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A Look Back at Ernest Solvay



INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

InChI, *the* Chemical Identifier ►

Suffixes and the Naming of Elements ►



From the Editor

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A Heartfelt Congratulations to OPCW

On 11 October 2013, the Norwegian Nobel Committee announced that this year's Nobel Peace Prize will be awarded to the Organization for the Prohibition of Chemical Weapons (OPCW) for its extensive efforts to eliminate chemical weapons.

This is a great and important recognition for an organization that works so diligently to make the world a safer place. I am humbled to



relay IUPAC's heartfelt congratulations to our OPCW colleagues for this fantastic and well-deserved recognition for their tireless work to free the world of chemical weapons.

In recent years, IUPAC has been privileged to work with OPCW, both in contributing technical expertise to the review conferences of the Chemical Weapons Convention (CWC)

and in developing educational resources on the multiple uses of chemicals. As recently as the July-Aug 2013 issue of *Chemistry International*, Leiv K. Sydnes contributed a feature outlining IUPAC's involvement with OPCW over the last 12 years. That feature was triggered by the recent IUPAC Technical Report (in the April 2013 *Pure and Applied Chemistry*) titled "Impact of Scientific Developments on the Chemical Weapons Convention," released in advance of the Third Review Conference of the CWC held last April.

In 2004, the president of IUPAC and the director general of the OPCW agreed on a joint project on chemistry education, outreach, and the professional conduct of chemists; see IUPAC project 2004-048-1-020. As an outcome of this project, the need for peer-reviewed educational materials was clearly identified. In response, a set of web-based materials to be used by educators and students has been created and published online at www.iupac.org/multiple-uses-of-chemicals or <http://multiple.kcvs.ca>. The approach was to start with the beneficial uses of chemicals, give examples of the misuse and abuse of chemicals, and then provide basic information about the Chemical Weapons Convention, ending with the need for and examples of existing codes of conduct.

The Nobel recognition to OPCW contributes to validating IUPAC's mission "to advance the worldwide aspects of the chemical sciences and to contribute to the application of chemistry in the service of Humankind." Today, I feel proud of being a chemist and helping IUPAC members to take part in these Union activities.

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PS: This year-end issue will be the last one to be carefully edited and paginated by my colleague Chris Brouwer. After 12 years of making *CI* "pubsimple," Chris is venturing into new communication challenges working at Cornell University. My thanks to you Chris, and best wishes.

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IUPAC Should Make Itself Known

by Nicole Moreau



After nearly six years as an officer of IUPAC, this is my last column. I will try to tell how much I enjoyed this period, and also express some ideas to improve our Union. I have been very happy in IUPAC, because the experience of serving as a volunteer in an international organization is so very different than working in a laboratory. Above all, there is no competition, no struggle, only a willingness to work with one another—colleagues but not competitors—for the good of Chemistry. I found that serving as an officer of IUPAC was a stimulating complement to my rich, but busy professional life. I feel lucky to have worked with an incredible variety of IUPAC colleagues—different nationalities, disciplines, professions. And, of course, many of these colleagues are now friends.

About 20 years ago, in the NAO of France, the Comité National Français de la Chimie, I was the representative of the Centre National de la Recherche Scientifique. In 1995, I attended the IUPAC General Assembly in Guilford (UK) as a member of the French delegation. I confess that I have no remembrance of that assembly, although I know that I conscientiously attended the whole session. Then, things become less blurry: the 1997 GA in Geneva with Fischli as president, then Berlin in 1999 with Jortner as president (an impressive voice indeed). However, I have clear memories of the Council and its votes only as far back as Ottawa in 2003, with the huge electricity blackout. With a meeting every two years, time passes rapidly, but it took a rather long time for me to become really aware of the way IUPAC works. It is not normal, and I suppose that after each Council, several NAO representatives have the same impression of having attended something complex and not well understood. This is one of the things that has to be changed in IUPAC.

I feel lucky to have worked with an incredible variety of IUPAC colleagues—different nationalities, disciplines, professions. And, of course, many of these colleagues are now friends.

At the end of IYC, when I was fortunate to be president of the Union, I felt frustrated, because I had no time to think of IUPAC, to try to find solutions for some problems I saw, small or more important, real or imaginary. But now, I understand that it has been for me a unique opportunity to meet numerous people in our NAOs. When I was invited to attend a scientific meeting, generally the “nth” congress of the National Chemical Society, I was very eager to prepare a presentation explaining, as well as I could, what our Union is, the way it works, and what we can offer to our members, but also what we can expect from our members. I began all of these presentations, each one an improvement I hoped over the preceding one, with some history of the Union, proud to say that we are older (1919) than the International Council for Science (1931)!

I cannot thank enough all the people I met on these trips; they did much more than simply pay my expenses. I received real kindness and friendship, curiosity, kind words, and compliments about IUPAC, but also advice, complaints, and criticisms. My hosts were pleased to show me a translation of a nomenclature book, a stamp made for IYC, the work of the country to celebrate the year. From these contacts I received many good ideas, but it was a little

too late to put many of them into practice since 2011 was also the last year of my presidency.

So, what to do, which ideas emerged?


- The first point is a regret rather than one idea: Why were we unable to inform everyone who celebrated the International Year of Chemistry, that it was thanks to IUPAC, and not only to UNESCO, that we had such a celebration? In some countries with extensive IYC celebrations, there was hardly a mention of IUPAC.
- In the congresses or national meetings of chemical societies around the world, even in countries that are part of IUPAC, very few people know about IUPAC. There are few opportunities to explain what IUPAC is: at the biennial IUPAC Congress and Council and at regular IUPAC-sponsored conferences. Why, as was the case not so many years ago, could we not have a poster with a description of IUPAC? Of course, in principle,

- at each IUPAC-sponsored conference, someone should make a short talk about the Union, but this is not always done. And if this talk is made at the wrong moment, if the allocated time is only a few minutes, it is done for nothing. A poster has many more chances to be seen, and with the multiple tools we have now, it is easy to have more than one and put them in strategic places. We should be using the meetings of the regional federations to meet people and explain IUPAC. At the very beginning of the Council, the president or another officer (why not the past president, who is very idle at his/her last Council) could begin his or her talk with a presentation about the Union: every two years, we have new delegates from the NAOs and also new members in our divisions and committees; it is likely that some of them are not very aware of the way IUPAC works, and have a poor understanding of its rules and bylaws.
- People complain that they cannot find in our website the useful documents describing IUPAC, such as “hints2.2,” and how the cost and advantages to becoming a member. There should be on the homepage of the website a navigation that takes users to a membership page. And, on that page, why not provide a presentation that could be useful not only to our active members, but also to our friends on each continent, who are ready to help us to recruit new NAOs or members? This presentation should clearly explain the benefits to being a member country, but it should also describe where and how their dues are allocated. In addition, our rules and bylaws should be easier to find.
 - We could and should produce short brochures about IUPAC that can then be translated into the languages of different countries. These brochures, with short and well-thought text, could be posted on our website for translation by our member countries.
 - The way we spend our money and the way in which members of our divisions and committees are chosen should be more transparent. This is a matter that was frequently brought to my attention as president of IUPAC. This is a very delicate point, and to bring up the subject within IUPAC is not a good way to make friends! The problem is not the quality of the new division members, whom are generally excellent. However, excellent

scientists from some of our NAOs are frequently overlooked because they are not known by the people electing the new members.

- There is also the problem of national representatives in the divisions. Generally, they never attend meetings, because the division pays only for titular members. Ideally, NAOs, which often complain that they are not listened to enough, would help pay for their national representatives to attend some division meetings. However, not all countries can pay for this. A way to remedy this problem would be for divisions to involve national representatives in their projects.
- IUPAC needs to attract young and new members. The Union needs to expand its affiliate program and enlarge its network. The value and benefits of such an affiliation need to be reassessed to ensure that IUPAC can sustain its activities and at the same time continue to function under an open access model.

There are also things that IUPAC should be aware of, such as the fact that ICSU holds its general assembly only every three years. The president is generally the one who attends, but as the president's mandate is only two years, sometimes a president never has the opportunity to attend. We could, as is the case for some other Unions, have a representative to ICSU. Such an approach could be extended to other strategic partners.

Finally, people within IUPAC should become more knowledgeable about the Union. To be a member of IUPAC is not only to be conscientious in one's job as a member of a division or a committee, it is also to understand what makes this Union so useful to the global community, so important for the discipline. In order for IUPAC to fulfill its role, it needs members who are convinced and conversant about its importance. 

Nicole J. Moreau <nj.moreau@free.fr> was IUPAC vice president in 2008–2009, president in 2010–2011, and past president for 2012–2013. She has been a member of the Bureau since 2000 and a member of the Executive Committee since 2006. She is also general secretary of the French National Committee for Chemistry. Since January 2012, she is a member of the Executive Board of ICSU, the International Council for Science.

A Look Back at Ernest Solvay

On the 150th Anniversary of the Solvay Company

On 20 September 1913, Ernest Solvay gathered family and relatives, colleagues and employees, as well as scientists and academics, in his Brussels headquarters to celebrate a double jubilee. Officially, it was to commemorate the 50th anniversary of the founding of “Société Solvay & Cie,” but the celebration had a private tone as well, since in 1863 he had also married Adèle Winderickx. In Ernest’s eyes, however, this was more of a huge family gathering, including both “ma famille naturelle” and “ma grande famille industrielle” as he described them in his address launching the ceremony. Indeed, from the very beginning, Ernest and his brother Alfred Solvay insisted on running the business as a family firm. Even when the Société Solvay became an international operation, the company maintained close relationships with the plants dispersed all over the world. Either the firm or the family—which had become immensely rich and was active in philanthropy—invested heavily in local education and social welfare.

The presence at the double jubilee of eminent scientists and representatives of renowned learned societies from many different countries, can only be explained by an important aspect of Ernest Solvay: his deep attraction to science. Having already secured wealth for his family, he had started to use his fortune to revolutionize science. He did this through his own scientific work, outside the frame of academic institutions, and by providing extensive support to the work and enterprises of others, much better rooted and reputed in the scientific community. It is in this specific context, that the founding of the International Institute for Chemistry should be viewed as one of Ernest Solvay’s greatest achievements.



Archetype of the Inventor-Entrepreneur

by Nicolas Coupain

As one of the most prominent Belgian inventor-entrepreneurs and individual sponsors of science, Ernest Solvay’s legacy is immense. Recent research in the archives of both the Solvay company and the Solvay family has renewed the state of knowledge on Ernest Solvay’s endeavors, achievements, and networks.

Ernest Solvay was the son of a quarry master in a rural



Ernest and Alfred Solvay
Solvay Heritage Collection

area 30 km south of Brussels. His family was part of the local bourgeoisie. At the Christian boarding school where he and his younger brother Alfred were enrolled, he showed great interest in physics and chemistry, to which he had been initiated by his professor, brother Macardus. His father expected him to become an engineer, but this ambition was shattered by a pleurisy that forced him to bed at the age of 17. Ernest Solvay thus continued to learn by self-teaching and started his professional career earlier than expected, first as accountant in the family shop,

then as “apprentice-manager” in his uncle’s gas plant at Saint-Josse (Brussels). There, he spent part of his time supervising workers, and another part experimenting on the concentration of ammonia liquors that

were lost in the production of gas. During his free time, he attended public lectures given by the chemist Henri Bergé and frequented the Musée de l'industrie with assiduousness. Then came his "eureka moment": by mixing salt with ammonia and carbonic acid gas in his experimentation room, he obtained sodium carbonate. What he apparently didn't know when he filed a first patent in 1861 was that this reaction had already been theoretically described by several chemists, and that a few entrepreneurs had tried to set up the process at an industrial scale without success in France, Germany, England, and even Belgium. This ignorance turned out to be a blessing: it is thanks to it that Ernest Solvay, age 23, undertook the many steps that lead to the creation of Solvay & Cie in 1863. He formed a small team including his brother Alfred, and their childhood mate Louis-Philippe Acheroy, launched a pilot plant in Schaerbeek (Brussels), obtained funds from his father, analyzed the economics of the soda ash market, and requested the necessary authorizations. When the first technical and financial obstacles arose (i.e., the discovery of anterior patents) Ernest Solvay demonstrated his ability to surround himself with talented people who pushed him a step forward. In Guillaume Nélis, Eudore Pirmez, and Valentin Lambert, he found three business angels who not only brought him extra seed money, but also their network, political influence, and expertise in law, commerce, and industry. It is this enlarged—although still limited—team that "converted the try" into a lasting success.

Technical stabilization of the ammonia-soda process was also reached by taking advice from renowned scientists, which Ernest Solvay employed as industrial consultants before it became a widespread practice. Next to Henri Bergé, Professor Louis Melsens became a regular correspondent, while the eminent chemist Jean Stas was consulted several times. August Kékulé, founder of the first university research laboratory in Belgium, exchanged several letters with Ernest Solvay, in which he indicated his intrigue with this mysterious Solvay who seemed to succeed in imposing his ammonia-soda process. At this stage, these random relationships had more to do with personal connections than with a systematic collaborative enterprise. Nonetheless, they were part of a gradual convergence, under the influence of the German model, between the science of universities and industries.

More than a mere inventor, Ernest Solvay soon proved to be a skillful entrepreneur eager to develop a business out of his soda process. In a visionary document written in 1865 when the company was still close

to bankruptcy, Ernest Solvay claimed his ambition to exploit his process in surrounding industrial powers instead of leaving to others the chance to copy it.

One of the Earliest Multinational Companies

A striking feature of the Solvay group's history is the rapidity and extent of its international expansion. Less



The Solvay Soda Process

The Solvay process consists of treating salt brine with ammonia and then carbon dioxide, producing sodium bicarbonate and ammonium chloride. The ammonium chloride is usually combined with lime to produce ammonia (recycled) and calcium chloride.

The Solvay process was one of the first examples of a gas-liquid reaction successfully scaled up. Its success resided in a tall gas absorption tower in which carbon dioxide bubbled up through a descending flow of brine, together with efficient recovery and recycling of the ammonia. In comparison with the older Leblanc process—invented by the Frenchman Nicolas Leblanc, but mainly used by British companies—the Solvay process was more efficient and less polluting. It also yielded a purer soda ash. However, originally, it only enabled the production of sodium carbonate, whereas the Leblanc process provided a full set of substances, among them sodium sulphate, chlorine, hydrochloric acid, bicarbonate of soda, and soda crystals. Another difference is that the Solvay process was a continuous one, whereas the Leblanc worked in batch. This meant that Solvay had to have a better command of all the technical details of the production process since it could not be stopped.

A Look Back at Ernest Solvay

than a quarter of a century after its creation, it was industrially active in all major developed countries. This expansion took place in two phases. Before 1880, the poorly financed Belgian-based company hesitatingly tested different formulas: the construction of a wholly-own plant in France (Dombasle); the grant of a license in Great-Britain (to Brunner, Mond & Co); and the buying of an existing plant in Germany (Wyhlen). These methods proved expensive, uncertain, or time-consuming. In a second step, the already well-established Solvay & Cie opted for joint-venture agreements with local entrepreneurs in the United States (Syracuse), Russia (Berezniki), and Austria-Hungary (Ebensee), and then turned to that solution in Germany and Great-Britain as well. Spain, Italy, and other countries were taken up soon after. The whole formed a cohesive group built on strong interpersonal links between managers, engineers, employees, and, to a certain extent, even workers. At its center, the Brussels headquarters defined both the technical and commercial strategies. Conversely, responsibility on operations was largely left in the hands of local managers.



