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MULTIPLE USES OF CHEMICALS

INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

Synthesis at the Interface of ►
Chemistry and Biology

CHEMISTRY International

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International Union of Pure and
Applied Chemistry (IUPAC)

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DE GRUYTER

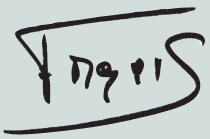
From the Editor

Every day, we all make choices. In reviewing "Multiple Uses of Chemicals—IUPAC and OPCW Working Together Toward Responsible Science" (feature p. 9), we are presented with a website resource that explores the beneficial uses, misuses, and abuses of multi-use chemicals, both historically and presently. This educational material considers how to make responsible choices in chemistry and what it means to practice chemistry responsibly. If the topic intrigues, I recommend that you read these pages, visit the website, and preview the video. Most informative, the video showcases the hands-on workshop held last year during the IUPAC Congress in Istanbul and explores how to use the resource by examining how chemists/students make choices. This project builds on the premise that education and outreach are key to prevent the abuse of chemical substances. While such a topic might seem far from the concerns of chemical warfare, it is really not a big leap to teach chemists and teachers about the importance of regulatory agencies such as the Chemical Weapons Convention and the creation of codes of conduct. In that context, the "About" section of the website ends with the following statement: "Each of us as scientists and citizens have a responsibility to ensure responsible uses of the chemical substances that are important to every aspect of our everyday lives."

This CI issue presents other choices and contents to reflect on. One is about the definition of the mole. A task group has set its goal to review the proposed definitions of fundamental chemical quantities and their impact on chemical communities. Various input is called for and you might choose to share your perspective.

Another choice is one that you can make by stepping up more actively in IUPAC committees: the timeline for the next elections cycle and the call for nominations is announced on p. 14. If you are able to commit time and expertise to IUPAC activities and willing to be nominated, you should consider contacting your NAOs and/or the current committee officers of the group that is of most interest to you.

One last choice that you can make, and a personal call, is to return some feedback about CI. IUPAC is interested in learning how you read this newsmagazine and why, what section is of interest, etc. While a survey is being prepared that will be shared via iupac.org, you can also email me, subject line "Why I read CI," and return your comments.



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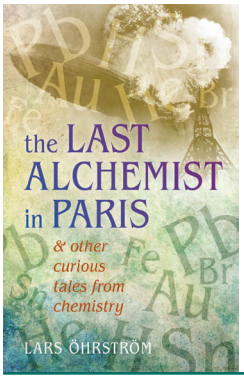

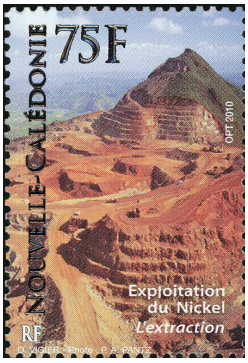

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Treasurer's Column

A Time for Renewal

by John Corish

After the difficult financial times that we have experienced in recent years we are now in a period with the opportunity for recovery, renewal, improvement, and growth. In better times it is too easy to coast along on the wave taking the comfortable pathways and to fail to critically examine the benefits and costs of decisions. One of the better outcomes of a recession is that it sharpens critical functions by making necessary a general examination and questioning of every choice made. Even the magic of our chemistry could not empower IUPAC to complete immunity from the global financial malaise and, as I have reported previously, two of our income streams—those from publications and investments—have inevitably been reduced. It also has been an expensive few years for us with the excitement and success of the International Year of Chemistry still fresh in our thoughts.

How are we now renewing ourselves and planning new growth into the future? Dealing first with the two declining income streams, we have entered into a partnership with De Gruyter publishers for the production of *Pure and Applied Chemistry* and *Chemistry International*. The complex change of publisher at the beginning of this year has been accomplished smoothly and our newly-appointed Acting Secretary General, Colin Humphris, is leading a very close and active liaison with our new partners to complete the transition and to iron out any wrinkles remaining in the new arrangements. With respect to our investments, the Finance Committee meeting in February advised that we undertake an examination of our portfolio with a view to adopting a somewhat more aggressive, though still prudent, investment policy and this has been done. Again we are currently in discussion, this time with professional financial advisors, so that our portfolio will be more actively managed and we will maximize the returns on our funds.

The Finance Committee also recommended that the Union make every effort to control our expenditures and this is being implemented in every aspect of our business, for example in the day-to-day expenses at the Secretariat and in our postage and other communication costs. In response to the recommendation, the Bureau at its recent meeting tasked a group to examine the schedule for our larger meetings such as the General Assembly to ensure that they are both efficient and economical and provide the best possible value for money—the changes recommended will be seen in the next General Assembly in 2015 in Korea. The guidelines for the reimbursement of travel and subsistence expenses have also been revised for this biennium so that receipts must now be furnished for all claims submitted. This will provide a proper set of records for our annual audit as well as ensuring that everyone is fairly and correctly reimbursed for their expenses up to the *per diem* limit. In terms of growth, the Bureau recommended the acceptance of applications from four new NAOs and IUPAC extends a very warm welcome in 2014 to Colombia, Costa Rica, Kazakhstan, and Senegal. The Membership Relations Committee will continue to actively seek and encourage additional new members to join us.

(continued on page 8)

Dr. Lynn Soby appointed IUPAC Executive Director

On 24 July 2014, the officers of IUPAC announced the appointment of Dr. Lynn Soby as IUPAC Executive Director.

Dr. Soby is a chemistry graduate who gained a PhD in Macromolecular Science and Engineering and an Executive MBA in the Management of Technology from Case Western Reserve University. She received a MS in Chemistry from Ohio University and a BS in Chemistry from Boston College. She has held senior positions in industrial research and in technology development with BF Goodrich and Avon Products companies, which included actively setting up research and technical organizations in many countries around the world. She has worked as a business analyst and most recently held the position of Vice President Innovation and Commercialization at Research Triangle Institute (RTI) International in North Carolina.

Dr. Soby brings a valuable blend of science, technology, and business administration to the role of Executive Director at a time of change for IUPAC as the Union approaches its centenary. The officers are sure the IUPAC community will welcome Dr. Soby to her new role and are all looking forward to working with her.

Synthesis at the Interface of Chemistry and Biology*

by Peter G. Schultz

The feature that perhaps most distinguishes chemistry from the rest of the sciences is the ability of chemists to control the structure of matter at the molecular level. Unfortunately, we are not nearly as adept at the synthesis of molecules with defined functions as we are at the synthesis of molecules with defined structures. As the focus of chemistry increasingly shifts from structure to function, chemists will need to develop better strategies to efficiently generate molecules, and systems of molecules, with desired physical, chemical, or biological properties in order to meet the biomedical, energy, and environmental needs of the future. Indeed this challenge represents one of the great opportunities for synthesis in the coming years. One direction we can turn for help is Mother Nature: after all, living organisms carry out a remarkable array of complex functions using natural molecules and molecular assemblies. With this theme in mind, the focus of our work has been to exploit nature itself, i.e., use the synthetic strategies, molecules, and biosynthetic machinery of living organisms, together with more traditional chemical approaches, to generate molecules with properties that might be difficult to realize by chemical strategies alone.

An Expanded Genetic Code

As an illustration of this notion we asked the question whether our molecular level understanding and chemical/biological tools are sophisticated enough to begin to manipulate the genetic code itself, i.e., generate organisms that genetically encode 21 or more amino acids. Although the functional groups contained in the 20 amino acid code might be sufficient for life, they might not be optimal. Consequently, the development of a general method that allows us to genetically encode additional amino acids beyond the canonical 20 might facilitate the evolution of proteins, or even entire organisms, with new or enhanced properties. Moreover, the ability to incorporate amino acids with defined steric/electronic properties and chemical reactivity at unique sites in proteins should provide powerful new tools for exploring protein structure and function; much the same way physical organic chemists use synthesis to understand the chemical reactivity of organic molecules.

The incorporation of additional amino acids into proteins directly in a living organism requires the following new components of the protein translational machinery: a unique tRNA- codon pair, a corresponding aminoacyl-tRNA synthetase, and significant intracellular levels of the unnatural amino acid. To ensure that the unnatural amino acid is incorporated with high fidelity the tRNA must not be recognized by the endogenous aminoacyl-tRNA synthetases (aaRS) of the host but still function efficiently in translation (an orthogonal tRNA). Moreover, this tRNA must deliver the novel amino acid in response to a unique codon that does not encode any of the common 20 amino acids. This codon can be either one of the degenerate stop codons (e.g., an amber nonsense codon) or an efficient four-base frameshift codon. Another requirement for high fidelity is that the cognate aminoacyl-tRNA synthetase (an orthogonal synthetase) aminoacylates the orthogonal tRNA but does not aminoacylate any of the endogenous host tRNAs. Furthermore, this synthetase must aminoacylate the tRNA with only the desired unnatural amino acid, and not with any of the large number of endogenous amino acids of the host organism. Similarly, the unnatural amino acid cannot be a substrate for the endogenous synthetases if it is to be incorporated uniquely in response to its cognate codon. To this end we used a combination of structure-based design and large libraries of tRNAs and aminoacyl-tRNA synthetases, together with a series of positive and negative selections, to generate unique tRNA/aaRS pairs specific for the amino acid of interest. The positive selection is based on chloramphenicol resistance, which is conferred by the suppression of an amber mutation at a permissive site in the chloramphenicol acetyltransferase gene only in the presence of the unnatural amino acid. The negative selection uses the toxic barnase gene with amber mutations at permissive sites and is carried out in the absence of the unnatural amino acid to eliminate aaRS mutants that aminoacylate endogenous amino acids. This selection scheme and more facile variants have been used to develop orthogonal tRNA/aaRS pairs that are capable of selectively inserting one or more unnatural amino acids into proteins in *E. coli* in response to nonsense and/or four-base frameshift codons (with a cognate tRNA containing an expanded anticodon loop) in good yields (>1 g/L) and with high translational fidelities. This system has been

*Essay based on the presentation of the first "Chemistry for the Future Solvay Prize" awarded to Professor Peter G. Schultz on 4 December 2013. See more on page 5.

Solvay Prize presentation at the Academy in Brussels on 4 December 2013

expanded to both yeast and mammalian cells; in addition transgenic flies and worms with a 21 amino acid code have been created. Most recently a "synthetic" *E. coli* strain has been generated in which the TAG codon has been deleted and used to uniquely specify unnatural amino acids.

On the order of 100 unnatural amino acids with novel chemical, biological, and physical properties have been genetically encoded in living organisms. These include amino acids with novel steric/packing and electronic properties for mechanistic studies; photo-cross-linking amino acids which have been used to probe protein-protein and protein-nucleic acid interactions in vitro or in vivo; keto, diketo, acetylene, azide, thioester, and boronate containing amino acids that contain functional groups with unique chemical reactivity which have been used to site-specifically introduce a large number of biophysical probes, tags, and drugs into proteins in vitro or in vivo; redox-active amino acids to modulate electron transfer in proteins; photocaged and photoisomerizable amino acids to photoregulate cellular processes; metal-binding amino acids for catalysis, protein folding and regulation; amino acids that contain NMR probes or fluorescent or IR-active side chains as local probes of protein structure and dynamics in vitro and in vivo; α-hydroxy acids and D-amino acids as probes of backbone conformation and hydrogen-bonding interactions; and sulfated amino acids and mimetics of phosphorylated amino acids as probes of protein post-translational modifications. Clearly this list will be further expanded to include many additional amino acids with novel chemical, physical, and biological properties.

In addition, we are beginning to examine the influence of an expanded genetic code on the evolution of peptides and proteins with new or enhanced properties. For example, a modified phage display system was used to evolve germline antibodies in strains that genetically encode sulfotyrosine. We found that antibodies containing the unnatural amino acid outcompeted the other variants in binding HIV gp120. In a second experiment we generated a library of cyclic peptides containing unnatural amino acids using an intein-based method for cyclization. In a selection system based on inhibiting protease activity for cell survival, cyclic peptides containing an aryl ketone side chain were evolved that inhibited HIV protease by a novel mechanism involving formation of a Schiff base with a surface lysine residue and thereby destabilizing the protein. Most recently, we generated a library of β-lactamase mutants in which residues throughout the protein were randomly mutated to UAAs. In a selection scheme based on resistance to ceftazidime we isolated mutants containing UAAs with enhanced catalytic activity relative to the wild type protein, or canonical amino acid variants. Finally, we have also successfully "synthesized" an autonomous 21 amino acid bacterium that both biosynthesizes and genetically encodes the unnatural amino acid, p-aminophenylalanine. It will be of interest to compare its evolutionary fitness to that of wild-type *E. coli*. Thus, by seamlessly integrating the complex translational machinery of living cells with new chemistries and *in vitro* evolution methods, we have overcome an evolutionary constraint imposed by the universality of the genetic code. This advance may allow the generation of proteins and perhaps even living organisms with novel or enhanced properties, and underscores the power of co-opting (rather than mimicking) Nature to create novel new functions.

