

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

# CHEMISTRY

## International

September-October 2011  
Volume 33 No. 5



**From the Wings  
of Butterflies**

**The Kilogram in the “New SI”**

**Berzelius’ Discovery of  
Selenium**



# From the Editor

## CHEMISTRY International

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

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Once upon a time, a young man named Ed from Springfield, Massachusetts, had a striking encounter with nature and became fascinated with butterflies. To his eyes, their wings' colors were magic. So, he embarked upon a life-time search to elucidate the structure of these pigments and discovered that their chemistry holds a key to the betterment of the human condition . . .

This story, continued on page 4, comes to us from Edward C. Taylor, A. Barton Hepburn Professor of Organic Chemistry Emeritus at Princeton



University. Taylor's enduring interest in heterocyclic chemistry lead to numerous new synthetic methodologies and new compounds that are potent inhibitors of cell growth, exhibiting therapeutic activity against some tumors. One of these compounds is now a cancer drug approved around the world for treatment of mesothelioma and second-line lung cancer.

This story is surely one that can inspire young people and generate enthusiasm for the creative future of chemistry. The story is one of fascination, frustration, and good fortune. There was no way to tell back in the 1940s that a fascination with the wing pigments of butterflies would turn into such a life-saving drug. And while not every chemist will see the fruits of his/her research translated into something as striking as a life-saving drug, they all have the power to contribute in their own way to the advancement of chemistry for the benefit of mankind. As we celebrate the International Year of Chemistry 2011, we are reminded that the challenges are important and numerous. May the IYC motto, "Chemistry—our life, our future," be a message of empowerment to a new generation of scientists.

As of now, Taylor and his colleagues are still active with research projects focused on the design and synthesis of new inhibitors and studies aimed at understanding toxicity. Set in the magnificent Frick Chemistry Laboratory at Princeton, they are busy researchers and, yet, one could say that . . . *they all lived happily ever after* . . .

Fabienne Meyers

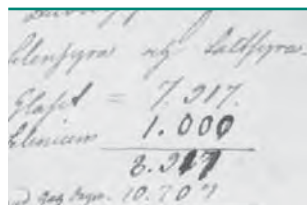
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Cover: Edward C. Taylor, A. Barton Hepburn Professor of Organic Chemistry Emeritus, in his lab at Princeton. See feature on page 4. Courtesy of Princeton University, photograph by Denise Applewhite.

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## Better than “Steady as She Goes”

by *John Corish*



**P**erturbations to the normal course of events, whether they carry a positive or a negative aspect, are always interesting. They disturb the steady as she goes and often boring routine character of our lives and, particularly if they are significant,

engender innovative thought and action to ensure that the enterprise affected continues on its way and prospers. There have been two significant perturbations to the financial life of the Union during the past 12 months and both are still running their courses. The first and very positive of these is the International Year of Chemistry which has brought us many strategic opportunities as well as some formidable challenges. The IYC has made and will continue to make 2011 a particularly active and exciting year for the Union and has very much sharpened our sensitivity to the need to promote and demonstrate the beneficial societal impact of our subject and of our own work as its international union. The second, and more difficult perturbation, is the continuation of the worldwide depression, which is impossible to ignore and which in many instances removes the luxury of certainty and plenty and makes it necessary to struggle to keep afloat and to maintain even core activities.


The recent financial performance of the Union can be properly and fairly assessed only in the light of these major factors as they have indeed had some influence on the manner in which we conduct our business. They are also interlinked because the IYC brought the necessity to raise sponsorship to support our program of international events and the facility with which sponsorship can be won for any purpose is affected by a general dearth of discretionary funds. Given these circumstances we have done very well and the finances of the Union will certainly emerge at the end of this year in a reasonably healthy state.

In respect to the IYC, the decision taken was to make a maximum of half a million U.S. dollars available to support the year, but with the proviso that as much of this as was possible, ideally all of it, be recovered from sponsorship. This funding was directed to be applied to support the Cornerstone Events, namely the Paris Opening Ceremony, the General Assembly in Puerto Rico, and the Closing Ceremony in Brussels, as well as the IYC website and other additional central costs that fell on the Secretariat. Because of its international character and appeal to young chemists, funds have also been provided to the Global Water Experiment. The outcome was that sufficient sponsorship was raised by the two local organizing committees at the Paris and Brussels events to cover their costs. These costs in total exceeded USD 800 000 and the organizers deserve our congratulations and gratitude for their superb efforts. Further sponsorship in excess of USD 400 000 as well as considerable sponsorship in kind were raised centrally. Even though the year still has several months to run, it is becoming clear that the Union itself will spend less than USD 250 000. It is still too early to know the final outcome, but this is clearly the time to say a very sincere thank you to all our sponsors who have supported and made possible our IYC program.

The additional activities of the International Year of Chemistry have given us the impetus to think in a wider context, but it is important to emphasize that there has been no let up in the work of the divisions and committees who have, during 2011, carried through a full program of our essential core activities. We have, however, realized that there is a much bigger world out there that we can and need to influence and that if we want to do this effectively we will have to increase our resources. The great value of the duality of our mandate—for pure and applied chemistry—has also been very apparent during the IYC. When used imaginatively this is more conducive to arousing the interest of non-chemists in our outreach activities. Therefore, we must continue to encourage and foster interactions and joint activities that bring the pure and applied sides of our subject together. The experience of winning sponsorship and working with our sponsors is another valuable lesson for the future.

Since there is not likely to be a more appropriate opportunity for some time to utilize our Strategic Opportunities Fund, it has been used to fund some of the projects comprising the IYC activities. Because of

the surge of events there has also been a faster than usual general uptake of project funds. Our income streams have stood up reasonably well despite the recession, but with our investment portfolio requiring careful monitoring. As I have reported on other occasions the prudent nature of the composition of that portfolio, our maintenance of both U.S. dollar and Euro accounts, and the varied nature of our holdings have again allowed us to do just about as well as could be expected in the global financial climate. It would be comforting to be able to say that we have emerged from this difficult period, but the market turbulence

continues. Nevertheless, we should now look forward with confidence to the improved financial possibilities that must come soon. When they do, we will need to maintain our increased and improved program of work and, as we have undoubtedly done this year, to continue to do better than “steady as she goes.” 

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

## Stamps International

See also [www.iupac.org/publications/ci/indexes/stamps.html](http://www.iupac.org/publications/ci/indexes/stamps.html)

### Avogadro's True Legacy

The centennial of Marie Curie's Nobel Prize in Chemistry, which she received in 1911 for the discovery of radium and polonium, has been extensively (and deservedly) publicized during the International Year of Chemistry. Many other scientific anniversaries are also worth remembering this year, such as the 50th anniversary of the first successful generation of the element lawrencium by a team led by Albert Ghiorso at the Lawrence Berkeley National Laboratory. The year 2011 also marks the 100th anniversary of the discovery of superconductivity by the Dutch physicist Heike Kamerlingh Onnes (1853-1926), who was rewarded

with the Nobel Prize in Physics for his seminal work only two years after the phenomenon was first observed. And the American chemist Melvin Calvin (1911-1997) ought to be remembered this year for the centenary of his

*“Volumi eguali di gas nelle stesse condizioni di temperatura e di pressione contengono lo stesso numero di molecole.”*

birth but, more importantly, for the 50th anniversary of the Nobel Prize in Chemistry with which he was honored for his influential work on the assimilation of carbon dioxide in plants.

The stamp illustrated herein was issued back in 1956 to commemorate the 100th anniversary of the death

of Amedeo Avogadro (1776-1856), the Italian savant whose name is most commonly associated with the number of elementary entities or particles in a mole (i.e., Avogadro's number or constant) but who had nothing to do with the experimental determination of such value. Instead, Avogadro's key contribution, stated in an insightful essay published exactly 200 years ago, consisted of suggesting that “equal volumes of gases at the same temperature and pressure contain equal numbers of molecules” and implied that the ratio of the densities of two gases is directly related to the ratio of their molecular weights. Avogadro's law, as it is now known, written in his native language, is shown together with his portrait and signature on the stamp above. Significantly, Avogadro's ability to ascertain the difference between atoms and molecules also helped solve the problem of assigning the correct molecular formulas to pure substances, which had afflicted the theories of his contemporaries Joseph Louis Gay-Lussac and John Dalton, and thus played a key role in the development of the modern concepts of atomic structure and molecular bonding.



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

# From the Wings of Butterflies

## The Discovery and Synthesis of Alimta

by Edward C. Taylor

The following essay describes in broad terms the history of the discovery of Alimta. It was written as a part of a brochure celebrating the dedication of Princeton's magnificent new chemistry building, completed by the end of 2010. The building, recognized as perhaps the finest, best-equipped, and designed facility for academic chemistry research in the country, was financed by royalties to Princeton from sales of Alimta by Eli Lilly & Co., to whom Princeton had given an exclusive license. The article was addressed to a general audience; my lecture in Glasgow<sup>1</sup> filled in the organic and heterocyclic chemistry involved in the extensive explorations that finally led to the discovery and synthesis of Alimta.

I have often been asked how an interest in the lovely white, yellow, and red pigments in the wings of butterflies could have led to the discovery of Alimta. For an answer, we have to go back 64 years to the fall of 1946, when I entered graduate school at Cornell University to major in organic chemistry. In searching for a possible thesis topic, I ran across an article in *Science* describing the isolation, properties, and structure of a strange compound that the researchers from the pharmaceutical company Lederle had isolated from human liver. It had the totally unexpected property of being necessary for the growth of a number of microorganisms. During their structural investigations of this compound, they found that its core was made up of two fused six-membered rings that constituted six carbon atoms and four nitrogen atoms, a core that had only been observed before as pigments in the wings of butterflies, and in the skins of tropical fish.

Shortly before I began my scientific studies, Robert Purrmann, a young organic chemist at the University of Munich, had taken up a problem that had frustrated

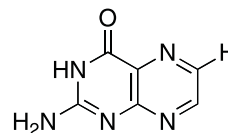
some of the best organic chemists in Europe over a period of 50 years. This was the elucidation of the structures of the white and yellow pigments in butterfly wings. Purrmann finally managed to identify and subsequently synthesize both the white pigment of the white cabbage butterfly and the gorgeous yellow pigment of the brimstone butterfly, and he published these results in *Liebig's Annalen der Chemie* in 1941.

Purrmann's paper came to the attention of the Lederle chemists who were struggling with the structure of the compound from human liver. To their amazement, the two-ring core of the Lederle compound was almost identical to the butterfly wing pigments described by Purrmann. This coincidence of structure between the butterfly wing pigments and the core of the liver compound that was essential for the growth of bacteria struck me as stunningly bizarre, and I decided at that moment to devote my Ph.D. thesis to a study of the so-called pterin heterocyclic core and related heterocycles—where they come from in nature, their properties, both physical and biological, and methods for their preparation.

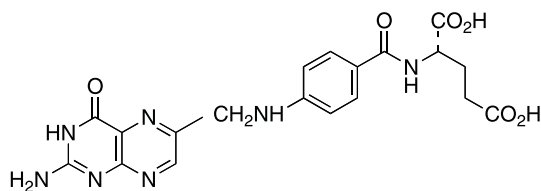
Upper right: pterin core that I studied as a part of my Ph.D. work.

Lower right: structure described in Purrmann's paper in 1941.

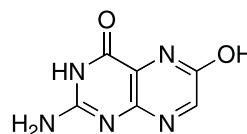
Below: compound isolated from liver by Lederle scientists and reported in *Science*.



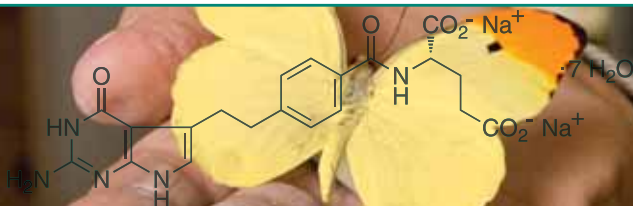
The Pterin Ring System



The Growth Factor from Human Liver  
Folic Acid



The Yellow Wing Pigment from the Brimstone Butterfly



I therefore spent the next three years working with these fascinating, frustrating compounds. It was abundantly obvious from the beginning of this project why it had taken more than 50 years before the structure of even the simplest of the butterfly wing pigments could be elucidated, for these compounds were not easy to work with. Their solubility, for example, rivaled that of Vermont granite, so that spectroscopic studies were difficult, and combustion analysis to determine molecular composition was seldom reliable because of the reluctance of these compounds to burn. (There was even a patent granted at that time for the use of related compounds as furnace liners.)

As it turned out, my choice of this area of organic chemistry for study proved to be extremely fortunate, for it led to a lifelong fascination with heterocyclic chemistry, and proved to be an invaluable training in the techniques of working in this experimentally challenging field.

At the same time that I was pursuing my thesis work at Cornell, the scientists at Lederle Laboratories reasoned, on the basis of the antimetabolite theory that was at that time a guiding principle of drug research, that it might be possible to develop a new group of antibacterial agents. If the structure of the liver compound could be modified, they hoped that bacteria might treat the modified compounds as if they were essential for its growth. Bacterial growth, however, should actually be inhibited because the modified structure would not function in the same way as the original. So Lederle made a change in the structure of the liver compound by substituting one nitrogen atom for an oxygen atom to give a compound called aminopterin, and replacing a hydrogen by a methyl group in the latter compound to give methotrexate. These new compounds indeed proved to be powerful antibacterial agents.

The compound isolated from human liver was shown to be the same substance that, albeit not identified structurally, had earlier been found in various leafy vegetables such as spinach, and was therefore named "folic acid" in 1941.

In 1948, it was found by others that aminopterin and methotrexate were effective in bringing about remissions in acute lymphoblastic leukemia in children. This startling revelation of the antitumor effects of blocking the action of folic acid immediately excited worldwide interest, for both the antibacterial and the antitumor activity of aminopterin and methotrexate were shown to be due primarily to blocking the action of a specific enzyme dihydrofolic acid reductase (DHFR)

essential for the ultimate biosynthesis of both DNA and RNA in cells. These discoveries are considered to be the beginning of modern cancer chemotherapy.

A fundamental problem associated with this approach to cancer chemotherapy was the lack of specificity (for cancer cells rather than normal cells) of any of the DHFR inhibitors thus far discovered, and this held true for a number of newer DHFR inhibitors that were found during the following several decades. During this time, however, much was learned about the multiple roles of folate-derived coenzymes in cellular metabolism, and it became increasingly clear that a better approach might be to search for inhibitors of some of the other folate-dependent enzymes involved in other aspects of cellular biosynthetic processes. By this time some 20 such processes had been identified. One indication that this was a fertile area for potential drug development was the discovery in 1957 of 5-fluorouracil (5-FU), which blocked an enzyme known as thymidylate synthase that is key to the biosynthesis of DNA. Further insights included the discovery of the essential role of a different enzyme that catalyzes the conversion of monoglutamates such as folic acid itself, as well as aminopterin and methotrexate, to polyglutamates.

My own role in these decades-long developments from the 1946–48 discoveries was minor. After receiving my Ph.D. from Cornell, I spent a year in Zürich, Switzerland studying with Nobelist Professor Leopold Ruzicka under a National Academy of Sciences postdoctoral fellowship. In 1950, I studied at the University of Illinois as a postdoctoral fellow, where I was appointed to the faculty in 1951. I accepted a position at Princeton in 1954, and have been there ever since. Although I retained my fascination with the folic acid arena, and continued to work with the heterocyclic ring systems that had so fascinated me in graduate school, I spent most of the following several decades enjoying myself hugely in explorations of many diverse areas of chemistry such as photochemistry, organometallic chemistry, synthetic methodology, and the total synthesis of natural products, most of them quite unrelated to butterfly wing pigments.

It was not until the middle 1970s that I returned to cancer chemotherapy as a specific research goal. The incentive was the accumulation by others of much additional information on the complex pathways by which drugs such as methotrexate enter the cell, undergo activation and deactivation, and can be retained in or eliminated from the cell, as well as an

## From the Wings of Butterflies

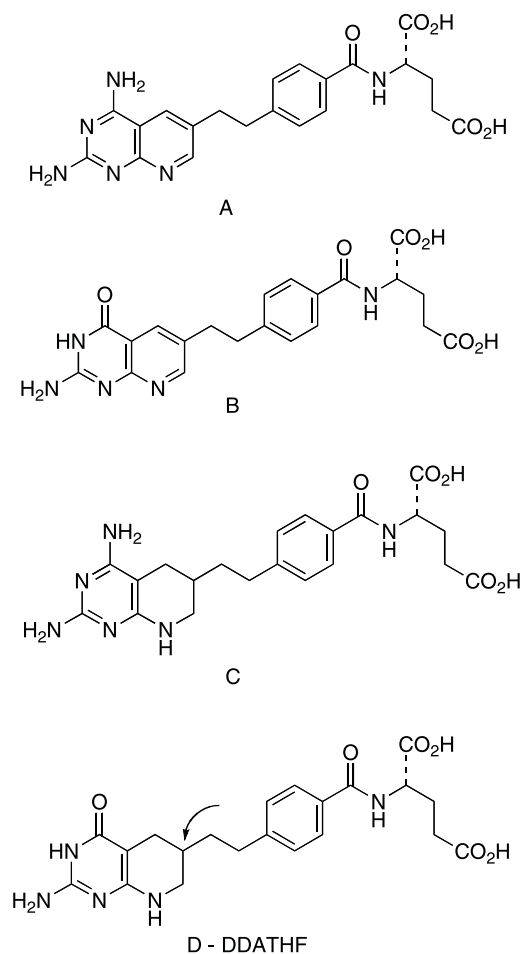
understanding of the other multiple roles played by folate-dependent enzymes.