Today, Solvay produces Rare Earths, mixed oxides and aluminas.

The extensive international presence of Solvay proved to be a strong asset at different levels, the first being technology. The efficient circulation of technical information was performed in a very structured, although secretive, way. All improvements made in any plant of the group were made available to others. Engineers were encouraged to travel to foreign plants and to meet their counterparts. Most of all, an advanced system of benchmarking was put in place as of 1875 between the Central Technical Department and the production sites in order to analyze and compare in great detail the pro-

The History of Solvay Revealed in Two Books

From Ernest Solvay's grand discovery in 1863 to the Group that we know today, all major developments have been captured among the pages of two books published this year. These works are the labor of three historians—Kenneth Bertrams, Nicolas Coupain, and Ernst Homburg—to whom Solvay opened its archives for the very first time. The more exhaustive of the two books is edited in English by Cambridge University Press (ISBN: 9781107024809), and counts 630 pages, relating in full detail the evolution of the company. The second is an abridged and less scientifically technical version which was published in English (ISBN 9781107607576), French, and Dutch. It includes a fascinating 52-minute documentary (subtitled in 14 languages) depicting a story of entrepreneurship, survival, and the interweaving of industry with history's most powerful moments.

ductivity and profitability of each plant. This instilled a healthy rivalry among sites. International collaboration also permitted Solvay to select and improve a winning electrolysis technology at the end of the 1890s, which opened the way to the production of chlorine and an alternative way of producing caustic soda from salt.

At the commercial level, each subsidiary could be supported in its fight with local competitors by its sister companies, which could squeeze them by flooding the market and making prices fall. This advantageous position enabled the Solvay group to exert lasting control on the various national alkali markets from the mid-1880s on. The strategy could be thought of as the "iron hand in a velvet glove" approach: instead of forcing the producers using the old-fashioned Leblanc process to shut down without delay, Solvay allowed them to keep their production level for a while, reserving to itself future increases in the market. In this way, Solvay discouraged its competitors from upgrading their technology. Beginning in 1891, after having won commercial battles in all its territories, the Solvay companies governed an unofficial international alkali cartel. In 1913, Solvay & Cie and its associated companies formed the largest chemical group worldwide, with 32 plants pro-



Archetype of the Inventor-Entrepreneur

ducing 2 millions tons of alkalis and employing 25 000 collaborators.

A Long-Lasting Family Business

Solvay & Cie was incorporated as a limited partnership (“société en commandite”), a status offering several advantages, including that of maintaining the firm’s independence, as shares could be transferred only with the consent of the partners, thereby ensuring the closed nature of the company. Nor was there any obligation to publish earnings figures. “To live happy, live hidden” could have been another motto of Solvay’s owners. At the creation in 1863, a vast majority of shares was held by the silent partners. Eudore Pirmez’ family owned 40 percent; Guillaume Nélis, 18 percent; Valentin Lambert, 9 percent; and Gustave Sabatier, 7 percent. The Solvay brothers only held 25 percent. As years went by, this repartition evolved in favor of the Solvay brothers (and their family), who got the opportunity to have their annual variable bonuses converted into shares. From 1882 on, the Solvay family owned more than 60 percent of the shares.

In this protected system, descendants of the founding brothers succeeded one another at the Solvay helm. To ensure that successors were appropriately skilled, sons were pushed towards civil engineering, and it was customary for the expected successors to undertake a full traineeship. When blood ties reached their limits, in-laws were brought in. Two notable exceptions confirmed the rule: Prosper Hanrez and Edouard Hannon, the first two “Masters of the Solvay technique” (technical managers) were the only two non-family “gérants” until the transformation of Solvay into a joint-stock company (“société anonyme”) in 1967. They had been appointed by Ernest Solvay himself. Today, the executive committee is fully composed of salaried managers. The “founding families,” a vast group of about 2500 people still own a substantial part of the shares and mainly exert their influence at the Board of Directors.

Nicolas Coupain <nicolas.coupain@solvay.com> is a historian and scientific advisor at Solvay S.A. He is the co-author of *Solvay—History of a Multinational Family Firm* (Cambridge University Press, 2013).



A Dynamic Website: www.solvay150.com

Imagined as a time machine, this dedicated website allows visitors to discover the major periods in the evolution of the Group. Short films, anecdotes, monthly articles, and captivating iconography that evolve through the passing of each era: in an effort to enchant each visitor, nothing has been left to chance. In addition, the site serves as a common place for event organizers to announce, illustrate, and convey through social media the range of events taking place throughout the Group’s sites around the world.

A New Science Prize

The premiere edition of the Chemistry for the Future Solvay Prize, taking place at the end of the year in Brussels, will honor breakthrough scientific discoveries that will help build the chemistry of tomorrow. Awarded every two years, it will be accompanied by a grant of EUR 300 000. A delegation of the Group’s researchers will be invited to the ceremony.

On 26 September 2013, Solvay announced that the first “Chemistry for the Future Solvay Prize,” will be awarded to Professor Peter G. Schultz, professor at the Scripps Research Institute in California, and Director of the California Institute for Biomedical Research, for his work at the interface of chemistry and the life sciences.

 www.solvay.com/en/media/press_releases/20130926-solvay-prize.html

The Solvay Chemistry Council, and the International Institute of Chemistry

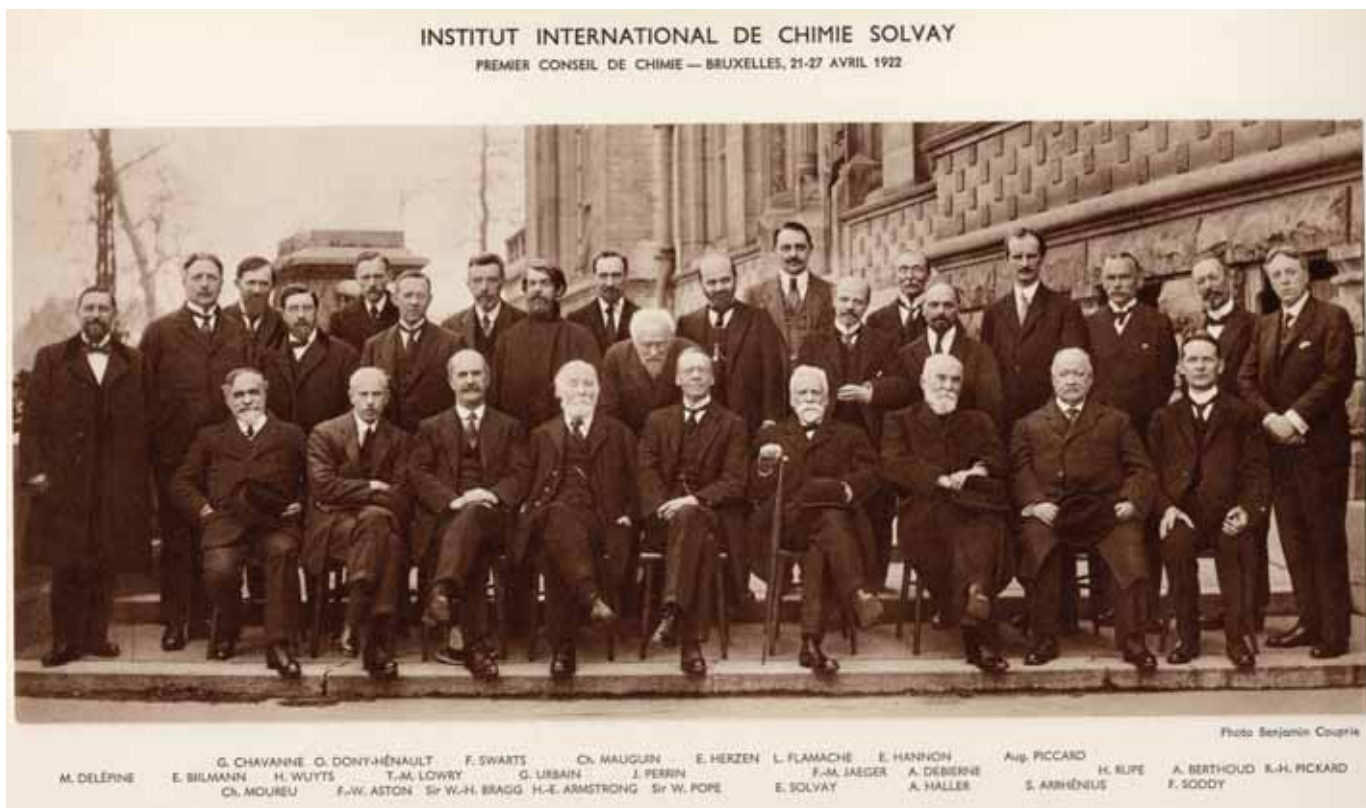
by Brigitte van Tiggelen

Until his death in 1922, Ernest Solvay remained a tutelary figure at the head of the company; even more so following the premature death of his brother Alfred in 1894. However, starting in the 1880s, he had left day-to-day management and turned increasingly to another of his consuming passions: scientific progress.

Ernest Solvay was passionate about Science and Progress. Actually, he believed that well-governed Science would and could only serve Progress, the ultimate goal of which was to elucidate all the laws of nature, including the laws governing living organ-

isms and human societies, and then use all these laws to govern the whole of society for the good of all. Very much in the positivist frame of thought, these laws once discovered were to be as mechanical and absolute as the laws of physics and chemistry. With this perspective in mind, Solvay started a huge program as soon as his industrial enterprise didn't need his constant and close care, a program whose specific outcomes, be it in his own work and publication, or in his scientific support and foundation, would otherwise seem scattered, not to say eclectic.

Following this vision à la Comte of a universe governed by rational laws, his main fields of interest and activities became physical chemistry (or a mix of physics and chemistry, with a strong emphasis on thermodynamics), physiology (or experimental medicine based on advanced biology and the use of physical chemical notions and instruments), and sociology (as the positive study of human societies and their evolution). The latter is very telling about the general approach of Ernest Solvay to philanthropy, since he believed that through a better understanding of "social laws," one could avoid the painful episodes



Ernest Solvay surrounded himself with renowned chemists, several of whom paved the way for IUPAC, namely Charles Moureu (France), first IUPAC president (1920-22); George Chavanne (Belgium), vice president; Sir William Pope (UK), second IUPAC president (1923-25); and Einaar Biilmann (Denmark), fourth IUPAC President (1928-1934).

The Solvay Chemistry Councils

of “chaotic” revolutionary unrest and assure the well being of every human being. In his opinion, this was, after all, the real goal of evolution for humanity. What is more striking is that his unwavering optimistic nature not only maintained him in his own scientific conceptions until the end of his life, despite numerous criticisms by some intellectuals and the cautious or polite silence of others, but that it also led him to believe that the goal was near, and that he, as a philanthropist, could provide guidelines to scientists to focus on his program, both in form and content.

Solvay’s personal philosophy was well articulated in his own mind, and he clearly envisioned a sort of metaphysical succession, tackling systems from the most simple to the most complex: solving the mystery of matter first, then revealing the functioning of living bodies, and ending by unveiling the hidden mechanisms of the behavior of human societies. Despite this well-articulated program, he devoted himself to all steps at once, with no particular schedule, as the inspiration and the personal encounters would emerge.

His scientific philanthropy followed the same logic. Solvay made a lot of donations in a rather opportunistic manner (both for him and the receivers), to organizations as diverse as the University of Nancy (founding of an electrochemical and physicochemical institute), the University of Paris, the University of Genève, and the Belgian Chemical Society. But his philanthropy and close relationship to the Université Libre de Bruxelles was of another nature, and closer to his progressive program. After having granted subsidies to specific research, he successively established in 1893 an Institute for Physiology under the guidance of Paul Héger, in 1894 an Institute of Social Sciences, and in 1903 a Business School. At this point, chemistry and physics, seemed to have been left behind.

An International Organization for Chemistry

Up until then, Solvay hadn’t yet created or subsidized a foundation that would be international in scope and essence, although he had contributed generously to institutions outside of Belgium. At that time, there were only a few international organizations, for instance, the International Association of Academies founded in 1899, a sort of federation of all scientific academies that held its first meeting in Paris in 1899. In 1907, Solvay supported Paul Otlet’s creation of the Office Central des Associations Internationales, and on the occasion of the Universal Exhibition of 1910 held in Brussels, he was asked to play a prominent role,

and agreed to the founding of an International Union that would link all international associations. However, there was nothing yet specifically for chemistry, or physics.

Through his own personal fascination for the concept of energy, Ernest Solvay had contacted Wilhelm Ostwald, who shared his views on sociology and internationalism. A Nobel Prize winner and the founder of chemical physics, Ostwald had reached the end of his scientific and academic career, but was obsessed with the rational organization of chemistry on an international level. For a time, he believed he had met the Maecenas who would sponsor his project, which he called the “Office International de Chimie.” His plan, however, turned out to need the support of other chemical societies, and this is how the first international organization for chemistry, the International Association of Chemical Societies (IACS) was born. To some extent, this organization can be considered IUPAC’s ancestor. Since, at that time, French was also an international language, and Europe was at the forefront of science, the new organization was actually known as the Association Internationale des Sociétés Chimiques (AICS). Although Russian, Japanese, and American societies were represented, meetings only took place in European countries (see also “The Formation of the International Association of Chemical Societies,” B. Van Tiggelen and D Fauque, *Chemistry International*, Jan-Feb 2012, www.iupac.org/publications/ci/2012/3401/2_vantiggelen.html).

The enthusiasm of the delegates who met successively in Paris and Berlin, however, failed to secure the funding necessary for the new organization, which was aimed at standardizing scientific results and their communication within the chemical community. Thanks to the good relationship between Albin Haller and Solvay, the later decided to fund the enterprise, starting with an initial donation of 250 000 francs and then 55 000 francs every year for 29 years, provided that the Association held all of its meetings in Brussels. This is why the third congress, originally planned for

Honoring Innovation

At the “Innovation @ Solvay” event held 16–18 October 2013, around 500 Solvay employees from around the world shared their knowledge, skills, and projects, and competed for an internal Innovation Award. And, as it took place in Brussels, these innovators were able to join in the program of activities for the 150th anniversary planned during the same timeframe.

A Look Back at Ernest Solvay

A Rich Program of Events Around the Globe

From 6-18 October 2013, Solvay's Brussels Campus sprang to life with a wealth of anniversary activities centered on a spectacular live artistic performance illustrating Solvay's history and future. Key stakeholders, shareholders, and personnel were invited to these performances. Their Royal Highnesses King Philippe and Queen Mathilde of Belgium (below) also attended a special VIP evening.