Harnessing the Immune System

Another example of synergy between chemistry and biology in the generation of molecules with novel functions is the development and application of diversity-based synthetic strategies, an approach inspired by the sophisticated combinatorial and mutational mechanisms by which antibodies are evolved to recognize foreign antigens with high affinity and selectivity. The notion that this natural diversity can be used to create novel chemical function was first illustrated with the generation of catalytic antibodies. Rather than attempting to design a synthetic host that selectively binds a substrate of interest and then modify it with catalytic auxiliaries, it was realized that one could

simply co-opt the immune system to generate a highly selective natural host in the form of an antibody combining site. To generate a selective catalyst rather than a selective receptor, stable transition-state analogues (rather than substrates) were used as antigens on the basis of the Pauling notion that enzymes evolve maximum binding affinity to the transition state of a reaction. The early experiments by Lerner and co-workers and in our own laboratory involved the generation of esterolytic antibodies using phosphonate/phosphate transition-state analogues. Other approaches have since been developed to generate catalytic antibodies, including covalent catalysis, proximity effects, and general acid-base catalysis (thereby allowing us to dissect the contribution of each of these factors to biological catalysis). Using these approaches, antibodies have been generated that catalyze a wide array of chemical reactions, from acyl transfer and redox reactions to pericyclic and photochemical reactions with specificities and, in some cases, rates rivaling those of enzymes.

The detailed characterization of the immunological evolution, three-dimensional structures, and mechanisms of catalytic antibodies has also helped to dissect and quantify the relationship between binding energy and catalysis in the evolution of catalytic function. Indeed the use of transition-state analogues to elicit catalytic antibodies provided "proof by synthesis" of the Pauling notion of enzymatic catalysis. In another example, a "ferrochelatase" antibody, which catalyzes the efficient insertion of metal ions into porphyrin (the last step in heme biosynthesis), was generated

Chemistry for the Future Solvay Prize

On 4 December 2013, the presentation of the first "Chemistry for the Future Solvay Prize" took place in Brussels at the prestigious Palace of the Academy of Sciences and Arts in Belgium. This prize created by Solvay in 2013 is to reward every two years a major scientific discovery that could shape tomorrow's chemistry and help human progress.

After the welcome address by Nicolas Boël (Chair of the Board of Solvay), the laureate Peter G. Schultz was invited on stage to receive the superb crystal trophy and the 300000 € prize from the hands of Jean-Pierre Clamadieu (Solvay CEO).

The large audience from scientific, academic, and political circles in Belgium had responded to the invitation of Solvay to congratulate Peter Schultz in the presence of US ambassador Mrs. Denise Campbell Bauer and to enjoy a Science and Innovation event.

Prof. Hakan Wennerstrom (University of Lund, Sweden), Chair of the Prize Jury, reminded us of the scope and goals of this new international award. After a short recap of Peter Schultz's career, he highlighted the scientific work and his great originality particularly in the field of stem cell differentiation techniques and modification of biochemical processes of life to incorporate unnatural amino acids into proteins.

To complete this "Science and Innovation" afternoon, Peter Schultz discussed the scope of his research. As a wonderful scientist and teacher, he managed to attract the public's attention and showed many potential applications of his work in medicine and chemistry.

Then, as a chemist himself, the Belgian Prime Minister Elio di Rupo stressed the initiative of Solvay and emphasized the role of science and research in our modern society and industry to respond to the changes and needs of our world.

And finally, to illustrate the "Spirit of Innovation" Bertrand Piccard, a third generation explorer of our planet, invited us virtually into the cockpit of "Solar Impulse" (around the world solar airplane) stimulating the public by its dynamism and inspiring messages.

A high level meeting, a great laureate.... See you in 2015!

www.solvay.com/en/innovation/solvay-prize/ceremony

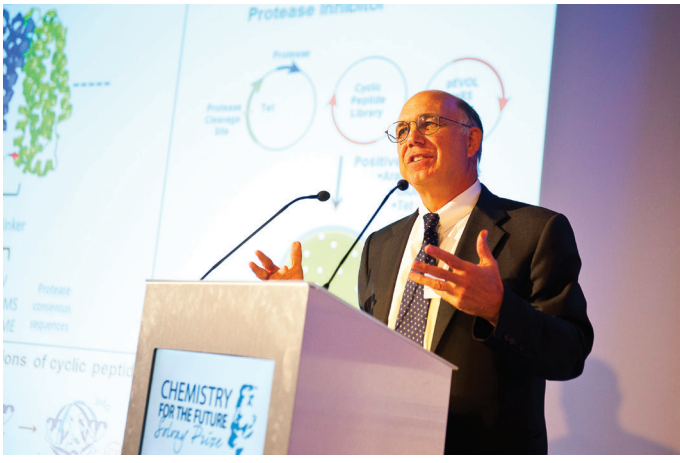
Price-giving of the award to the Laureate Professor Peter G. Schultz, by Solvay CEO Jean-Pierre Clamadieu (left)

against an N-methyl porphyrin, which mimics the distorted porphyrin ring of the putative transition state for metalation. The crystal structure of the Michaelis complex indeed showed that the substrate is bound in a strained conformation, providing the first direct structural evidence for the theory of substrate strain proposed by Haldane over 70 years ago. The characterization of catalytic antibodies has also provided fundamental insight into the mechanisms by which the immune system itself evolves selective receptors. For example, the first detailed structural comparisons of germline and affinity-matured antibodies revealed the critical role of structural plasticity (in addition to genetic diversity) in determining the tremendous binding potential of the germline antibody repertoire. Germline antibodies appear to have a high degree of intrinsic combining site conformational flexibility (reminiscent of the chemical instruction theory of the immune response proposed by Haurowitz and Pauling) which allows them to bind multiple, distinct ligands in different conformational states. That conformational state which binds a specific antigen is then locked and further refined by somatic mutations which occur during affinity maturation (not protein folding as proposed by Pauling). Structural and biophysical analyses of the immunological evolution of catalytic antibodies also pointed to the critical role of mutations distal to the active site in controlling the binding and catalytic activity of proteins through complex networks of side chain and backbone interactions. Indeed these studies underscore a key aspect of diversity-based synthetic strategies—the fact that analyses of the relationship between molecular structure and properties in molecules obtained by combinatorial methods often lead to new chemical insights which further increase our ability to generate new molecular function from basic chemical principles.

Diversity-based Synthesis

The demonstration that the vast structural diversity of antibody molecules can be redirected with proper chemical instruction to generate selective catalysts illustrated the utility of molecular diversity (the antibody repertoire in this case) as a new, biologically inspired "synthetic strategy" to create novel chemical properties. Shortly thereafter, libraries of other biomolecules were designed and synthesized in order to identify molecules with new or enhanced functions. These included the use of phage display libraries to generate peptides, proteins, and antibody fragments with novel specificities, and libraries of random RNA sequences (including those containing unnatural bases with novel functional groups) to identify RNAs that selectively bind ligands with high affinity, that catalyze chemical reactions such as acyl or phosphoryl transfers, or whose structure and transcription is regulated by the binding of small synthetic molecules. Today, combinatorial strategies are impacting many areas of chemistry. This method is particularly valuable when theory has insufficient predictive power to guide molecular design with precision, and quickly provides large amounts of experimental data to guide additional experiments and/or theoretical predictions.

One particularly illustrative example is the application of diversity-based approaches to the generation of solid-state materials with novel properties. The properties of many functional materials, such as high-temperature superconductors, heterogeneous catalysts, ferroelectric materials, magnets, and even structural materials, arise from complex interactions involving the host structure, dopants, defects, and morphology, all of which are highly dependent on composition and processing. Unfortunately, our current level of theoretical understanding does not generally allow one to predict the structures and resulting properties of these materials. Given the large number of elements in the periodic table that can be used to



make compositions consisting of up to six elements, the universe of possible new compounds with interesting physical and chemical properties remains largely unexplored; combinatorial synthetic methods represent a powerful way for experimentalists and theorists alike to more effectively mine this huge chemical space for interesting new materials properties. The first application of combinatorial methods to materials science involved the synthesis and screening of libraries of thin-film copper oxides to identify high-temperature superconductors. More recently, a variety of thin

film, solution-based and physical methods (e.g., ball milling) have been used to make libraries of diverse solid state materials. In addition, a large number of scanning or parallel detection systems have been developed for rapidly screening materials libraries for optical, electronic, magnetic, adsorptive, or catalytic properties of interest. This combinatorial approach to materials discovery, is now practiced in many industries and has led to new olefin polymerization and oxidative catalysts, hydrogen storage materials, separations materials, dielectrics, phosphors, etc. and is now being applied to the optimization of complex integrated devices such as lithium ion batteries, solar cells, and computer chips. Indeed with the challenges we now face finding new environmentally friendly energy sources, combinatorial methods are likely to play a critical role in the development of enabling new materials. These include new hydrogen and methane storage materials, fuel cell catalysts, photovoltaic devices, CO_2 sequestrants, and high-energy-density batteries. This will likely be best achieved by a synergistic use of combinatorial approaches, more conventional solid-state chemistry, and theory.

Regenerative Medicine and Neglected Disease

Another particularly powerful application of combinatorial strategies, involves the synthesis of diverse libraries of nonoligomeric synthetic molecules. Just as large libraries of antibodies are genetically assembled from families of V, D, and J gene segments, it was realized that libraries of small organic molecules could be efficiently assembled from chemical building blocks. Although there are many examples of the rational design of biologically active small molecules, it remains a challenge to design a priori molecules that selectively activate or inhibit a desired enzyme or receptor, or modulate a specific cellular signaling pathway, regulatory circuit, or transcriptional program. As a consequence, the screening of synthetic chemical libraries offers a highly effective approach to identify biologically active molecules, especially molecules with novel cellular activities, which may not be predicted or even conceived of in hypothesis-driven experiments. However, with the increased availability and decreased cost of chemical libraries and the power of modern screening technologies, the question arises as to which opportunities should the academic chemistry community pursue with these new tools? One answer is to focus on those areas of biology which are still poorly understood and, as a consequence, there exists a real need for small molecules as *in vitro* and *in vivo* probes; another is to focus on major unmet medical needs that have been largely ignored by industrial research efforts due to perceived risk or financial considerations.

A timely example (of both) is regenerative medicine, in which new cells (e.g., neurons, muscle, chondrocytes, etc.) are generated to replace tissues lost to degenerative diseases or aging. To this end, we and others are carrying out cell-based screens to identify molecules that control cell fate. For example, we have carried out image-based screens with one class of adult stem cells, hematopoietic stem cells (HSCs), to identify molecules that control self-renewal and differentiation (HSCs are adult stem cells that give rise to all the blood lineages such as macrophages, B and T cells, platelets, red blood cells, etc.). Molecules have been identified that are able to significantly expand cord blood HSCs in an undifferentiated state by antagonizing the aryl hydrocarbon receptor. These compounds will likely produce a robust source of HSCs for the large number of cancer, blood, and autoimmune disease patients for which no matched donors exist. In another experiment we have used image-based screens to identify a molecule that induces the selective neurogenesis of neural progenitor cells in vitro and in vivo in the rat dentate gyrus. This compound acts by selectively binding the centrosomal protein TACC3, which has been previously implicated in regulating the balance between progenitor cell renewal and differentiation. This and other such molecules may ultimately lead to new treatments for neurodegenerative disease. We have also identified molecules that selectively induce mesenchymal stem cells (adult stem cells which normally give rise to osteoblasts, adipocytes, and chondrocytes) to undergo osteogenesis to form bone, or chondrogenesis to form cartilage. The chondrogenic molecule, kartogenin, functions by blocking the interaction of the cystolic protein filamin A with the transcriptional coactivator CBF-β. CBF-β then traffics to the nucleus and selectively upregulates the expression of the master transcriptional regulator, Runx1. These molecules have shown excellent efficiency upon intra-articular injection in rodent osteoarthritis models. More recently, a molecule has been identified from image-based screens of oligodendrocyte precursor cells that induce their selective differentiation to oligodendrocytes. These molecules show excellent efficacy and function in both in vitro and in vivo by inducing remyelination of axons, rather than by an immunosuppressive mechanism.