One of my first major new projects in this field involved the synthesis of 5,10-dideazaaminopterin (A), 5,10-dideazafolic acid (B), and the corresponding tetrahydro derivatives C and D (see figure to right). Compound D, 5,10-dideazatetrahydrofolic acid, subsequently became known by its acronym DDATHF. The deletion of two of the nitrogen atoms of aminopterin, folic acid, and their tetrahydro derivatives would be expected both to lower basicity and increase lipophilicity, and we therefore anticipated that these compounds might have different biological properties as a result. Of particular potential interest was D because, as a variant of tetrahydrofolic acid and not aminopterin, it might satisfy the requirements of a new type of inhibitor. For one thing, this new inhibitor would have to be accepted by the cell as a “normal substrate” for all of the transport and activation processes that were now understood to be essential for inhibitory activity. In addition, it had to function as a pseudo substrate for the enzymes involved in one-carbon atom transfers in cellular metabolism. Its structure, however, precluded its possible function as a one-carbon acceptor; i.e., it could not participate in any of the one-carbon transfer reactions known to be critical for the syntheses, *inter alia*, of purines and thymidylate, and therefore both DNA and RNA.

At this time, I had been for many years a consultant to both the medicinal chemistry and the process development programs at Eli Lilly & Co. in Indianapolis, Indiana. As a consequence, we knew each other well, and they readily agreed to subject these new potential antitumor candidates to initial evaluation. So I sent samples of these compounds to them, and crossed my fingers.

The first response I received was a curious one. Lilly reported that something appeared to be amiss with their tests, and they asked if I could send them an additional sample of D. Fortunately, there was a bit more, but not much more, of the compound, and I sent it to Lilly.

Their next response, however, was a very excited apology. It appeared that nothing had been wrong with the first tests, but Lilly could not believe them and assumed that the tests were faulty. My compound D was one of the most active antitumor agents they had ever seen, and brought about 95–100 percent inhibition of growth in a broad range of tumors in mice and in human tumor xenografts. In addition, it was fully



active against tumors that were resistant to methotrexate, indicating that it was acting to block tumor growth by a totally different mechanism. Further examination of this compound by Lilly showed convincingly that it killed tumor cells by blocking *de novo* purine biosynthesis within cells, thus preventing DNA and RNA biosynthesis.

It was clear that we had an extraordinarily exciting compound on our hands, and that we might be on the brink of a major breakthrough. Princeton does not have a medical school and thus could not provide a base for various aspects of the drug development process, let alone for clinical trials. We needed an active collaboration with a partner with extensive experience in drug development and with an active cancer program in place. A Princeton/Lilly collaboration was a natural one to investigate this exciting lead, and this was quickly agreed upon. I was to head up the chemistry effort, while Lilly took on the basic biochemical and pharmacological studies that are so critical for guiding



## The Discovery and Synthesis of Alimta

the synthetic work, as well as the overall organization of this collaborative effort.

It seemed highly unlikely that DDATHF (compound D), whose extraordinary activity served to launch this collaborative program, would prove to be the ultimate structure of choice. We therefore embarked on what amounted to a classical SAR, or structure-activity-relationship study, where structural changes are made systematically, and each new compound emerging from this work is then evaluated. Every portion of the structure of DDATHF was probed in the hope that a picture of an optimal structure might emerge. We had to bear in mind that every change in structure can affect solubility, absorption, bioavailability, metabolism, partition coefficients, toxicity, possible activity against other biological targets, stability (pharmacokinetic and biochemical properties), as well as resonance, inductive effects, electronic distribution, chemical reactivity and stability, shape, size and bond angles,  $pK_a$  and hydrogen bonding capacity (chemical properties). Furthermore, the effect of a change in one part of the molecule can modify or cancel what might have appeared to be a potentially useful change in another part of the molecule.

For me, this program proved to be a veritable playground for explorations of heterocyclic chemistry, since it called for the synthesis of many new ring systems and required the discovery of many new chemical transformations. Over the next four years, at least 800 new antitumor candidates were designed and synthesized, at Princeton and at Lilly, and each compound had to be thoroughly evaluated. To our astonishment, DDATHF itself proved to be one of the two most active compounds, another being a variation of DDATHF in which a thiophene ring replaced the benzene ring in the bridge region (see structure D).

One unavoidable step in the synthesis of both of these compounds was reduction of a substituted pyridine ring. As we had carried it out, the hydrogen addition was not stereospecific and resulted in the formation of two diastereomers. Because we wanted to evaluate the pharmacological properties of the individual diastereomers, the two diastereomers of DDATHF (and of the second, thiophene-containing candidate) had either to be separated and evaluated separately, or individually synthesized. In discussions with Lilly, it was decided that Lilly would undertake the

separation challenge, while Princeton would tackle the synthesis challenge.

At Lilly, my principal chemical collaborator, Dr. Joe Shih, succeeded in the separation of the two diastereomers of DDATHF. The yields were extremely low: diastereomer 1 was obtained only in 3–5 percent yield, and diastereomer 2 was obtained in 15 percent yield. The latter was chosen to be the clinical candidate and was named lometrexol. Some time later, the two diastereomers of the thiophene-containing candidate were also separated by Dr. Shih, and one of the two, named LY309887, was also chosen for clinical trial. However, preparing sufficient quantities of these materials for clinical trials appeared to be a herculean task, since the reduction step, followed by the mandatory separation of diastereomers (in very low yield), occurred late in a multistep total synthesis.

*... to our amazement and delight, this new compound proved to be a veritable bombshell when it was evaluated at Lilly.*

Although the single diastereomer 2 indeed went into clinical trial, an alternative approach to its preparation was a high priority.

While Lilly was struggling with the separation problems, I tried at Princeton one approach

after another to devise a stereospecific strategy for the preparation of diastereomer 2 alone. After many, many failures, I decided to dodge the problem entirely by designing a new candidate that could not exist in two diastereomeric forms. This approach required the design of a compound that did not possess the stereogenic carbon atom that was responsible for the two diastereomers resulting from the pyridine reduction step. To accomplish this, I focused on a new ring system that retained as many of the structural features of DDATHF as possible so I could assess the impact of the new ring system on activity. However, there was no way one could predict the consequence of what amounted to a very significant change in the structure of DDATHF, and the abandonment of some of the structural features that we had already determined to be critically important for activity.

Certain fragments of our projected new target compound were already in hand, and this facilitated the design and implementation of its synthesis. Dr. Dietmar Kuhnt joined my group at that time as a post-doc, and I asked him to prepare the compound. And to our amazement and delight, this new compound proved to be a veritable bombshell when it was evaluated at Lilly.

## From the Wings of Butterflies

After extensive attempts by both Princeton and Lilly to improve on this compound, we found that this was still the most active compound in the series, and it was chosen for clinical trials. This compound is now known as Alimta.

Most striking was its remarkable activity against thymidylate synthase (TS). This folate-dependent enzyme is required for the biosynthesis of thymidine, and thus DNA, and finding an effective inhibitor of TS was considered at that time to be the Holy Grail for cancer researchers. Furthermore, our new compound also proved to be an inhibitor of several other folate dependent enzymes including dihydrofolate reductase and glycinamide ribonucleotide N-formyltransferase. It was therefore, in essence, and all by itself, the equivalent of a cocktail of antitumor agents, with the advantages of the usual antitumor cocktail (a combination of different drugs with different targets of action) but without its disadvantages (a combination of the toxicities of each drug in the mixture).

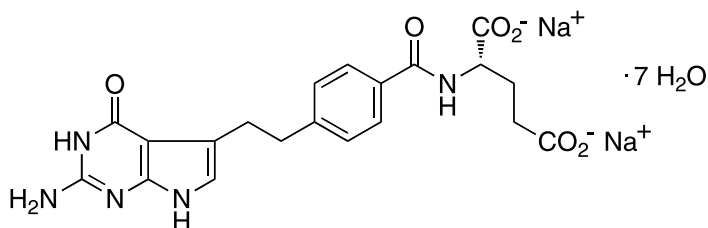
The transformation of Princeton's new clinical candidate compound into an effective and successful cancer drug has been described as possessing all of the elements of a great action movie - overcoming obstacles, detective work, perseverance and, ultimately, a triumph for patients. It was the result of the remarkable scientific collaboration between Princeton and Lilly that should stand as a model of what can be possible when academia and industry truly work together.

Everyone was ecstatic when early clinical trials showed that almost all solid tumors examined responded to Alimta. Perhaps the most remarkable of all the responses was that with malignant pleural mesothelioma, the devastating lung cancer caused primarily by exposure to asbestos. No clinically effective treatment for mesothelioma was previously known.

The results of clinical trials in mesothelioma were so promising that even before the drug was approved, the FDA allowed Lilly to provide it free of charge to more than 1000 medically eligible patients through a compassionate use program.


Many obstacles lay ahead. For instance, in the last phase of stability testing, glass particles appeared in the vials of Alimta. These particles were caused by a totally unexpected interaction of liquid Alimta and the glass. Lilly scientists quickly reconstituted the drug into a new powdered formulation. In addition, during a Phase I clinical trial, some patients reacted to Alimta administration with skin rash. Lilly found that this effect could be mitigated by the addition of a low dose of oral steroids to the treatment regimen.

In 2004, Alimta, in combination with cisplatin, received its first FDA approval for the treatment of malignant pleural mesothelioma when surgery was not an option. Within five years, Alimta received three more



Alimta™

approvals for the treatment of advanced nonsquamous non-small cell lung cancer. Through these clinical trials, researchers have shown that tumor histology can be used to determine which NSCLC patients may benefit from Alimta treatment.

Today, Lilly is continuing studies of Alimta in combination with other therapies and in new tumor types at cancer centers around the world. 

Edward C. Taylor <etaylor@princeton.edu> is A. Barton Hepburn Professor of Organic Chemistry Emeritus at Princeton University. Taylor's career has involved pioneering studies in organic synthesis methodology, organometallic chemistry, natural products, and medicinal chemistry.

1. Glasgow was the site of the 23rd International Congress on Heterocyclic Chemistry held 31 July-4 August 2011. Other papers presented at the ICHC-23 will appear in the IUPAC journal *Pure and Applied Chemistry*.

# The Kilogram in the “New SI”

For good reason, chemists regularly follow progress made by the Bureau International des Poids et Mesures (BIPM) toward the so-called “New SI.” The International Committee for Weights and Measures (CIPM) of the BIPM continues to ponder over the redefinition of the kilogram, which is the only base unit of the SI still tied to an artifact. CIPM drafted a Resolution for consideration this coming October at the General Conference on Weights and Measures (CGPM) meeting, noting its intention to redefine four of the SI base units, namely the kilogram, the ampere, the kelvin, and the mole, in terms of invariants of nature. The new definitions would be based on fixed numerical values of the Planck constant ( $h$ ), the elementary charge ( $e$ ), the Boltzmann constant ( $k$ ), and the Avogadro constant ( $N_A$ ), respectively. In order to encourage communication, awareness, and debate on the possible revision of the SI, BIPM has provided key draft documents on its website at [www.bipm.org/en/si/new\\_si](http://www.bipm.org/en/si/new_si).

Readers of *CI* have been informed of these developments and in several instances Ian Mills, IUPAC representative on CIPM Consultative Committee on Units (CCU) and president of CCU, has reviewed the issues; see “An Update on the Kilogram” (*CI* Sep-Oct 2005, pp. 12-15); “Amount and Substance and the Mole,” I. Mills and M. Milton (*CI* Mar-Apr 2009, pp. 3-7); “What is a Mole? Old Concepts and New” by Jack Lorimer, “A Fixed Avogadro Constant or a Fixed Carbon-12 Molar Mass: Which One to Choose?” by Y. Jeannin, and “Closing Comment” by Ian Mills (*CI* Jan-Feb 2010, pp. 6-11).

In this two-part feature, Albert C. Censullo et al. start with a review of the status of the kilogram and their understanding of it and end by offering an alternative proposal. In part II, Ian Mills responds by reviewing the rationale behind the proposed new SI, the concept of explicit-constant definitions, and the implications of the definitions of both the kilogram and mole.



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

## Part I—From the Current “Kilogram Problem” to a Proposed Definition

*by Albert C. Censullo, Theodore P. Hill, and Jack Miller*

**T**he metric system of measurements has served the international scientific and technical communities well since its inception over 200 years ago. By the mid 1800s, three so-called “base units” were in place, for measuring distance, mass, and time (centimetre, gram, second, or CGS system). These base units evolved into the metre, kilogram, and second (MKS system). The ampere became the fourth base unit in 1946. In 1954, the kelvin and candela became new base units. Finally, in 1971, the mole became the seventh base unit, for amount of substance. The definitions of each base unit have undergone continuous evolution, corresponding to improvements in measuring capabilities, and recognition of shortcomings of

prior definitions. As stated by BIPM, “The SI is not static but evolves to match the world’s increasingly demanding requirements for measurement.”

Of the seven base units in existence today, only one of them is based on a physical artifact. The current definition for the kilogram is embodied in *Le Grand K*, the platinum-iridium cylinder maintained by the BIPM in Sèvres, near Paris. Comparisons with virtually identical artifacts suggest that the mass of *Le Grand K* may have changed by 50 micrograms, or possibly even more, from its date of creation in 1884. Starting with the 1963 redefinition of the second and the 1983 redefinition of the metre, there has been a call to replace the definition of the kilogram with a more suitable one, using some “invariant of nature” to replace the artifact kilogram.<sup>1</sup> Since the perceived weakness of the current SI definitions of other units such as the ampere, mole, and candela “derives in large part from their dependence on the kilogram . . . the definition of the kilogram is thus central to the more general problem of improving the SI.”<sup>2</sup> This so-called “kilogram problem” is the subject of this paper.

# The Kilogram in the “New SI”

## Current Proposed Definition for the Kilogram

Following the success of the redefinition of the second and the metre, a revision of the entire system of measurements was envisioned, based on defining units based on fundamental constants. As stated in the current draft *SI Brochure* for the proposed new SI,<sup>3</sup> “The present definitions of the seven base units are made in terms of the values of seven fundamental constants that are believed to be true invariants throughout time and space, available to anyone, anywhere, at any time, who wishes to realize and make use of the values of the units to make measurements.”

Effort was made to maintain style consistency in the new definitions. The proposed definitions belong to a class known as “explicit-constant definitions.” In the draft proposal, each definition is linked to a specific fundamental constant and states explicitly the numerical value of the fixed constant. Underlying principles and laws of physics are intended to allow the definition of the unit to become apparent. According to BIPM,<sup>1</sup> “The metre is the length of the path travelled by light in vacuum during a time interval of  $1/299\,792\,458$  of a second.” In that case, the relationship between speed, time, and distance is obvious, and easily comprehended. As will be seen, this is not quite the case for the new kilogram definition.

A set of preliminary proposals under consideration by BIPM for redefining the kilogram began appearing in the literature five or six years ago.<sup>2,4</sup> The idea put forth involved the establishment of either an “electronic kilogram” or an “atomic kilogram,” whose definition would be based on fixing the value of either of two constants, Planck’s constant or Avogadro’s constant, respectively. Eventually, redefinition via Planck’s constant, the electronic kilogram, became the recommended approach by the Consultative Committee on Units and it was forwarded on to the BIPM. This has been verified by the BIPM’s release of the draft chapter 2 of the 9th edition of the *SI Brochure* in which the proposed new definition for the kilogram is as follows:

“The kilogram, kg, is the unit of mass; its magnitude is set by fixing the numerical value of the Planck constant to be equal to exactly  $6.626\,068\,563 \times 10^{-34}$  when it is expressed in the unit  $\text{s}^{-1} \text{m}^2 \text{kg}$ , which is equal to  $\text{J s}$ .”

(The “X” refers to as-yet-unspecified additional digits.)

The indirect implied relationship between the kilo-

gram and Planck’s constant is not immediately apparent from the definition, and requires knowledge of both special relativity and quantum mechanics.<sup>5,6</sup>

Mills et al.<sup>2</sup> present a case for dramatic changes to the SI system of units. They noted that the most important quality of newly defined units was that the defining quantity should be a true invariant of nature. The International Committee for Weights and Measures of the BIPM called for the widest possible publicity be given to these ideas among the scientific and user communities (94th meeting in October 2005). Other important factors were as follows: (a) practical realization of definition should be possible anywhere, at anytime; (b) definition should be readily comprehensible to students in all disciplines; and (c) continuity of definition should be preserved, for consistency with older definition.