Since the acquisition of Rhodia by Solvay in 2011, the new Group is the largest chemical group in France. As such, another special event was organized in early November in Lyon, which is the cradle of Rhodia (formerly part of the Rhône-Poulenc Group). Around 10 000 visitors discovered the "Solvay Techno Lab," where they could learn about Solvay's chemistry while having fun.

Each Group site worldwide was also encouraged to organize local events, in order to involve a maximum number of collaborators.

London in September 1913, was eventually held in Brussels at the special request of Ernest Solvay, where it coincided with other anniversaries he intended to celebrate with splendor: 50 years since the foundation of his company (Solvay et Cie) and a golden milestone in his own marriage.

The Solvay Chemistry Councils and the International Institute for Chemistry

Though this meeting bore the same title as the famous Physics Council that had taken place in 1911, the scope and the organization of the Chemistry Council were


almost the opposite. For the first Solvay council in physics, Solvay had insisted first on having a set of scientific questions on a specific and totally new topic, "Questions d'actualité de théorie cinétique" (kinetic theory of matter) and second, on selecting the speakers according to their potential expertise on these topics, rather than on their academic record or national provenance. For sure, Solvay himself made sure that there wasn't an overrepresentation of German scholars, and that a certain balance was kept between scientists from Germany, France, and Great Britain, but the criteria of selection was based on the relevance of their research rather than on their national identity. And the story is well known about how Albert Einstein, Paul Langevin, Jean Perrin, Marie Curie, Ernest Rutherford, Hendrik-Antoon Lorentz, Henri Poincaré, Max Planck, and many other reputed physicists participated in what Einstein described as a "Witches Sabbath." On the contrary, for the 1913 chemistry meeting, each national chemical society was invited to delegate up to three representatives and the topics were not of a scientific nature, but concerned rather the management of the international circulation of chemical knowledge.

Highly satisfied with the first Physics Council, and willing to ensure the permanence of these councils, Solvay established in 1912 the "Institut International de Physique Solvay" (International Institute for Physics founded by Solvay), whose aim was not only to organize the next councils but also to provide fellowships for young Belgian scholars, and distribute funding to investigators around the world on research topics that were close to Solvay's scientific obsessions. This foundation is still vigorous and organized last year a series of scientific and public events to commemorate the hundredth anniversary of its creation. Not surprisingly, Solvay wished to establish a similar foundation for chemistry, "Institut International de Chimie Solvay" (International Institute for Chemistry founded by Solvay), but in this case, it was founded prior to the first Chemistry Council and very much along the same line as its physics counterpart, completely oblivious to the striking divergence of the chemistry meetings from the physics meetings.

The subsequent history of the chemistry councils shows, however, the limitations of a model that had been so successful for a particular part of physics that was laying the foundations of quantum and relativity theories, that very part that revolutionized physics and beyond at the beginning of the twentieth century. Indeed, the chemical community had already many more opportunities to meet and discuss, in varied

The Solvay Chemistry Councils

places and according to diverse themes, and the state of the field was such that it was very difficult to identify a set of hot topics that such a meeting would actually be able to solve. Also to be noted is the heavy influence of physical chemistry: many members of the program committee in charge of selecting topics and speakers were actually scientists close to the Physics Institute, and to a certain extent expanded the questions deliberated there into the Chemistry Institute. As a result, the Chemistry Councils of 1922 and 1925 debated themes such as isotopes, valency, electronic theory of matter, and X-ray diffraction to “see” into solid matter. These new phenomenon or concepts pretty much polarized discussion between “true” chemists (organic chemists who felt untouched by these new developments) and those who were adamant to promote cross-fertilization between phys-

ics and chemistry. Recurring for instance, was the discussion around the concept of element and that of valence, as a sort of collateral output of these gatherings. Only after 1930 did the chemistry councils actually focus on one specific theme, be it the constitution and configuration of organic molecules, the chemical and biological reactions of oxygen. And eventually, the 1937 council, dedicated to vitamins and hormones, had the same percentage of current or future Nobel prize winners, as its physics counterpart. 

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Stamps International

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

We've Come a Long Way from Soda Ash, Baby!

Soda ash (sodium carbonate, Na_2CO_3) is one of the most important and ubiquitous commodity chemicals in the world. A whopping 53 million tonnes of the compound were produced worldwide in 2012, a figure that is equivalent to more than seven kilograms per person! About half of it is used for making the common (or “soda-lime”) glass found in windowpanes and containers, and the rest goes towards the manufacture of soaps and detergents, water softening agents, as an alternative base to the more corrosive sodium hydroxide (caustic soda), and a myriad of other applications.

There is ample archeological evidence suggesting that soda ash mined from dry lake beds or extracted from the ashes of burnt seaweeds was already used for making glass ornaments and vessels in Ancient Egypt and the Roman Empire. The advent of the Industrial Revolution led to a significant increase in demand for soda ash and the development of synthetic procedures for its preparation became necessary. The most successful was the process developed from 1861 by Ernest Solvay (1838-1922), a Belgian industrial chemist and founder (in 1863) of the company that still bears his surname today. Even though increasing amounts of soda ash are currently obtained from natural deposits of trona, nearly three-quarters

of the world's output are still generated by the original Solvay process, a tribute to the legendary ingenuity and entrepreneurship of its namesake. Furthermore, Solvay S.A. has grown to become a global company with net sales of 12.4 billion euros in 2012 and a diversified product portfolio that includes functional polymers, rare earth materials, silica, caustic soda, flavors and fragrances, hydrogen peroxide, chlorinated and fluorinated derivatives, and many other specialty and bulk chemicals.

The stamp illustrated in this note portrays Ernest Solvay and was issued in 1955 as part of a set honoring distinguished Belgian scientists and inventors, a cohort that also included Leo Baekeland (1863-1944), a pioneer of the plastics industry, and Jean-Jacques Dony (1759-1819), who developed a process for the industrial production of pure zinc.

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



InChI—the IUPAC International Chemical Identifier

Current Status and Future Development in Relation to IUPAC Activities

by *Andrey Yerin, Alan McNaught, and Stephen Heller*

The IUPAC International Chemical Identifier (InChI) is a non-proprietary, machine-readable chemical structure representation format enabling electronic searching, and interlinking and combining, of chemical information from different sources. It was developed from 2001 onwards at the U.S. National Institute of Standards and Technology under the auspices of IUPAC's Chemical Identifier project. Since 2009, the InChI Trust, a consortium of (mostly) publishers and software developers, has taken over responsibility for funding and oversight of InChI maintenance and development. Funding and responsibility for scientific aspects of InChI development remain with the IUPAC Division VIII (Chemical Nomenclature and Structure Representation) and InChI Subcommittee.

The many potential uses of InChI may not be immediately apparent to many chemists, since it was developed to be handled by computer tools, not by human beings. Its role as a unique chemical identifier is analogous to the role of a barcode in general commerce—while not intended for reading or generation by humans, the identifier provides a unified electronic encoding for chemicals, which can be built upon by various computer services to collect, search, and exchange chemical information. Its chemical “intelligence,” single source, and vendor neutrality mean that InChI functions as a chemical barcode, giving to every chemist instant and reliable access to the electronic world of chemistry. However, the InChI is not supposed to be a replacement for established means of identification, like names or registration numbers, but a very powerful addition to the chemist's arsenal of tools for dealing with chemical informatics.

The Most Significant IUPAC Initiative for e-Chemistry

Current chemistry is now practically “paper free” and critically dependent on computer tools, from the planning of an experiment to the publication of the results, not to mention chemical calculations and modeling, which have significant practical importance but are performed exclusively in the virtual space of computer memory. However IUPAC's activities in the area of e-chemistry have been extremely limited hitherto. In fact, there is little else apart from the JCAMP-DX vendor-independent file format from the Committee on Printed and Electronic Publications (CPEP) Subcommittee on Spectroscopic Data Standards, developed to exchange spectroscopy and chromatography data, and some recommendations on spectroscopic data standards. InChI is probably the most important and relevant IUPAC activity in relation to e-chemistry needs; its facilities are readily available via the desktops of virtually every chemist dealing with chemical structures. Hardly any other IUPAC activity is available for electronic use by the whole of the chemistry community.

A Chemical Informatics Tool

Searching of existing publications and data is now impractical without the use of electronic databases. An efficient way of finding specific chemical information is vital both for science and industry. However, although ways to search publications by bibliographic and other textual data are straightforward and well implemented, searching data by chemical structure is so far not standardized and still significantly vendor dependent.

InChI and especially its fixed-length-hash-representation InChIKey provide unique tools for indexing and searching structure-related information suitable both for huge chemical databases and for specific scientific papers in electronic form. However, their introduction into the chemical literature is slow, perhaps inevitably. Both InChI and InChIKey can be used now to search over the internet but they still give fewer hits than searches by chemical name. Nevertheless, the take-up of InChI continues to grow and chemists are becoming increasingly aware of its advantages in facilitating dissemination, collection, indexing, and retrieval of chemical information. In this way, InChI serves the



The InChI Trust launched a four-part video series to explain the International Chemical Identifier (InChI): www.youtube.com/watch?v=rAnJ5toz26c.

whole chemical community and the InChI Project thus fits perfectly the aims of IUPAC.

InChI and Structure Representation

The InChI text string is an algorithmically generated, unique encoding of a chemical structure. InChI encoding includes built-in algorithms for recognition of possible mistakes in chemical structures—atom valence states, connectivity, and definition of stereoconfiguration. For example, omitted indication of stereoconfiguration for tetrahedral stereocenters and double bonds is explicitly designated in an InChI string and this allows such mistakes to be detected.

Correct operation of the InChI software is dependent on correct electronic input of the structure concerned. While common organic compounds have well-agreed representation conventions, there is still a lack of standards for representing many other classes of chemicals, especially in electronic form. There are many available chemical drawing tools, ranging from desktop programs to web-based applets, but the tools and conventions are still vendor-dependent especially for classes of chemicals with poorly defined representation standards.

Further development and wider adoption of InChI as a vendor-neutral structure identifier will force chemical drawing software producers to conform to InChI procedures and unify their representation conventions and encoding of chemical structures. Thus, InChI needs and allows involvement of chemical software vendors in development of unified structure representation standards via the combined resources of Division VIII and the InChI Trust. In this sense, the InChI project can be treated as an interface between IUPAC and chemical software vendors for development of unified conventions for electronic representation of chemical structures.

In Relation to Chemical Nomenclature

Traditional chemical nomenclature is aimed at development of conventions for naming chemical substances in a human-friendly common language. Current chemistry often deals with molecules that are very complex,

and conventional nomenclature developments lead to long, scarcely pronounceable names derived from large sets of rules. This complexity prevents most chemists from assigning chemical names manually and software tools are now very useful for chemical name generation. Thus, even the development of classical nomenclature needs to take into account electronic representation and computer naming tools.

A consequence of this complexity is that such systematic names are no more human-friendly than the corresponding InChI text strings generated from the chemical structure. From this point of view, InChI may be considered as a special kind of nomenclature allowing explicit definition of a chemical compound. A very important aspect is that traditional chemical nomenclature is largely structure dependent and inherits most of the limitations of structure discrepancies mentioned above. InChI still has some areas, for example complex tautomers, that need further development, but being significantly substance aimed, InChI by design does not have such limitations. The involvement of Division VIII is highly desirable for development of principles to deal with multiple structure representations. At the same time, InChI concepts can be useful for development of nomenclature for chemical structures represented in delocalized form.

InChI text strings can hardly be treated as a replacement for conventional chemical names but they are far more suitable for identification of chemicals in various electronic media. Any chemist with any level of nomenclature knowledge and any chemical software available will be able to generate the same unique InChI text string for the same chemical structure. InChI can be treated as an additional type of nomenclature and needs no less attention from IUPAC than traditional nomenclature.

Current State and Further Development

The InChI project is now quite mature and provides a well-developed set of tools adopted by many open access and commercial chemical media (www.iupac.org/inchi). Most prominent examples include the Royal Society of Chemistry (ChemSpider), Chemical Abstracts Service (SciFinder), and the U.S. National

Institutes of Health (PubChem). Existing services allow retrieval of data for chemical compounds including many experimental and predicted properties, environmental and biomedical data, spectra, and links to patents, articles, and other databases. Facilities for InChI generation are already present in practically all chemical drawing programs allowing chemists to use various InChI-based tools.

Although well developed and tested for organic structures, InChI still needs further development to other areas of chemistry. Each new area needs first of all the development of a unified electronic representation with essential involvement of IUPAC resources to ensure the choice of chemically intelligent and widely acceptable conventions.

Current InChI projects are aimed at extension of InChI tools to treat more complex cases of tautomerism, and development of conventions for representation and treatment of inorganic, organometallic, coordination, and polymer structures. The project on encoding of chemical reactions is an example of InChI extension to more complex chemical objects.

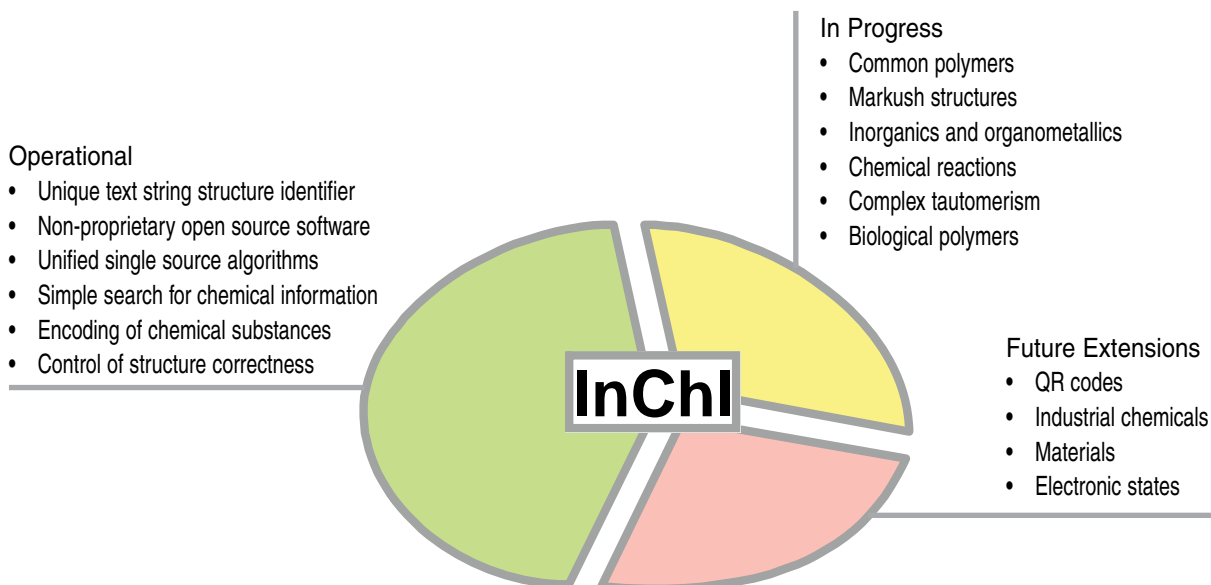
Another important and challenging area is the handling of biochemical structures and especially biological macromolecules such as peptides and proteins. This task will need significant work to develop new procedures and standards of electronic representation for biomacromolecules and will require the involvement not only of IUPAC and InChI Trust resources but also joint work with the International Union of Biochemistry and Molecular Biology (IUBMB) and with chemical software vendors.

