minor differences in the placements of locants, e.g., poly(pyridine-3,5-diylthiophene-2,5-diyl) is poly(3,5-pyridinediyl-2,5-thiophenediyl) in the CAS registry, but otherwise polymers are named using similar methods to those of IUPAC.^{14,15}

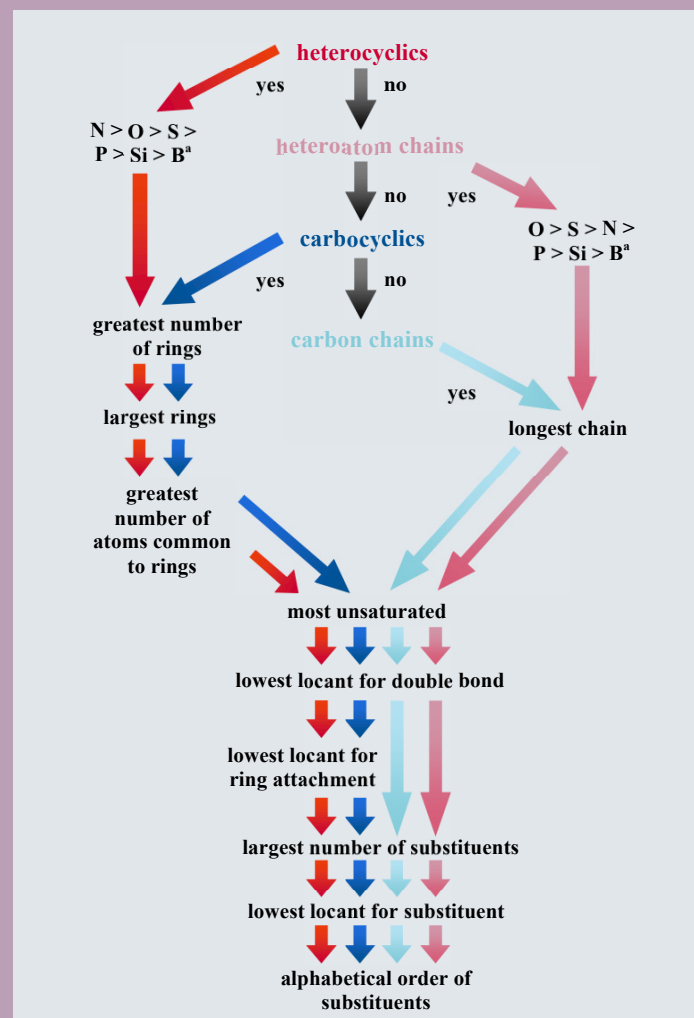


Figure 1 The order of subunit seniority. The senior subunit is at the top centre. Subunits of lower seniority are found by following the arrows. The type of subunit, be it a **heterocycle**, a **heteroatom chain**, a **carbocycle**, or a **carbon chain**, determines the colour of the arrow to follow.⁸ Other heteroatoms may be placed in these orders as indicated by their positions in the periodic table.⁸

¹⁰ IUPAC. *Pure Appl. Chem.* **65**, 1561–1580 (1993).

¹¹ IUPAC. *Pure Appl. Chem.* **57**, 149–168 (1985).

¹² IUPAC. *Pure Appl. Chem.* **66**, 2469–2482 (1994).

¹³ IUPAC. *Pure Appl. Chem.* **80**, 277–410 (2008).

¹⁴ *Macromolecules*, **1**, 193–198 (1968).

¹⁵ *Polym. Prepr.* **41**(1), 6a–11a (2000).