## Criticism of the Proposed SI

In the past year or two, there has been increasing discussion appearing in the literature by members of the international scientific community on the proposed system referred to by BIPM as the “New SI.”

The Consultative Committee on Units’ recommendation, which IUPAC supports, is to define the mole as the amount of substance of specified elementary entity, such that the Avogadro constant is exactly  $6.022\,141\,79 \times 10^{23}$  per mole.<sup>2</sup> This means that a mole contains Avogadro’s number of entities. The result of this assignment is that the molar mass of  $^{12}\text{C}$  will no longer be fixed by definition, but will be an experimental quantity.

Leonard<sup>7</sup> points out a “compatibility condition” that naturally exists between Planck’s constant, Avogadro’s constant, and the mass of the carbon-12 atom, such that  $h N_A = K_c M(^{12}\text{C})$ , where  $K_c$  is a combination of constants:  $K_c = (c_0/2)(1/R_\infty)[m_e/m(^{12}\text{C})]\alpha^2$ . He points out that any two of the quantities ( $h$ ,  $N_A$ ,  $M(^{12}\text{C})$ ) may be fixed, but the third must be related by the aforementioned compatibility condition. If we wish to maintain  $M(^{12}\text{C})$  as exactly 12, either  $h$  or  $N_A$  must be determined experimentally; they cannot both be assigned exact values. If both  $h$  and  $N_A$  are fixed (as in the proposed New SI definition), the mass of the carbon-12 atom will no longer be fixed, but becomes a quantity to be determined (and re-determined) experimentally, as higher precision techniques may eventually allow. This variance of what chemists normally consider invariant causes its own “kilogram problem.”

Dissenting from the CCU view, Jeannin<sup>8</sup> noted the present definition of the mole (amount of substance containing as many entities as there are atoms in 0.012 kg of carbon-12) implies a fixed molar mass of carbon-12  $M(^{12}\text{C})$  as exactly 12 grams/mole. This definition requires that the unit of mass (kilogram) must be defined prior to defining the mole. The proposed definition<sup>2</sup> de-couples the mole from the kilogram, which was viewed as desirable. However, the three values for Planck's constant ( $h$ ), the Avogadro constant ( $N_A$ ), and carbon-12 molar mass,  $M(^{12}\text{C})$ , are still linked. This presents a dilemma to the chemist, who tends to think of the carbon-12 atom as a "true invariant of nature," perhaps the ultimate invariant of nature.

Khrushchov<sup>6</sup> compares defining the kilogram in terms of either  $h$  or  $N_A$ . He describes the watt-balance method for producing an "electronic kilogram," based on the equation relating electrical and mechanical power that may be written as  $mgv/K = h/4$ . By fixing the value for  $h$ , the mass may be "measured," based on other known constants and experimental variables (velocity, voltage, and current) which have very small uncertainties. He states, "the basis of this definition will not be a natural invariant, such as the mass of a carbon atom, but an artificially created electro-mechanical device, the watt balance, with a large number of sources of systematic uncertainty."<sup>6</sup> As of this date, discrepancies between experimental values for Planck's constant determined by U.S. and U.K. watt balance teams have not been resolved.

The alternative "atomic kilogram" is based on an exact value for Avogadro's number, so an accurate count of a large number of atoms must be made. The current method for obtaining this number is based on a crystalline silicon sphere, and complications of this experiment include uncertainties in isotopic abundance of the silicon atoms, as well as impurities and defects in the crystal, and adsorbed surface oxides. Khrushchov and his colleagues find an atomic kilogram "logically consistent and intuitive, which makes it convenient for use in education." They propose the definition: the kilogram is the exact mass of  $N_A/0.012$  free atoms of carbon-12, where  $N_A$  must be a multiple of 12 so that the gram and kilogram will contain an integral number of atoms. They conclude "new definitions of the units of mass and amount of substance should be based on a fixed value of the Avogadro constant<sup>9</sup> and the mass of the carbon atom." We share this view.<sup>5</sup>

Milton et al. outlined several key aspects desired in an updated SI system.<sup>10</sup> They recognized the need for a

dynamic measuring system, responsive to scientific and technological advances, that is responsive to the needs and views of the scientific community of users. As stated in that article, "Any new definition must be comprehensible to this audience . . ." The New SI System's reliance on quantum standards, intended to reduce the uncertainty in measurements, limits the realization of the definitions to highly specialized experimentations with equipment that is not readily available. For example, to realize the new definition of the kilogram, a watt balance is often suggested as the *mise en pratique*. There are only a few of these expensive and complex devices in the global metrology community. This hardly fulfills the BIPM directive that "The new definitions will be referenced to true invariants of nature, and may be realized by anyone, anywhere, at any time."<sup>11</sup> Milton et al. find that the redefinition of the kilogram is premature, and potentially dangerous to the integrity of the SI System. Their [2007] conclusion, "At present, there is insufficient experimental evidence to justify any proposed resolution of the 'kilogram problem' . . ." should serve as a caution to those interested in any potential immediate redefinition of the kilogram.

A number of issues concerning the "New SI" have been raised in the summary article by G. Price.<sup>11</sup> Some objections include: difficulty in explaining definitions to new users of the SI system (including beginning students in the physical sciences); continued use (rather than clarification) of the confusing term "amount of substance"; increasing interdependency of base units (making systematic errors more difficult to detect, and complicating the redefinition of any single unit); likely inconsistencies produced by fixing the exact values of many physical "constants" (unless the exact "correct" values for all of these constants happened to be fortuitously chosen). The author refers to the new kilogram definition in this way: "the most obvious source of confusion in the New SI will be the definition of the kilogram, which no longer makes any reference to any real mass of any kind, artifactual or natural."

### A Constructive Alternative

As an alternative to the proposed electronic kilogram, a concrete atomic kilogram has been described.<sup>5</sup> There, some of the perceived shortcomings associated with the proposed New SI definition are described in detail. In lieu of that definition, an alternate formulation based on fixing Avogadro's constant is proposed, which is pedagogically simpler, and is based on a true

# The Kilogram in the “New SI”

invariant of nature, the carbon-12 atom. Under this definition,

“a kilogram is the mass of  $84\,446\,889^3 \times 1000/12$  unbound atoms of carbon-12 at rest, in their ground state.”

The factor of 1000 is, of course, a necessary requirement that results from the use of the kilogram (rather than the gram) as the unit of mass. This definition fully satisfies the desirable qualities of unit redefinition, (a), (b), (c) above. It has the added advantage of maintaining the value of the carbon-12 atom at its exact value of 12, ensuring that tables of atomic masses will not need to be periodically adjusted.

We hope that the scientific community has adequate opportunity to review and propose alternative definitions for the kilogram, as well as other SI units, before any changes are promulgated. A delay in producing a “New SI” seems to be a perfectly acceptable alternative for the present.

## References

1. *SI Brochure* 8th edn, Bureau International des Poids et Mesures, SI; [www.bipm.org/en/si](http://www.bipm.org/en/si)
2. I.M. Mills, P. Mohr, T. Quinn, B. Taylor, and E. Williams, *Metrologia* **43** 227–46 (2006).
3. BIPM draft of new SI, 2010 [www.bipm.org/utis/common/pdf/si\\_brochure\\_draft\\_ch2.pdf](http://www.bipm.org/utis/common/pdf/si_brochure_draft_ch2.pdf)
4. I.M. Mills, P. Mohr, T. Quinn, B. Taylor, and E. Williams, *Metrologia* **42** 71–80 (2005).
5. T.P. Hill, J. Miller, and A.C. Censullo, *Metrologia* **48** 83–86 (2011).
6. A. Khrushchov, *Meas. Tech.* **53** 583–91 (2010).
7. B. Leonard, *Metrologia* **43**, L3–L5 (2006).
8. Y. Jeannin, “What is a Mole?: Old Concepts and New (continued)” *Chem. Int.* **32** (1) 8–11 (2010).
9. R.F. Fox and T.P. Hill, “An exact value for Avogadro’s number,” *Am. Sci.* **95** 104–107 (2007).
10. M. Milton, J. Williams, and S.J. Bennett, “Modernizing the SI: towards an improved, accessible and enduring system”, *Metrologia* **44**(5) 356–364 (2007).
11. G. Price, “A skeptic’s review of the New SI,” *Accred. Qual. Assur.* **16** 121–132 (2011).

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## Part II—Explicit-Constant Definitions for the Kilogram and for the Mole

by Ian Mills

Censullo et al. suggest the following changes to the present proposals for the new SI. They prefer explicit-unit definitions over the proposed explicit-constant definitions of all the units. They would prefer the kilogram to be redefined to fix the mass of an atom, such as the carbon 12, rather than to fix the value of the Planck constant. They would prefer the mole, and hence the Avogadro constant, to be defined to fix the molar mass of carbon 12 (which is the current definition) rather than by defining the mole explicitly by specifying the number of entities in a mole, and thus fixing the numerical value of the Avogadro constant. Each of these issues is discussed in turn below. A more detailed discussion can be found in reference 1. The copy of Resolution A for the 24th CGPM to be held in October 2011,<sup>2</sup> and the FAQs,<sup>3</sup> are also relevant; both are available on the BIPM website.

### Explicit-constant versus explicit-unit definitions

The distinction between explicit-unit and explicit-constant definitions may be illustrated by the present definition of the metre. The more familiar explicit-unit definition reads:

**The metre is the length of path travelled by light in vacuum in 1/299 792 458 of a second.**

Exactly the same definition expressed in the proposed explicit-constant form reads:

**The metre, m, is the SI unit of length; its magnitude is set by fixing the numerical value of the speed of light in vacuum to be equal to exactly 299 792 458 when it is expressed in the unit m s<sup>-1</sup>.**

The advantage of the explicit-constant format is that it emphasizes the reference constant used in the defini-

## Part II

tion, which in this case is the speed of light, and which actually defines the unit metre per second rather than the metre. It also avoids suggesting that the definition of the metre is realized by measuring the speed of light, which is not the case. The definition of a unit should be distinguished from its realization (described as the *mise en pratique* for the unit), because experiments to realize a definition may change as experimental techniques develop, and new experiments may be devised. The definition of the metre, for example, is actually realized by combining sophisticated laser experiments with interferometry, which are not simple to describe, rather than by measuring the speed of light.

Explicit-constant definitions emphasize the fundamental importance of the reference constants used to define the units, rather than the base units themselves, which are less important. They also allow a simple definition of the entire system of units in a single sentence by specifying the exact numerical values of seven reference constants, as illustrated in the Resolution A proposed by the CIPM, and also in reference.<sup>1</sup> It is important to note that the seven reference constants must be taken together to define the system. This is the most fundamental approach to defining the system of units, and it makes no reference to the base units—which indeed are not needed to define the system of units. These are the reasons why the CIPM prefer the explicit-constant format for all the definitions.

### Choosing the reference constant to define the kilogram

The proposed explicit-constant definition of the kilogram in the new SI reads:

**The kilogram, kg, is the SI unit of mass; its magnitude is set by fixing the numerical value of the Planck constant to be equal to exactly 6.626 068 ...  $\times 10^{-34}$  when it is expressed in the unit  $\text{s}^{-1} \text{m}^2 \text{kg}$ , which is equal to J s.**

This defines the unit of action,  $\text{s}^{-1} \text{m}^2 \text{kg}$ , rather than the unit of mass, the kg. But when taken as part of the complete set of reference constants, in which the second s is defined by fixing the caesium hyperfine frequency and the metre m by fixing the speed of light, it is seen that fixing the Planck constant  $h$  defines the kilogram.



*Mechanism of the BIPM watt balance under construction at the BIPM at Sèvres.  
(Reproduced with permission from BIPM.)*

The alternative to using  $h$  as the reference constant would be to use the mass of an atom, probably the carbon 12 atom,  $m(^{12}\text{C})$ , or another atom, or even the mass of the electron. It is certainly true that this would have the advantage of being easier to comprehend and to teach. However choosing  $h$  has other advantages which the CIPM judge to be more important. There are two main reasons for preferring to use  $h$  as the reference constant.

The first is that in the new SI it is proposed to fix both  $h$  and  $e$  (where  $e$  is the elementary charge, the charge on a proton). This would result in exactly known values for the Josephson constant  $K_J = 2e/h$  and the von Klitzing constant  $R_K = h/e^2$ , which are used to interpret Josephson effect measurements of electromotive force and quantum Hall measurements of electrical resistance. These are now universally used for all precise electromagnetic measurements, and if the values of  $K_J$  and  $R_K$  were exactly known it would bring all electrical measurements into the SI. The present practice is to use the conventional values  $K_{J-90}$  and  $R_{K-90}$  that were the best estimates of these constants in 1990, in order to ensure international consistency in electrical units. But these conventional values are

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not consistent with the other SI units. For this reason, workers in the field of electromagnetism are strongly in favor of fixing  $h$  and  $e$ , and they are a very important community.

The second reason is that the  $c$ ,  $h$ , and  $e$  are the most fundamental constants of physics, in relation to relativity, quantum mechanics, and quantum electronics respectively. It is the overall objective of the new SI to base all our units on the fundamental constants of nature, and these three constants top the list. Since we are choosing a system of units for the world that may last for many years, there are compelling reasons for choosing the most fundamental constants of physics as the reference constants to be fixed.

It is important to add that an alternative definition in terms of the mass  $m(^{12}\text{C})$  would be only very slightly different from the definition in terms of  $h$ , because of the fundamental relation of physics:

$$\frac{h}{m(^{12}\text{C})} = \frac{\alpha^2 c}{2R_\infty} \left( \frac{m_e}{m(^{12}\text{C})} \right) \quad (1)$$

That relation does not involve any units; it expresses relations between the values of the quantities involved that must be satisfied whatever units are used.<sup>1</sup> The product of factors on the right hand side is known at present with a relative standard uncertainty of less than  $1 \times 10^{-9}$ , which is more than an order of magnitude smaller than the present uncertainty in  $h$  or  $m(^{12}\text{C})$ . Thus,  $h$  may be calculated from  $m(^{12}\text{C})$ , and, hence, fixing  $h$ , or fixing  $m(^{12}\text{C})$ , are almost equivalent definitions. The CIPM prefers the definition to fix  $h$ , for the reasons described above. This definition will be realized by using any experiment that at present may be used to determine  $h$ , such as either a watt-balance, or the XRCd experiment on a silicon 28 sphere to determine  $h$  from  $m(^{28}\text{Si})$  using equation (1) above where  $m(^{12}\text{C})$  is substituted both sides by  $m(^{28}\text{Si})$ . The change to the new definition of the kilogram will not be made until the value of  $h$  determined by these experiments agree to a few parts in  $10^8$  (at present the best experimental results differ by about a part in  $10^7$ ).

Censullo et al. argue that these experiments involve expensive and complicated equipment; although this is clearly true, it is also true that this criticism applies to experiments to realize any of the definitions of SI units at the level required for modern quantum physics.

## Choosing the Reference Constant to Define the Mole

There are two quantities which are currently used to quantify the amount of a pure chemical sample in a manner that is proportional to the number of molecules, or entities, in the sample. The first is simply to use the quantity *number of entities*, denoted  $N$ , which is dimensionless, or of dimension 1. The second is to use the quantity *amount of substance*,  $n$ , which is regarded as a base quantity in the system of quantities and units currently adopted in chemistry. Amount of substance thus has its own unit in the SI, the mole, symbol mol. The two quantities  $N$  and  $n$  are related by the equation

$$n = N/N_A \quad (2)$$

where the conversion factor  $N_A$  is the Avogadro constant. These statements are true regardless of how the mole is defined. The unit 1 for the quantity  $N$  does not need to be defined, because it is simply the unit of a count, which is 1.

There are two alternative ways of defining the mole to be considered. The first is to use the molar mass of carbon 12 as the reference constant, thus fixing exactly the value of the molar mass  $M(^{12}\text{C})$ . This is the definition in the current SI; expressed in explicit-constant form it would read:

**The mole, mol, is the SI unit of amount of substance of a specified elementary entity, which may be an atom, molecule, ion, electron, any other particle or a specified group of such particles; its magnitude is set by fixing the numerical value of the molar mass of carbon 12 to be equal to exactly 0.012 when it is expressed in the unit kg/mol.**

The second is to use the Avogadro constant as the reference constant, thus fixing exactly the value of  $N_A$ . Expressed in explicit-constant form it would read:

**The mole, mol, is the SI unit of amount of substance of a specified elementary entity, which may be an atom, molecule, ion, electron, any other particle or a specified group of such particles; its magnitude is set by fixing the numerical value of the Avogadro constant to be equal to exactly 6.022 141 ...  $\times 10^{23}$  when it is expressed in the unit mol<sup>-1</sup>.**




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The CIPM is recommending that the second definition should be adopted. The reasons are that the first definition links the mole to the kilogram, whereas the second definition is independent of the other base units. The second definition is also regarded as simpler to comprehend, and to teach, and  $N_A$  is regarded as a more fundamental constant than  $M(^{12}\text{C})$ , which is not tied to any particular atom.