Support by Industry and Public Organizations

Being structure-based, InChI encoding is at the same time a more powerful identifier than the structure itself. The existence of several ways of graphically representing the same chemical substance often prevents recognition of the equivalence of different tautomers, mesomers, and alternative protonation variants, creating difficulties for chemical data search and indexing. Built-in recognition of multiple structure representations of the same substance allows InChI to serve as a substance identifier rather than a structure identifier and makes InChI more useful for identification of chemicals than a single chemical structure. However, industrial chemistry still awaits better support from InChI since industrial chemicals are often impure substances or mixtures that lack agreed representation and encoding conventions.

Currently, most official registration systems include support of chemical structures in addition to textual data such as registration numbers and chemical names. Being free from the shortcomings of chemical structure representations and aimed at substances, InChI is ideally suited for application in substance registration and regulations. Several government organizations already use InChI tools internally and some plan to make InChI and InChIKey an integral part of their registration systems.

An important industrial application concerns patents that deal with the special structure representation commonly referred to as a Markush structure. The general principles for InChI support of Markush struc-



tures are already developed within the corresponding IUPAC project and await funding for implementation. It should be noted that there are currently no IUPAC recommendations on Markush representation. The support of Markush representation by InChI tools will significantly improve the applicability of InChI in patents.

While the development of InChI tools now involves only Division VIII resources, the acceptance of InChI by industry and government authorities needs involvement of other IUPAC bodies, primarily the IUPAC Committee on Chemistry and Industry (COCI) and the Committee on Printed and Electronic Publications (CPEP).

Extended IUPAC Involvement

The development of InChI projects is currently covered by the InChI Trust (see www.inchi-trust.org) and IUPAC Division VIII funds assigned to projects having general chemical importance. The degree of InChI acceptance critically depends on rapid extension of coverage to all classes of chemicals and integration of InChI tools into a wide variety of commercial and open-access, chemistry-oriented services. Wide acceptance of InChI depends upon better involvement of IUPAC resources, including support by other IUPAC bodies and international organizations.

Proposed Actions

It is clear that InChI and InChIKey have already become an important part of chemical space and serve well the needs of the chemical community. Any doubts about their usefulness were resolved long ago. However, the current implementation needs extension to other classes of chemicals and more active promotion of InChI to assure its position as the universal identifier for all chemicals dealt with by all types of scientific and industrial enterprise.

To be in accord with the current highly computerized nature of activities in chemistry, any IUPAC actions and special projects must be initiated to assure correct and uniform coverage of all areas of chemistry in electronic and printed media. However, the current subject-based divisional structure is not conducive to the development of such projects, and there is no budget assigned specifically to e-chemistry. Perhaps the best way forward would be to reorganize CPEP into an e-chemistry committee or even a division and provide it with a suitable project budget.

To extend IUPAC activities to fulfill the needs of e-chemistry and to ensure further successful develop-

ment of InChI, the following actions should be considered by the appropriate IUPAC bodies:

1. recognize the importance of IUPAC involvement in various e-chemistry projects. Consider organization of a new IUPAC body responsible for fulfilling the needs of electronic chemistry and chemical informatics (CPEP initially, then higher authorities)
2. take into account computer representation and treatment of chemical data in the development of all IUPAC recommendations. (all divisions, committees, and especially ICTNS (i.e., the Interdivisional Committee on Terminology, Nomenclature and Symbols))
3. recognize and support the InChI project as the most significant IUPAC activity in the area of e-chemistry (all IUPAC bodies)
4. ensure involvement of the divisions and the InChI Subcommittee in extension of InChI to cover additional classes of chemicals (Inorganic Chemistry (Div II), Organic and Biomolecular Chemistry (Div III), Polymer (Div IV), and Div VIII)
5. investigate the possibility to extend InChI to cover biochemicals, including peptide and nucleic acid sequences (Divisions VIII and III, and IUBMB and the Joint Commission on Biochemical Nomenclature)
6. promote InChI and InChIKey to industry and regulatory authorities as identifiers for regulation and registration of chemical compounds (CPEP, COCI)

Some of these matters are already under consideration by IUPAC authorities. We hope that the proactive involvement of IUPAC in InChI and other e-chemistry projects (e.g., the development of chemical ontologies) will ensure that the Union maintains a leading role in the development of standards for chemistry that keep pace with the ever-increasing speed of advances in information technology.

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2014 IUPAC-SOLVAY International Award for Young Chemists Announced

The 2014 IUPAC-SOLVAY International Award for Young Chemists is intended to encourage outstanding young research scientists at the beginning of their careers. The awards are given for the most outstanding Ph.D. theses in the general area of the chemical sciences, as described in a 1000-word essay. The award, which is now generously sponsored by Solvay, succeeds the IUPAC Prize for Young Chemists.

IUPAC will award up to five prizes annually. Each prize will consist of USD 1000 cash and travel expenses to the next IUPAC Congress. In keeping with IUPAC's status as a global organization, efforts will be made to assure fair geographic distribution of prizes.

The awards will be presented biennially at the IUPAC Congress. Each awardee will be invited to present a poster on his/her research and to participate in a plenary award session, and is expected to submit a review article for possible publication in *Pure and Applied Chemistry*.

Applications may be submitted, as described below, to the IUPAC Secretariat. In addition, some IUPAC National Adhering Organizations are soliciting applications in their own countries, frequently in conjunction with a national award. In such cases, applications may be submitted to the NAO or to the Secretariat (not both). The list of NAOs is available. Applications will be judged by a committee of eminent scientists appointed by the president of IUPAC.

Procedures for the 2014 Award

- Entrants must have received the Ph.D. (or equivalent) degree, or completed all Ph.D. requirements including successful defense of the doctoral thesis, during calendar 2013 in any of the countries that are members or associate members of IUPAC. Entrants need not be citizens or residents of one of these countries at the time the application is submitted.
- The research described in the entrant's thesis must be in the field of the chemical sciences, defined as "chemistry and those disciplines and technologies that make significant use of chemistry."
- The IUPAC Prize recognizes only work that was performed while the entrant was a graduate student.
- Application requires submission of a completed entry form, together with the material listed in items e. and f. The entry form and supporting material should be submitted by e-mail whenever feasible.
- An essay must be submitted by the entrant that describes his or her thesis work and places it in perspective relative to current research in the chemical sciences. The essay must be written in English by the entrant and may not exceed 1000 words. [For applications submitted through NAOs, a national language may be permissible, and the NAO will assist in translation to English. The announcement by the appropriate NAO should be consulted.]
- Two supporting letters (sent by e-mail if feasible) are required, one from the thesis adviser and/or chairman of the thesis committee and one from an additional faculty member who is familiar with the applicant's thesis work. These letters should comment on the qualifications and accomplishments of the applicant and the significance of the thesis work.
- Complete applications must be received at the IUPAC Secretariat by **1 February 2014**.

IUPAC Secretariat E-mail: secretariat@iupac.org

CHEMRAWN VII Prize for Atmospheric and Green Chemistry—Call for Nominations

IUPAC is now seeking nominations for the 2014 CHEMRAWN VII Prize for Atmospheric and Green Chemistry. The CHEMRAWN VII Prize was first announced in August 2008 and since, has been awarded in 2010 and 2012 at the IUPAC International Conference on Green Chemistry held those years.



The prize of USD 5000 is granted to a young investigator (less than 45 years of age) from a developing country who is actively contributing to research in green chemistry and atmospheric chemistry. The prize was awarded to Nouredine Yassaa (Algeria) in 2010 and to Rashimi Sanghi (India) in 2012.

Nominations for the 2014 prize must be submitted by **22 March 2014**.

Each nomination should include a CV and two letters of support, plus a brief summary of accomplishments illustrating the contributions of the applicant to research in green chemistry and atmospheric chemistry. Complete applications should be sent by email to the IUPAC Secretariat <secretariat@iupac.org> before the submission deadline.

The selection committee comprises the chair of the IUPAC Committee on Chemical Research Applied to World Needs, CHEMRAWN, the president of the Organic and Biomolecular Chemistry Division, and the chair of the Subcommittee on Green Chemistry. The next award will be presented at the 5th IUPAC International Conference on Green Chemistry, 17–21 August 2014, Durban, South Africa.

For further information, please contact Prof. Leiv K. Sydnes, chair of CHEMRAWN, at <leiv.sydnes@kj.uib.no>.

DSM Materials Sciences Award 2014—Call for Nominations

In partnership with IUPAC, Royal DSM has issued a call for nominations for the DSM Materials Sciences Award 2014 for research in the field of “Polymer Mechanics and Rheology.” The award, which carries a cash prize of EUR 50 000, forms part of DSM’s Bright Science Awards Program and has been established to recognize and reward excellence in innovative research in the materials sciences.

Scientists from around the world who have made major contributions to fundamental or applied research in this field of polymer physics can be nominated for the award. A prime requirement is that the candidate’s research must have significantly advanced the world’s understanding and knowledge of key questions in the field specified. An international judging committee will review the nominations and select the winner.

Candidates for the award can be put forward by nomination only and may not nominate themselves.

The award recipient will be required to deliver an award lecture on his/her research work.



Nominations must be made using the nomination form. The deadline for submissions is **7 February 2014**.

The award will be presented at the IUPAC World Polymer Congress 2014 to be held at the International Convention and Exhibition Centre, Chiang Mai, Thailand, 6–11 July 2014.

Contact Edith de Kreek <edith.kreek-de@dsm.com> to receive this nomination form and for further information regarding the award. The nomination form, together with supporting documents should be sent by email to Edith de Kreek.

 www.dsm.com/content/solutions/awards/en_US/materials-sciences.html

Standard Atomic Weights Revised

The IUPAC Commission on Isotopic Abundances and Atomic Weights (II.1) met under the chairmanship of Dr. Willi A. Brand, at the Scientific and Technological Research Council of Turkey in Gebze, prior to the IUPAC General Assembly in Istanbul, Turkey, in August 2013. Following its meeting, the commission recommended changes to the standard atomic weights of 19 chemical elements. The IUPAC Council, at its meeting on 14–15 August, approved these changes. The changes are the result of cooperative research supported by the U.S. Geological Survey, IUPAC, and other contributing commission members and institutions.

The standard atomic weights of cadmium, molybdenum, selenium, and thorium have been changed based on recent determinations of terrestrial isotopic abundances. In addition, the standard atomic weights of 15 elements have been revised based on the new assessment of their atomic masses by the International Union of Pure and Applied Physics.

The following changes in the standard atomic weights have been made:

Element	From	To
aluminium (aluminum)	26.981 5386(8)	26.981 5385(7)
arsenic	74.921 60(2)	74.921 595(6)
beryllium	9.012 182(3)	9.012 1831(5)
cadmium	112.411(8)	112.414(4)
caesium (cesium)	132.905 4519(2)	132.905 451 96(6)
cobalt	58.933 195(5)	58.933 194(4)
fluorine	18.998 4032(5)	18.998 403 163(6)
gold	196.966 569(4)	196.966 569(5)
holmium	164.930 32(2)	164.930 33(2)
manganese	54.938 045(5)	54.938 044(3)
molybdenum	95.96(2)	95.95(1)
niobium	92.906 38(2)	92.906 37(2)
phosphorus	30.973 762(2)	30.973 761 998(5)
praseodymium	140.907 65(2)	140.907 66(2)
scandium	44.955 912(6)	44.955 908(5)
selenium	78.96(3)	78.971(8)
thorium:	232.038 06(2)	232.0377(4)
thulium	168.934 21(2)	168.934 22(2)
yttrium	88.905 85(2)	88.905 84(2)

These changes in the standard atomic weights will be published in a new "Table of Standard Atomic Weights 2013," which will be published in *Pure and Applied Chemistry* in 2014. The revised values for atomic weights can be found online at the website of the Commission on Isotopic Abundances and Atomic Weights (www.ciaaw.org).

The commission has also resolved to reclassify thorium from a mono- to a bi-isotopic element owing to the significant abundance of the thorium-230 isotope in deep seawaters. The commission also recommended a new standard value for the isotope ratio of uranium, $N(^{238}\text{U})/N(^{235}\text{U}) = 137.8(1)$, in naturally occurring terrestrial materials.

The importance of determining precise atomic weights has long been recognized, resulting in the creation of the International Atomic Weights Committee in 1899. IUPAC has overseen the periodic evaluation and dissemination of standard atomic-weight values since its formation in 1919.

For more information, contact Dr. Juris Meija <juris.meija@nrc.ca>, secretary of IUPAC Commission II.1.

2013 International Chemistry Olympiad

The 45th International Chemistry Olympiad (IChO) was held in Moscow, Russia, from 15–24 July 2013. The competition involved 291 secondary school students representing 73 countries from all over the world. The participants were assigned a number of tasks in both practical and theoretical chemistry and were scored based upon their command of chemistry, creativity, and experimental skills.

"The Chemistry Olympiads are all about emotion: the thrill of getting to know a new country, the apprehension of looking forward to the Olympiad, the anticipation of the results and, finally, the unbelievable feeling of being the winner," said Alexey Zeifman, graduate of the MSU Chemistry Department, the absolute winner of IChOs in 2004 and 2005.

It was the third time Moscow State University hosted the International Chemistry Olympiad. The oldest Russian university, it bears the name of the renowned Russian scientist, encyclopedist, and chemist Mikhail Lomonosov, whose 300th anniversary was celebrated worldwide last year following a UNESCO declaration.

The winning chemists were awarded at the Closing Ceremony in the Great Assembly Hall of M.V. Lomonosov Moscow State University. The IUPAC cer-

The Russian organizers of the 2013 IChO pass the IChO flag to their colleagues from Hanoi, Vietnam, which will host the 2014 Olympiad.





A platter of gold medals before the awards ceremony.

tificates were presented by Natalia Tarasova, a member of the IUPAC Executive Committee, to Chun-Yi Chen from Chinese Taipei (the best score in the Practical exam, 36.32 points of 40) and to Yuyang Dong from China (the best score in the Theoretical exam, 53.89 point of 60), who also became the absolute winner of the 45th IChO (85.09 points of 100).

 www.icho2013.chem.msu.ru

IUPAC Selects De Gruyter as Partner for its Scientific Publications

IUPAC has entered into an exclusive agreement with academic publisher De Gruyter for the publication of its academic journal, *Pure and Applied Chemistry* (PAC) and its newsmagazine, *Chemistry International* (CI). Beginning in 2014, the journal and the newsmagazine will be published by De Gruyter in print and electronic form.

Pure and Applied Chemistry publishes monthly, highly topical scientific articles at the forefront of all aspects of pure and applied chemistry. It is also the designated medium for publication of recommendations, technical reports on standardization, recommended procedures, data compilations, and collaborative studies of IUPAC bodies. The scientific journal is edited by IUPAC and overseen by a prestigious advisory board.

Chemistry International publishes bi-monthly news about IUPAC and its chemists, publications, recommendations, and conferences, and the work of its commissions and committees. The news magazine has a circulation of more than 6,000 scientists and institutions worldwide.