Another exciting opportunity for the academic

community to exploit chemical libraries and screening technologies that is not generally competitive with pharmaceutical or biotechnology research interests is in the area of orphan and neglected diseases. For example, there exist both a large research opportunity and a major unmet medical need with respect to molecules that kill persistent Mycobacterium tuberculosis (the biology of persistors is largely unknown), or molecules that target nonessential host factors that are required for viral replication (HIV, HCV, Dengue, etc.), but which will not mutate rapidly. To this end, we recently identified a molecule from a cell-based biofilm screen using Myobacterium smegmatis that kills both replicating and nonreplicating Mtb as well as XDR drug resistant strains. These molecules down-regulate key mycobacterial persistence genes, and function by inhibiting two activities—the cell wall biosynthetic enzyme DprE1 and the biosynthesis of an essential molybdenum cofactor. Analogues of this compound show excellent activity in chronic models of Mtb in rodents. In addition, there are a large number of orphan diseases (type I diabetes, muscular dystrophies, spinal muscular atrophy, childhood cancers, Rett syndrome, Fragile X, Huntington disease, etc.) for which no good treatments exist. The identification of molecules that modulate these disease processes may ultimately lead to new therapies as well as provide new insight into the biology of many of these diseases.

Conclusion

Chemistry continues to evolve from its historical focus on molecular structure, reactivity, and synthesis to take on the challenge of making small and large molecules and even systems of molecules with tailored properties and functions. This requires improved theoretical and analytical tools, as well as innovative new synthetic strategies. Given the remarkable array of functions found in biological molecules, Mother Nature offers help in this regard through an approach to synthesis that seamlessly interfaces biology and chemistry. Hopefully, the examples illustrated above from our work, and the many other elegant examples in the literature, convey the exciting and highly relevant opportunities that exist for chemical synthesis at the interface of the chemical and biological sciences.

Peter G. Schultz <schultz@scripps.edu> is professor at The Scripps Research Institute and Director at the California Institute for Biomedical Research, in La Jolla, California.

Treasurer's Column

(continued from page 2)

Even if done grudgingly a Treasurer can sometimes admit that there are other things that are as important as and perhaps even more important than money to the lifeblood of an organization. Good communications among its members and with the world at large is one of these and, in terms of general renewal, the Bureau has set as a major objective for the coming year to have a new or updated website in place by the time of the General Assembly in August of 2015. A task force, which will consult widely with the membership to establish its needs, has been established under the leadership of Bonnie Lawlor, Chair of the Committee on Publications and Cheminformatics Data Standards. This will create the vision for the website and develop informed recommendations. Every organization also needs a constant supply of new volunteers to renew and keep its business abreast of the new developments. To this end, IUPAC is streamlining the election process whereby the membership of its Divisions and Standing Committees are chosen so that we have a more transparent and effective recruitment process. Another vital necessity for success is a coherent and far-seeing strategic plan for the future and the need has been identified to draw up a contemporary strategic plan for IUPAC that will better reflect our objectives and define how these can be achieved in the modern environment. Our President, Mark Cesa, is leading a group that is formulating a new strategic plan for IUPAC for the coming years to ensure that it continues to serve the world community of chemists in both academic and commercial endeavours and continues to provide the language and standards that our subject needs to further enhance its unique and vital contribution to the progress and betterment of humankind. An IUPAC renewal is indeed very much in the air.

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.

IUPAC and OPCW Working Toward Responsible Science

by Peter Mahaffy, Joseph Zondervan, Alastair Hay, Daniel Feakes, and Jonathan Forman

Imagine being a chemist in the summer of 1941, four years prior to the end of the Second World War. The pressure to use the powerful knowledge of chemistry in service of national and political interests is enormous. The end result? At the Auschwitz Nazi extermination camp, Zyklon B, an infamous weapon of mass destruction, is first used. Over the next four years it claims responsibility for the lives of several million people in the gas chambers of Auschwitz and other death camps. When mixed with water, Zyklon B releases hydrogen cyanide, which fatally interferes with the respiratory processes of those inhaling it. Hydrogen cyanide is a simple, triatomic molecule whose power for destruction is now burned into our global consciousness as a symbol of how badly things can go wrong when the tools of chemistry are misused. Prior to the Second World War, hydrogen cyanide had been used as a delousing agent and insecticide, and this toxicity inspired its use in designing a new way to kill people.

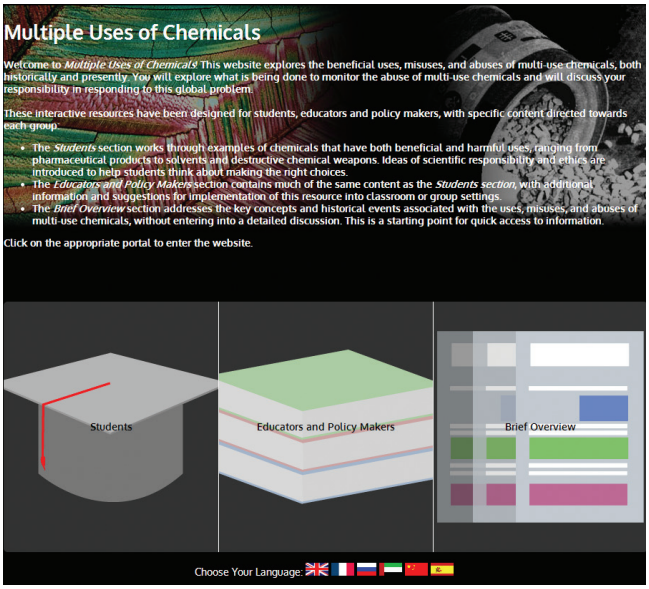
Making responsible choices can be a dilemma ... let's explore what it means to practice chemistry responsibly.

However, this story of a molecule does not end in the gas chambers, and it is more than a horror story of the misuse of a chemical substance. More than 70 years later, hydrogen cyanide is produced annually in million-tonne quantities. Most of that HCN is used in a variety of important and beneficial industrial processes, such as manufacturing paints, producing chelating agents, and synthesizing adiponitrile, a precursor to nylon. Hydrogen cyanide is a good example of a substance that can both improve the quality of life and be employed for destruction of life. Such is the nature of *multi-use chemicals—substances which can be used for a variety of applications, ranging from beneficial to harmful, and at other points along the spectrum between these extremes.*

Fast-forward to being a chemist or chemist-in-training 72 years after the use of Zyklon B. The pressure to misuse the power of multi-use chemicals is demonstrated again in the early morning hours of 21 August 2013, when the world watches in horror as sarin, produced from a variety of beneficial substances including isopropanol (rubbing alcohol) and a chemical compound used as a flame retardant, is unleashed on a civilian population in the East Ghouta suburbs of Damascus, Syria. A few months later, after mobilizing a global response to the Syria attack, the Organization for the Prohibition of Chemical Weapons (OPCW) is awarded the Nobel Peace Prize for its "extensive efforts to eliminate chemical weapons," many of which are created from multi-use precursors. As the implementing body for the Chemical Weapons Convention, the OPCW seeks to monitor and prevent the production of chemical weapons, as well as destroy existing chemical weapon stockpiles in any of its states parties. In his Nobel Peace Prize Lecture, OPCW Director-General Ahmet Üzümcü declares that it is the task of the OPCW "to consign chemical weapons to history, forever."

Educate and Raise Awareness

The desire to ensure that stories, such as those described here, about responsible choices regarding the multiple uses of chemicals are told to students, the public, and policy makers has provided the motivation for IUPAC and the OPCW to work together. Various initiatives have been supported for over a decade to give emphasis to education and awareness about the responsible practice of science. As emphasized in the Director-General's Nobel Peace Prize Lecture, organizations (such as the OPCW and IUPAC) need to



Homepage of www.iupac.org/multiple-uses-of-chemicals —the website designed to present educational material regarding the uses and misuses of multi-use chemicals, and to teach chemists and teachers about the importance of regulatory agencies such as the Chemical Weapons Convention and the creation of codes of conduct.

think "about how [they] can employ new communication tools to raise awareness of the need to practice responsible science, to instil the highest ethical standards in our future scientists and researchers."

The OPCW strives to achieve its goal "to consign chemical weapons to history, forever," through scientific work related to verification, international cooperation, and most recently, through education and outreach. Education is increasingly recognized as one of the first lines of defense to prevent the abuse of chemical substances, by equipping the public to respond to these issues. IUPAC is also concerned with ensuring that chemistry is practiced in a safe and beneficial way. IUPAC's vision is "to advance the worldwide aspects of the chemical sciences and to contribute to the application of chemistry in the service of humankind." To help ensure that chemistry acts "in the service of humankind," IUPAC works through its Committee on Chemistry Education to provide free educational resources to raise awareness about the responsible use of chemistry in modern society.

One concrete step toward raising awareness of the need to practice responsible science has been taken through a joint IUPAC-OPCW project (project 2005-029-1-050 and 2013-020-1-050) to create a set of interactive electronic materials, *Multiple Uses of Chemicals*. This website (www.iupac.org/multiple-uses-of-chemicals) introduces students, educators, and policymakers to the topic of multi-use chemicals, and discusses how they can be used for beneficial purposes and misused to create illegal drugs or even chemical weapons. The website also includes

Chemical Weapons: The Human Toll

A stark reminder of the importance of communicating responsibility with respect to multi-use chemicals comes from grasping the short- and long-term human toll of the use of chemical weapons in Syria in 2013 and Iran in the late 1980s. 1000 people (mainly civilians) were killed in the August 2013 sarin attack near Damascus. Still unknown are the number injured in this attack and the extent of continuing health problems. So far no investigations have addressed this issue. During the Iraq/Iran war chemical weapons were used extensively by Iraq against Iranian soldiers and civilians, and in 1988 by Iraq against its own Kurdish community. At least 7000 Kurds died from chemical weapons in these attacks. Most were civilians, including many women and children. Well over 7000 were injured and millions of Kurds fled across borders into neighbouring Iraq, Turkey and Syria out of fear of the effects of these agents. The number of people who still bear the scars of these attacks in Kurdish areas is also unknown. At least two chemical weapons, mustard gas and a nerve agent, possibly sarin, were used in the attacks. A nerve agent caused most of the fatalities. Iran still treats 30000 people, mainly former soldiers, for mustard gas related injuries. However, those being treated are the ones who were able to prove injury from mustard gas because of their army affiliations. Many others were not able to establish a causal link between mustard gas and their injuries, and have had to manage as best they can.

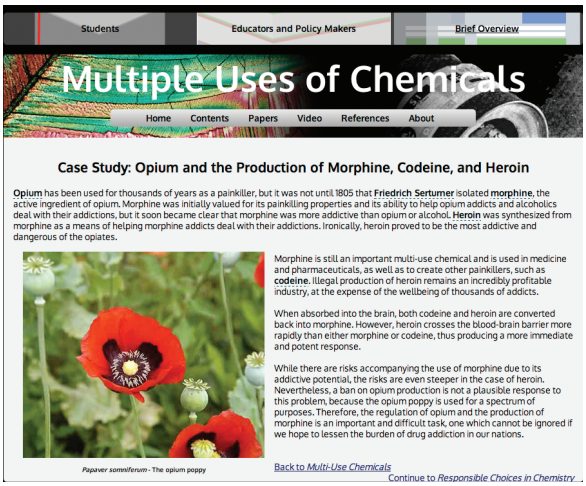
One of the major complications in making chemical weapons is the safety of the workforce involved in their manufacture, because of the potency of these substances. Creating these chemical weapons is within the reach of most competent chemists and the precursors are well known. It is, of course, illegal to do this and most countries have severe penalties for those who may be tempted. *Multiple Uses of Chemicals* was created, in part, to open the eyes of those who could be tempted, and to show them the destructive results that could result from their choices and actions.

video footage that demonstrates how this complex set of topics can be communicated in engaging and informative ways with educators and chemists. The joint project was led by Peter Mahaffy (Canada), and Alastair Hay (UK), and included other members of the OPCW Temporary Working Group on Education and Outreach: Jan Apotheker (Netherlands), Djafer Benachour (Algeria), Jo Husbands (USA), Robert Matthews (Australia), Ting-Kueh Soon (Malaysia), and Alejandra Suarez (Argentina). An interdisciplinary team of undergraduate students and faculty at the King's Centre for Visualization in Science (www.kcvs.ca), under the direction of Peter Mahaffy and Brian Martin, developed the educational materials, in close consultation with scientists and educational specialists from both IUPAC and the OPCW. Additional funding for the project was provided by the European Union through the OPCW.