At present,  $M(^{12}\text{C})$  is known exactly, and  $N_A$  is an experimentally determined constant with a relative standard uncertainty of  $5.0 \times 10^{-8}$  (using CODATA 2006 values of the fundamental constants). If we were to adopt the new SI recommended by the CIPM then  $N_A$  would be known exactly, and  $M(^{12}\text{C})$  would be an experimentally determined constant; it would still have the value 12 g/mol, but it would have a relative standard uncertainty of  $1.4 \times 10^{-9}$  (see table 2 in reference 1 below). The values and experimental uncertainty in the molar masses of other atoms would remain unchanged, because the contribution from the uncertainty in the relative molar masses is significantly greater than  $1.4 \times 10^{-9}$ . The actual atomic masses of the atoms are usually expressed on the atomic mass scale based on the mass of a carbon 12 atom  $m(^{12}\text{C}) = 12 \text{ u}$  exactly; none of the atomic masses expressed in either the unit u or in the kg would be changed by the new definition.

### Summary

The proposals for the new SI recommended by the CIPM involve using the fundamental constants  $h$ ,  $e$ , and  $N_A$  as three of the reference constants that would take fixed values in the new SI. The details of the proposed changes to the definitions of the units are explained in greater detail in reference 1. The overall effect of the changes will be to reduce the uncertainty with which almost all of the fundamental constants of physics are known by more than an order of magnitude, as shown in the table of uncertainties to the right.<sup>1</sup> In the new SI proposed by the CIPM, the unit of mass, in addition to all the other SI units, will be referenced to a true invariant of nature rather than a prototype artifact whose mass is known to be varying, perhaps by more than a part in  $10^7$  since it was adopted over a century ago. 

### References

1. I.M. Mills, T.J. Quinn, P.J. Mohr, B.N. Taylor and E.R. Williams, "Adapting the International System of Units to the 21st century," *Phil Trans Roy Soc* 2011 (in press).
2. BIPM 2011, Resolution A for the 24th meeting of the CGPM, *On the Possible Future Revision of the International System of Units, the SI*. [www.bipm.org/utis/common/pdf/24\\_CGPM\\_Convocation\\_Draft\\_Resolution\\_A.pdf](http://www.bipm.org/utis/common/pdf/24_CGPM_Convocation_Draft_Resolution_A.pdf)
3. BIPM 2011, Frequently Asked Questions about the New SI: [www.bipm.org/en/si/new\\_si/faqs.html](http://www.bipm.org/en/si/new_si/faqs.html)

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**Table of relative standard uncertainties for a selection of fundamental constants in the current SI and the new SI, multiplied by  $10^8$  (i.e., in parts per hundred million) (CODATA 2006)**

constant	current SI	new SI	constant	current SI	new SI
$m(K)$	0.0	5.0	$\alpha$	0.068	0.068
$h$	5.0	0.0	$K_J$	2.5	0.0
$e$	2.5	0.0	$R_K$	0.068	0.0
$k$	170	0.0	$\mu_0$	0.0	0.068
$N_A$	5.0	0.0	$\epsilon_0$	0.0	0.068
$R$	170	0.0	$Z_0$	0.0	0.068
$F$	2.5	0.0	$N_A h$	0.14	0.0
$\sigma$	700	0.0	$J \leftrightarrow \text{kg}$	0.0	0.0
$m_e$	5.0	0.14	$J \leftrightarrow \text{m}^{-1}$	5.0	0.0
$m_u$	5.0	0.14	$J \leftrightarrow \text{Hz}$	5.0	0.0
$m(^{12}\text{C})$	5.0	0.14	$J \leftrightarrow \text{K}$	170	0.0
$M(^{12}\text{C})$	0.0	0.14	$J \leftrightarrow \text{eV}$	2.5	0.0

Note: In this table the symbols denote the following constants:  $R$ : the molar gas constant;  $F$ : the Faraday constant;  $\sigma$ : the Stefan-Boltzmann constant;  $m_e$ : the electron mass;  $m_u$ : the unified atomic mass constant;  $m(^{12}\text{C})$ : the mass of a carbon 12 atom;  $M(^{12}\text{C})$ : the molar mass of carbon 12;  $\alpha$ : the fine structure constant;  $K_J$  and  $R_K$ : the Josephson and von Klitzing constants;  $\mu_0$  and  $\epsilon_0$ : the magnetic and electric constants;  $Z_0$ : the impedance of vacuum;  $N_A h$ : the molar Planck constant; and  $U_a \leftrightarrow U_b$ : the conversion factor between unit a and unit b.

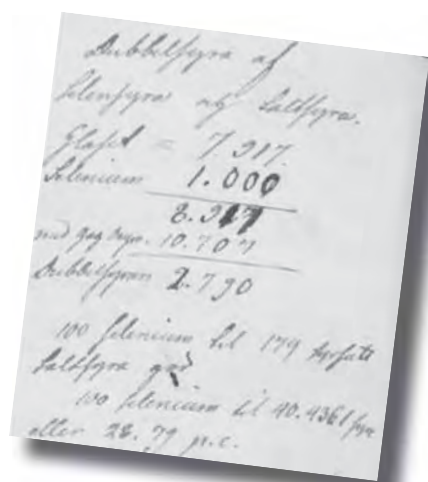
# Berzelius' Discovery of Selenium

*“Undersökning af en ny Mineral-kropp, funnen i de orenare sorterna af det vid Fahlun tillverkade svaflet.”<sup>1</sup>*

by Jan Trofast

## Swedish Discoveries of New Elements

Sweden has a long tradition of mining and assaying. As early as the mid-17th century, Sweden had a chemical laboratory devoted to the study of minerals and ores and the art of mineral analysis. The resulting research was often used to improve mining, iron, and steel production. During the first decades of the 19th century, Jacob Berzelius' laboratory in Stockholm became the center of these activities. From 1803 to 1843, Berzelius (1779-1848) and his Swedish pupils J.A. Arfvedson, N.G. Sefström, and C.G. Mosander discovered and characterized no less than 10 new elements. Many of these discoveries were made using a simple instrument—the blow pipe.<sup>2</sup>



*Determination of the composition of selenic acid. From Berzelius' laboratory notebooks, Ms. Berzelius, 24:6, Royal Swedish Academy of Sciences, Stockholm.*

### Elements Discovered by Swedish Chemists and Miners

Georg Brandt	cobalt	1735
Axel Fredrik Cronstedt	nickel	1751
Johan Gottlieb Gahn	manganese	1774
Carl Wilhelm Scheele	oxygen	1770s
Peter Jacob Hjelm	molybdenum	1782
Anders Gustaf Ekeberg	tantalum	1802
Jacob Berzelius	cerium	1803/4
	selenium	1818
	zirconium	1824
	silicon	1824
	thorium	1828
Johan August Arfvedsson	lithium	1817
Nils Gabriel Sefström	vanadium	1830
Carl Gustav Mosander	lanthanum	1839
	erbium	1843
	terbium	1843
Lars Fredrik Nilsson	scandium	1879
Per Theodor Cleve	holmium	1879
	thulium	1879

## The Gripsholm Chemical Factory

The first major chemical factory in Sweden was established in 1800 in a former distillery adjacent to the Castle of Gripsholm. Following drawn-out negotiations, the factory owners were granted the right to produce alcohol for the manufacture of acetic acid. At that time, one of the major uses of acetic acid was for the production of white lead paint. However, a poor business climate, unfair competition, and incompetent technical management forced the Gripsholm factory into liquidation in 1816. Fortunately, the factory was soon acquired at an auction by some businessmen and the chemists Johan Gottlieb Gahn (1845-1818), H.P. Eggertz, and Jac. Berzelius. Gahn's personal commitment to the business, persuaded Berzelius to join. Thus, three distinguished chemists became linked to the company. Berzelius had been one of the experts in settling disputes concerning the manufacturing rights of white lead. In a long letter to Gahn in late 1816, Berzelius discussed the chemical processes for the production of acetic acid and the improvements he considered necessary.<sup>3</sup>

As a devoted scientist, Berzelius was in principle disinterested in business, but in this particular case, he saw the potential to use scientific knowledge to establish a robust and profitable industrial business. He participated actively in matters in which he considered

himself capable of contributing. A typical example is the isolation of the new element selenium from the bottom sludge of the lead chambers used for sulfuric acid production.<sup>4</sup>

## The Discovery of Selenium

Berzelius and Gahn met at Gripsholm in August 1817. Berzelius spent more than one month there, studying, *inter alia*, technical issues related to the production of sulfuric acid and nitric acid (aqua fortis). The former owner of the factory, M. Bjuggren, had noted that a reddish sludge occurred in the lead chamber, only when pyrite (an iron sulfide) from the mine in Falun was used. The sludge was believed to be an arsenic compound and hence the Falun pyrite was avoided. However, Gahn and Eggertz both came from Falun and considered it interesting and important to use Falun pyrite. Therefore, Gahn and Berzelius—being the experts—tried to analyze the reddish sludge. By roasting 200 kg of sulfur they obtained about 3 g of a precipitate. Their subsequent chemical analysis of the sample indicated the possible presence of tellurium (discovered in mines in Transylvania in the 1780s). However, Berzelius doubted this result since tellurium had never been found in minerals from Falun. Nevertheless, he wrote about tellurium in letters to his close friends Alexandre Marcet and H.G. Trolle Wachtmeister in 1817.<sup>5</sup> In early 1818, Berzelius repeated

the experiments in his Stockholm laboratory and concluded that the sludge must contain a new element.

The new element had properties of a metal, and was similar to sulfur, initially suggesting it to be a new species of sulfur. In its metallic state, it had a brilliant grayish lustre. When heated by a candle using blow-pipe analysis, it burned with an azure-blue flame and emitted a strong odor of horseradish, typical of tellurium. This smell may initially have fooled Berzelius and Gahn.

Klaproth had assigned tellurium (Latin: tellus, earth) to Müller von Rechenstein's new element in 1784. Berzelius chose the name selenium (Greek: selene, moon) for the new element, noting its resemblance to tellurium. The naming was described (in Swedish):

*. . . skola beskrifvas vara en egen förut okänd brännbar mineral kropp, hvilken jag har kallat Selenium af Σελήνη, måna, för at dermed utmerka dess nära släktskap med Tellurium.*<sup>6</sup>

Berzelius was able to prove that selenium was indeed a new element after establishing its properties, as well as the properties of the compounds it formed with metals, oxygen, hydrogen, sulfur, phosphorus, and different salts. Due to the similarity between selenium and sulfur and tellurium, Berzelius carefully investigated the properties of these elements (e.g., their ability to form gaseous compounds and their reactivity towards oxygen and metals). In the appendix to the third volume of his *Textbook in Chemistry*, published in 1818, Berzelius gave the formulas of 90 different selenium compounds (58 selenias, 20 selenietum, and 12 hydroselenietum) together with the atomic weight of the element itself. A remarkably high number of compounds!

Berzelius tried to reduce the selenium salts to the pure metal in different ways, but found it difficult to obtain it in a pure enough form for an atomic weight determination. The impurities, mainly mercury, copper, tin, lead, zinc, arsenic, and iron were difficult to remove. Eventually, he managed to obtain beautiful crystals of selenium, still preserved in the Berzelius collection in Stockholm, that he used to determine the atomic weight. These crystals were featured on a stamp commemorating the 200th anniversary of the Karolinska Institutet, the medical school founded by Berzelius and others and where Berzelius was a professor for 25 years.



*Statue of Jacob Berzelius in Berzelii Park, Stockholm, Sweden.*

## Berzelius' Discovery of Selenium

According to Berzelius, selenium formed two oxides—selenic oxide and selenic acid. His analysis of selenic acid gave the following:

	Content of each element (by mass %)	Content % by mass of oxygen per 100 % selenium
Selenium	71.261	100
Oxygen	28.739	40.33

Selenic acid corresponds to what we today denote as selenious acid ( $\text{H}_2\text{SeO}_3$ ). Berzelius reported its anhydride ( $\text{SeO}_2$ ) and assumed the selenic acid contained two oxygen atoms per selenium. Today, this compound theoretically contains 28.84 percent by mass oxygen—a remarkably accurate analysis by Berzelius in 1818!<sup>7</sup>

Berzelius determined the atomic weight of selenium to be 495.91 (O=100), corresponding to 79.34 (O=16).<sup>8</sup> The value today is 78.96, which again shows the accuracy of his chemical analysis.

His analysis of seleniuretted hydrogen (hydrogen selenide) gave the correct formula:<sup>9</sup>

	Content of each element (by mass %)	Atomic mass	Corresponding formula
Selenium	97.4	495.91	= Se
Hydrogen	2.6	13.27	= 2H

Since selenium possessed a brilliant metallic lustre, Berzelius thought it should be considered a metal. He subdivided the metals into two classes, those that are capable of forming acids, and those that act as bases: "... I place selenium among the acidifiable metals near arsenic . . ."<sup>10</sup>

Berzelius experienced first hand the toxicity of the gaseous selenium compounds, particularly selenuretted hydrogen (hydrogen selenide). As a medical doctor, Berzelius carefully described the sensation:

*The gas has the odor of sulphuretted hydrogen gas [hydrogen sulfide], when it is diluted with air; but if it is breathed less diluted, it produces a painful sensation in the nose and a violent inflammation, ending in a catarrh, which continues for a considerable length of time. I am still suffering from having breathed, some days ago, a bubble*

*of selenuretted hydrogeous gas, no larger than a small pea. Scarcely had I perceived the hepatic taste in the fauces, when I experienced another acute sensation: I was seized with a giddiness, which, however, soon left me, and the sensibility of the schneiderian membrane was so far destroyed that the strongest ammonia produced scarcely any effect upon the nose.*<sup>11</sup>

Berzelius first announced the new element in a letter of 27 January 1818 to J.S.C. Schweigger in Germany, followed by a letter in April for immediate publication in his *Journal für Chemie und Physik*, XXI (1817), 342-344. In February, he sent descriptions to scientific



*Jacob Berzelius (1779-1848) from a daguerreotype taken by J.W. Bergström 1844. Royal Swedish Academy of Sciences, Stockholm. ©Lennart Nilsson, photography/Scanpix.*

friends including C.L. Berthollet<sup>12</sup> (published in *Annales de Chimie et de Physique*), A. Marcet (published in *Annals of Philosophy*) and H.G. Trolle Wachtmeister.<sup>13</sup> The comprehensive investigation of the discovery of selenium was finalized in April 1818 and published in *Ahandlingar i Fysik, Kemi och Mineralogi*, VI, (1818), 42-144.<sup>14</sup>

These *Ahandlingar* (Dissertations) were published in six volumes from 1806 to 1818 by Berzelius and a few of his friends as a practical way of publishing scientific results without being in conflict with other Swedish journals at the time. *Ahandlingar* contain the remarkable scientific achievements made by Berzelius during his most productive years. The discovery of selenium

## Berzelius' Discovery of Selenium

was also included in his *Lärbok i Kemien (Textbook in Chemistry)*, III (1818), 410–417, although the element had already been described in the second volume of the textbook. The discovery was further reported to the Royal Academy of Sciences in Stockholm by publications in its transactions for 1818.<sup>15</sup> Selenium was first isolated from Falun pyrite, but Berzelius also searched for selenium in other minerals. He found 38.5 percent selenium in “selen-copper” or selenite ( $\text{Cu}_2\text{Se}$ , later called Berzelianite) and also in eukairite ( $\text{AgCuSe}$ ) from Skrikerum in Sweden.

Selenium was discovered thanks to the curious, analytical, and observant mind of Berzelius at a time when he was also heavily occupied with teaching medical students and overseeing his busy chemical laboratory. Selenium is now known as a trace element, which is essential for important antioxidant systems, thyroid function, and the immune system.