“We look forward to some immediate benefits from this partnership. We expect to see an improved time to publication in *Pure and Applied Chemistry*, something that is very important to today’s researchers. In addition, both publications will have increased visibility at international scientific conferences, leading to an increase in readership,” said David Martinsen, chair of IUPAC’s Committee on Printed and Electronic Publications. As part of the transition, the PAC/CI Oversight Subcommittee will work with De Gruyter to enhance the presentation of both the journal as well as individual articles.

“The opportunity to publish two established and important journals as *Pure and Applied Chemistry* and *Chemistry International* is another step forward to further expand De Gruyter’s chemistry portfolio,” emphasized Anke Beck, president of publishing at De Gruyter. Karin Sora, senior editorial director for chemistry and material sciences, added, “The journals further strengthen our internationally oriented publishing program and extend our collection of journals.”

“We are very pleased to work together with IUPAC. This collaboration further underlines our concept of building partnerships with the most influential societies worldwide,” Anke Beck concluded.

“De Gruyter is an ideal partner for our publishing activities. We are looking forward to working together with them,” said René Deplanque, IUPAC Secretary General.

The academic publishing house De Gruyter has a history spanning over 260 years. The Berlin-based group of companies releases over 1,250 new titles each year in the fields of medicine, the humanities, natural sciences, and law, in addition to more than 650 journals and digital media publications. The De Gruyter Group includes the publishing houses Versita, Birkhäuser, Oldenbourg Wissenschaft, and Akademie.

 www.degruyter.com

A Global Framework for Implementing Consistent Ecological Risk Assessment for Pesticides for Sustainable Agriculture

In order to increase food production to feed the world's growing population, there has been an exponential growth in agricultural outputs during the last decade, which has boosted pesticide use significantly in many scientifically emerging regions of the world. With increased pesticide application, the potential ecological impact has become a growing concern. Although in many countries ecological risk assessments (ERAs) are routinely carried out before pesticides can be registered for use, in scientifically emerging regions the science and application of ecological risk assessment is still in its early stages. There is a strong interest from scientists and regulators in these regions to utilize existing datasets and models to begin the process of ERA to examine the potential risks to natural resources in sensitive areas. This is a task where international cooperation among scientists can be extremely effective in transferring knowledge and skills. In order to address this, a project entitled "A Global Framework for Implementing Consistent Ecological Risk Assessment of Pesticides for Sustainable Agriculture" was launched to identify and prioritize the key issues related to pesticide ecological risk assessment in these regions.



Participants at the ERA Workshop, 15–16 September 2012, Beijing, China.

The scope of this project included:

- the development of an integrated framework and guidance document for the application of ecological risk assessment methodologies that can be applied to the pesticide regulatory process
- the production of appropriate training materials
- the organization of workshops to promote and transfer current scientific knowledge about ecological risk assessments

These goals have now been achieved and the first of the workshops was held 15–16 September 2012

in Beijing, China, in conjunction with the 8th IUPAC International Workshop on Crop Protection Chemistry and Regulatory Harmonization. The second was held 25–26 May 2013 in Bogota, Colombia, in conjunction with the 4th Latin American Pesticide Residue Workshop (see next report). The objective of the ERA workshops was to provide focused training on ERA methodologies and exchange information with local scientists and regulators for consistent and risk-based ERA practices.

Each workshop had 30 to 40 attendees from academia, government agencies, and industrial organizations. Twelve presentations were given by members of the IUPAC Chemistry and the Environment Division (Div VI) Advisory Committee on Plant Protection Chemistry and were specifically tailored to cover the following topics: ERA overview in the USA and EU; ecological hazard identification, exposure assessment, risk characterization, uncertainties in risk estimation, probabilistic risk assessment, principles for scenario development, integration of local conditions, and risk perception, communication, and management.

In Beijing, two additional presentations were given by the Chinese regulatory agency ICAMA and the Nanjing Institute of Environmental Science, which provided a thorough update of the current development status for pesticide ERA in the country. In Bogota, additional presentations were made on behalf of CropLife Latin America dealing with regulatory principles and the current status of ERA in Colombia. During, and at the end of the workshops, discussions were held among all enthusiastic participants on good modeling practices, recommendations on scenario development, model testing, and validation.

After the workshop all participants received copies of the presentations together with supplementary guidance documentation on the development of ERAs. It was agreed that this was a very worthwhile initiative and participants appreciated the chance to discuss ecological risk assessment with scientists and experts in the field of ERA development and for the net working opportunities that the workshops enabled and which will be useful for discussing any future questions that might arise.

For more information, contact Task Group Chair John B. Unsworth <Unsworth@aol.com> (consultant, UK) or member Wenlin Chen <wenlin.chen@syngenta.com> (Syngenta Crop Protection, LLC., USA).

 www.iupac.org/project/2010-056-1-600

Latin American Pesticide Residue Workshop Food and Environment

The primary objectives of this project are to:

- identify and prioritize the key regional issues related to pesticide residues in crops in Latin America for both local and export consumption
- facilitate exchange of information and ideas regarding harmonized approaches available for the scientific evaluation and regulation of pesticide residues in crops and the setting of MRLs
- develop recommendations for advancement of crop protection chemistry, with reference to treated crops, in Latin America

The 4th Latin American Pesticide Residue Workshop was held in Bogota, Colombia, 26–29 May 2013. This event brought together academics, researchers, companies in the agrochemical industry, government agents responsible for monitoring and regulation of residues in food and environment, and suppliers of analytical equipment and supplies. The workshop attracted over 400 participants and featured leading scientists as speakers.

Over more than four days, the workshop offered 32 lectures, two round tables, and two poster sessions with around 140 posters. The scientific program was supplemented by satellite courses in which participants received training in topics such as risk assessment, methodologies, instrumentation, and GLP in pesticides residues laboratories. In addition, the workshop offered nine technical seminars, as well as an exhibition of analytical instrumentation, laboratory equipment, and supplies.

During the two round tables the participants received recommendations regarding harmonized approaches available for the scientific evaluation and regulation of pesticide residues and recommendations for troubleshooting in pesticide residue analysis.

For more information, contact Task Group Chair Jairo Arturo Guerrero Dallos <jaguerrero@unal.edu.co>.

 www.iupac.org/project/2012-017-1-600



Participants listen to an ERA presentation at the workshop in Bogota, Colombia, May 25–26, 2013

Evaluated Kinetic Data for Atmospheric Chemistry

The project task group on Evaluated Kinetic Data for Atmospheric Chemistry met in Montreux, Switzerland, on 12–14 June 2013; participants were R.A. Cox, M. Ammann, J.N. Crowley, M.J. Rossi, J. Troe, and T.J. Wallington (chair). Updates to the over 1000 data sheets covering gas phase and heterogeneous phase reactions of importance in atmospheric chemistry were discussed.

The task group prepared, submitted for publication, and published a comprehensive evaluation of heterogeneous reactions on solid surfaces. The publication is M. Ammann, et al., “Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry: Volume VI—Heterogeneous Reactions with Liquid Substrates,” *Atmos. Chem. Phys.*, 13, 8045–8228, 2013; <http://dx.doi.org/10.5194/acp-13-8045-2013>.

The evaluation covers the heterogeneous processes involving liquid particles present in the atmosphere with an emphasis on those relevant for the upper troposphere/lower stratosphere and the marine boundary layer, for which uptake coefficients and adsorption parameters have been presented on the IUPAC website since 2009.

The article consists of an introduction and guide to the evaluation, giving a unifying framework for parameterization of atmospheric heterogeneous processes. Summary sheets containing the recommended uptake parameters for the evaluated processes are provided. The experimental data on which the recommendations are based, are provided in data sheets in separate appendices for the four surfaces considered: liquid water, deliquesced halide salts, other aqueous electrolytes, and sulfuric acid. A total of 79 chemical processes are covered in Volume VI.

The six snapshot volumes are readily accessible from http://www.atmos-chem-phys.net/special_issue8.html. The Atmospheric Chemistry website that once was based in Cambridge, UK, <http://www.iupac-kinetic.ch.cam.ac.uk>, has a new home at <http://iupac.pole-ether.fr>, which is supported by CNRS (France).

For more information, contact Task Group Chair Tim J. Wallington <twalling@ford.com>.

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

Provisional Recommendations

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

Nomenclature of Flavonoids

Flavonoid structures, found in nature or obtained by synthesis, have become more and more complex, and a guide for aglycone names is provided here to permit the construction of the names for their polyglycosylated species with clarity and conciseness.

A joint working party of IUPAC/IUBMB members has prepared these recommendations, which establish rules for the general nomenclature of flavonoids, providing examples of acceptable trivial names, and

names derived from trivial names, together with semi-systematic and fully systematic names that follow the published IUPAC recommendations.

Comments by 28 February 2014

Amelia P. Rauter
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 www.iupac.org/project/2009-018-2-800

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Terminology of Metal–Organic Frameworks and Coordination Polymers (IUPAC Recommendations 2013)

Stuart R. Batten, et al.

Pure and Applied Chemistry, 2013
Vol. 85, No. 8, pp. 1715–1724

A set of terms, definitions, and recommendations is provided for use in the classification of coordination polymers, networks, and metal–organic frameworks (MOFs). A hierarchical terminology is recommended in which the most general term is coordination polymer. Coordination networks are a subset of coordination polymers and MOFs a further subset of coordination networks. One of the criteria an MOF needs to fulfill is that it contains potential voids, but no physical measurements of porosity or other properties are demanded per se. The use of topology and topology descriptors to enhance the description of crystal structures of MOFs and 3D-coordination polymers is furthermore strongly recommended.

 <http://dx.doi.org/10.1351/PAC-REC-12-11-20>

Glossary of Terms Used in Medicinal Chemistry. Part II (IUPAC Recommendations 2013)

Derek R. Buckle, et al.

Pure and Applied Chemistry, 2013
Vol. 85, No. 8, pp. 1725–1758

The evolution that has taken place in medicinal chemistry practice as a result of major advances in genomics and molecular biology arising from the Human Genome Project has carried with it an extensive additional working vocabulary that has become both integrated and essential terminology for the medicinal chemist. Some of this augmented terminology has been adopted from the many related and interlocked scientific disciplines with which the modern medicinal chemist must be conversant, but many other terms have been introduced to define new concepts and ideas as they have arisen. In this supplementary Glossary, we have attempted to collate and define many of the additional terms that are now considered to be essential components of the medicinal chem-

ist's expanded repertoire. (Part I is published as *Pure Appl. Chem.* 70(5), 1129–1143 (1998); <http://dx.doi.org/10.1351/pac199870051129>)

 <http://dx.doi.org/10.1351/PAC-REC-12-11-23>

Assessment of Theoretical Methods for the Study of Hydrogen Abstraction Kinetics of Global Warming Gas Species During their Degradation and Byproduct Formation (IUPAC Technical Report)

Ponnadurai Ramasami, et al.

Pure and Applied Chemistry, 2013
Vol. 85, No. 9, pp. 1901–1918

Global climate change is a major concern as it leads to an increase in the average temperature of the earth's atmosphere. The existence and persistence of some gaseous species in the atmosphere contribute to global warming. Experimental techniques are used to study the kinetics and degradation of global warming gases. However, quantum mechanical methods are also useful for the kinetic and radiative forcing study of global warming species and can precede experimental investigations. Research has also been targeted to develop more adapted procedures using ab initio and density functional theory methods. This report provides a global perspective, in simplified manner, of the theoretical studies of the degradation of gas species in the atmosphere with an emphasis on the hydrogen abstraction kinetics of global warming gas species during their degradation and byproduct formation. En route, the results obtained from these studies are analysed and compared with experimental data where available. Our analyses indicate that the theoretical predictions are in agreement with experimental findings but the predicted parameters are dependent on the method being used. Theoretical methods are used to predict the thermodynamic parameters of reactions, and, with relevance to this report, the global warming potential index can also be calculated. This report can be useful for future investigations involving global warming gaseous species while providing suggestions on how computations can fill in data gaps when experimental data are unavailable.

 <http://dx.doi.org/10.1351/PAC-REP-10-02-38>

Use of Abbreviations, Enclosing Marks, and Line-Breaks

by Jeffery Leigh

The use of abbreviations sometimes causes more problems for a reader than is strictly necessary. The current free use of acronyms in texting has exaggerated these problems. In chemistry, care must always be taken to write in terms that are as clear as possible for any potential reader, and certain rules should always be followed in an attempt to achieve this. For the purposes of this article, the words abbreviation and acronym may be used interchangeably.

IUPAC has suggested a set of guidelines for the employment of abbreviations in chemistry texts ("The Use of Abbreviations in the Chemical Literature, Recommendations 1979," *PAC*, 1980, **52**(9), 2229–2232). These recommendations suggest that "there are great advantages in defining all abbreviations . . . in a single conspicuous place in each paper . . . preferably near the beginning in a single list." Included in these recommendations is a suggestion that no abbreviations should be used in titles or abstracts. The use of abbreviations in formulae is often preferable to the use of recommended names, but in such cases an accompanying definition may be absolutely necessary.

In English texts, there are certain abbreviations that are generally understood by all chemists, though thought should be given as to whether this will be true for speakers of other languages. Abbreviations such as thf (for tetrahydrofuran) may be self-evident to an English speaker but not to, say, a German or Hungarian speaker. Abbreviations for more complex organic groups should generally be defined. Generally accepted English abbreviations include those for organic substituent groups such as Ph, Me, Et, Pr, and Bu, though whether specific variants of qualified versions, such as *t*-Bu or Bu^t, are preferred may be a matter of editorial style. Care should be exercised, because it is sometimes not evident whether an abbreviation such as Bz is meant to indicate benzyl or benzoyl or even benzene.

Inorganic chemists also generally have problems with abbreviations, especially for the names of ligands in the formulae of coordination complexes, because specific rules for producing abbreviations from systematic names are not generally available and lists of recommended abbreviations cannot be complete and comprehensive. The new *Principles* goes some way to deal with this by providing a long list containing the names of some of the commonest ligands, their rec-

ommended abbreviations, and the names from which the abbreviation was derived. For example, the abbreviation acac, derived from the non-standard name acetylacetonate, may be widely understood, though the current recommended IUPAC systematic name is 2,4-dioxopentan-3-ide. Some general principles for developing suitable abbreviations are also presented.

Polymers also have names that are often abbreviated, especially when the use is to define unequivocally a given material rather than to convey a detailed chemical structure. This is especially true in industry and commerce, names such as PTFE and PVC being common examples. Whereas IUPAC nomenclature methods can be used unequivocally to name specific polymers, the accepted abbreviations are often not based upon systematic names but upon trivial names, and many of the users of the abbreviations may not be chemists anyhow. The new *Principles* contains a discussion on polymer nomenclatures, including a list of the most widely used names and abbreviations. In addition, the subject of abbreviation is still a matter for discussion in particular areas, as demonstrated recently by Brimble et al. in "Rules for Abbreviation of Protecting Groups (IUPAC Technical Report)," *PAC*, 2013, **85**(1), 307–313.