A Versatile Online Resource

Following best practices in the design of electronic learning materials, the *Multiple Uses of Chemicals* website resource was made with interactivity in mind, implementing a variety of case studies and role-playing scenarios to communicate information effectively. To engage a wide range of audiences while delivering content appropriate to each type of user, the resource starts with three separate portals: *Brief Overview, Students*, and *Educators and Policymakers*.

The *Brief Overview* displays the major features of the resource, and is highly condensed for easy navigation through the site. The *Students* portal targets secondary and post-secondary chemistry classes, and can be used to stimulate discussions of scientific responsibility and integrity in the context of applications of



various concepts in general and organic chemistry, or to support courses in ethics. Interactive resources for students include role-playing scenarios, case studies, and a variety of personal and discussion questions. The *Educators and Policymakers* section contains tips for implementing the resource into presentations or classroom discussions, as well as a list of learning outcomes for each topic, supplementary resources such as worksheets for students, and links to other websites that may be useful in preparing presentations or lectures.

The website is divided into four major sections: *Multi-Use Chemicals*, *Responsible Choices in Chemistry*, *Convergence of Chemistry and Biology,* and *Codes of Conduct*. The majority of the content is in the first two sections, where users are introduced to the concept of multi-use chemicals and the problems associated with their regulation and distribution.

The *Multi-Use Chemicals* section explores the concept of multi-use chemicals, starting with three case

Complementary OPCW Education and Outreach Resources

In addition to the Joint IUPAC/OPCW Multiple Uses of Chemicals resources, the OPCW has published other resources, exploring the history and science behind chemical warfare agents:

• **Fires** is a documentary film series exploring the historical context for chemical weapon use, abuse, regulation, and prevention, while also investigating the motivations and inspirations for both the producers and monitors of chemical weapons. Find it at: www.thefiresproject.com

• **Chemistry in Conflict** is an educational module for high school students, designed to introduce students to chemical weapons, the Chemical Weapons Convention, and ethics in science. It provides both a rich context for educating in chemistry, and historical background to the production and regulation of chemical weapons. A diverse set of activities, case studies and exercises facilitate instructor implementation. Feedback is currently being incorporated into the resource, after which it will be made freely and publicly available. (See OPCW Today, Dec 2013 (same as ref.3), pp. 25-26.)

studies on the production of illegal drugs. It is unlikely that most university students have given much thought to the production of chemical weapons. However, they may have been tempted by the easy money which can be obtained from synthesizing illegal drugs from readily available precursors, especially when their syntheses are so simple. Workshops have shown that introducing multi-use chemicals through examples of the synthesis of illegal drugs is relevant to most audiences, and effectively stimulates discussion of scientific ethics and responsibility. Three case studies are presented: the production of heroin from extracts of the opium poppy; the preparation of methamphetamine from ephedrine and other precursors; and the synthesis of methylenedioxymethylamphetamine (ecstacy) from safrole. Each of these case studies displays not only the availability but also the industrial importance of the precursors to these drugs, showing that the regulation of these drugs is not simply a matter of banning their precursors, as this would prevent the production of a variety of important industrial and consumer products. Rather, the prevention of illegal drug production requires strict monitoring of these precursors, so as to not restrict the beneficial applications of these substances. This section then explores the historical use of chemical warfare agents through a slideshow of photographs showcasing their first modern use in the First World War to their recent use in Syria. This helps to emphasize both the historical devastation and modern relevance of the production of chemical warfare agents. Following this are four case studies on the production of chemical weapons, three on the production of Zyklon B, mustard gas, and sarin gas from their multi-use precursors, hydrogen cyanide, thiodiglycol, and glyphosate, respectively, and one on the potential bacterial production of the lethal natural product, saxitoxin.

The *Responsible Choices in Chemistry* section explores what it means to practice chemistry responsibly, as well as individual responsibilities of both chemists and non-chemists to understand and address the misuse of multi-use chemicals. Users first explore an individual role-playing scenario, where they have the option to choose what they consider to be an appropriate response to a given scenario, and then continue to choose decisions in this way as the scenario continues to unfold, introducing deeper complexity and moral ambiguity. Following this, the user can explore both the successes and challenges of national and international efforts to regulate the production of chemical and biological weapons.

Group discussion during the IUPAC Congress in Istanbul, August 2013.

The third section, *Convergence of Chemistry and Biology,* explores the areas of overlap between the disciplines of chemistry and biology. The blurring of boundaries between chemistry and biology has enabled better understanding of biochemical pathways and exploited molecular biology for medical applications, and is also responsible for new industrial products and methods of production. However, this convergence also poses a new concern for chemical and biological warfare, especially when having two separate multilateral regimes for chemical and biological weapons leaves ambiguity as to the responsibility of each to monitor these convergent areas. Users explore the possible scenario of converting a brewery into a chemical weapons laboratory that uses genetically modified yeast to produce a chemical weapon. While this area of convergence has previously been largely unexplored, OPCW considered the implications of this convergence through a Temporary Working Group of the OPCW Scientific Advisory Board. This working group met four times between 2011 and 2013 to investigate the technological and scientific developments which are accelerat-

In WWI trench warfare, mustard gas was used against the Allied Forces.

ing the convergence of these disciplines. Their findings are available on the OPCW website.

The final section of the resource is *Codes of Conduct*, which explores the relevance of both aspirational and enforceable codes of conduct for the regulation and distribution of multi-use chemicals. This is implemented through the use of another interactive "decision tree," as well as examples of the effects and power of various codes of conduct.

By interacting with the resource, users can engage in discussions of scientific ethics while learning or reinforcing chemistry concepts such as structure-function relationships. It is through this context-based learning that both chemistry information can be better communicated and the relevance of topics such as scientific ethics and codes of conduct can be more extensively understood and appreciated.

Resource for Workshops

The *Multiple Uses of Chemicals* resource has been piloted at several workshops for chemists and educators, including the August 2013 44th IUPAC World Chemistry Congress in Istanbul. The workshop, held just a week before the sarin incident in Syria, confronted participants with several role-playing scenarios, such as being a post-graduate student who is short of money but is familiar with the production of methamphetamine. Attendees were asked whether they would be curious to see if the synthesis was possible, whether they would tell others if they were successful, whether they would try again if they failed their first attempt at synthesis, and what circumstances would tempt them to sell the drugs. Participants discussed these questions in small groups, facilitated by the workshop directors, to see how innocent and seemingly harmless initial intentions can lead to dangerous or even criminal behaviour, all through a simple set of seemingly naturally connected decisions. The video of this workshop has been posted on the multiple-uses website, to give presenters tips for implementing the resource into their presentations and discussions. Another workshop was held at an OPCW regional meeting on responsible use of chemicals in Argentina in April 2014, and a workshop is planned for the 5th IUPAC Conference on Green Chemistry in Durban, South Africa, 17-21 August 2014. The resource is also being used in university contexts to provide ethics training for both undergraduate and graduate students in North America and Europe, and has been used with the Associate Programme at OPCW.

Peter Mahaffy <peter.mahaffy@kingsu.ca> is Professor of Chemistry at the King's University College Edmonton, Canada, Co-director of the King's Centre for Visualization in Science, and Past-Chair of IUPAC's Committee on Chemistry Education. Joseph Zondervan is a fourth-year undergraduate chemistry student at the King's University College, and was the lead student researcher at the King's Centre for Visualization in Science, working on preparation of the Multiple Uses of Chemicals site. Alastair Hay <A.W.M.Hay@leeds.ac.uk> is Professor of Environmental Toxicology at the University of Leeds, England. He has worked on chemical weapons issues for more than 35 years and conducted six investigations of real and alleged chemical weapon use. Peter Mahaffy and Alastair Hay are members of the OPCW Temporary Working Group on Education and Outreach, and have worked together on developing and implementing educational materials related to multiple uses of chemicals since the 2005 Joint IUPAC/OPCW Oxford workshop. Daniel Feakes <Daniel.Feakes@opcw.org> is the Strategy and Policy Adviser in the Office of Strategy and Policy at the OPCW. He is the Secretary to the OPCW Temporary Working Group on Education and Outreach in Science and Technology Relevant to the Chemical Weapons Convention. Jonathan Forman <Jonathan.Forman@opcw.org> currently holds a post of science policy adviser at the OPCW. Prior joining OPCW in March 2013, Forman worked in Silicon Valley for several biotechnology companies developing molecular diagnostic and bioanalytical assay technologies for genomic, immunoassay, and cell capture applications.

Resources and References

1. Multiple Uses of Chemicals website: www.iupac.org/multiple-uses-of-chemicals or http://multiple.kcvs.ca/
2. IUPAC Project 2013-020-1-050 "Updating, Piloting, and Disseminating Educational Material for Raising Awareness of the Multiple Uses of Chemicals and the Chemical Weapons Convention" www.iupac.org/project/2013-020-1-050
3. Multiple Uses of Chemicals: Choices for Chemists and the Public By Alastair Hay and Peter Mahaffy, *OPCW Today*, December 2013, Vol.2 , No 5, pp. 23-24; www.opcw.org/documents-reports/opcw-today (the entire issue is on education and outreach and also includes a coverage of OPCW winning the Nobel Peace Prize)
4. Video message by OPCW Director-General Ahmet Üzümcü at the 44th IUPAC World Chemistry Congress in Istanbul, Turkey, which took place from 11 to 16 August 2013; www.youtube.com/watch?v=fWIX2lB8cSc (or via www.youtube.com/user/opcwonline)
5. Video of the workshop led by Dr. Alastair Hay and Dr. Peter Mahaffy at the IUPAC 44th World Chemistry Congress in Istanbul, August 2013 on how to use Multiple Uses of Chemicals in a workshop for chemistry educators; www.youtube.com/watch?v=HJ2psAWflso
6. IUPAC, OPCW, and the Chemical Weapons Convention by Leiv K. Sydnes, *Chemistry International*, July-August 2013, pp.4-8; DOI: 10.1515/ci.2013.35.4.4.

IUPAC Elections for the 2016–2017 Term

Every two years, IUPAC holds an election for its officers and committee members. About 120 individuals are to be elected or reelected either as Titular Members, Associate Members, or National Representatives. Information concerning the voting process and the role of each kind of member is contained in the Union bylaws (see www.iupac.org/home/about/organizational-guidelines.html).

Any qualified individual who is interested in being nominated is invited to contact his/her National Adhering Organization (NAO) and/or the current committee officers. The next election will cover a two- or four-year term that will start in 2016. Every division committee and standing committee will have vacancies.

As part of the nomination procedure, NAOs are invited to submit curriculum vitae for each nominee to the IUPAC Secretariat no later than **31 March 2015**. Elections for each committee will take place during the second trimester of 2015 and the 2016–2017 memberships for all committees will be finalized during the next IUPAC General Assembly in August 2015. Individuals interested in becoming officers on the IUPAC Bureau should contact their NAOs. Nominations for officers have a different timeline and can only be made by an NAO. Officer elections will take place at the Council Meeting during the next General Assembly.

Contact information for all NAOs and division and standing committee officers is available on the IUPAC website, or upon request at the IUPAC Secretariat; e-mail <secretariat@iupac.org>; tel.: +1 919 485 8700; fax +1 919 485 8706; www.iupac.org

Winners of the 2014 IUPAC-SOLVAY International Award for Young Chemists

In May 2014, IUPAC and Solvay announced the winners of the 2014 IUPAC-SOLVAY International Award for Young Chemists presented for the best PhD theses in the chemical sciences as described in 1000-word essays.

The five Winners are:

- **Keary Mark Engle**, USA/UK - The Scripps Research Institute, La Jolla, California, USA, joint with University of Oxford, UK
- **Albert C. Fahrenbach**, USA—Northwestern University, Evanston, Illinois, USA
- **Yohei Ishida**, Japan - Tokyo Metropolitan University, Japan
- **Ahmad Masarwa**, Israel - Technion-Israel Institute of Technology, Haifa, Israel
- **Rodrigo Andreas Vargas Jentzsch**, Switzerland - University of Geneva, Switzerland

The Winners will each receive a cash prize of USD 1000 and travel expenses to the 45th IUPAC World Chemistry Congress, 9-14 August 2015, in Busan, Korea. Each prizewinner is also invited to present a poster at the IUPAC Congress describing his/her award-winning work and to submit a short critical review on aspects of his/her research topic to be published in *Pure and Applied Chemistry*. The awards will be presented to the winners during the Opening Ceremony of the Congress.