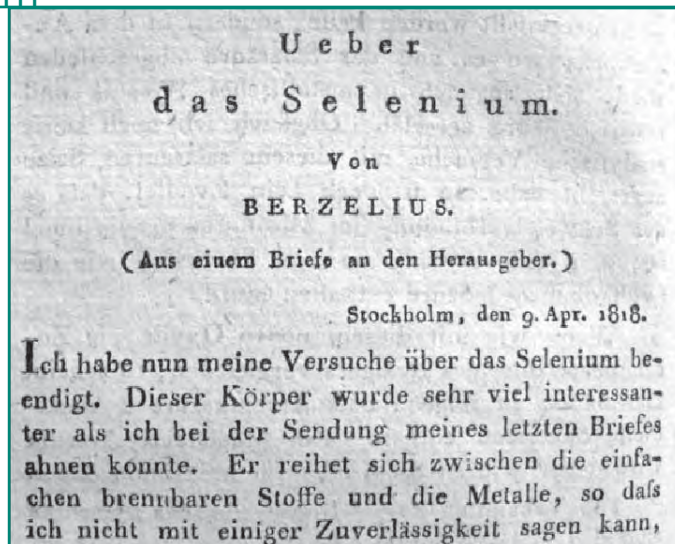
The discovery of selenium—just one example of Berzelius' many accomplishments—further established his reputation as one of the world's leading chemists of the 19th century. He revised the chemical nomenclature and in 1813 introduced the atomic notation system based on the Latin names of the elements, which, in principle, is still in use. He allowed these symbols to design the number of mass units given by the atomic mass of the particular element. Using this formalism, he could construct elegant and simple empirical formulas describing the composition (in mass %) of a given chemical compound. This important innovation finally translated chemistry into the language of atomic theory. For several decades, Berzelius dominated his scientific field more than any other chemist since. 🌱

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**Acknowledgement:** I would like to express my gratitude to Anders Kallner and Lars Ivar Elding for their support and great interest in the work of Berzelius and his contemporaries.

### Notes and References

1. “Investigation of a New Mineral, Found in the Impure Varieties of Sulphur, Manufactured at Fahlun”
2. U. Burchard, The History and Apparatus of Blowpipe Analysis, *The Mineralogical Review*, 25 (1994), 251–277.
3. Letter from J. Berzelius to J.G. Gahn 7 Oct. 1816, *Jac. Berzelius Brev*, IV:2 (1922), 140–142.
4. The laboratory notebooks describing the experiments on the discovery of selenium performed by Jac. Berzelius together with drafts to different publications



*The letter of 9 April 1818 from Jac. Berzelius to J.S.C. Schweigger was published in Journal für Chemie und Physik, bd XXI (1817), 342.*

- on selenium are kept at the Royal Swedish Academy of Sciences, Stockholm—Ms. Berzelius 24:6; 24:8 and 27:25:1-2.
5. Letter from J. Berzelius to A. Marcet 23 Sept. 1817, *Jac. Berzelius Brev*, I:3 (1914), 155–159.
  6. ... should be described to be a characteristic, not previously known, combustible mineral body, which I have called Selenium, derived from Σελήνη, moon, in order to indicate its resemblance with Tellurium.” Ms Berzelius 27:25:1, Royal Swedish Academy of Sciences, Stockholm.
  7. In his laboratory notebook Berzelius gave the value of the oxygen content as 28.79%!
  8. Jac. Berzelius et al., *Afhandlingar i Fysik, Kemi och Mineralogi*, VI, (1818), 42–144, particularly 68–74.
  9. *Ibid.*, 79.
  10. Letter from J. Berzelius to A. Marcet 6 February 1818, published in *Annals of Philosophy*, XI, (1818), 447–449.
  11. Letter from J. Berzelius to A. Marcet 6 February 1818. Marcet wrote on 25 March to John Bostock in order for the information to be published (*Annals of Philosophy*, XI (1818), 291–93).
  12. Letter from J. Berzelius to C.L. Berthollet 9 Feb. 1818. The selenium work was published in *Annales de Chimie et de Physique*, 9 (1818), 160–180, 225–267, 337–365.
  13. Letter from J. Berzelius to H. G. Trolle Wachtmeister 17 February 1818, published (ed. J. Trofast) in *Brevväxlingen mellan Herr Professorerna Jac. Berzelius och Hans Excellens H.G. Trolle Wachtmeister*, part 1 (1998), 40–42.
  14. A complete translation into English was published in *Annals of Philosophy*, XIII (1819), 401–412; XIV (1819), 97–106, 257–265; 420–427; XV (1820), 16–27.
  15. Jac. Berzelius, *Kongl. Vetenskapsakademiens Handlingar*, (1818), 13–22.

## 2012 Thieme–IUPAC Prize—Call for Nominations

**T**he Thieme–IUPAC Prize is presented every two years at the IUPAC International Conference on Organic Synthesis (IUPAC–ICOS). The 2012 ICOS will be held 1–6 July in Melbourne, Australia. The prize is awarded to a scientist under 40 years of age whose research has had a major impact in synthetic organic chemistry.

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

The Thieme–IUPAC Prize was awarded to Stuart L. Schreiber in 1992, Paul Knochel in 1994, Eric N. Jacobsen in 1996, Andrew G. Myers in 1998, Alois Fürstner in 2000, Erick M. Carreira in 2002, John F. Hartwig in 2004, David W. C. MacMillan in 2006, F. Dean Toste in 2008, and Phil S. Baran in 2010.

Proposals must be accompanied by a biographical sketch of the nominee, a list of the candidate's 10 most significant publications, and a statement of how the candidate's research has had a major impact on the field of synthetic organic chemistry. The material should be submitted by e-mail no later than **9 December 2011** to [marcus.white@thieme.de](mailto:marcus.white@thieme.de) and will be confidentially forwarded to an independent selection committee.

 [www.thieme-chemistry.com/our-service/thieme-iupac-prize.html](http://www.thieme-chemistry.com/our-service/thieme-iupac-prize.html)

## 2012 IUPAC Richter-Prize—Call for Nominations

**T**he IUPAC Subcommittee on Medicinal Chemistry and Drug Development has announced that the call for nominations for the 2012 IUPAC–Richter Prize is now open. The prize is awarded to an internationally recognized scientist, preferably a medicinal chemist, whose activities or published accounts have made an outstanding contribution to the practice of medicinal chemistry or to an outstanding example of new drug discovery.

Applications for the prize should be received by nomination only, with just one person needing to serve in that capacity, although a total of five individu-

als should be listed as referees overall. The package must be submitted electronically and should contain a complete résumé, a professional autobiography of not more than two pages, and a one-page summary of what the individual considers to be his/her activities, accomplishments, and/or publications that have had the most significant impact upon the field of medicinal chemistry.

The deadline for nominations is **31 December 2011**. Nomination materials should be submitted by e-mail to the IUPAC Secretariat at [secretariat@iupac.org](mailto:secretariat@iupac.org).

The 2012 IUPAC–Richter Prize will be presented in June 2012 at the ACS National Medicinal Chemistry Symposium at the University of Arizona, Tucson, USA, where the recipient will also give a plenary lecture on the subject of his/her research. The recipient is required to repeat the lecture at a medicinal chemistry symposium in Europe.

Previous IUPAC–Richter Prizes were awarded to Malcolm F.G. Stevens in 2006, to Jan Heeres in 2008, and to Arun K. Ghosh in 2010.

The prize was established by a generous gift from the Chemical Works of Gedeon Richter Plc. (Budapest, Hungary) to acknowledge the key role that medicinal chemistry plays in improving human health.

 [www.iupac.org/publications/ci/2011/3305/iw2\\_richterprize.html](http://www.iupac.org/publications/ci/2011/3305/iw2_richterprize.html)

## Crop Protection Chemistry Award Reminder

**N**ominations are due 1 December 2011 for the 2012 IUPAC International Award for Advances in Harmonized Approaches to Crop Protection Chemistry.

Presented by the IUPAC Division on Chemistry and the Environment, the award recognizes individuals in government, intergovernmental organizations, industry, and academia who have exercised personal leadership for outstanding contributions to international harmonization for the regulation of crop protection chemistry.

Awardees receive a USD 3000 honorarium plus travel and per diem reimbursement to attend the award presentation ceremony. Corporate sponsorship for the award is provided by Dow AgroSciences.

 [www.iupac.org/publications/ci/2011/3302/iw5\\_award.html](http://www.iupac.org/publications/ci/2011/3302/iw5_award.html)



## James Flack Norris Award to Peter Mahaffy

**T**he Northeastern Section of the American Chemical Society is pleased to announce that Prof. Peter Mahaffy is the recipient of the 2011 James Flack Norris Award for Outstanding Achievement in the Teaching of Chemistry. Within the classroom, Mahaffy is known for his highly effective and innovative teaching methods including his commitment to helping students, educators, scientists, and the general public to observe the intricate connections between science and their everyday lives.

Mahaffy was instrumental in establishing and co-directing the King's Centre for Visualization in Science which has allowed him to continue his development of digital learning resources that help learners see and understand scientific concepts that would otherwise be difficult to visualize. Each month, over 10 000 learners from over 70 countries contribute to their chemical understanding by visiting <[www.kcvs.ca](http://www.kcvs.ca)> where they access information on topics ranging from elementary science to chemistry, physics, and climate change science. During the International Year of Chemistry, Mahaffy has interacted with and learned from chemists and educators from around the world, observing the imaginative solutions they bring to the many challenges faced by scientists. The award will be formally presented to Mahaffy at the 10 November 2011 meeting of the Northeastern Section.

## In Memoriam

**Frederick William Sunderman Jr.**, B.S.c., MD, died 1 April 2011 in Middlebury, Vermont, at the age of 79. Bill was a founding member of the IUPAC Division of Clinical Chemistry in 1972. He served as chair of the Commission on Toxicology from 1972–1981 and as division president from 1981–1985. He remained active

in IUPAC for some years afterwards and was elected an Emeritus Fellow of the Division of Chemistry and Human Health in 2010.

Sunderman was born in Philadelphia and graduated with his MD in 1955. After a period as a lieutenant in the U.S. Navy, where he served as chief of the Clinical Chemistry Service at the U.S. Naval Medical School in Bethesda, he began his distinguished academic career as a scientist and teacher with a professorship at Thomas Jefferson University in Philadelphia. In 1968, he moved to Farmington, Connecticut, where he was a professor and chair of pharmacology, nutrition, and toxicology at the University of Connecticut Medical School until his retirement in 1997. Sunderman remained active in retirement, as a research professor of pathology at the University of Vermont and a visiting scholar in chemistry and biochemistry at Middlebury College. He published 258 research papers, 87 reviews, and 18 books, mostly in the area of metal toxicology. He was for many years the world's leading authority on nickel toxicology and in 1992 received an IUPAC Achievement Award for his research on nickel. He is remembered fondly by many as an always enthusiastic and supportive colleague and mentor.

**Kazuyuki Horie**, "Kaz," died on 29 April 2011 in Tokyo. Professor emeritus of The University of Tokyo and retired professor of Tokyo University of Agriculture and Technology, Horie was a longtime member of the IUPAC Polymer Division and in particular its Subcommittee of Polymer Terminology. He became an associate member of the Macromolecular Division in its Nomenclature Commission in 1996, becoming a titular member in 1998. He continued when the Macromolecular Division became the Polymer Division and then became a member of the Subcommittee on Polymer Terminology.

Horie was particularly active in many projects of the subcommittee and he was also involved in the translation of IUPAC recommendations into Japanese. He successfully initiated IUPAC projects and contributed significantly to many of them, including two recent projects: Guidelines for the Abbreviation of Polymer Names and the Glossary of Terms Related to Thermal and Thermomechanical Properties of Polymers. IUPAC has lost not only a knowledgeable member and a distinguished scientist but a true friend and a perfect ambassador of his country and its scientific community.

 [www.iupac.org/publications/ci/2011/3305/iw5\\_inmemoriam.html](http://www.iupac.org/publications/ci/2011/3305/iw5_inmemoriam.html)

## Using Process Mapping to Support (analytical) Laboratory Processes

The objectives of this new project of the Analytical Chemistry Division is to utilize process mapping for understanding, controlling, and documenting laboratory activities. Process mapping is a technique for graphically mapping and representing all steps of a complete system that form strings and/or networks of individual processes. The main purpose of applying process mapping in any complex activity is (1) to provide a common vision of the entire system and connectivity of its components, and to (2) emphasize any problem areas and opportunities that can be defined.

Since process mapping is suitable for complex and connected procedures, it can be used to analyze, optimize, and troubleshoot (with use of graphical mapping tools) any laboratory processes, from sample reception and analytical procedure to quality testing and reporting. The preliminary step to map a process is to collect information about all complex processes and see how well each process functions. It helps to identify risks and potential errors at each step. The process mapping itself will use this information to clarify the specific roles and contributions of each process participant.

This tool will be useful for any laboratory, irrespective of whether the quality standards are already implemented (accredited laboratories) or not (not-accredited laboratories). It is important to realize that process mapping does not substitute for any international quality standards (e.g., ISO 1025, ISO Guide 34, GLP, etc.). It is a step towards improving laboratory management by providing a unifying view of the entire process and allowing for reengineering of the management approach.

Creating a process map of all laboratory processes is a milestone (Milestone 1) for development/upgrade of the dedicated and optimized Laboratory Information Management Systems (LIMS) (Milestone 2). This allows implementation of the fully-fledged interactive research and management platform providing efficient and quality-assured tools for defining, assigning, and reserving tasks and activities, for monitoring progress to task-, data-, and report-levels at all stages, and for assuring the quality of measurement results and data, as well as identifying opportunities for continual improvement.

For more information, contact Massoud Malek <[m.malek@iaea.org](mailto:m.malek@iaea.org)>.

 [www.iupac.org/web/ins/2010-061-2-500](http://www.iupac.org/web/ins/2010-061-2-500)

## Sustainable Education and Environmental Development (SEED) in Latin America: Reflections on the Roots of Green Chemistry

Nowadays, the importance of the green chemistry movement is widely recognized around the world.<sup>1</sup> The goal of the Sustainable Education and Environmental Development (SEED) in Latin America project is to clarify the basis for, and discuss the applications of, green chemistry in Latin America, by establishing a continent-wide network. There are several, national green chemistry projects in developing countries, but this network would cover all of Latin America.

Since its inception in October 2009, the SEED has promoted a series of events and produced and distributed teaching and scientific material about green chemistry in Latin America. SEED has facilitated regular activities and contacts among Latin-American researchers and the most important worldwide networks in green chemistry. Following are some of the many courses and lectures organized by SEED in the past two years:

- 4th Regional Meeting of Biocatalysis and Biotransformation, Montevideo, Uruguay (December 2010)
- 31st Chemistry Summer School of Federal University of São Carlos, São Carlos, Brazil (February 2011)
- 37th Buenos Aires International Book Fair, Buenos Aires, Argentina (April 2011)
- 12th International Forum of Education of Science and Technology, Buenos Aires, Argentina (April 2011)

SEED has also helped improve communication among the green chemistry community through the launch of the SEED website, the introduction of a social network for “Green Chemistry Argentina” and the “Brazilian Network of Green Chemistry,” translation of the book *Green Chemistry: Fundamentals and Applications*<sup>2</sup> from Portuguese to Spanish, and publication of the book *Green Chemistry: New Habits to Learn*.<sup>3</sup>

Last but not least, the SEED network is also responsible for the organization of the 4th International IUPAC Conference on Green Chemistry (4th ICGC) to be held 25–29 August 2012 at Foz do Iguaçu, which is at the Brazilian border with Argentina and Paraguay. The conference is intended to provide opportunities for interdisciplinary debate across scientific and tech-





**SEED members at the 38th Journey of Young Researchers, Santa Fe, Argentina—Universities of the Group Montevideo Association (from left): Horacio Thomas, Jorge Sambeth, Gustavo Romanelli, Patricia Vazquez, Vania Zuin, and Arlene Correa.**

nological fields among researchers from Latin America and other countries about recent findings in green chemistry.

Considering all of its recent activity, one could say that the roots of the SEED group are growing healthfully.

#### References

1. P. Tundo, R.H. Rossi (Ed.), *Green Chemistry in Latin America*. Venice: INCA/IUPAC (2004).
2. A.G. Correa, V.G. Zuin (Ed.), *Química Verde: Fundamentos e Aplicações*. São Carlos: EdUFSCar (2009).

For more information, contact Patricia Vazquez <[vazquez@quimica.unlp.edu.ar](mailto:vazquez@quimica.unlp.edu.ar)>, Arlene Correa <[agcorrea@ufscar.br](mailto:agcorrea@ufscar.br)> or Vania Zuin <[vaniaz@ufscar.br](mailto:vaniaz@ufscar.br)>.

 [www.iupac.org/web/ins/2009-014-2-300](http://www.iupac.org/web/ins/2009-014-2-300)

## UNESCO/IUPAC Postgraduate Course in Polymer Science

The 15th run of the UNESCO/IUPAC Postgraduate Course in Polymer Science began in October 2010 and will conclude in July 2011 with the workshop Careers in Polymers III organized by the Institute. Five students from the following countries have been attending the course: Kazakhstan, Serbia, Vietnam, and Poland. In March, the mid-term seminar was held at which the students reported on the results of their research projects. More than half of the projects are likely to result in publications in international journals or communications at meetings.

Preparations for the 16th course are nearly complete. Out of the large number of applicants, 10 have

been nominated from India, China, Uruguay, Poland, Bulgaria, and Ukraine. The course will start in October 2011 and will be concluded in July 2012.

Cumulative results of the 15 runs held so far are as follows: 120 graduates, 20 nationalities, 173 publications in international journals, 306 communications at international meetings, and 2614 citations (all as of December 2010).