The IUPAC names of natural products are often rather long and complicated. For example, most people can identify what is meant by an acronym such as DNA, though each person probably understands its significance only in as much detail as is needed. Certainly the IUPAC name would only confuse most people, as well as consuming much time and space in presentation. In addition, IUPAC is not the only international body concerned with the nomenclature of materials such as DNA. Biochemical nomenclature is often based upon trivial names, and bodies such as the International Union of Biochemistry and Molecular Biology (IUBMB) are involved in developing and publishing recommendations, the latest IUBMB recommendations dating from 1992. There is a joint IUPAC/IUBMB committee that considers matters of interest to both Unions, including nomenclature problems. Amino acids, carbohydrates, and peptides, as well as nucleic acids, have generated their own specific nomenclatures, and all are dealt with in the new *Principles*, which provides references for those seeking more information.

Enclosing marks and line breaks are in common use throughout chemical literature. However, though their use may be defined quite clearly by nomenclaturists, their employment is often not consistent. The correct use is important when a sequence of enclosures is being used because these marks are employed in

nomenclature as a hierarchy, dictating which set of marks enclose which. The principal enclosing marks are parentheses, (), sometimes simply called brackets or round brackets, curly brackets, { }, also often called braces in U.S. texts, and square brackets, []. These are the principal marks used, and though some others may be found in specialized literature, these are those used by chemists. However, the order in which they are used depends upon the specific context.

In organic nomenclature generally and in inorganic names (but not formulae) the sequence to be employed is {{{{ () }}}}} or (), [()], {{{ () }}, {{{ () }}}}, {{{{()}}}} {{{{()}}}}. It will rarely be necessary to use a longer set than this. However, in formulae, and perhaps unfortunately, a different sequence is employed. One reason for this is the universal practice of enclosing the formulae of coordination entities, whether positively or negatively charged, or neutral, in square brackets. The sequence thus becomes [], [()], {{{ () }}, {{{{()}}}}, {{{{{{ ()}}}}}, {{{{{{ ()}}}}}}, etc. This sequence, as printed, raises another question often posed when writing long names and formulae: Is the break at the end of the line in the fifth member of the last sequence simply an accident arising from the particular line and word length, or is it an intended break, so that the item is meant to read {{{{()}}}}? From the context, it is clearly the latter.

It is not possible here to describe all types of use of enclosing marks, and there may be some more specialized instances when minor variations to the above sequences are used. For example, polymer chemists employ an abbreviated hierarchy, which suffices for most general presentations of polymer formulae, namely {{{ () }}, and there are other occasions when enclosing marks can help, even when their use is not mandatory. For example, simple parentheses may be used to distinguish terms such as trioxido, O₃²⁻, from tri(oxido), (O²⁻)₃. Such uses often amount to common sense. Clearly, the writer of names and formulae must be aware of the precise context in which the enclosing marks are being used, and select the appropriate sequence. All these matters are dealt with in *Principles*.

Principles also uses a specific device to deal with the problems sometimes posed by line-breaks. This device is not part of any IUPAC recommendation, but this writer has found it very useful and recommends it for consideration by the community as a whole. Many of the names, systematic or otherwise, employed by chemists contain hyphens to isolate and indicate distinct parts of the name. This is particularly common

in names for organic compounds. They are often very long, and as written or printed contain a line-break, because it is not always possible or convenient to write a given name entirely on a single line. Since such names often contain hyphens anyhow, it may not be clear whether the hyphen at the end of a printed line is part of the name or simply indicates a line-break.

Take, for example, the following name:

(1R*,3R*,5R*)-[(1S)-sec-Butoxy]-3-chloro-5-nitro-cyclohexane

Is the hyphen at the line end part of the name or should the final part read: nitrocyclohexane?

An inorganic example would be undecahydro-7,8-dicarba-*nido*-undecaborate(2-).

The hyphen at the end of the line poses a similar question. In *Principles* these names would appear as follows,

(1R*,3R*,5R*)-[(1S)-sec-Butoxy]-3-chloro-5-nitro-►
cyclohexane

and, in the inorganic example, undecahydro-7,8-►
dicarba-*nido*-undecaborate(2-)

The symbol ► used as a line-break makes it clear that the hyphens are indeed part of the name and not imposed by typographical considerations. *Principles* contains many examples of the use of this device, and consideration of its adoption is recommended to the English-speaking chemical community. Whereas experienced chemists may not feel the need for such a device, the same will not be true for students, which is why it was employed in *Principles*. The use and value of such a device may vary from language to language and, as Bernardo Herold showed in *CI*, 2013, **35**(3), 12-15, translations of chemistry texts and formulae between different languages raise all sorts of problems, for some of which this kind of device might also be useful.

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

Naming Superheavy Halogen and Noble Elements

by Brett F. Thornton and
Shawn C. Burdette

Chemists have fought vigorously for exceptionally small details of linguistic consistency. In 1813 André Ampere suggested to Humphry Davy to name an as-yet-unisolated element fluorine, because it was derived from the mineral fluorospar.¹ Davy accepted Ampere's suggestion, as it was already clear that fluorine was in some ways chemically like chlorine. Later, Ampere realized he'd made a mistake: chlorine, bromine, and iodine were all named from Greek adjectives describing a property of the element (yellow-green, stinks, and violet-colored, respectively), but fluorospar was a *source* of the element, not a *property*, and thus it was linguistically unsuitable for a halogen name. Ampere resolved to fix this, and suggested phthorine as the name of the element, using a Greek adjective meaning destroyer.² Davy, who was no stranger to naming elements and had written extensively about correct nomenclature, responded that this wasn't sufficient reason to rename the element, leaving us with a barely perceptible irregularity in the halogen names. When astatine was named over a century later, the Greek adjective tradition was remembered—the parent Greek adjective means unstable.³ For two centuries, the English suffix for halogens has been *-ine*. In many other languages the halogens lack *any* suffix; in Swedish, for example, the halogens are fluor, klor, brom, jod, and astat. English is the official language of IUPAC, and therefore our focus of discussion.

IUPAC will likely soon accept the discoveries of elements 117 and 118. These new elements lie in the halogen and noble gas groups of the periodic table, and will therefore be an expectation to other recently discovered superheavy elements. How should this new halogen and noble gas be named? Should the naming follow tradition in using *-ine* (halogen) and *-on* (noble gas) suffixes? The existing IUPAC element-naming rules, which incorporate lessons of past discovery priority controversies,⁴ are designed to avoid disagreements. The rules acknowledge historical tradition, and explicitly allow naming an element for a mineral, a property of the element, a place, a mythological or

astronomical concept or object, or a scientist⁵; however, the rules do not include the two-century long tradition of distinguishing between metals and non-metal elements using the element's suffix⁶ (Figure 1).

Beginning in 1953, IUPAC's element-naming rules included "new metallic elements should be given names ending in *-ium*."⁷ This formalized tradition: the suffix of every metal discovered in the past 220 years is either *-um* or *-ium*. The updated 2002 rules changed this earlier guideline slightly by stating "the names of all new elements should end in '*-ium*'." No official statement had ever been made regarding the suffixes of non-metals or metalloids prior to 2002; however, non-metal suffixes *are* longstanding traditions. Except for helium, every non-metal discovered in the past 225 years has either an *-on* or *-ine* suffix.

A cursory glance at the diagonal line separating the metals and non-metals in the p-block may hint that elements 117 and 118 are metallic. But the dividing line is an unreliable approximation: even in period 6, bismuth is *less* metallic than polonium.⁸ Further, relativistic effects impart interesting properties in heavy elements, and the effects are expected to become more pronounced in transactinide elements. Predictions had long held that element properties might not fit periodic law expectations in the 7th row, but this has not been borne out by experiments. Rf, Db, Sg, Bh, Hs, and Cn have been shown to fit well into their groups, though not in all properties.⁹ For flerovium, initial chemical experiments have been inconclusive and predictions suggested it could be a liquid or gas, and even inert.¹⁰ Predictions and chemical studies have been both divergent and convergent. Cn and Fl are expected to show the strongest deviation from periodic trends due to relativistic effects, later period 7 elements should be less impacted.

The chemistry of elements beyond Fl, including 117 and 118, will require new isotopes of these elements to be created before they can be studied¹¹; however, both will probably be named before such studies are completed. Livermorium (element 116) was named before its chemical properties were characterized.¹² Helium too was named prior to any chemical studies, after it was detected in the solar spectrum and thought to be metallic. Similarly, Berzelius believed the metalloid selenium was a metal, and thus used an *-ium* suffix. Naming elements before chemical characterization has been proven to be problematic. If the discoverers knew the location of helium and selenium in the periodic table, they might have chosen different suffixes. What if the chemistry of a new element is not

<div style="display: flex; justify-content: space-between; align-items: flex-start;"> <div style="width: 45%;"> <p>H</p> <p>Li Be</p> <p>Na Mg</p> <p>K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge As Se Br Kr</p> <p>Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb Te I Xe</p> <p>Cs Ba La Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn</p> <p>Fr Ra Ac Rf Db Sg Bh Hs Mt Ds Rg Cn Uut Fl Uup Lv Uus Uuo</p> </div> <div style="width: 45%;"> <p>He</p> <p>B C N O F Ne</p> <p>Al Si P S Cl Ar</p> </div> </div>																	
<div style="display: flex; justify-content: space-between;"> <div style="width: 45%;"> <p>metals with -ium/-um suffix</p> <p>non-metals and metalloids without -ium suffix</p> <p>metals without -ium suffix discovered before 1789</p> <p>non-metals and metalloids with -ium suffix discovered after 1789</p> <p>unnamed, expected to be metals</p> <p>unnamed, possible non-metals</p> <p>systematic non-metal suffix</p> </div> <div style="width: 45%;"> <p>Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu</p> <p>Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Lr</p> </div> </div>																	

Figure 1: Periodic table showing the different suffixes for metals and nonmetals.

yet available or accessible? Is there a way to preserve the distinct suffixes? One possibility would be to use the electronic definitions of transition metals, and non-metals, halogens and noble gases. Element 117 lacks one electron in its 7p shell; element 118 has six 7p electrons. The reactivity of those electrons could be seen as a separate matter, so even if element 118 was later found to bond vastly more than its lighter group members, it would still be grouped with the noble elements. This is not a perfect solution: had Cn and Fl turned out to have noble gas characteristics, as was once predicted, should they have received the *-on* suffix?

We hope that IUPAC and the discoverers of elements 117 and 118 will consider all the pertinent factors—history, tradition, chemistry—when choosing an appropriate suffix for these elements. The inconsistency between early theoretical predictions and later chemical experiments in transactinide elements provide a cautionary tale against assuming elements 117 and 118 will definitively not possess halogen- and noble gas-like properties, respectively. There are exceptions amongst the element suffixes, but the traditional practices have great utility in enabling quick recognition of element groups; *-ium* means metal and *-ine* means halogen by virtue of having been used in this manner for over two centuries. Changing these traditions degrades the usefulness the existing names: giving an *-ium* suffix to halogen and noble gas elements diminishes the meaning of *-ium* for metal and non-metal names alike. The element suffixes have meaning, and there is value in preserving them. We suggest officially systematizing the element name suffixes for halogens and noble elements (*-ine* and *-on*).

Brett F. Thornton is at the Department of Geological Sciences and Bolin Centre for Climate Research, Stockholm University, Stockholm, Sweden. Shawn C. Burdette is at the Department of Chemistry and Biochemistry, Worcester Polytechnic Institute, Worcester, Massachusetts, USA.

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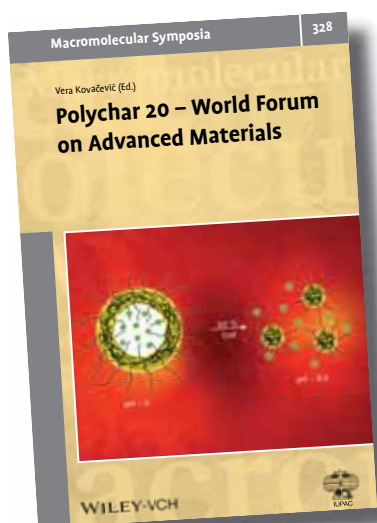
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Polychar 20

Macromolecular Symposia, Vol 328, June 2013
edited by Vera Kovacevic

This volume of *MS* includes a collection of manuscripts submitted to Polychar 20, the World Forum on Advanced Polymeric Materials that was held in Dubrovnik, Croatia, from 26–30 March 2012. A report of that conference was prepared by Vera Kovacevic and Michael Hess and published in *C/* (Sep-Oct 2012 issue, www.iupac.org/publications/ci/2012/3405/cc3_26.03.12.html).

 <http://dx.doi.org/10.1002/masy.201370018>



Solubility Data Series

To date, the Subcommittee on Solubility and Equilibrium Data (SSED) has published 99 volumes in the Solubility Data Series. Volumes 66 to 99 were published in the *Journal of Physical and Chemical Reference Data* (JPCRD) under the title of the IUPAC-NIST Solubility Data Series. From 2012 to 2013, six new volumes were published, either as a single manuscript or in parts, making a total of 12 articles published in JPCRD during this period. Citations to these publications are presented in the table below. For quick access, visit <http://jpcrd.aip.org/> and search IUPAC-NIST Solubility Data Series.

See <http://jpcrd.aip.org/> and search IUPAC-NIST Solubility Data Series.