The essays describing the 2014 Winners' theses may be found on the IUPAC web site and cover a wide range of subject matter:

- Dr. Engle: (1) Ligand-Accelerated Catalysis in Palladium(II)-Mediated C–H Functionalization; and (2) Hydrogen-Bonding Effects on the Reactivity of Fluoride Anion
- Dr. Fahrenbach: Molecular Switches Based on Donor-Acceptor, Radical and Coulombic Interactions – From Solution, to Solid-State to Application
- Dr. Ishida: Artificial Light-Harvesting System by Supramolecular Host-Guest Assemblies
- Dr. Masarwa: Selective Metal-Mediated C-C Bond Activation of Strain Compounds: Application to Challenging non-Natural Product Synthesis
- Dr. Vargas Jentzsch: Anion Transport with Anion-π Interactions and Halogen Bonds

There were 55 applications from 20 different countries. The Prize Selection Committee comprised members of the IUPAC Bureau with a wide range of expertise in chemistry. Professor Kazuyuki Tatsumi, former IUPAC President, chaired the committee. The 2014 International Award for Young Chemists is the first sponsored by Solvay and is intended to encourage outstanding young research scientists at the beginning of their careers. In making their decisions, the jury was keen to recognize a global representation of the awards in line with the pool of applications.

In view of the many high-quality applications, the Committee also decided to give four Honorable Mention Awards to:

- Yoichi Hoshimoto, Japan - Osaka University, Japan
- Frank A. Leibfarth, USA – California Institute of

Technology, Pasadena, California, USA
- Robert J. Macfarlane, USA - Northwestern University, Evanston, Illinois, USA
- Xuemei Sun, China - Fudan University, Shanghai, China

The recipients of Honorable Mention Awards will receive a copy of the *Principles of Chemical Nomenclature – A guide to IUPAC Recommendations*. The book is published by Royal Society of Chemistry (UK) and offered with the compliments of RSC Publishing.

Now in its 15th year, the International Award for Young Chemists has steadily attracted bright young chemists. Everyone is invited to review the latest collection published in *Pure and Applied Chemistry* covering last year's awards, which appeared in January 2014. Also, in 2011, *PAC* published a special issue, fittingly subtitled "Perspectives and Challenges" inviting winners of the very early years of the prize. IUPAC is proud of its commitment to engage and encourage young scientists. Hopefully, the contents of these *PAC* issues will inspire and enthuse readers with fascinating insights into new and emerging aspects of chemical sciences.

Applications for the 2015 Prizes are now being solicited; application deadline is 1 February 2015.

www.iupac.org/news/news-detail/article/2015-iupac-solvay-international-award-for-young-chemists-announced.html

Steven V. Ley wins 2014 IUPAC-ThalesNano Prize in Flow Chemistry

University of Cambridge professor Steven V. Ley (Cambridge, UK) is the 2014 recipient of the IUPAC-ThalesNano Prize in Flow Chemistry. The award was presented on 25 June 2014 at the International Conference on Microreaction Technology (http://www.imretconferences.com) in Budapest, by former IUPAC Committee of Chemistry and Industry (COCI) Chair Prof. Michael Droescher and Dr. Ferenc Darvas for ThalesNano and for the Flow Chemical Society.

This award was established in 2012 by a generous gift from the Hungarian Technology company ThalesNano Inc. to acknowledge the key role that flow chemistry plays in improving chemical processes. The prize of 7500 USD goes to an internationally recognized scientist whose activities or published accounts have made an outstanding contribution to the practice of flow chemistry. ThalesNano also provides support for travel by the recipient to the prize ceremony. The prize is awarded biannually, and ThalesNano will provide the funds for the first 10 years.

Steven V. Ley (center) receiving his award from Michael Droescher (right) and Dr. Ferenc Darvas (left).

Professor Ley receives this award for his outstanding contribution and creative work in methodologies for organic synthesis, especially in multi-step synthesis in continuous flow chemistry reactor systems. With his work in flow chemistry, published in over 80 papers, Prof. Ley contributed several landmark discoveries. His success has also been fueled by continued instrument development in flow chemistry with commercial organizations.

Flow chemistry focuses on synthesis of functional molecules, which plays an important role in modern society. However, the labor intensive and wasteful synthesis practices of the past are no longer acceptable. Prof. Ley began a campaign in the early 1990s to develop enabling technologies to improve the synthesis process. By demonstrating the power of immobilized reagents and scavengers he was able to achieve multi-step synthesis in a clean fashion, avoiding the wasteful practices of chromatographies, crystallizations, distillations, and water washes or extraction. He demonstrated that these systems could be incorporated with automation into continuous flow processes to achieve multi-step synthesis with minimum purification and work up.

Prof. Ley has received more than 50 major prizes and awards, many distinguished named lectureships and visiting professorships. He has served in many international and national appointments and committees.

www.iupac.org/news/latest-news

The InChI Team presented with the 2014 Chemical Structure Association (CSA) Trust Mike Lynch Award

The 2014 Chemical Structure Association (CSA) Trust Mike Lynch Award is being presented to the "InChI Team," namely Steve Heller, Steve Stein, Alan McNaught, Dmitrii Tchekhovskoi, and Igor Pletnev.

This award is given tri-annually to someone who has made outstanding contributions to education, research, and development activities that facilitate the storage, processing, and retrieval of information about chemical structures, reactions, and properties. Dr. Andreas Barth, Chair of the CSA Trust, stated that it is an honor to acknowledge the work in the conception and development of the IUPAC International Chemical Identifier, InChI.

The Award ceremonies took place during the 10th International Conference on Chemical Structures held in Nordwijkerhout, in The Netherlands, 1-5 June 2014.

www.int-conf-chem-structures.org

www.csa-trust.org

Data Citation Principles

Sound, reproducible scholarship rests upon a foundation of robust, accessible data. For this to be so in practice as well as theory, data must be accorded due importance in the practice of scholarship and in the enduring scholarly record. In other words, data should be considered legitimate, citable products of research. Data citation, like the citation of other evidence and sources, is good research practice and is part of the scholarly ecosystem supporting data reuse. In support of this assertion, and to encourage good practice, a set of guiding principles for data citation has been developed by the "Data Citation Synthesis Group."

The "Data Citation Synthesis Group (www.force11.org/node/4785) is a cross-team committee leveraging the perspectives from the various existing initiatives working on data citation to produce a consolidated set of data citation principles (based on the Amsterdam Manifesto, the CODATA-ICSTI Task Group report and other sets of principles provided by others) in order to encourage broad adoption of a consistent policy for data citation across disciplines and venues. The group has reviewed the existing efforts and made a set of recommendations in a Joint Declaration of Data Citation Principles released earlier this year at www.force11.org/datacitation

The Data Citation Principles cover purpose, function, and attributes of citations. These principles recognize the dual necessity of creating citation practices that are both human-understandable and machine-actionable. As the preamble to those eight short consensus principles states, they are not meant as a blueprint for implementation of data citation policies and practices, but as high-level guidance for any organization and sector to develop and then implement a data citation protocol. These principles integrate the emerging consensus of several different international groups working in the data citation arena. The principles were broadly reviewed and discussed over the past several months.

The Group is seeking endorsements of these principles by the worldwide research community. See the endorsement page:

www.force11.org/datacitation/endorsement

2015 Year of Soils and Year of Light

The United Nations has approved 2015 as the Year of Soils. This will be an unique opportunity to raise the profile of soils and celebrate soil science. The IUSS has formed an ad-hoc committee that will coordinate and organize all activities for this special year. Many activities are being planned. Please submit activities and all your ideas to the IUSS President elect Rainer Horn: rhorn@soils.uni-kiel.de

www.fao.org/globalsoilpartnership/iys-2015/en/

The United Nations has also declared that the year 2015 will be the International Year of Light and Light-based Technologies (IYL2015). With light-science and its applications, the potential for collaboration is very broad. Do not hesitate to contact the IYL2015 organizers to explore collaboration possibilities. For more information, please contact Joe Niemela (light2015@ictp.org).

INTERNATIONAL YEAR OF LIGHT 2015

www.light2015.org.

The Project Place

A critical review of the proposed definitions of fundamental chemical quantities and their impact on chemical communities

The objective of this project is to provide a Technical Report containing a critical review of the definitions for the quantity amount of substance and its unit, mole, as well as the related unit of the quantity mass.

The work will consist of the compilation of existing published work related to the definition of the quantity amount of substance, its unit, and the consequence of these definitions on the unit of the quantity mass. The compilation will be reviewed critically with the aim of assembling all possible elements in order to judge the adequateness of the existing definitions or new proposals. Compilation and critical review shall rely on the broadest spectrum of interested IUPAC members. Therefore, all divisions will be invited to participate in the project, as well as the Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS) and Committee on Chemistry Education (CCE). All task group members will have a mandate to speak on behalf of their corresponding communities. External experts will be consulted.

The task group is scheduled for discussions in the Consultative Committee for Amount of Substance, or Comité consultatif pour la quantité de matière (CCQM) and the International Bureau of Weights and Measures (BIPM) on the new definition of the mole. A time horizon of 2015 for establishing a firm position of IUPAC with regard to this question is adequate for further decisions to be taken by CCQM, the International Committee for Weights and Measures or Comité international des poids et mesures (CIPM), and the General Conference on Weights and Measures (Conférence Générale des Poids et Mesures, CGPM).

In June 2014, the task group initiated a survey to collect opinions and comments by the IUPAC National Adhering Organizations (NAOs). The questionnaire focuses on the current definition of the mole, the new definition of the mole, the current definition of the quantity amount of substance, and the current name of the quantity amount of substance. NAOs are asked to reply **no later than 1 October 2014**. The questionnaire is available from the project webpage below.

For more information, contact the Task Group Chair Jürgen Stohner <sthj@zhaw.ch> or email <mole@iupac.org>

www.iupac.org/project/2013-048-1-100

On the definition of the mole

In 1971, the 14th General Conference of Weights and Measures resolved to define the mole as "the amount of substance of a system which contains as many elementary entities as there are atoms in 0.012 kilogram of carbon 12..." In addition, "when the mole is used, the elementary entities must be specified and may be atoms, molecules, ions, electrons, other particles, or specified groups of such particles." This is the current definition of the mole.[1]

In 2011, the 24th General Conference of Weights and Measures proposed a revision of the SI. As a consequence of this, the redefinition of the mole is necessary and its magnitude will be set "by fixing the numerical value of the Avogadro constant to be equal to exactly 6.022 14X × 10^{23} when it is expressed in the SI unit mol^{-1}." The symbol X represents one or more additional digits to be added to the numerical value of N_A. This is the proposed new definition of the mole.[2]

Mole is the name of the SI base unit (symbol mol) for the base quantity *amount of substance* (symbol *n*) which is defined in IUPAC documents (e.g. IUPAC Green Book, 3rd Edition, 2nd Printing 2008)[3] using the expression $n = N/N_A$, where N is the number of entities, and N_A is the Avogadro constant. Similarly, the SI Brochure (8th Edition 2006)[1] provides the following definition of the quantity *amount of substance*:

"Amount of substance is defined to be proportional to the number of specified elementary entities in a sample, the proportionality constant being a universal constant which is the same for all samples ... This constant is called the Avogadro constant, symbol N_A or L ... the relation is $n = N/N_A$. ... the Avogadro constant has the coherent SI unit reciprocal mole."

References

1. www.bipm.org/en/si/si_brochure/
2. www.bipm.org/en/CGPM/db/24/1/
3. www.iupac.org/home/publications/e-resources/nomenclature-and-terminology/quantities-units-and-symbols-in-physical-chemistry-green-book.html

Basic Terminology of Crystal Engineering

Crystal engineering is the design and synthesis of functional crystalline structures, based on a bottom-up approach from smaller building blocks. Crystal engineering is a fascinating new subject that has expanded rapidly in the last 20 years. It is also attracting the interest of the chemical and pharmaceutical industry. It overlaps with supramolecular chemistry, X-ray crystallography, materials science, and solid-state chemistry, but is a distinct discipline in itself. The subject goes beyond the traditional divisions of organic, inorganic, and physical chemistry; this makes for an eclectic blend of ideas, techniques, and strategies.