The course has become a global activity. Students from all continents except Australia and North America have graduated. The average publication output is more than one paper in an impacted journal, two conference communications, and about 22 citations per graduate. Of course, the distribution of scientometric hits per individual is very non-uniform. In several cases, a productive long-term co-operation has developed between the institute and the graduate's mother institution. In the last five years, 12 graduates became doctoral students at Czech universities. Graduation from the course often enhanced professional promotion in the home countries of the graduates. The course contributes to a positive image of IUPAC both inside and outside the professional community at virtually no cost for the Union.

For more information, contact Task Group Chair, Pavel Kratochvíl <[krat@imc.cas.cz](mailto:krat@imc.cas.cz)> or visit <[www.imc.cas.cz/en/imc/unesco.html](http://www.imc.cas.cz/en/imc/unesco.html)>.

 [www.iupac.org/web/ins/2010-015-1-400](http://www.iupac.org/web/ins/2010-015-1-400)

## Common Values of Nuclear Electric Quadrupole Coupling Terms for Appropriate Nuclei in Functionalized Hydrocarbons

Numerous common functionalized hydrocarbon chains contain quadrupolar nuclei,  $I > \frac{1}{2}$ , such as chlorine and nitrogen. These groups include halocarbons, acyl chlorides, nitriles, amines and amides. High resolution spectroscopy affords the measurement of nuclear electric quadrupole coupling constants for these nuclei within the molecule of interest. These constants are essentially the product of the nuclear electric quadrupole moment and the electric field gradient at the nuclei. The electric field gradient is informative for several reasons. First, the magnitude of the electric field gradient can be interpreted, via a simple model, in terms of the ionicity and/or hybridization of

## The Project Place

the bonding orbitals involving the quadrupolar nuclei. Second, these quantities can be directly linked to analogous values determined through nuclear magnetic resonance spectroscopy. Third, these “tight” quantities provide useful benchmark data for high-level computational chemistry methodologies.

We have already established that there are somewhat “standard” nuclear quadrupolar coupling constants for chlorine in various acyl chlorides  $\chi_{zz} \sim -60$  MHz, and furthermore, these values differ from the chlorine nuclear quadrupole coupling constants in perfluoroacyl chlorides,  $\chi_{zz} \sim -65$  MHz.

In this context, the task group for this project will scour the literature to determine more “standard” values. These data will be compiled, interpreted, and discussed.

For more information, contact Stephen Cooke < [sacooke@unt.edu](mailto:sacooke@unt.edu) >.

 [www.iupac.org/web/ins/2010-048-3-100](http://www.iupac.org/web/ins/2010-048-3-100)

## 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.*

### Guidelines for Reporting of Phase Equilibrium Measurements

Recommendations are given for reporting in the primary scientific literature of measurements involving phase equilibrium. The focus is on documentation issues, and many of the recommendations may also be applied to the more general fields of thermodynamic and transport properties. The historical context of the work and specific plans for implementation of the recommendations are discussed.

#### Comments by 31 October 2011

Robert D. Chirico  
National Institute of Standards & Technology  
Physical and Chemical Properties Division  
Thermodynamics Research Center, 838.01  
Boulder, Colorado, USA 80305-3328  
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 [http://media.iupac.org/reports/provisional/abstract11/chirico\\_311011.html](http://media.iupac.org/reports/provisional/abstract11/chirico_311011.html)

### Glossary of Terms Used in Immunotoxicology

The primary objective of this Glossary of Terms Used in immunotoxicology is to give clear definitions for those who contribute to studies relevant to immunotoxicology but are not themselves immunologists. This

applies especially to chemists who need to understand the literature of immunology without recourse to a multiplicity of other glossaries or dictionaries. The glossary includes terms related to basic and clinical immunology insofar as they are necessary for a self-contained document, and particularly terms related to diagnosing, measuring, and understanding effects of substances on the immune system. The glossary consists of about 1200 terms as primary alphabetical entries, and annexes of common abbreviations, examples of chemicals with known effects on the immune system, autoantibodies in autoimmune disease, and therapeutic agents used in autoimmune disease and cancer. The authors hope that among the groups that will find this glossary helpful, in addition to chemists, are toxicologists, pharmacologists, medical practitioners, risk assessors, and regulatory authorities. In particular, it should facilitate the worldwide use of chemistry in relation to occupational and environmental risk assessment.

#### Comments by 30 November 2011

Douglas M. Templeton  
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Toronto, ON M5S 1A8, Canada  
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 [http://media.iupac.org/reports/provisional/abstract11/templeton\\_301111.html](http://media.iupac.org/reports/provisional/abstract11/templeton_301111.html)

## Soils Contaminated with Explosives: Environmental Fate and Evaluation of State-of-the-Art Remediation Processes (IUPAC Technical Report)

Dimitrios Kalderis, et al.

*Pure and Applied Chemistry*, 2011

Vol. 83, No. 7, pp. 1407–1484

An explosion occurs when a large amount of energy is suddenly released. This energy may come from an over-pressurized steam boiler, from the products of a chemical reaction involving explosive materials, or from a nuclear reaction that is uncontrolled. In order for an explosion to occur, there must be a local accumulation of energy at the site of the explosion, which is suddenly released. This release of energy can be dissipated as blast waves, propulsion of debris, or by the emission of thermal and ionizing radiation. Modern explosives or energetic materials are nitrogen-containing organic compounds with the potential for self-oxidation to small gaseous molecules ( $N_2$ ,  $H_2O$ , and  $CO_2$ ). Explosives are classified as primary or secondary based on their susceptibility of initiation. Primary explosives are highly susceptible to initiation and are often used to ignite secondary explosives, such as TNT (2,4,6-trinitrotoluene), RDX (1,3,5-trinitroperhydro-1,3,5-triazine), HMX (1,3,5,7-tetranitro-1,3,5,7-tetrazocane), and tetryl (*N*-methyl-*N*-2,4,6-tetranitro-aniline).

 <http://dx.doi.org/10.1351/PAC-REP-10-01-05>

## Discovery of the Elements with Atomic Numbers Greater than or Equal to 113 (IUPAC Technical Report)

Robert C. Barber et al.

*Pure and Applied Chemistry*, 2011

Vol. 83, No. 7, pp. 1485–1498

The IUPAC/IUPAP Joint Working Party (JWP) on the priority of claims to the discovery of new elements 113–116 and 118 has reviewed the relevant literature pertaining to several claims. In accordance with the criteria for the discovery of elements previously established by the 1992 IUPAC/IUPAP Transfermium Working Group (TWG), and reinforced in subsequent IUPAC/IUPAP JWP discussions, it was determined

that the Dubna-Livermore collaborations share in the fulfillment of those criteria both for elements  $Z = 114$  and 116. A synopsis of experiments and related efforts is presented.

 <http://dx.doi.org/10.1351/PAC-REP-10-05-01>

## Defining the Hydrogen Bond: An Account (IUPAC Technical Report)

Elangannan Arunan, et al.

*Pure and Applied Chemistry*, 2011

Vol. 83, No. 8, pp. 1619–1636



and

## Definition of the Hydrogen Bond (IUPAC Recommendations 2011)

*Ibid*, Vol. 83, No. 8, pp. 1637–1641

The term “hydrogen bond” has been used in the literature for nearly a century now. While its importance has been realized by physicists, chemists, biologists, and material scientists, there has been a continual debate about what this term means. This debate has intensified following some important experimental results, especially in the last decade, which questioned the basis of the traditional view on hydrogen bonding. Most important among them are the direct experimental evidence for a partial covalent nature and the observation of a blue-shift in stretching frequency following  $X-H\cdots Y$  hydrogen bond formation ( $XH$  being the hydrogen bond donor and  $Y$  being the hydrogen bond acceptor). Considering the recent experimental and theoretical advances, a novel definition for the hydrogen bond is recommended that takes into account the theoretical and experimental knowledge acquired over the past century. This definition insists on some evidence. Six criteria are listed that could be used as evidence for the presence of a hydrogen bond.

The Technical Report and Recommendations are published back to back in *PAC*, providing both a detailed account and a straightforward definition.

 <http://dx.doi.org/10.1351/PAC-REP-10-01-01>  
 <http://dx.doi.org/10.1351/PAC-REC-10-01-02>

## Making an imPACT

### Polyaniline: The Infrared Spectroscopy of Conducting Polymer Nanotubes (IUPAC Technical Report)

Miroslava Trchová and Jaroslav Stejskal  
*Pure and Applied Chemistry*, ASAP article  
published online 10 June 2011

Polyaniline (PANI), a conducting polymer, was prepared by the oxidation of aniline with ammonium peroxydisulfate in various aqueous media. When the polymerization was carried out in the solution of strong (sulfuric) acid, a granular morphology of PANI was obtained. In the solutions of weak (acetic or succinic) acids or in water, PANI nanotubes were produced. The oxidation of aniline under alkaline conditions yielded aniline oligomers. Fourier transform infrared (FTIR) spectra of the oxidation products differ. A group of participants from 11 institutions in different countries recorded the FTIR spectra of PANI bases prepared from the samples obtained in the solutions of strong and weak acids and in alkaline medium within the framework of an IUPAC project. The aim of the project was to identify the differences in molecular structure of PANI and aniline oligomers and to relate them to supramolecular morphology, viz. the nanotube formation. The assignment of FTIR bands of aniline oxidation products is reported.

 <http://dx.doi.org/10.1351/PAC-REP-10-02-01>

### Metrological Traceability of Measurement Results in Chemistry: Concepts and Implementation (IUPAC Technical Report)

Paul De Bièvre et al.  
*Pure and Applied Chemistry*, ASAP article  
published online 15 June 2011

This IUPAC study aims at formulating recommendations concerning the metrological traceability of a measurement result in chemistry. It is intended to provide the chemical measurement community with a consistent view of the creation, meaning, and role of metrological traceability and its underpinning concepts. No distinction is made between measurement results obtained in "high metrology" and in the "field."

A description is given of the calibration hierarchies needed in different circumstances to arrive at metrological traceability along a metrological traceability chain. Flow charts of generic calibration hierarchies are presented as well as a variety of examples. The establishment, assessment, and reporting of metrological traceability are discussed, including the provision of metrological references by a metrological institutional framework and the role of interlaboratory comparisons.

 <http://dx.doi.org/10.1351/PAC-REP-07-09-39>

### Volatile Organic Compounds in Pesticide Formulations: Methods to Estimate Ozone Formation Potential

Mazyar Zeinali et al.  
*Atmospheric Environment* 45 (2011) 2404e2412;  
doi:10.1016/j.atmosenv.2011.02.015

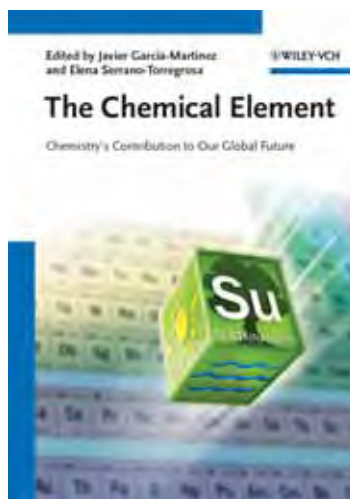
The environmental fate and toxicity of active ingredients in pesticide formulations have been investigated for many decades, but relatively little research has been conducted on the fate of pesticide co-formulants or inert. Some co-formulants are volatile organic compounds (VOCs) and can contribute to ground-level ozone pollution. Effective product assessment methods are required to reduce emissions of the most reactive VOCs. Six emulsifiable concentrate pesticide products were characterized for percent VOC by thermogravimetric analysis (TGA) and gas chromatography/mass spectrometry (GCeMS). TGA estimates exceeded GCeMS by 10–50% in all but one product, indicating that for some products a fraction of active ingredient is released during TGA or that VOC contribution was underestimated by GCeMS. VOC profiles were examined using TGAeFourier transform infrared (FTIR) evolved gas analysis and were compared to GCeMS results. The TGAeFTIR method worked best for products with the simplest and most volatile formulations, but could be developed into an effective product screening tool. An ozone formation potential (OFP) for each product was calculated using the chemical composition from GCeMS and published maximum incremental reactivity (MIR) values. OFP values ranged from 0.1 to 3.1 g ozone g<sup>-1</sup> product. A

(continued on bottom of page 27)

## The Chemical Element— Chemistry's Contribution to Our Global Future

Javier Garcia-Martinez and  
Elena Serrano-Torregrosa (editors)  
ISBN: 978-3-527-32880-2, 396  
pages, June 2011

Following the UN Millennium Development Goals, the authors examine the nine most critical areas, including energy, climate, food, water, poverty, education, and health. All of the authors are opinion leaders in their fields or high-ranking decision makers in national and international



institutions. This book provides an intellectual basis for the future development of chemistry. It is aimed at a wide readership including students, professionals, engineers, scientists, environmentalists, and anyone interested in a more sustainable future.

The book contains a foreword by IUPAC President Nicole Moreau and Julia Hasler (UNESCO Focal Point for IYC) and an epilogue by Jeffrey Sachs (director of The Earth Institute).

 [www.thechemicalelement.com](http://www.thechemicalelement.com)

## Macromolecular Symposia

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

### Macromolecular Complexes

Volume 304, June 2011  
doi: 10.1002/masy.201190016

Issue edited by Juan Costamagna, Franco M. Rabagliati, and Bernabé L. Rivas

This volume includes 16 invited contributions from the 13th IUPAC International Symposium on Macromolecular Complexes held at Termas de Chillán, Concepción, Chile, from 15 to 17 November 2009.

### Polymer-Solvent Complexes and Intercalates (POLYSOLVAT-8), Volume 303, May 2011

doi: 10.1002/masy.201190012

Issue edited by Jean-Michel Guenet

This volume includes 18 selected papers from the

international conference POLYSOLVAT-8 on Polymer-Solvent Complexes and Intercalates, which took place at the Institut Charles Sadron in Strasbourg (France) from 5–8 July 2010.

### POLYCHAR-18 World Forum on Advanced Materials

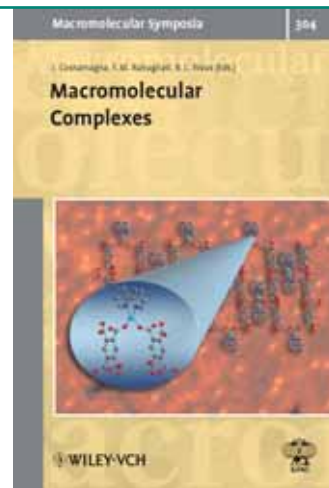
Volume 298, December 2010  
doi: 10.1002/masy.201190000

Issue edited by Werner Mormann

This volume includes papers from the 18th World Forum on Advanced Polymeric Materials held in Siegen, Germany, 7–10 April 2010.

Full text is available online.

 <http://onlinelibrary.wiley.com/journal/10.1002>



(continued from page 26)

24-h VOC emission simulation was developed for each product assuming a constant emission rate calculated from an equation relating maximum flux rate to vapor pressure. Results indicate 100% VOC loss for some products within a few hours, while other products containing less volatile components will remain in the field for several days after application. An alternate method

to calculate a product OFP was investigated utilizing the fraction of the total mass of each chemical emitted at the end of the 24-h simulation. The ideal assessment approach will include: 1) unambiguous chemical composition information, 2) flexible simulation models to estimate emissions under different management practices, and 3) accurate reactivity predictions.

This publication serves as the final outcome of IUPAC project 2006-011-1-600.

## Bookworm

### Heavy Elements—a special issue of *Radiochimica Acta*

Volume 99, No. 7-8, 2011

*Preface by Jens Volker Kratz, editor (reproduced below)*

This special issue of *Radiochimica Acta*, published in celebration of the International Year of Chemistry 2011, is devoted to the man-made transuranium elements which, at this time, represent almost a quarter of the Periodic Table of the Elements. The journal's editors asked eminent scientists working in the field of transuranium elements to write review articles on subjects such as the syntheses of the heaviest elements, their nuclear structure both from a theoretical and an experimental point of view, as well as on their chemical properties, which are also of both theoretical and experimental interest.

The heaviest elements owe their stability to nuclear shell effects without which they would not exist. Shell closures for deformed nuclei at neutron numbers  $N=152$  and  $N=162$  are well established. The location of the next spherical shell after the lead shell is still an open question. There is experimental evidence that the long-favored magic proton number  $Z=114$  is not the center of the predicted "island of stability," which means that the search for the next spherical proton-shell closure continues. Equally exciting are the chemical properties of the heaviest elements: They exhibit increasing nuclear charge on relativistic effects in the electron shell, giving them chemical properties that

deviate in a non-linear way from the properties of their lighter homologues in the periodic table. A most striking example is element 114 (eka-lead) which, due to the relativistic contraction and energetic stabilization of its radially symmetric  $7s^2$  and  $7p_{1/2}^2$  valence-electron orbitals constituting a relativistic electron-shell closure, is gaseous in its elemental state.