Volume	Authors, titles, and references to recent SDS publications in the <i>Journal of Physical and Chemical Reference Data</i>
93	J. Eysseltová and R. Bouaziz, IUPAC-NIST Solubility Data Series. 93. Potassium Sulfate in Water, <i>JPCRD</i> 41, 01303 (2012).
94	T. Mioduski, C. Guminski, and D. Zeng, IUPAC-NIST Solubility Data Series. 94. Rare Earth Metal Iodides and Bromides in Water and Aqueous Systems. Part 1. Iodides, <i>JPCRD</i> 41, 013104 (2012).
95 (1)	A. De Visscher, J. Vanderdeelen, E. Königsberger, B.R. Churagulov, M. Ichikuni and M. Tsurumi, IUPAC-NIST Solubility Data Series. 95. Alkaline Earth Carbonates in Aqueous Systems. Part 1. Introduction, Be and Mg, <i>JPCRD</i> 41, 013105 (2012).
95 (2)	A. De Visscher and J. Vanderdeelen, IUPAC-NIST Solubility Data Series. 95. Alkaline Earth Carbonates in Aqueous Systems. Part 2. Ca, <i>JPCRD</i> 41, 023105 (2012).
96 (1)	M. Góral, D. G. Shaw, A. Maczynski, B. Wisniewska-Gocłowska and P. Oracz, IUPAC-NIST Solubility Data Series. 96. Amines with Water. Part 1. C4 to C6 Aliphatic Amines, <i>JPCRD</i> 41, 043106 (2012).
96 (2)	M. Góral, D. G. Shaw, A. Maczynski, B. Wisniewska-Gocłowska and P. Oracz, IUPAC-NIST Solubility Data Series. 96. Amines with Water. Part 2. C7 to C24 Aliphatic Amines, <i>JPCRD</i> 41, 043107 (2012).
96 (3)	M. Góral, D. G. Shaw, A. Maczynski, B. Wisniewska-Gocłowska and P. Oracz, IUPAC-NIST Solubility Data Series. 96. Amines with Water. Part 3. Non-Aliphatic Amines, <i>JPCRD</i> 41, 043108 (2012).
97	P. Fogg and A. Skrzecz, IUPAC Solubility Data Series. 97. Solubility of Higher Acetylenes and Triple Bonded Derivatives, <i>JPCRD</i> 42, 013102 (2013).
98 (1)	W.E. Acree, Jr. IUPAC-NIST Solubility Data Series. 98. Solubility of Polycyclic Aromatic Hydrocarbons in Pure and Organic Solvent Mixtures: Revised and Updated. Part 1. Binary Solvent Mixtures, <i>JPCRD</i> 42, 13103 (2013).
98 (2)	W.E. Acree, Jr. IUPAC-NIST Solubility Data Series. 98. Solubility of Polycyclic Aromatic Hydrocarbons in Pure and Organic Solvent Mixtures: Revised and Updated. Part 2. Ternary Solvent Mixtures, <i>JPCRD</i> 42, 13104 (2013).
98 (3)	W.E. Acree, Jr. IUPAC-NIST Solubility Data Series. 98. Solubility of Polycyclic Aromatic Hydrocarbons in Pure and Organic Solvent Mixtures: Revised and Updated. Part 3. Neat Organic Solvents, <i>JPCRD</i> 42, 13105 (2013).
99	W.E. Acree, Jr. IUPAC-NIST Solubility Data Series. 99. Solubility of Benzoic Acid and Substituted Benzoic Acids in Both Neat Organic Solvents and Organic Solvent Mixtures, <i>JPCRD</i> 42, 033103 (2013); http://dx.doi.org/10.1063/1.4816161 (525 pages)

Conference Call

On the New Definition of the Mole

by *Roberto Marquardt*

The CCQM (**Comité Consultatif pour la Quantité de Matière**) held its 19th meeting on 18–19 April 2013, at the Bureau international des poids et mesures (BIPM) in Sèvres, Paris. One point of the agenda included a discussion about the new definition of the mole. I was invited to represent IUPAC Interdivisional Committee on Nomenclature, Terminology and Symbols (ICTNS) Chair Ron Weir. Ales Fajgelj was also present representing IUPAC.

Martin Milton, director of BIPM, gave a short update on the subject. He mentioned the CCQM12-27 document that contains CCQM internal information regarding the mise-en-pratique and potential assessment methods of the numerical value of the Avogadro constant. It was mentioned that the Consultative Committee for Units of the International Committee for Weights and Measures would hold a meeting in June 2013 where further discussion on the issue would continue.

The general impression was that the urgency of fixing the new definition of the unit mole has given way to a broader discussion on this subject. It seems that CCQM is not hurrying for a new definition now. The ideas regarding the mise-en-pratique are not uncontested among members of the meeting.

Bernd Güttler from PTB (Physikalisch-Technische Bundesanstalt, Braunschweig, Germany) made a suggestion to include results of the so-called Avogadro project into the mise-en-pratique of the mole. The international Avogadro project aims at the redetermination of the Avogadro constant and is based on measurements of a single crystal sphere of Si enriched in 28-silicon [*Phys. Rev. Lett.* 106, 030801 (2011); <http://dx.doi.org/10.1103/PhysRevLett.106.030801>]. This approach allows for a description of a practical realization of the mole based on counting atoms in a crystal and a fixed Avogadro constant. The exact wording of the proposal is currently further discussed. This presentation received quite a broad support from the participants who found it elegant and adequate for teaching.

Willie May, president of CCQM, said that chemists were not sufficiently consulted prior to the publication

of the proposal of a new definition of the mole. He suggested that a symposium should be organized on one of next CCQM meetings, where opponents to the proposed redefinition could express their concerns.

I reiterated the position of ICTNS/IUPAC in the form expressed under point 11 of the 141th meeting of the Executive Committee in October 2009 (see www.iupac.org/fileadmin/user_upload/standing/ec/141_ec.pdf and also Jan-Feb 2010 *CI*, p. 6, www.iupac.org/publications/ci/2010/3201/2_lorimer.html). I said that IUPAC should be involved in further discussions of CCQM regarding the new definition of the mole, and that the official representative of IUPAC should be invited to attend the symposium, if it takes place. I finally asked on behalf of IUPAC to have a copy of the sentence formulated by Bernd Güttler.

The report of the 19th Meeting of the CCQM is now available at www.bipm.org/utills/common/pdf/CCQM19.pdf.



Macromolecules and Materials

The **12th Annual UNESCO/IUPAC Workshop and Conference on Macromolecules and Materials** was held in Stellenbosch, South Africa, 24–28 March 2013. The organizing committee comprised of H Pasch (Chair), L Klumperman, AJ van Reenen, PE Mallon and Aneli Fourie (University of Stellenbosch, Department of Chemistry & Polymer Science, South Africa).

The conference drew 151 attendees, including 53 students, representing 32 countries other than South Africa. Other western countries represented were Australia, Austria, Belgium, Brazil, Canada, China, Czech Republic, Egypt, France, Germany, Hungary, Iran, Iraq, Israel, Italy, Japan, Saudi Arabia, Malaysia, Nepal, Nigeria, Poland, Republic of Korea, Russia, South Korea, Spain, Switzerland, Thailand, The Netherlands, Turkey, United Kingdom, USA, and Venezuela.

The conference was opened by T.E. Cloete, vice rector, research and innovation, University of Stellenbosch and H. Pasch, IUPAC Representative, Department of Chemistry and Polymer Science, University of Stellenbosch, South Africa.

The workshop featured 6 talks and the conference offered 47, of which 6 were plenary speakers, 17 invited speakers, and 32 oral submissions, by experts in their

Conference Call

field, recording the state-of-the-art in various fields, often encompassing the last few years of research.

In addition to IUPAC, the following organizations have given considerable support, either financial or in kind:

- Sasol Polymers Corporate
- Kansai Plascon South Africa
- African Sun Media, University of Stellenbosch

Papers are being collected for peer review for plenary, invited, and oral presentations for publication in a volume of *Macromolecular Symposia*.

 <http://academic.sun.ac.za/unesco/>

Polymer Spectroscopy

by Daniela Illnerova

This year, the **19th European Symposium on Polymer Spectroscopy** (ESOPS19) was held on 7–11 July 2013, at the Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic in Prague. It was organized simultaneously as the 77th Prague Meeting on Macromolecules.

The ESOPS 19 conference was organized by Dr Jiří Spěváček and Dr Jiří Dybal under the auspices of IUPAC. It attracted 100 participants from 25 countries and brought together both young and experienced researchers, as well as many students. At the opening ceremony, the attendees were welcomed by František Rypáček, Director of the IMC, and co-organizer of the conference, Jiří Dybal. The Official IUPAC Representative, Pavel Kratochvíl from the Institute of

Macromolecular Chemistry, Academy of Sciences of the Czech Republic outlined the activities of IUPAC in general and its Polymer Division in particular.

The conference highlighted all fields of spectroscopy (infrared, NIR, Raman, fluorescence, NMR, EPR, mass spectroscopy, X-ray, dielectric and mechanical spectroscopy), from theoretical and fundamental aspects to recent advances and novel developments in characterization and analysis of polymers. The scientific program consisted of 9 invited lectures, 28 short contributed lectures, and 60 poster presentations. Invited lectures were of excellent quality and covered all aspects of polymer spectroscopy.

The conference featured the following invited lectures:

- Bernhard Blümich, Germany (Polymer analysis by compact NMR)
- Dariush Hinderberger, Germany (EPR spectroscopy on nitroxides: a simple method to elucidate molecular and nanoscale processes in thermoresponsive polymers)
- Isao Noda, USA (Two-dimensional correlation spectroscopy study of polymers)
- Vladimír Baumruk, Czech Republic (Vibrational optical activity of (bio)polymers), Daniele Cangialosi, Spain (Dielectric and calorimetric spectroscopy to unravel dynamics and physical aging in nano-structured polymers)
- Yukihiro Ozaki, Japan (Low-frequency Raman and THz spectroscopy studies on higher-order structures of poly-(R)-3-hydroxybutyrate and nylons)
- Monika Schönhoff, Germany (Pulsed field gradient NMR diffusion in colloid and polymer science: transport of ions in polymer electrolytes and of active molecules in carrier particle dispersions)



Group photo of participants in the 19th European Symposium on Polymer Spectroscopy.

Conference Call

- Sergei Kazarian, UK (Emerging applications of spectroscopic imaging to polymers)
- Marek Potrzebowski, Poland (Slow and very fast MAS solid state NMR study of biopolymers)

The conference was held in a friendly and stimulating atmosphere. The participants followed the presentations with great interest, which was reflected in fruitful discussion. Poster presentations were accompanied with selected specialties of Czech cuisine and beer.

The scientific committee selected the following poster presentations for awards, which were bestowed at the conference dinner:

- “Two-dimensional molecular orientation analysis of poly(L-lactic acid) and poly(hydroxybutyrate) spherulites using FT-IR imaging method” presented by Yuta Hikima, Japan
- “Temperature-dependent structural changes and intermolecular hydrogen bonds in Nylon 6 studied by low-frequency Raman and Terahertz spectroscopies and Quantum chemical calculation” by Erika Onishi, Japan
- “NMR study of transition behaviour of amphiphilic block copolymers composed of poly(ethylene glycol) and poly(N-isopropylacrylamide) in water” presented by Mr Rafal Konefał, Czech Republic

Apart from scientific work, the participants enjoyed a relaxed atmosphere at the welcome reception, conference dinner, and in the guided walk in Prague, which included interesting sights such as the historical halls of the Strahov Library and the Old Town Hall with the famous Astronomical Clock.

Nonlinear Optical Spectroscopy as a Probe of Polymer Surface Structure

by *Dennis K. Hore*

It was an honor to receive a 2013 CNC-IUPAC Travel Award that enabled me to participate in the 19th European Symposium on Polymer Spectroscopy, Prague, 7-11 July 2013. My group at the University of Victoria uses unique aspects of laser beams to interrogate the structure of molecules that find themselves at the interface between a solid and liquid phase. One of the overarching goals of our research program (<http://web.uvic.ca/~dkhore>) is to characterize the conformational changes that proteins undergo when they land

The CNC-IUPAC Travel Awards

Dennis Hore's participation in this IUPAC symposium was an integral part of his CNC-IUPAC Travel Award. The Canadian National Committee/IUPAC travel awards were established in 1982 to enable young Canadian scientists to present their research at IUPAC-sponsored conferences outside continental North America. Applicants should be within 10 years of having obtained their Ph.D. The awards are sponsored jointly by the Canadian National Committee, IUPAC's company associates, and the Gendron Fund, which was established in memory of a noted Canadian chemist who organized a highly successful IUPAC congress in Vancouver, British Columbia in 1981. Although many IUPAC member countries have national committees that handle liaison with IUPAC, to the best of our knowledge, the Canadian National Committee is the only one that operates a travel awards program. See www.cnc-iupac.ca/awards_e.html for more details and future announcements.

on hydrophobic surfaces such as polymers. Protein-polymer interactions are important in a wide range of chemical applications, such as enhanced separation technologies, enzyme immobilization in biosensors, and in the biocompatibility of implant materials. Polymeric materials are found in the body in the form of sutures, catheters, vascular stents, and organ repair components. Many polymers that have the best mechanical properties for their task are hydrophobic; water would bead up on their surfaces. This is a problem when such materials are in contact with bodily fluids as proteins, in their native conformation, are folded in a manner that buries their hydrophobic components in their cores, exposing hydrophilic residues to their aqueous environment. When such proteins encounter artificial hydrophobic surfaces, they may unfold upon contact in order to maximize hydrophobic interactions, resulting in loss of function and disease. For decades, researchers have been working on ways to circumvent these issues, for example, by modifying the surface of the polymer components to render them hydrophilic. Although there is empirical data to assist in this effort, there is surprisingly little understanding of what the altered structures of the proteins are, when on the polymer surfaces.



This is where the Hore group fits in, developing a combination of experimental and modeling tools that can probe this elusive interfacial environment with extreme specificity and structural detail. In one of our experiments, a visible and an infrared laser are overlapped at the polymer-solution interface. When certain symmetry requirements are met, one visible and one infrared photon are annihilated, and a new photon is born. This is a very rare occurrence but, as a result of energy conservation, we can know which colour of light to expect in the detector channel. Since momentum must also be conserved, and the frequencies and angles of approach of the two incident laser beams are known, we additionally know where to position the detector. We then use the symmetry requirements of the process and manipulate the laser beam polarizations to work backwards, ultimately arriving at the structure of the molecules responsible for the optical interaction.

Although there is much interest and attention on the proteins, two other species deserve attention, as they are equally important in accounting for the adsorbed structure. The first is the solvent—water molecules in region within about 15 Å from the surface, have a net orientation and hydrogen bonding network significantly different from that in the bulk aqueous phase. The second important player is the hydrophobic surface itself. In the case of proteins on polymers, one is describing a macromolecule on macromolecule interaction. Although the bulk structure of the polymer may be well characterized, its surface structure—in terms of the number and types of chemical functional groups and their orientation—may be a completely different story. Furthermore, the surface of many polymers has been shown to differ depending on the nature of the solvent, necessitating in situ studies. Nonlinear vibrational spectroscopy is ideally suited to probing components of polymer main and side chains at the material's surface. We have recently applied our techniques to show that ester methyl groups are directed away from the poly(methyl methacrylate) surface, thereby providing a molecular rationalization of the material's weak hydrophobicity.

The 19th European Symposium on Polymer Spectroscopy brought together 100 participants from 25 countries, with representation from academia and industry. This meeting struck a balance between experiment and theory, and resulted in many hours of stimulating conversation outside of the technical sessions. I was particularly interested in the presentations

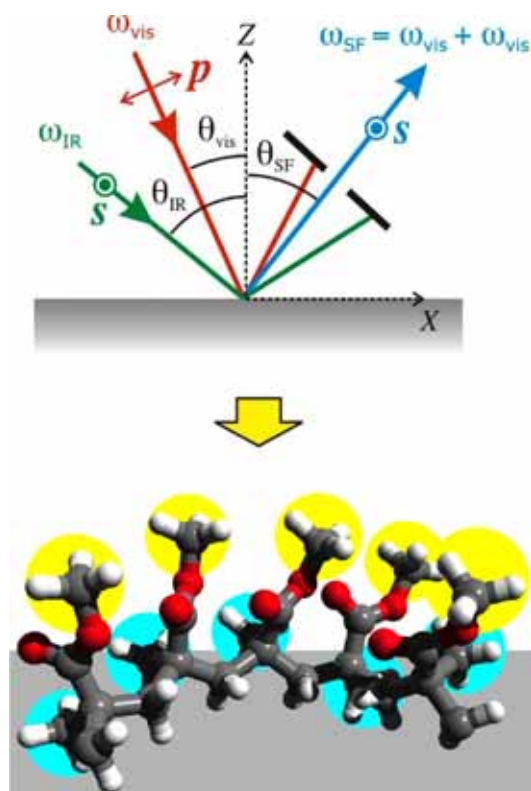


Figure caption: Nonlinear vibrational spectroscopy measurements utilizing different beam polarizations may be combined with molecular simulations to yield detailed structural information about polymer surfaces.

on infrared and Raman spectroscopy and microscopy, and the discussions on chemometrics and spectral processing, including correlation techniques. However, I also appreciated the opportunity to learn about magnetic resonance and EPR of polymers, as those topics are outside of my daily experience. I am grateful for the opportunity to have attended this excellent meeting.