The diversity in focus and scientific basis of the researchers in the field has led to numerous terminology practices that are not consistent among research groups, causing confusion and unnecessary conflicts.

The purpose and scope of this project is to provide a basic glossary of terms for this rapidly evolving, highly interdisciplinary field, to identify and debate open questions, and to point out new directions.

The objectives of this project are: to produce guidelines for terminology (glossary of terms) in the area of crystal engineering; to ensure that these guidelines are accepted by a large group of leading researchers in the field; and to have these guidelines implemented or referred to in the instructions to authors of leading crystal engineering journals.

In May 2014, the Task Group secured a grant from ICSU and proceeded with a kickoff workshop held concurrently with the 1st International Symposium on Halogen Bonding (ISXB-1) in Porto Cesareo (Lecce, Italy), 18-22 June 2014 (see http://www.isxb-1.eu/symposium-program/satellite-event.html). The project is being advertised in major meetings relevant to related fields, including the recent 23rd Congress and General Assembly of the International Union of Crystallography (IUCr) held in Montreal, Canada, 5-12 August 2014.

Next year, 30-31 August 2015, an international workshop open to the public will be organized for consideration of public comments, presentation, and dissemination of results; the workshop will be a satellite event, part of the 29th European Crystallography Meeting organized in Croatia.

For more information, contact the Task Group Chairs Pierangelo Metrangolo <pierangelo.metrangolo@polimi.it> or Giuseppe Resnati <giuseppe.resnati@polimi.it>

www.iupac.org/project/2012-044-1-100

Implementation of InChI for chemically modified large biomolecules

The IUPAC International Chemical Identifier (InChI) algorithm is now well established as a powerful means of denoting the basic chemical structure of a well-defined, small (<1024 atoms) organic molecule as a unique machine-readable character string, suitable for electronic data storage, searching, and exchange. The IUPAC Division VIII InChI Subcommittee is now starting work on a complete overhaul of the InChI algorithm, i.e. the beginning of plans for a second version of InChI. A crucial part of this work is intended to address the known shortcomings of the current InChI algorithm pertaining to the handling (or lack thereof) of various types of biological substances. Chemically modified sequences are becoming very important in life science research both as tools and as products. Chemically modified biologics range from siRNA sequences, established therapeutics such as Levimir and Byetta for diabetes, to the growing area of antibody drug conjugates (ADCs). There is currently no standard approach for the naming of chemically modified biologics; this constitutes a tremendous opportunity for InChI to become established as the naming technology.

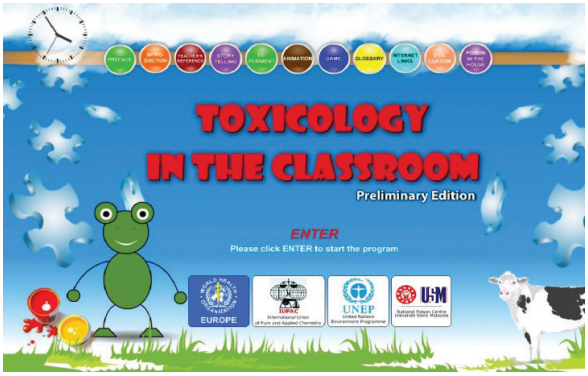
For more information, contact the Task Group Chair Keith Taylor <Keith.Taylor@accelrys.com>

www.iupac.org/project/2013-010-1-800

Toxicology in the Classroom II

This new project is based on a recently completed IUPAC project 2004-045-1-700 "Training of School Children on Pesticides and Health" that was designed to raise awareness among young children about the potential adverse effects of chemicals and, in the process, help reduce the careless use of pesticides. Toxicology in the classroom (Toxiclaro for short) is a multimedia resource that will help teachers educate their students about pesticides and health. Toxiclaro is a virtual toolbox, offering training materials, a curriculum, and resources such as games, experiments, and a virtual house to explore—all of which provide for a basic understanding of toxicology and awareness of the need for protective and precautionary measures.

Task group members prepared an experimental design for teaching the dose response principle in the classroom. This experiment makes use of the suppression of seed growth by copper sulfate. A test run was



conducted in Malawi and came up with several very valuable observations and recommendations to review and refine the existing material. Experimental amendments were made and the results were used for the computer animation.

The project was also an expansion of a project of the International Programme on Chemical Safety (IPCS) of the World Health Organization. The IPCS multilevel course aims at training different groups of people in the sound management of pesticides. The course material addresses trainers and technical and medical personnel. The Toxiclaro project aimed to expand this approach to young people, educating them about protecting themselves from the harmful effects of pesticides and hazardous chemicals, and developing a safety culture for the future (feature published in *Chem. Int.* Nov-Dec 2009 pp. 17-20).

The Toxiclaro initiative originated from the Chemistry and Human Health (IUPAC Division VII) and the working group formally met to plan the project in May 2005 at the Federal Agency for Risk Assessment, Berlin, Germany. Several meetings followed and the Toxiclaro package was finally developed in a joint effort involving IUPAC, WHO, UNEP, and the Universiti Sains Malaysia.

It was pilot tested in both urban and rural schools in Argentina, Ghana and Malaysia. Presentations on Toxiclaro were held during the annual congress of the Asia Pacific Association of Medical Toxicology in Chandigarh (2008) and Hong Kong (2012); Toxiclaro was also presented at the 2011 conference in Carpi/Italy of the Collegium Ramazzini. It won two awards (gold medal and special) at the Malaysia Technology Exposition in Kuala Lumpur in February 2013.

Toxiclaro is currently available via the UNEP website www.unep.org/chemicalsandwaste/UNEPsWork/Pesticides/ToxicologyintheClassroom/tabid/104445/

Toxicology in the classroom – Teacher's edition

Following the pilot testing of Toxiclaro in schools the Teacher's edition was developed in a printed format to support teaching in schools where access to computers and audio-visual equipment are limited.

Toxicology in the classroom – Children's edition

The Children's edition was developed after a workshop held in Malaysia in late 2011. The content follows closely with that of the Teacher's edition but included simple text and many illustrations. This book contains a storytelling section incorporating 11 comic strips intended to further illustrate the understanding of chemical risks to human health and the environment.

Interactive Multimedia CD-version

The original CD version has now been updated to incorporate the experience's gained from the pilot trials.

Toxiclaro has now been translated into Spanish and Polish. Further translations are envisaged.

The new IUPAC project aims to produce a second version with new toxicological content that will pay particular attention to the understanding of chemical risks to human health and the environment. The project will strengthen the association of IUPAC with educational material relating to the safe use of chemicals.

Comments and recommendations are welcome. For more information contact Task Group Chairman Wayne A. Temple <wayne.temple@otago.ac.nz>.

www.iupac.org/project/2013-023-1-700

Abbreviations of polymer names and guidelines for abbreviating polymer names (IUPAC Recommendations 2014)

Jiasong He, et al
Pure and Applied Chemistry, 2014
Volume 86, Issue 6, pp 1003–1015

Abbreviations are commonly used by authors of manuscripts to avoid repetition of lengthy polymer names, and for the benefit of the editors and readers of scientific and professional journals and other written material. People working within industry use a well-established ISO list of abbreviations of polymer names which contains more than 100 entries (138 in ISO 1043-1:2011). In fact, mainly selected on the basis of the scale of production, the ISO abbreviations are used in industry, standards, trade, and legislation. On the other hand, scientific and professional journals in the polymer field deal with hundreds of polymers annually, including many new ones, some with complicated structures. Thus, IUPAC has also recognized the importance of abbreviations and has published recommendations on the use of common abbreviations for polymer names.

This document provides some basic rules and guidelines regarding the use and creation of abbreviations for the names of polymers. An extended list of currently used abbreviations for polymers and polymeric materials is appended.

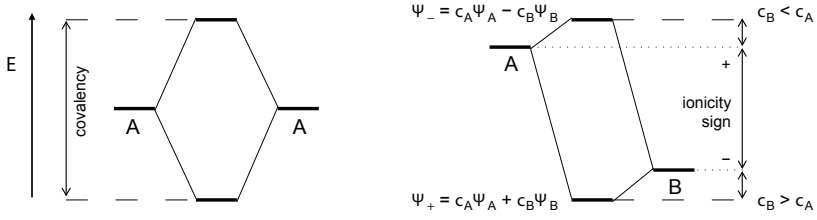
http://dx.doi.org/10.1515/pac-2012-1203

Toward a comprehensive definition of oxidation state (IUPAC Technical Report)

Pavel Karen, Patrick McArdle, and Josef Takats
Pure and Applied Chemistry, 2014
Volume 86, Issue 6, pp 1017–1081

A generic definition of oxidation state (OS) is: "The OS of a bonded atom equals its charge after ionic approximation." In the ionic approximation, the atom that contributes more to the bonding molecular orbital (MO) becomes negative. This sign can also be estimated by comparing Allen electronegativities of the two bonded atoms, but this simplification carries an exception when the more electronegative atom is bonded as a Lewis acid. Two principal algorithms are outlined for OS determination of an atom in a compound: one based on composition, the other on topology. Both provide the same generic OS because both the ionic approximation and structural formula obey rules of stable electron configurations. A sufficiently simple empirical formula yields OS via the algorithm of direct ionic approximation (DIA) by these rules. The topological algorithm works on a Lewis formula (for a molecule) or a bond graph (for an extended solid) and has two variants. One assigns bonding electrons to more electronegative bond partners, the other sums an atom's formal charge with bond orders (or bond valences) of sign defined by the ionic approximation of each particular bond at the atom. A glossary of terms and auxiliary rules needed for determination of OS are provided, illustrated with examples, and the origins of ambiguous OS values are pointed out. An electrochemical OS is suggested with a nominal value equal to the average OS for atoms of the same element in a moiety that is charged or otherwise electrochemically relevant.

http://dx.doi.org/10.1515/pac-2013-0505



The essence of the adopted ionic approximation based on how the valence orbitals participate in the bonding MO. The mixing coefficients c_A and c_B refer to the atomic-orbital wavefunctions ψ_A and ψ_B in a MO as linear combination of atomic orbitals (MO-LCAO) approach.

Solubility of Nonsteroidal Anti-inflammatory Drugs (NSAIDs) in Neat Organic Solvents and Organic Solvent Mixtures

William E. Acree

J. Phys. Chem. Ref. Data 43, 023102 (2014)
IUPAC-NIST Solubility Data Series, Volume 102

This IUPAC-NIST Solubility Data Series volume reviews experimentally determined solubility data for 33 nonsteroidal anti-inflammatory drugs (NSAIDs) dissolved in neat organic solvents and well-defined binary and ternary organic solvent mixtures retrieved from the published chemical and pharmaceutical literature covering the period from 1980 to the beginning of 2014. Except for aspirin (2-acetoxybenzoic acid) and salicylic acid (2-hydroxybenzoic acid), very little physical and chemical property data are available in the published literature for NSAIDs prior to 1980. Solubility data are compiled and critically reviewed for aclofenac, celecoxib, dexibuprofen, diclofenac, diflunisal, etoricoxib, fenbufen, fentiazac, flufenamic acid, flurbiprofen, ibuprofen, indomethacin, ketoprofen, ketorolac, lornoxicam, mefenamic acid, meloxiam, nabumetone, naproxen, niflumic acid, nimesulide, phenylbutazone, piroxicam, rofecoxib, sodium diclofenac, sodium ibuprofen, sodium naproxen, sodium salicylate, tenoxicam, tolfenamic acid, and valdecoxib.

http://dx.doi.org/10.1063/1.4869683

To access recent volumes in the Solubility Data Series, visit http://jpcrd.aip.org/ and search IUPAC-NIST Solubility Data Series

IUPAC Empfehlungen

The German National Adhering Organization, the Deutscher Zentralausschuss für Chemie, through one of its component Societies, the Gesellschaft Deutscher Chemiker, regularly arranges for the translation and publication of selected IUPAC Reports and Recommendations in the journal *Angewandte Chemie*.