The first transuranium element, neptunium was discovered in 1940. The intervening decades have seen great changes in science in general, and very large increases in understanding and new concepts of the transuranium elements in particular. The techniques used to synthesize the heaviest elements have changed dramatically and involve, at this time, powerful heavy-ion accelerators. The detection techniques have been improved in a very sophisticated way. They allow us to detect single atoms and to assign their mass and charge numbers unequivocally. New theoretical concepts have been devised and continuously improved and have provided guidance for new attempts. The aim of this special issue is to convey the essence of the ideas and the spirit of theory and experiment that characterizes the study of these elements. It covers heavy-element discoveries, nuclear properties, nuclear structure and nuclear synthesis reactions, chemical properties, and experimental techniques. It is intended to serve as an up-to-date primer for the transuranium elements and as a convenient source of the key publications in this fascinating field of chemical research.

 [www.oldenbourg-link.com/toc/ract/99/7-8](http://www.oldenbourg-link.com/toc/ract/99/7-8)

### The African Journal of Chemical Education, second issue announced

In addition to Temechegn Engida's editorial providing a mid-year review of IYC 2011 in Africa, this issue includes a series of timely and topical papers

 [www.faschem.org](http://www.faschem.org)

#### AFRICAN JOURNAL OF CHEMICAL EDUCATION AJCE



Vol. 1, Number 2, July 2011



A Publication of

# Conference Call

## World Forum for Advanced Materials

by Michael Hess

The **19th World Forum for Advanced Materials**, POLYCHAR 19, was held in Kathmandu, the capital of Nepal, which started on 20 March 2011 with the Short Course on Polymer Characterization and ended on 24 March. This IUPAC-sponsored event was organized by Rameshwar Adhikari and his team from the Tribhuvan University Kathmandu and by the Nepal Polymer Institute Kathmandu.

The conference began with a traditional Nepalese inauguration ceremony that took place in the Open Theatre of the Park Village Resort Hotel. Chaired by the vice chancellor of Tribhuvan University, Madhab Prasad Sharma, the ceremony received much public attention because it featured a welcome address by the Right Honourable Prime Minister of Nepal, Jhala Nath Khanal. In his address, he stressed the relevance of holding this globally important materials science meeting in Nepal during the International Year of Chemistry. The Opening Ceremony was closed with a welcome address by a representative of the IUPAC Polymer Division. The conference was broadcast and publicized by several national Nepali media including Himalayan Television, Kantipur Television, Nepal Television, radios stations, and the Nepali national daily and weekly newspapers.

The scientific program covered a broad range of materials science topics with sessions focussing on Predictive Methods and Simulations, Nano-and Smart Materials, Electrical and Dielectrical Properties, Surfaces, Interfaces and Tribology, Mechanical Properties and Performance, Rheology and Processing, Structure-Properties Relationships, Materials Synthesis and Characterization, Biomaterials, and Materials for Energy and Recycling. In total, there were 137 oral contributions and 117 posters with 382 registered participants from 46 countries. The six keynote speakers represented six continents.

The conference began with a Short Course in Polymer Characterization, a traditional one-day tutorial taught by distinguished specialists. Chaired by Valerio Casuin (University of Padova, Italy) and Sven Henning (Fraunhofer institute for Micromechanics, Halle, Germany), it covered a wide range of topics. Following



*Byung-Wook Jo, Chosun University, Korea, with his Paul J. Flory Polymer Research Prize.*

is a brief sampling: Polymer Tribology (Witold Brostow, University of North Texas, Denton, USA), Polymer Characterization by Scattering Techniques (Jean-Michel Guenet, Institute Charles Sadron, Strasbourg, France), Dynamic-Mechanical and Calorimetric Analysis of Polymers (Michael Hess, University of Siegen, Germany), Chromatographic Characterization of Polymers (Dusan Berek, Slovak Academy of Sciences, Slovakia), and Trends in Chemistry of Nanocomposites (Anatolii D. Pomogailo, Russian Academy of Sciences, Moscow, Russia). Participants were provided with hand-outs of the teaching material and the lecturers were available for discussions throughout the duration of the conference.

It is always difficult to select specific contributions from the multitude of excellent presentations reflecting the wide span of aspects of Materials Science. One main focus of POLYCHAR 19 certainly was systems related with submicron structures in different fields of materials science. "Nano" was the magical term in many contributions that sneaked into all fields mentioned above, as these examples show:

- Greiner (Marburg, Germany): "All-Biodegradable Functional Water-Stable Polymer Nanofibre Nonwovens by Green Electrospinning"
- H. Schönherr (Siegen, Germany): "Block-Copolymer Nanocapsules for Advanced Wound Management- Fabrication, Structure, and Properties"
- B. Hsiao (New York, USA): "Highly Efficient Nanofibrous Membranes for Water Purification"
- L. Leibler (Paris, France): "Creating and Controlling Structure and Dynamics on Nano- and Meso Scales Yields Self-Healing"
- M. Matsuo (Dalian, China): "Electric-and Dielectric Properties of Nano-Composites Prepared by Gelation/Crystallization from Solution"
- J.-J. Pireaux (Namur, Belgium): "Spectroscopic Characterization of Hybrid Organic-Inorganic" Materials at the Nanoscale

As these lecture titles clearly show, the conference tended to focus on structure, properties, and applications of nanoscopic systems and environmental and bio-medical applications. There were vivid discussions throughout the breaks and at the end of each day.

## Conference Call



The highlight of each POLYCHAR conference is the distribution of awards before the closing ceremony. The prestigious Paul J. Flory Polymer Research Prize that was given ex aequo to Byung-Wook Jo of Chosun University in Korea and to Alejandro Mueller of Universidad Simón Bolívar in Venezuela for their outstanding contributions to the field of polymer drugs and confined crystallization in nanostructured polymers, respectively.

POLYCHAR's International Materials Science Prize was given to Sven Henning, Fraunhofer Institute for Materials Mechanics, Halle, Germany, for his contributions to electron microscopy of nano-structured polymers and biomaterials.

Three IUPAC Poster Prizes were awarded:

- Rujirat Longloiert (Chulalongkorn University, Bangkok, Thailand): "Novel Silica Source for Synthesis of MCM-48 via Sol-Gel Process"
- Marília M. Horn (Universidade de São Paulo, São Carlos): "Rheological Characterization of Chitosan/Starch Blends: Variation in Polyols and Amylopectin Content"
- Mykola Borzenkov (Lviv Polytechnic National University, Lviv): "Novel Surface Active Monomers Based on Tert-Butylperoxy-6-Hydroxyhexanoate"

The Jürgen Springer and the Bruce Hartmann Prize for Young Scientists went to:

- Chengcheng Yang (University of Pisa, Pisa): "Designed Coating Surfaces from Water-Borne Semifluorinated Polymer Particles Obtained by Cyclodextrin-Assisted Emulsion Polymerization"
- Tea Datashvili (University of North Texas, Denton, Texas, USA): "Well-Ordered SiO<sub>2</sub> Rods and Recycled Polyethylene + Silica Functionalized Wood Composites"

The Carl Klason Prize for the best Students' Presentation were awarded to the following students:

- Guy Mechrez (Israel Institute of Technology, Haifa): "High-Elongation MWNT Networks: Preparation, Characterization and Nanostructuring"

- Larisa Dobircan (University of Rouen, France): "Acoustic Properties of a 100% Natural Composite Reinforced by Bamboo Fibers"
- Severene Rose (ESPCI, Paris): "Nano-Hybrids PDMA/Silica Hydrogels: From Structure to Properties"

Diplomas of Distinction for their excellent scientific work and presentation of it were handed out to:

- Nicolaas Christiaan Basson (University of Stellenbosch, Stellenbosch): "The Effect of Compatibilizer on the Properties of Impact Polypropylene/Pinus Radiata Wood Polymer Composites"
- Paramjit Kaur (Thapar University, Patiala, Punjab): "Synthesis of Polylactide under Inert Atmosphere and Vacuum"
- Santosh Khanal (Tribhuvan University, Kathmandu): "Preparation and Properties of Styrene-Isoprene-Styrene (SIS) Triblock Copolymer Based Nanocomposites"

The conference was sponsored by the Tribhuvan University, Kathmandu, Nepal Academy of Science and Technology, the LECAP Laboratory of Prof. Jean-Marc Saiter, University of Rouen, France, the Third World Academy of Sciences and Technology, the Nepal Tourism Board, the Park Village Hotel & Resort, Kathmandu, Nepal Polymer Institute, Kathmandu, the University Grants Commission, Nepal, the International Centre for Theoretical Physics, the Alexander von Humboldt Foundation, Germany, the Polymer Standards Service, Germany, and Gulf Air, Bahrain.

The name POLYCHAR stands for polymer characterization and dates back to the days when it was an annual event at the University

of North Texas in Denton, Texas. Over the years it has expanded to cover the whole range of polymeric materials as well non-polymeric materials science. In 2004, POLYCHAR was held in Guimarães, Portugal, the first time outside Texas. It was followed by Singapore in 2005, Nara (Japan) in 2006, Buzios (Brasil) in 2007, Lucknow (India) in 2008, Rouen (France) in 2009, Siegen (Germany) in 2010. POLYCHAR 20 is scheduled for 26-30 March 2012 in Dubrovnik, Croatia.



*Prof. Alejandro Mueller (right), Universidad Simón Bolívar, Caracas, Venezuela, receiving the Paul J. Flory Polymer Research Prize from Michael Hess (left).*



### Functional Polymeric Materials & Composites

by Harald Pasch and Aneli Fourie

The 11th Annual UNESCO/IUPAC Conference on Functional Polymeric Materials & Composites, which took place 27–29 April 2011 at the Stellenbosch Institute for Advanced Studies, South Africa, attracted 143 participants who took part in its program focused on synthesis, characterization, properties, and application. Attendees represented 29 countries other than South Africa. Delegates from the African continent were from Zimbabwe. The total number of students who actively participated was 46 (they were from 12 historically black universities). Other Western countries represented were Austria, Australia, Brazil, Belgium, Canada, Czech Republic, Denmark, Germany, Iraq, Italy, India, Iran, Japan, France, Mauritius, Malaysia, New Zealand, Nigeria, Poland, Philippines, The Netherlands, Ukraine, Russia, Saudi Arabia, South Korea, Sweden, UK, and USA.

The UNESCO/IUPAC Conference was opened by T.E. Cloete, dean of the Faculty of Science, University of Stellenbosch, and H. Pasch, IUPAC representative, Department of Chemistry and Polymer Science, University of Stellenbosch.

A UNESCO/IUPAC Workshop was held on 26 April that featured seven invited talks. The conference itself featured 47 talks, of which 6 were plenary speakers, 21 invited speakers, and 20 oral submissions. In addition there was a lively poster session featuring 53 posters, especially popular for student presentations. Three poster prizes were awarded to the following young scientists (M.Sc./Ph.D. level):

- Best Poster: S.S. Ndlovu, University of the Free State, South Africa, “The Effect of Utilizing Thermally Degraded LDPE as a Compatibilizer in LDPE/Wood Composites”
- Second Best Poster: Christina Schmid, Karlsruhe Institute of Technology, Germany, “Switching from RAFT to ROP: A Facile Route to Complex and Sulphur-Free Macromolecular Architectures”
- Third Best Poster: Margaretha Brand, University of Stellenbosch, “Solution Crystallization Analysis by Laser Light Scattering: Applications to Polyolefins”

The topics of the workshop and conference lectures can be found online at the address below.

The following organizations provided considerable support, either financial or in kind:

- Sasol Polymers Corporate,
- IUPAC
- Mondi Packaging SA
- Plascon South Africa (Pty) Ltd.
- African Sun Media

Papers are being collected for peer review for inclusion in *Macromolecular Symposia*.

The organizing committee comprised H. Pasch, L. Klumperman, A.J. van Reenen, P.E. Mallon, and Aneli Fourie, all from the Department of Chemistry & Polymer Science at the University of Stellenbosch.

 <http://academic.sun.ac.za/unesco/Conferences/Conference2011>

### Applied Thermodynamics

by Anthony R.H. Goodwin

The 25th European Symposium on Applied Thermodynamics (ESAT) was held at St. Petersburg State University, St. Petersburg, Russia, 24–27 June 2011. The local organizing committee was chaired by Natalia Smirnova and Alexey Victorov. ESAT was organized under the auspices of the Working Party on Thermodynamics and Transport Properties of the European Federation of Chemical Engineering, founded in 1953.

ESAT was founded by the late Helmut Knapp, formerly of the Technical University of Berlin, to stimulate discussion among Europeans practicing thermodynamics. The first ESAT was held in Berlin in 1974 and it has been held annually except when it occurs in the same year as Properties and Phase Equilibria for Product and Process Design, which convenes every three years. This conference has among its objectives the following: (1), bring together engineers and scientists from universities, industry, and research institutes to discuss chemical engineering thermodynamics; and (2), consider future applications, offer solutions for current problems, and discuss the present state of the art of thermodynamics.

Panoramic view of Stellenbosch, South Africa.



## Conference Call

ESAT has grown to be a truly international event with about 290 participants at the most recent conference (see group photo below), with contributions from European countries as well as Africa, Canada, China, India, Iran, Israel, Japan, Mexico, Russia, Argentina, United Arab Emirates, and the USA. There were nine oral and two poster sessions that included process product design, molecular thermodynamics, ionic liquids, surfactants, polymers and biological systems, interfacial phenomena, phase equilibria and thermophysical data measurement, analysis and predictive tools, and petroleum fluids. Following is a sampling of the 16 plenary and invited lectures:

- G. Kontogeorgis, Danish Technical University, Denmark, presented “Industrial Requirements for Thermodynamics and Transport Properties—Before and Now.”
- A. Galindo, Imperial College London, UK, presented “Phase Behaviour, Solubility and Salting Out in Aqueous Solution: SAFT Approaches and Computer Simulations.”
- Mikhail Anisimov, University of Maryland, USA, presented “Liquid Water: A State Between Two Critical Points.”
- M. Francisco, University of Santiago de Compostela, Spain, presented “Desulfurization of Fuel Oils by Solvent Extraction with Ionic Liquids.”
- J.P. Martin Trusler, Imperial College London, UK, presented “Fundamental Equation of State for Solid Phase I of Carbon Dioxide.”
- E. Voutsas, National Technical University of Athens, Greece, presented “Phase Equilibrium in Natural Gas Mixtures.”
- K. Saito, University of Tsukuba, Japan, presented “Restricted Dynamics of Hydrocarbon Chain in the Lamellar Phase of Lipid-Water Systems.”

As the conference was held during the International Year of Chemistry, it was particularly pertinent that ESAT was sponsored by IUPAC and held at St. Petersburg State University, where Dmitri Ivanovich Mendeleev produced the first periodic table. The conference included a presentation by C. Nieto de Castro describing the impact of Mendeleev on a wide variety of chemical topics. Anthony R.H. Goodwin, titular member of the IUPAC Physical and Biophysical Chemistry Division, addressed the delegates on behalf of IUPAC.



*Anthony R.H. Goodwin, a titular member of the IUPAC Physical and Biophysical Division, addresses the delegates on behalf of IUPAC.*

A significant number of oral presentations and posters were given by students. Eight awards were

given for posters: (a), the Helmut Knapp Junior award, which is granted by ESAT for the best poster; (b), two from Nertzsich for the best application of calorimetry and thermal analysis; and (c), five from the International Association for Chemical Thermodynamics, which is an IUPAC Associated Organization, for posters presented by Young Scientists. On this occasion, the Helmut Knapp award was presented by Prof. E. Neau, President of the ESAT International Steering Committee, to S. Tsyrlunikov who is a M.Sc. student from St. Petersburg State University. Recipients of the IACT Poster Awards were as follows: (I), Ali Eslamianesh, France; (II), Nuno Garrido, Portugal; (III), Mickael Simond, France; (IV), Deepa Subramanian, U.S.A.; and (V), Maya Trofimova, Russia. In addition, the highly coveted EFCE WP-TTP Award of Excellence for Thermodynamics and Transport Properties, for achievement during a Ph.D. was presented by Prof. Dohm to Dr. M. Francisco in recognition of her Ph.D. thesis entitled “Desulfurization of Fuel Oils by Solvent Extraction with Ionic Liquids.”



## Where 2B & Y

### Greening Education

19–21 October 2011, Karlsruhe, Germany

A three-day **International Greening Education Event**, 19–21 October 2011, Karlsruhe, Germany, will take participants through the need for greening education and then discuss effective initiatives that educational institutions can take to make sustainability an integral part of teaching and learning. The event provides an exclusive forum to examine how global warming, climate change, and other environmental concerns are reshaping education globally. Conference participants and lecturers will deliberate on the role of academia in making the world cleaner, greener, and more sustainable. The conference program will cover cutting-edge

issues in greening education and share best practices from around the world in respect to education for sustainability.