Dennis Hore <dkhore@uvic.ca> received his Ph.D. from Queen's University under the mentorship of Profs. Almeria Natansohn (Queen's, Chemistry) and Paul Rochon (Royal Military College, Physics). His dissertation examined the photo-induced orientation of light-responsive polymers. He was then a postdoc in Prof. Geri Richmond's group at the University of Oregon, studying surfactant and water structure at the air–water interface. In 2006 he joined the Department of Chemistry at the University of Victoria. His research interests are centered on characterizing the structure of molecules adsorbed at solid surfaces.

Where 2B & Y

Sensing Change

1 July 2013–2 May 2014
Philadelphia, Pennsylvania, USA

On 1 July 2013, the Chemical Heritage Foundation (CHF) opened a new art exhibit titled *Sensing Change*, which will be on display until May 2014, both in CHF's Hach Gallery in Old City and through offsite installations in Center City Philadelphia. What motivates artists and scientists to observe and investigate our environment? How do creative professionals in both fields make visible largely invisible processes, such as wind patterns and air quality? What methods and instruments have been used to sense shifts in our climate over time? *Sensing Change* explores these important questions.

"The exhibit brings art into conversation with science to ask the question, 'how do we know our environment?' And from there it provokes a conversation about the experience of the world around us," said Jody Roberts, director of the Center for Contemporary History and Policy at CHF. "These works beautifully compliment the rich heritage that is at the core of CHF's collections—instruments and artifacts that have changed what we know about our world and how we know it."

Sensing Change aims to highlight the intersection of art and science. Featured artists use their

work to interpret scientific findings, historical records, and their own observations to bridge the divide between what can be seen in daily life to larger global changes. Their work creates a space for conversations emerging out of a renewed sense of place.

Sensing Change is a comprehensive exhibit, giving audiences access through a variety of channels. Guests may wish to see the artwork in person by visiting the Hach Gallery, engage in a First Friday program or community outreach event, listen to CHF's podcast *Distillations* for a themed series surrounding *Sensing Change*, or participate online via the website and social media platforms.

 <http://sensingchange.chemheritage.org>



Test of Particle Falls at the Wilma Theater.

Photo © Greg Benson.

Chemical Schemas, Taxonomies, and Ontologies

16–20 March 2014, Dallas ACS meeting

The development of chemical information in the digital era has benefited from fundamental work on classification of molecules and structure. Facilitating the integration of chemical knowledge with other areas and disciplines is greatly helped by the use of formal and informal taxonomies, and potentially by the technologies of the semantic web including schemas and ontologies.

The organizers of this Joint CINF-RSC CICAG Symposium encourage presentations on all aspects of

the construction, deployment and use of these semantic technologies and other approaches to desegregation by academic and industrial research groups. One aim of this symposium is to find a common ground to approach IUPAC and create an internationally agreed Digital environment for 21st Century Chemistry.

CINF is the Chemical Information Group of the American Chemical Society; CICAG is the Chemical Information and Computer Applications special interest group of the (UK) Royal Society of Chemistry.

For more information, contact Jeremy Frey at <J.G.Frey@soton.ac.uk>.

 http://abstracts.acs.org/chem/247nm/meetingview.php?page=session&par_id=617

Chemical Education and Research for Sustainable Development

3–4 April 2014, Colombo Sri Lanka

The Institute of Chemistry Ceylon is completing its 40th year of formal tertiary chemical education in Sri Lanka. So far, the institute has produced 867 chemistry technicians and 905 graduate chemists, a unique achievement for a professional body. It is anticipated that by the end of 2013, it will have produced over 1000 professional graduate chemists and 925 technicians.

From its inception, the institute has received guidance from the U.K. Royal Society of Chemistry. In March 2013, following consideration of extensive documentation and a site visit in 2012, the institute received formal accreditation from the RSC. To mark this landmark event, the Institute of Chemistry Ceylon has convened an international conference on the theme

“Professional Chemical Education and Research for Industrial Development and Sustainable Economic Growth in a Knowledge Based Economy” in Colombo on 3–4 April 2014.

This forum will enable a review and re-evaluation of both programs with a view to making them even stronger, effective, and productive and make them even more relevant to contemporary needs in a knowledge-based economy. Strengthening the woefully inadequate secondary education system in chemistry will be also part of the agenda and school-teachers will be encouraged and expected to participate very actively. An opportunity is also available for presentation of research papers in the areas of Chemical Education as well as other areas in chemical sciences, including industrial and similar research.

See Mark Your Calendar for more information.

 www.ichemc.edu.lk

MicroREaction Technology

23–25 June 2014, Budapest, Hungary

The next event of the IMRET “International Conferences on MicroREaction Technology” conference series will be held in the historic city of Budapest, Hungary, from 23–25 June 2014. IMRET13 will be organized by the Flow Chemistry Society in collaboration with Akadémiai Kiadó, a Wolters Kluwer company, publisher of the *Journal of Flow Chemistry* and co-organizer of the society’s FROST conference series.

IMRET2013 will consist of presentations on the following topics:

- fundamentals: fluidics, mixing, mass, and heat transfer
- process data acquisition, kinetics and chemical analysis; materials aspects, micro- and nanostructures and micro- and nanoparticles
- flow chemistry
- catalysis
- process optimization and intensification

- flow plants—process design and control
- fine and commodity chemical synthesis
- advanced material synthesis
- energy, biomass conversion, and thermal systems
- food, personal care, and other applications

The International Conferences on MicroREaction Technology (IMRET) is a scientific conference series in the field of micro process engineering and the sciences of microreactors that started in Frankfurt am Main, Germany, in 1997. Since then, 12 IMRET conferences have been organized by various well-recognized societies and institutes.

By organizing IMRET13, the Flow Chemistry Society aims to strengthen the bridge between micro-process technology and flow chemistry, and help their integration into everyday practices throughout the world by delivering the latest knowledge and making it available for the entire micro-process technology and chemistry communities.

 www.flowchemistrysociety.com

Modern Physical Chemistry for Advanced Materials

26–30 June 2014, Kharkiv, Ukraine

The organizing committee has received agreements from V.N. Karazin Kharkiv National University and National Academy of Sciences of Ukraine to support the Modern Physical Chemistry for Advanced Materials Conference, 26–30 June 2014, Kharkiv, Ukraine. This is the second conference organized by chemists of Kharkiv National University in collaboration with colleagues from other countries under the sponsorship of IUPAC and NAS of Ukraine; the first one took place in Kharkiv in 2007 (see May–June 2008 *CJ*). The main goals of the conference are as follows:

- to survey the status of modern physical chemistry in Ukraine
- to strengthen the international collaboration of Ukrainian physical chemists
- to develop the physico-chemical foundations of modern material science, technology, and ecology

The conference schedule anticipates already about 20 plenary and invited lectures, which will be delivered by scientists from Brazil, France, Germany, UK, Japan, Ukraine, and USA.

In addition, the following subsections are planned:

- new materials
- organized solutions (supramolecular chemistry, nanochemistry, microreactors, macromolecules, sensors). green chemistry
- electrochemistry and solution chemistry (thermodynamics; physico-organic chemistry; electrochemistry; spectroscopic methods)
- ecotoxicological aspects of nanotechnology
- theoretical chemistry.

Brief abstracts (one page) should be submitted to <beketov2014@karazin.ua>.

See Mark Your Calendar for more information.

 www-chemo.univer.kharkov.ua/beketov2014

Cheminformatics: An International Intercollegiate Online Course

The ACS Division of Chemical Education Committee on Computers in Chemical Education (CCCE) is organizing an intercollegiate Online Chemistry Course in cheminformatics, chemical information sciences, and literature in collaboration with the ACS Division of Chemical Information, IUPAC Committee on Chemistry Education, and RSC ChemSpider. This will be the 6th online course the CCCE has organized since 1996. It will be offered in the fall of 2014 and the fall of 2015. The CCCE is looking for faculty who would like to offer

this course to students in their home institutions.

OLCCs are hybrid courses involving collaborative teaching between expert online guest lecturers and local faculty facilitators (instructors of record—the class is part of their teaching assignment). Prior to offering the course, the faculty facilitators will have a chance to work with cheminformaticians and experts in chemical information to develop customized instructional content. The experts will be available to interact directly with their students when the course is offered.

Further information is available at the development web list below.

 <http://olcc.ccce.us>

2014

12-17 January 2014 • Carbohydrate • Bangalore, India

27th International Carbohydrate Symposium (ICS 2014)

Prof. N. Jayaraman, Indian Institute of Science, Department of Organic Chemistry, Bangalore 560 012, India
Tel.: +91 80 2293 2578, E-mail: ics27@orgchem.iisc.ernet.in, www.ics2014bangalore.in

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

Chemistry Conference for Young Scientists 2014

Prof. Thomas Vranken, Universiteit Hasselt, Institute of Materials Research, Martelarenlaan 42, B-3500 Hasselt
Belgium, E-mail: thomas.vranken@chemcys.be, www.chemcys.be

2-5 March 2014 • Heterocyclic Chemistry • Gainesville, Florida, USA

15th Florida Heterocyclic and Synthetic Conference (FloHet-2014)

Prof. Alan R. Katritzky, University of Florida, Department of Chemistry, Gainesville, FL 32611-7200, USA, Email:
katritzky@chem.ufl.edu, <http://www.arkat-usa.org/conferences-flohet-others>

5-7 March 2014 • Applied Chemistry • Rajagiriya, Sri Lanka

International Conference on Applied Chemistry 2014

Prof. S. Sotheeswaran, Institute of Chemistry Ceylon, Adamantane House, 341/22 Kotte Road, Rajagiriya, Sri
Lanka, Email: sotheeswaran@hotmail.com, www.fnu.ac.fj/newsite/images/stories/conference/index.html

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

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

Prof. Ramanee D. Wijsekera, University of Colombo, Department of Chemistry, P.O. Box 1490, Colombo 3, Sri
Lanka, E-mail: ramanee@chem.cmb.ac.lk, www.ichemc.edu.lk

7-10 April 2014 • Polymer Characterization • Matieland, South Africa

22nd International Conference on Polymer Characterization—World Forum on Advanced Materials

Prof. Peter Mallon, University of Stellenbosch, Department of Chemistry & Polymer Sciences, Private Bag X1,
Matieland, 7602, South Africa, Email: pemallon@sun.ac.za, <http://academic.sun.ac.za/POLYCHAR>

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

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

Prof. Tatiana Birshtein, Russian Academy of Sciences, Institute of Macromolecular Compounds, Bolshoi Pr. 31
RF-199004 Saint Petersburg, Russia, E-mail: birshstein@imc.macro.ru, www.macro.ru

10-13 June 2014 • Polymers and Organic Chemistry • Timisoara, Romania

15th International Conference on Polymers and Organic Chemistry

Prof. Corneliu M. Davidescu, Deputy Rector, University of Timisoara, 2, Victoriei Square, RO-30006 Timisoara,
Romania, Email: corneliu.davidescu@chim.upt.ro

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

Modern Physical Chemistry-2014 (MPC '14)

Dr. Olexander Lebed, Department of Physical Chemistry, Karazin Kharkiv National University, Svoboda Square
4, UA-61022 Kharkiv, Ukraine, E-mail: beketov2014@karazin.ua, www-chemo.univer.kharkov.ua/beketov2014

29 June-4 July 2014 • Organic Synthesis • Budapest, Hungary

20th International Conference on Organic Synthesis

Monika Bondar, Hungarian Chemical Society, H-1015 Budapest, Hattyú u. 16. II/8.
E-mail: icos20@mke.org.hu, www.icos20.hu

6-11 July 2014 • Macro • Chiang Mai, Thailand

IUPAC World Polymer Congress (MACRO 2014)

Wild Blue Congress Organizer, 19/2 Ekkamai 10, Sukhumvit 63, Wattana, Bangkok 10110.
E-mail: info@wildblueorganizer.com, www.macro2014.com

6–11 July 2014 • Solid State Chemistry • Trencianske Teplice, Slovakia

11th International Conference on Solid State Chemistry

Prof. Milan Drábik, Slovak Academy of Sciences, Institute of Inorganic Chemistry, Dúbravská Cesta 9, SK-845, 36 Bratislava, Slovakia, Email: uachmdra@savba.sk, www.ssc2014.sav.sk

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

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

Prof. Judith C. Poë, University of Toronto, Mississauga, Department of Chemical & Physical Sciences, 3359 Mississauga Road, Mississauga, ON L5L 1C6, Canada, E-mail: judith.poe@utoronto.ca, www.icce2014.org

13–18 July 2014 • Photochemistry • Bordeaux, France

XXVth IUPAC Symposium on Photochemistry

Dr. Dario M. Bassani, Université de Bordeaux, ISM, UMR 5255, 351, Cours de la Libération, F-33400 Talence, France, E-mail: d.bassani@ism.u-bordeaux1.fr, www.photoiupac2014.fr

13–18 July 2014 • Organometallic Chemistry • Sapporo, Japan

XXVth International Conference on Organometallic Chemistry (ICOMC 2014)

Prof. Munetaka Akita, Hokkaido University, Catalysis Research Centre, Sapporo 060-0811, Japan. Tel.: +81 117 069 149, E-mail: tamotsu@cat.hokudai.ac.jp, www.ec-pro.co.jp/icomc2014

21–25 July 2014 • Solubility Phenomena • Karlsruhe, Germany

16th International Symposium on Solubility Phenomena and Related Equilibrium Processes (ISSP-16)

Prof. Marcus Altmaier, Karlsruhe Institute of Technology, Institute of Nuclear Waste Disposal, Hermann von Helmholtz Platz, 1, D-76344 Eggenstein-Leopoldshafen, Germany, Email: marcus.altmaier@kit.edu

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

13th International Congress on Pesticide Chemistry

Dr. Kenneth D. Racke, Dow Agrosciences, 9330 Zionsville Road Building 308/2E, Indianapolis, IN 46268, USA
E-mail: kracke@dow.com, www.iupac2014.org

10–15 August 2014 • Physical Organic Chemistry • Ottawa, Canada

22nd International Conference on Physical Organic Chemistry

Paul M. Mayer (Local Organizing Committee)

E-mail: pmmayer@uOttawa.ca, <http://events.science.uottawa.ca/icpoc22/welcome.html>

17–21 August 2014 • Green Chemistry • Durban, South Africa

5th International Conference on Green Chemistry

Prof. Liliana Mammìno, Department of Chemistry, University of Venda, P/Bag X5050, Thohoyandou 0950, South Africa, Email: sasdestria@yahoo.com, www.saci.co.za/greenchem2014

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