For more information, please visit the journal website: http://onlinelibrary.wiley.com/journal/10.1002/(ISSN)1521-3757/homepage/iupacemp/index.html

Suggestions for themes and experts are welcomed; e-mail contact: angewandte@wiley-vch.de

IUPAC Recommendations recently translated in German include:

- Definition of the halogen bond (IUPAC Recommendations 2013), *Angew. Chem*. 2014, 126, No. 24, 6391-6392 (DOI: 10.1002/ange.201309626)
- Terminology for aggregation and self-assembly in polymer science (IUPAC Recommendations 2013), *Angew. Chem*. 2014, 126, No. 11, 3078-3091 (DOI: 10.1002/ange.201304087)

Provisional Recommendations

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

Nomenclature and Graphic Representations for Chemically Modified Polymers

A new source-based nomenclature system is described which indicates that a particular polymer has been chemically modified. A connective within the name of a polymer, -mod-, is introduced for this purpose as in poly[(A)-mod-(B)]. The system is intended to be used in accordance with source-based naming of polymers but also provides for the use of structure-based names when it is unavoidable. It embraces: (1) modification of a constitutional unit into another, the unique structure of which is known; and (2) a more general modification of a constitutional unit resulting in any one of a number of possible structures. In addition, a new symbol, ~>, is proposed for use in graphic representations of the structure of modified polymers.

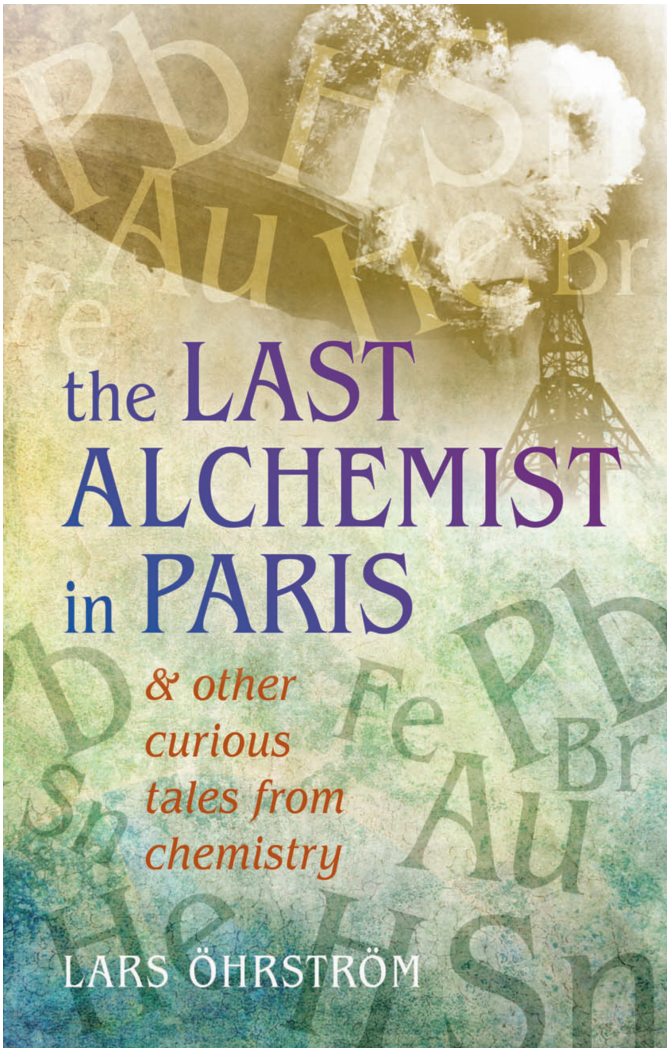
Comments by 31 December 2014
Richard G. Jones
kapitimana@gmail.com
http://www.iupac.org/project/1999-051-1-800

The Last Alchemist in Paris

by Lars Öhrström
Oxford University Press, 2014, xiv + 257 p.

reviewed by Juris Meija

Like most popular science books of chemistry, *The Last Alchemist in Paris* is a collection of stories where chemistry of elements intertwines with the cultural history of recent or distant times. A problem common to many popular chemistry books is that either good chemists are usually not good historians, or that good historians are usually bad chemists. Öhrström is certainly a good chemist and in this book he also demonstrates a passion and respect for history.



By now, most of us have heard the tale of "Napoleon's buttons," the chemical "romance" of the soldiers' tin buttons crumbling to dust in the cold Russian winter of 1812, aiding the defeat of the French army. Fact or fiction? To answer this question, Öhrström does not exercise the popular copy-paste approach to writing and research. Rather, he draws from contemporary and historic records and offers an exemplary dive into the crux of this story. It also helps that he has seen the infamous buttons and has participated in the investigation of the recently discovered mass grave of the grand army in Lithuania. His analysis of facts, rumors, and opinions is a first-rate example of critical thinking, research, and scientific journalism. Overall, this book offers an inspiring tour behind the scientific backdrop of so many cultural scenes of our lives.

"In this book you will find out the answers to important and interesting socio-chemical questions."

The book is inspiring. I can imagine, for example, a young reader and aspiring scientist performing alkaline hydrolysis of cloves in mom's kitchen in anticipation of conjuring the scent of nutmeg. Öhrström also has a good sense of humor. There are plenty of witty subtitles and comments: mining, he writes, has been around ever since Snow White and the Seven Dwarfs, and for easy reference he approximates the chloride-to-bromide amount ratio in seawater as 666:1 (can't argue with that). On a more serious side of things, this book has the intellectual muscle. In this book you will find out the answers to important and interesting socio-chemical questions. Why were the zeppelins not filled with the non-flammable helium a century ago and why should we resist buying those useless helium-filled party balloons. Most importantly, you will find out how to tell apart a diamond from the coveted cubic zirconia.

Juris Meija is Titular Member of the IUPAC Interdivisional Committee on Terminology, Nomenclature and Symbols and Chair of the IUPAC Commission on Isotopic Abundances and Atomic Weights.

On the Use of Italic and Roman Fonts for Symbols in Scientific Text*

by Ian Mills

Scientific manuscripts frequently fail to follow the accepted conventions concerning the use of italic and roman fonts for symbols. An italic font is generally used for emphasis in running text, but it has a quite specific meaning when used for symbols in scientific text and equations. The following summary is intended to help in the correct use of italic fonts in preparing manuscript material.

1. The general rules concerning the use of italic (sloping) fonts or roman (upright) fonts are presented in Section 1.3.2., p. 5 and Section 4.1, p. 103 in the IUPAC Green Book [1], in relation to mathematical symbols and operators. These rules are also presented in the International Standards ISO 31 (successively being replaced by ISO/IEC 80000), ISO 1000 [2], and in the SI Brochure [3].

2. The overall rule is that symbols representing physical quantities or variables are italic, but symbols representing units, mathemathical constants, or labels are roman. Sometimes there may seem to be doubt as to whether a symbol represents a quantity or has some other meaning (such as a label): a good general rule is that quantities, or variables, may have a range of numerical values, but labels cannot. Vectors, tensors, and matrices are denoted using a boldface (heavy) font, but they should still be italic since they are still quantities.

Examples:

The mass of my pen m = 24 g = 0.024 kg. The electric field strength $\boldsymbol{E}$ has components E_x, E_y, and E_z. The Planck constant h = 6.626 068 96(33) $\times 10^{-34}$ J s.

3. The above rule applies equally to letter symbols from both the Greek and the Latin alphabet, although authors often appear to resist putting Greek letters into italic.

Example:

When the symbol μ is used to denote a physical quantity (such as mass or reduced mass) it should be italic, but when it is used in a unit such as the microgram, μg, or when it is used as the symbol for the muon, μ (see 5 below), it should be roman.

4. Numbers and labels are roman (upright), since they are not physical quantities.

Example:

The ground and first excited electronic states of the CH_2 molecule are denoted

$...(2a_1)^2(1b_2)^2(3a_1)^1(1b_1)^1$, $\tilde{X}\ ^3B_1$, and

$...(2a_1)^2(1b_2)^2(3a_1)^2$, $\tilde{a}\ ^1A_1$, respectively.

The π-electron configuration and symmetry of the benzene molecule in its ground state are denoted: $...(a_{2u})^2(e_{1g})^4$, $\tilde{X}\ ^1A_{1g}$. All these symbols are labels and are roman.

5. Symbols for elements in the periodic table should be roman, since they are not physical quantities. Similarly the symbols used to represent elementary particles are always roman. (See, however, paragraph 9 below for the use of italic font in chemical-compound names.)

Examples:

H, He, Li, Be, B, C, N, O, F, Ne, ... for atoms; e for the electron, p for the proton, n for the neutron, μ for the muon, α for the alpha particle, etc.

6. Symbols for physical quantities are single letters of the Latin or Greek alphabet. Exceptionally two letters are used for certain dimensionless quantities, such as the Reynolds number, *Re*. However the symbols are frequently supplemented with subscripts or information in brackets to further specify the quantity. Further symbols used in this way are either italic or roman depending on whether they represent physical quantities or labels.

Examples:

H denotes enthalpy, but H_m denotes molar enthalpy (m is a mnemonic label for molar, and is therefore roman).

C_p and C_V denote the heat capacity at constant pressure p and volume V, respectively; but $C_{p,m}$ and $C_{V,m}$ denote the *molar* heat capacity at constant p and V, respectively (note the roman m but italic p and V).

The chemical potential of argon might be denoted μ_{Ar} or μ(Ar), but the chemical potential of the ith component in a mixture would be denoted μ_i, where the i is italic because it is a variable index.

*The 1999 version of this document has been prepared by I.M. Mills and W.V. Metanomski and has since been available online. It was then slightly revised in 2007 and full text included in the GUIDELINES FOR DRAFTING IUPAC TECHNICAL REPORTS AND RECOMMENDATIONS and also in the 3rd edition of the IUPAC Green Book (ref. 1).

7. Symbols for mathematical operators are always roman. This applies to the symbol Δ for a difference, δ for a small difference, d for an infinitesimal difference (in calculus), and to capital Σ and Π for summation and product signs. The symbols π, e (base of natural logarithms), i (square root of minus one), etc. are always roman, as are the symbols for specified functions such as log (lg, ln or lb), exp, sin, cos, tan, erf, **div**, **grad**, **rot** (the operators div, grad and rot may be printed boldface since they represent a vector). Some of these letters are also sometimes used to represent physical quantities: then of course they should be italic, to distinguish them from the corresponding mathematical symbol.

Examples:

$\Delta H = H(\text{final}) - H(\text{initial})$; $(\mathrm{d}p/\mathrm{d}t)$ used for the rate of change of pressure; δx used to denote an infinitesimal variation of x. But for a damped linear oscillator the amplitude F as a function of time t might be expressed by the equation $F = F_0\exp(-\delta t)\sin(\omega t)$ where δ is the decay coefficient (SI unit: Np/s) and ω is the angular frequency (SI unit: rad/s). Note the use of roman δ for the operator in a small time interval δt, but italic δ for the decay coefficient in the product δt. Note that the products δt and ωt are both dimensionless, but are described as having the unit neper (Np = 1) and radian (rad = 1), respectively.

8. The fundamental physical constants are always regarded as quantities subject to measurement (even though they are not considered to be variables) and they should accordingly always be italic. Sometimes fundamental physical constants are used as though they were units, but they are still given italic symbols. An example is the hartree, E_h. However the electronvolt, eV, the dalton, Da, or the unified atomic mass unit, u, and the astronomical unit, ua, have been recognized as units by the Consultative Committee on Units of the BIPM and they are accordingly given roman symbols.

Examples:

c_0 for the speed of light in vacuum, m_e for the electron mass, h for the Planck constant, N_A or L for the Avogadro constant, e for the elementary charge, a_0 for the Bohr radius, etc. But for the electronvolt eV = $e \times$ V = 1.602 176 487(40) $\times 10^{-19}$ J, the symbol eV is roman.

9. Greek letters are used in some cases for certain purposes in systematic organic, inorganic, polymer, and biochemical nomenclature. These should be in roman (upright) type. They designate e.g. the position of substituents, double bonds, ligating-atom attachment and bridging mode in coordination compounds, end groups in structure-based names for polymers, and configuration in carbohydrates and natural products. Letter symbols for elements are italic when used in names indicating attachments to heteroatoms, e.g. *O*-, *N*-, *S*-, and *P*-. The italic element symbol *H* denotes indicated or added hydrogen [refs. 4 and 5].