This event also provides an excellent networking opportunity for academia, education, environmental, and sustainable development policy makers; senior members of academic institutions; representatives of government and non-governmental organizations and international development agencies; administrators and teachers; sustainable development practitioners; and environmental management professionals.

 [www.etchgermany.com/en/IGEE2011/igee2011.html](http://www.etchgermany.com/en/IGEE2011/igee2011.html)

### Macro 2012

24–29 June 2012, Blacksburg, Virginia, USA

The **2012 IUPAC World Polymer Congress** will take place on the beautiful campus of Virginia Tech in Southwest Virginia. The conference will reflect the profession, passion, and scientific vision of the Americas, including organizational leadership from Canada, Mexico, South America, and the USA. The event will provide an international forum for scientific discovery, professional networking, research collaboration, interdisciplinary education, and dissemination

of the most recent scientific advances. The campus of Virginia Tech is open to the global polymer community and welcomes contributions to the success of the program.

Now is the time for the entire polymer community to gather and synergistically address the many challenges that we face including energy, sustainability, health-care, safety, and emerging polymer technologies.

See **Mark Your Calendar** on page 35 for contact information.

 [www.macro2012.org](http://www.macro2012.org)

### Advanced Materials

26–30 March 2012, Dubrovnik, Croatia

POLYCHAR is a series of prestigious annual conferences, held throughout the world, at which participants review the latest research and developments in materials science and engineering. An integral part of the conference is the one-day Course on Polymer Characterization. The **POLYCHAR 20 World Forum on Advanced Materials**, 26–30 March 2012, Dubrovnik, Croatia, will focus on nanomaterials, smart materials, biomaterials, green materials, and materials for energy and recycling. Specific topics to be covered include predictive methods and simulations, structure-properties relationships, surfaces, interfaces, adhesion and tribology, materials synthesis, rheology and pro-

cessing, mechanical properties and performance, and electrical and dielectric properties.

The deadline for submission of abstracts is 15 October 2011.

See **Mark Your Calendar** on page 35 for contact information.

 [www.polychar20-croatia.com](http://www.polychar20-croatia.com)



## Conference Call

### Photochemistry

15–20 July 2012, Coimbra, Portugal

The XXIVth IUPAC Symposium on Photochemistry will carry on the excellent tradition of this series of conferences in Coimbra in July 2012. The meeting will provide a forum for presenting recent advances in all aspects of the field and will bring together members of the international photochemistry community. It will address topics in photochemistry that are likely to contribute to resolving some of the major problems of the 21st century, such as energy, the environment, and medicine.

The conference will offer a full range of plenary and invited lectures, oral contributions, and poster presentations. Confirmed plenary speakers include Guillermo C. Bazan (Santa Barbara), Anthony Harriman (Newcastle), Ben L. Feringa (Groningen), Tetsuro Majima (Osaka), Gregory D. Scholes (Toronto), Sebastião J. Formosinho/Luis G. Arnaut (Coimbra), Franco Scandola (Ferrara), Vivian W.W. Yam (Hong Kong), and the winner of the Porter Medal.

Topics to be covered will include the following:

- Organic and inorganic photochemistry from a synthetic and mechanistic point of view
- Solar energy conversion
- Photocatalysis, environ., & green photochemistry

- Materials science and engineering
- Supramolecular chemistry
- Photoactive nanoparticles and nanomaterials
- Photobiology, biophysics, and skin photochemistry
- Photochemistry in medicine
- Luminescent probes, sensors and imaging
- Spectroscopy and instrumentation
- Photochromism and photoswitching
- Industrial applications of photochemistry  
Photochemistry and cultural heritage

In addition, there will be a special Young Photochemists session that will include all aspects of photochemistry. A limited number of grants for young researchers will be made available.

The symposium will be held in the old city of Coimbra, well-known for its university, founded in 1290. Coimbra has a wide range of hotels and similar accommodations for all tastes. The city and the surrounding region offer various leisure, sporting, and cultural activities.

See Mark Your Calendar on page 36 for contact information.

 [www.photoiupac2012.com](http://www.photoiupac2012.com)

### Chemistry Education

15–20 July 2012, Roma, Italy

“Stimulating Reflection and Catalysing Change in Chemistry Education” will be the central theme for the 2012 joint meeting of the **International Conference on Chemistry Education and the European Conference on Research and Innovation in Chemical Education (ICCE-ECRICE)** in Rome, Italy, on 15–20 July 2012. It is only fitting that these two major international conferences in chemistry education meet together under the same roof, that of Rome, la città eterna, the eternal city.

ICCE 2012 will be the 22nd in a series that it is held every two years as an IUPAC sponsored conference.

In recent years, the ICCE met in Taipei in 2010, in Mauritius in 2008, in Seoul in 2006, and in Istanbul in 2004. ECRICE 2012 will be the 11th in a series that it is

also held every two years as an EuCheMS sponsored conference: ECRICE met in Krakow in 2010, in Istanbul in 2008, in Budapest in 2006, and in Ljubljana in 2004.

The discipline of chemistry education is constantly undergoing major developments that reflect the changing role of chemistry in our global society and the manner in which our science is perceived by the public. In so many new ways, the social, scientific, cultural, and didactic aspects of chemistry interact with each other and with other emerging disciplines such as museology, ethics, and communication science. The organizers would like the Roman conference to be remembered in the future as one that contributed to the growth of the quality of chemistry education around the world.

The organizers of the conference are assembling a high-level scientific program in an exceptional environment that will make ICCE-ECRICE 2012 a memorable event. See the website for more details.

See Mark Your Calendar on page 36 for contact information.

 [www.iccecrice2012.org](http://www.iccecrice2012.org)



# Mark Your Calendar

Upcoming IUPAC-sponsored events  
See also <http://www.iupac.org/indexes/Conferences>  
for links to specific event websites

## 2011 (after 25 September)

### 25–30 September 2011 • General and Applied Chemistry • Volgograd, Russia

*XIXth Mendeleev Congress on General and Applied Chemistry*

Prof. Alexander Navrotsky, Volgograd State Technical University, Polymer Chemistry Department, Lenin Avenue, 28, RF-400131 Volgograd, Russia, Tel.: +7 1 44 27 31 08, Fax: +7 1 44 27 38 34, E-mail: navrotsky@vstu.ru

### 27–29 September 2011 • Renewable and Sustainable Energy • Kuala Lumpur, Malaysia

*19th International ChemRAWN Conference on Renewable and Sustainable Energy from Biological Sources*

Prof. Ting-Kueh Soon, Institut Kimia Malaysia, 127 B Jalan Aminuddin Baki, Tam Tun Dr Ismail, 60000 Kuala Lumpur, Malaysia, Tel.: +60 3 7728 3272, Fax: +60 3 7728 9909, E-mail: soonk@ikm.org.my

### 5–7 October 2011 • Chemical Industry and Sustainability • Milano, Italy

*S-Chem: Chemistry Industry and Sustainability*

Prof. Angelo Albini, Università degli Studi di Pavia, Dipartimento de Chimica Organica, Via Taramelli 10 I-27100 Pavia, Italy, Tel.: +39 0 382 987 316, Fax: +39 0 382 987 323, E-mail: angelo.albini@unipv.it

### 11–14 October 2011 • Novel Materials and Their Synthesis • Shanghai, China

*7th International Symposium on Novel Materials and Their Synthesis*

Prof. Yuping Wu, Fudan University, Department of Chemistry, New Energy and Materials Laboratory, Shanghai 200433, China, Tel.: +86 21 545 664 223, Fax: +86 21 545 664 223, E-mail: wuyup@fudan.edu.cn

### 29 November–2 December 2011 • Medicinal Chemistry • Tokyo, Japan

*8th International Medicinal Chemistry Symposium*

Professor Yuusako Yokoyama, Toho University, Chiba, Japan

Tel.: +81 47 472 1589, Fax: +81 47 472 1595, E-mail: yokoyama@phar.toho-u.ac.jp

## 2012

### 6–9 January 2012 • Polymers and Organic Chemistry • Doha, Qatar

*14th International IUPAC Conference on Polymers and Organic Chemistry*

Prof Hassan S. Bazzi, Science Program Coordinator, Texas A & M University at Qatar, P.O. Box 23874, Doha, Qatar  
Tel.: +974 423 0018, Fax: +974 423 0060, E-mail: bazzi@tamu.edu

### 12–15 February 2012 • Polymer • Hobart, Australia

*33rd Australasian Polymer Symposium*

Prof Sébastien Perrier Director, Key Centre for Polymers and Colloids, School of Chemistry, University of Sydney, Sydney, NSW 2006, Australia, Tel.: +61 2 9351 3366, Fax: +61 2 9351 3329, E-mail: s.perrier@chem.usyd.edu.au

### 15–18 February 2012 • The Role of Chemistry for Sustainable Agriculture • Pusa, Delhi, India

*2nd International Conference on Agrochemicals Protecting Crops, Health and Natural Environment*

Dr. Najam A. Shakil, Indian Agricultural Research Institute, Division of Agricultural Chemicals, New Delhi 110 012, India, Tel.: +91 981 819 6164, Fax: +91 11 2584 3272, E-mail: iamshakil@gmail.com

### 26–30 March 2012 • Polymer Characterization • Dubrovnik, Croatia

*20th International Conference on Polymer Characterization - World Forum on Advanced Materials*

Dr Vera Kovacevic, University of Zagreb, Department of Chemical Engineering & Technology, Marulicev Trg., 19, HR-10000 Zagreb, Croatia, Tel.: +385 1 459 7188, Fax: +385 1 459 7260, E-mail: polychar20@fkit.hr

### 16–21 April 2012 • Chemical Sciences • Corfu, Greece

*12th Eurasia Conference on Chemical Sciences*

Prof Nick Hadjiliadis, University of Ioannina, Dept. of Chemistry, GR-45110 Ioannina, Greece  
Tel.: +30 2 651 008 420, Fax: +30 2 651 008 786, E-mail: nhadjis@uoi.gr

### 24–29 June 2012 • Macromolecules • Blacksburg, Virginia, USA

*44th International Symposium on Macromolecules - IUPAC World Polymer Congress*

Prof Timothy E. Long, Virginia Polytechnic University, Chemistry Dpt, VA 24061, USA  
Tel.: +1 540 231 2480, Fax: +1 540 231 8517, E-mail: telong@vtu.edu

### 1–6 July 2012 • Organic Synthesis • Melbourne, Australia

*19th International Conference on Organic Synthesis*

Prof Mark Rizzacasa, University of Melbourne, School of Chemistry, The Bio21 Institute, Melbourne, Victoria 3010, Australia, Tel.: +61 3 3844 2397, Fax: +61 3 3947 8396, E-mail: masr@unimelb.edu.au

## Conference Call

### 15–20 July 2012 • Photochemistry • Coimbra, Portugal

*XXIVth IUPAC Symposium on Photochemistry*

Prof Hugh D. Burrows, University of Coimbra, Dpt of Chemistry, P-3004 535 Coimbra, Portugal

Tel.: +351 239 854 482, FAX: +351 239 827 703, E-mail: burrows@ci.uc.pt

### 15–20 July 2012 • Change in Chemistry Education • Rome, Italy

*22nd International Conference on Chemical Education (ICCE) and 11th European Conference on Research In Chemical Education—Stimulating Reflection and Catalysing Change in Chemistry Education*

Prof. Luigi Campanella, Conference Chairman; Agency YES Meet, organizing secretariat, Tel: + 39 081 8770604,

Fax: + 39 081 8770258, E-mail: info@iccecrice2012.org

### 22–27 July 2012 • Carbohydrate • Madrid, Spain

*XVIth International Carbohydrate Symposium*

Prof Jesús Jiménez-Barbero, Centro de Investigaciones Biológicas, Consejo Superior de Investigaciones Ciencias, Ramiro de Maeztu 9, E-28040 Madrid, Spain

Tel.: +34 91 837 3112, Fax: +34 91 536 0432, E-mail: jjbarbero@cib.csic.es

### 5–10 August 2012 • Chemical Thermodynamics • Búzios, Brazil

*22nd International Conference on Chemical Thermodynamics and 67th Calorimetry Conference*

Prof. Watson Loh, Universidade de Estadual de Campinas, Instituto de Química, Caixa Postal 6154, Campinas, São Paulo 13083-970, Brazil, Tel.: +55 193 521 3001, Fax: +55 193 521 3023, E-mail: wloh@iqm.unicamp.br

### 25–29 August 2012 • Biomolecular Chemistry • Beijing, China

*9th International Conference on Biomolecular Chemistry*

Prof. Liangren Zhang, School of Pharmaceutical Sciences, Peking University Health Science Center, 38 Xueyuan Road, Beijing 100083, China, Tel.: + 86 10 82 802 491, Fax: + 86 10 82 802 638, E-mail: liangren@bjmu.edu.cn

### 9–13 September 2012 • Physical Organic Chemistry • Durham, United Kingdom

*21st International Conference on Physical Organic Chemistry*

Professor Ian H. Williams, Department of Chemistry, University of Bath, Claverton Down, Bath BA2 7AY, United Kingdom, Tel.: + 44 1225 386 625, Fax: + 44 1225 386 231, E-mail: i.h.williams@bath.ac.uk

### 15–20 September 2012 • Pesticide and Environmental Safety • Beijing, China !!New Dates!!

*4th International Symposium on Pesticide and Environmental Safety & 8th International Workshop on Crop Protection Chemistry and Regulatory Harmonization*

Prof. Zhang Jing, China Agricultural University, Centre for Chemicals Applications Technology, Yuanmingyuan West Road, Beijing 100193, China, Tel.: +86 10 6273 1456, Fax: +86 10 6273 3688, E-mail: zj810515@163.com

### 5–9 November 2012 • Mycotoxin • Rotterdam, Netherlands

*7th World Mycotoxin Forum and XIIIth International IUPAC Symposium on Mycotoxins & Phycotoxins*

Ms. Helena B. Bastiaanse (Program Coordinator), Bastiaanse Communication, P.O. Box 179, NL-3720 AD Bilthoven, Netherlands

Tel.: +31 302 294 247, Fax: +31 302 252 910, E-mail: helena@bastiaanse-communication.com

## Visas

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

## How to Apply for IUPAC Sponsorship

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

 [www.iupac.org](http://www.iupac.org)



# International Union of Pure and Applied Chemistry

Advancing the worldwide role of chemistry for the benefit of Mankind

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

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Secretary General: DAVID StC. BLACK (Australia)  
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## National Adhering Organizations

Australian Academy of Science (*Australia*)  
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Bangladesh Chemical Society (*Bangladesh*)  
The Royal Academies for the Sciences and Arts of Belgium (*Belgium*)  
Brazilian Chemistry Committee for IUPAC (*Brazil*)  
Bulgarian Academy of Sciences (*Bulgaria*)  
National Research Council of Canada (*Canada*)  
Sociedad Chilena de Química (*Chile*)  
Chinese Chemical Society (*China*)  
Chemical Society located in Taipei (*China*)  
Croatian Chemical Society (*Croatia*)  
Sociedad Cubana de Química (*Cuba*)  
Pancyprian Union of Chemists (*Cyprus*)  
Czech National Committee for Chemistry (*Czech Republic*)  
Det Kongelige Danske Videnskabernes Selskab (*Denmark*)  
National Committee for IUPAC (*Egypt*)  
Chemical Society of Ethiopia (*Ethiopia*)  
Suomen Kemian Seura—Kemiska Sällskapet i Finland (*Finland*)  
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Thieme Publishers, IUPAC, and the Editors of *SYNTHESIS*, *SYNLETT*, *SYNFACTS*, and *Science of Synthesis* announce the

# 2012 Thieme–IUPAC Prize in Synthetic Organic Chemistry



## Call for Nominations



The Thieme–IUPAC Prize is presented every two years on the occasion of the International Union of Pure and Applied Chemistry – International Conference on Organic Synthesis (IUPAC–ICOS). The 2012 ICOS will be held in Melbourne, Australia, on July 1–6. The prize is awarded to a scientist under 40 years of age whose research has had a major impact in synthetic organic chemistry.

### Prize € 5000

The Thieme–IUPAC Prize has been awarded to Stuart L. Schreiber in 1992, Paul Knochel in 1994, Eric N. Jacobsen in 1996, Andrew G. Myers in 1998, Alois Fürstner in 2000, Erick M. Carreira in 2002, John F. Hartwig in 2004, David W.C. MacMillan in 2006, F. Dean Toste in 2008, and Phil S. Baran in 2010.

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

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



**ICOS-19**  
Melbourne, Australia  
July 1–6, 2012  
[www.ICOS-19.com](http://www.ICOS-19.com)

### Nomination materials

should be submitted by e-mail no later than **December 9, 2011** to [marcus.white@thieme.de](mailto:marcus.white@thieme.de)

**Deadline: December 9, 2011**

For further information please visit [www.thieme-chemistry.com](http://www.thieme-chemistry.com)

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