Examples:

α-ethylcyclopentaneacetic acid

β-methyl-4-propylcyclohexaneethanol

[*N*, *N*'-bis(2-amino-κ*N*-ethyl)ethane-1,2-diamine-κ*N*] chloroplatinum(II)

tetracarbonyl(η^4-2-methylidenepropane-1,3-diyl) chromium

α-(trichloromethyl)-ω-chloropoly(1,4-phenylenemethylene)

α-D-glucopyranose

5α-androstan-3β-ol

N-methylbenzamide

O-ethyl hexanethioate

3*H*-pyrrole

naphthalen-2(1*H*)-one

References

1. Quantities, Units and Symbols in Physical Chemistry, the IUPAC Green Book, prepared for publication by E Richard Cohen, et al, 3rd Edition, Royal Society of Chemistry, Cambridge, 2007.
2. The ISO Standards Handbook, Quantities and Units, ISO, Geneva, 1993.
3. Le Système International d'Unités (the SI Brochure), 7th Edn. (French and English), BIPM, Sèvres, 1998.
4. Principles of Chemical Nomenclature,- A Guide to IUPAC Recommendations, 2011 Edition, edited by G J Leigh (RSC 2011, ISBN 978-1-84973-007-5).
5. Nomenclature of Organic Chemistry. IUPAC Recommendations and Preferred Names 2013, prepared by H A Favre and W H Powell (RSC 2013, ISBN 978-0-85404-182-4)

Radiochemistry

by Yuichiro Nagame

The Asia-Pacific Symposium on Radiochemistry (APSORC) was first held in Kumamoto (Japan) in 1997 with the objective of disseminating, together with the other Asia-Pacific countries, the latest study of radiochemistry into the world. The successive symposia in Fukuoka (Japan), Beijing (China), and then in Napa (U.S.A.) have increasingly made APSORC more cosmopolitan. The APSORC13, the 5th Asia-Pacific Symposium on Radiochemistry, took place in Japan after an interval of twelve years, was jointly held with the 57th Radiochemistry Symposium organized by Japan Society of Nuclear and Radiochemical Sciences. The symposium was held at "Kanazawa Bunka Hall" 22-27 September 2013 with a record-breaking attendance of 375 participants from 25 countries.

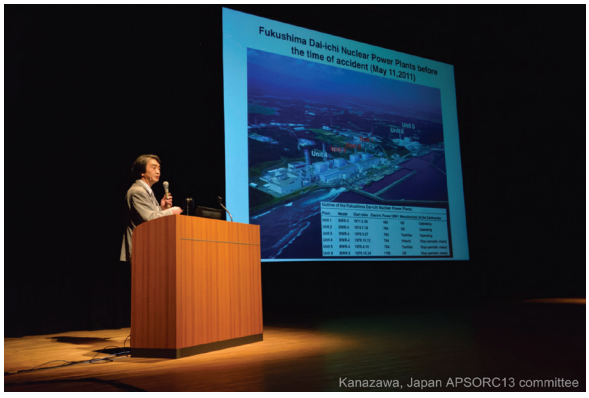
As this is the first APSORC after the accident of Fukushima Daiichi Nuclear Power Plant, issues related to the accident were discussed extensively. The topics covered were:

1. Fukushima issues
2. Education in nuclear and radiochemistry
3. Nuclear forensics
4. Nuclear energy chemistry
5. Nuclear chemistry
6. Actinide chemistry
7. Environmental radiochemistry
8. Radiopharmaceutical chemistry and nuclear medicine
9. Nuclear probes for materials sciences
10. Activation analysis
11. Application of nuclear and radiochemical techniques

The scientific program consists of 343 contributions (108 oral and 235 poster presentations) including 8 plenary talks and 25 invited talks. Among them, 144 presentations (61 oral and 83 poster presentations) were given by overseas presenters.

The symposium began with a commendation of the George Hevesy Medal Award followed by an award lecture. The George Hevesy Medal Award is the premier international award of excellence in radioanalytical and nuclear chemistry. It is named after George de Hevesy (1885-1966), who received the Nobel Prize for Chemistry in 1943 for his work on the use of isotopes as tracers in the study of chemical processes. The Medal is awarded to an individual in recognition of excellence through outstanding, sustained career achievements in the fields of pure as well as applied nuclear and radiochemistry, in particular applications to nuclear analytical chemistry. It was established originally in 1968 by the Journal of Radioanalytical and Nuclear Chemistry (JRNC) and Professor Tibor Braun (Editor-in-Chief of JRNC). Professor Dr. Hab. Rajmund S. Dybczyński of the Institute of Nuclear Chemistry and Technology, Warszawa, Poland, has been selected to receive the Hevesy Medal Award 2013 (HMA-13) in recognition of his significant contributions to the field

Hevesy Medal Award: R. Dybczynski (right) and A. Chatt (left, presenter)



Fukushima session: M. Yamamoto

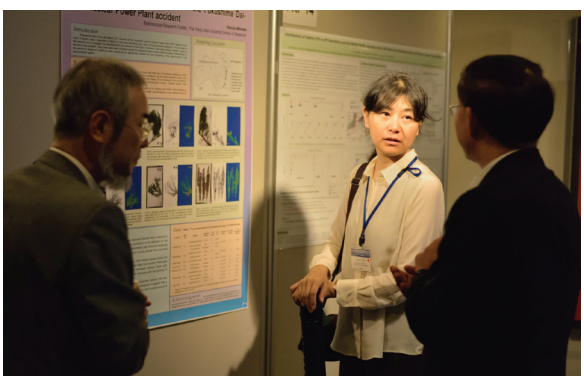
of radiochemical neutron activation analysis (RNAA), in particular for proposing the idea of "definitive" methods by RNAA, and to the certification of reference materials.

At the session on Fukushima issues, M. Yamamoto (Kanazawa University) gave a talk entitled "Overview of the Fukushima Daiichi Nuclear Power Plant (FDNPP) accident with amounts and nuclear compositions of the released radionuclides." This was to report a general description of the accident. I. McKinley (Switzerland), in his talk entitled "Fukushima challenges in perspective." emphasized the importance not only of decontamination of radioactive materials but also of distributing information on ongoing status of contamination and radiation education of general public. Other issues covered in the session include a report on radionuclides, such as iodine (I) and cesium (Cs), released in the early stage of the accident, current picture and emerging problems in decontamination of radioactive materials, migration behavior of radioactive I and Cs fallen into the environment, and so on. Furthermore, the following topics were discussed: the status of marine contamination and its future prospects using a model simulation based on the enormous amount of data on radioactive Cs released into the ocean, cross-reaction of nuclear fuel meltdown and water, research reports aiming at decommissioning plan of the disabled reactors, radioactivity measurement of waste, thermodynamic properties of melted fuel materials, etc. Issues related to the Fukushima accident were discussed broadly from ocean to lands, and extending to decontamination processes. The fact that 80 presentations (2 plenary talks and 5 invited talks, 14 oral presentations, and 59 poster presentations) were dealing with the issue represents much attention has been paid to the Fukushima issue.

In the session on Education in Nuclear and Radiochemistry, S. B. Clark (Washington State Univ.) covered importance of nuclear chemistry in the fields of nuclear energy, nuclear medicine and environmental related issues including radioactive disposals, and education of next generation radiochemists. In addition, an educational network system used in Europe called CINCH-II (Coordination of education and training In Nuclear Chemistry in Europe) was introduced. Nuclear forensics, a radiochemical analysis technique, is a newly developed research field in the last ten years, mainly in USA and Germany. This method is employed in analyses of confiscated illegal nuclear materials, aiming to specify an origin of the nuclear substance and a type of nuclear weapon used in the scene. Research on age determination of single Pu and Pu/U mixed oxide particles were reported at the session. From a nuclear security perspective, nuclear forensics plays a huge role. A few more presentations on this subject would be anticipated.

In the Nuclear Energy Chemistry session, Z. Chai (IHEP, China) talked about overview of nuclear energy chemistry in China, followed by A. Goswami (BARC, India) reporting a back-end process in India. Issues on a nuclear fuel cycle were discussed widely from chemical processes to technical development including separation of high-level liquid waste. In the actinide chemistry session, M. Denecke (UK) reported the latest result on speciation of actinide using synchrotron radiation. Recent progress in substantive actinide research including computational science, electrochemistry, and separation chemistry was represented in the session.

Topics related to superheavy elements, nuclear waste disposal and fuel cycle, radioisotope production, nuclear decay properties, and radiation detection technologies were discussed in the nuclear chemistry session. A plenary talk entitled "Advances in the production and chemistry of the heaviest elements" was



Poster session

given by A. Türler (Bern Univ.), presenting hot topics including naming of the newly found elements recognized by IUPAC and overview of gas-phase chemical research on element 114, flerovium (Fl). Atomic mass measurement of element 102, Nobelium (No) and 103, lawrencium (Lr) using SHIPTRAP, which is a combination device of a recoil separator, SHIP at GSI and an iron trap, was introduced as a newly innovative approach to the study of the heaviest elements. The study of more detailed physical and chemical properties of the heaviest elements by using atomic spectroscopic techniques is anticipated.

In the Environmental Radiochemistry session, S. Nagao (Kanazawa Univ.) gave a presentation on transport of particulate organic matter in river and coastal marine systems using radiocarbon. This serves as the application of radioisotopes in revealing environmental transport dynamics of particle materials. J. V. Kratz (Johannes Gutenberg Univ.) provided ultratrace analysis of long-lived radionuclides by resonance ionization mass spectrometry (RIMS). The session as a whole was substantial including presentations addressing Fukushima issues.

In the session of Radiopharmaceutical Chemistry and Nuclear Medicine, J. Hatazawa (Osaka Univ.) outlined the radiopharmaceutical development in the field of nuclear medicine and emphasized its significance in radiochemistry. He mentioned that it is worthwhile to challenge realization of "theranostics," a combination of diagnostics and therapeutics, for future radioactive drugs. S. Wilbur (Univ. Washington) reported on α-emitting radionuclides for medical use, which has drawn increasing attention recently. A particular focus was put on application of halogen, astatine 211At, and its importance in radiochemistry. He emphasized, in regard to α-emitting radionuclides, that more active involvement of radiochemists in the research of At is necessary to actualize clinical application.

In the session on Nuclear probes for materials science, H. Ueno (RIKEN, Japan) gave a plenary talk reporting development of the RI (radioactive ion) beam factory in RIKEN (RIBF) and the recent progress of nuclear physics owing to it, and, furthermore, the future prospects of research plans. The highly informative talk shows a potency of material physics employing various types of nuclear spectroscopic methods using RI beams.

In the session on Activation analysis, A. Chatt (Canada) gave an invited talk on radioactive annalistic speciation of arsenic, antimony and selenium. The session covered a broad range of the subject including the methods employing a prompt gamma-ray measurement, and a characteristic X-ray measurement generated from muonic nuclei. In the session on application of nuclear and radiochemical techniques, H. Harada (JAEA, Japan) reported the research result and foresight with the neutron reaction measurement device (ANNRI) at the J-PARC facility. Results presented in the session ranged from those associated with facilities and measurements to the fields of nanoscience and nuclide analyses. In the closing session, six young scientists were awarded for their poster presentations. Five days of conference were wrapped up on a high note. Proceedings of the symposium will be published in *Journal of Radioanalytical and Nuclear Chemistry*.

It is important to remember that the success of the symposium is primarily due to the unstinting support of many people. The supports, including sponsorships provided by 10 Japanese academic societies and 5 associations (2 autonomous bodies) and IUPAC, industrial exhibitions, advertisements contributed by 5 industrial firms, 14 endowments and volunteer efforts in Kanazawa, realized the prestigious symposium.

The APSORC international committee meeting was held during the symposium. The next symposium in 2017 following Japan, China, and USA is to be hosted in Korea (Jeju).

Yuichiro Nagame <nagame.yuichiro@jaea.go.jp> was Co-chair of APSORC13; he is Deputy Director General at the Advanced Science Research Center of the Japan Atomic Energy Agency.

POLYCHAR 22

by Michael Hess

POLYCHAR 22 World Forum on Advanced Materials was hosted 7-11 April 2014, by the Department of Chemistry & Polymer Science of the University of Stellenbosch in South Africa. Thus, for the first time in its history, our Forum took place in Africa. Earlier the conferences took place in Denton, Texas, (1992-2003), Guimarães, Portugal (2004), Singapore (2005), Nara (2006), Buzios, Rio de Janeiro (2007), Lucknow (2008), Rouen (2009), Siegen (2010), Kathmandu (2011), Dubrovnik (2012), and Gwangju (2013).

There were eight Conference Sessions:

- Nanomaterials and Smart Materials (15 contributions)
- Physical Morphology (15)
- Biomaterials and Green Materials (11)
- Materials Properties in Relation to Performance (11)
- Property Prediction and Simulation (11)

POLYCHAR 22, Stellenbosch, South Africa, 2014

- Processing, Rheology, and Mechanical Properties (11)
- New Developments in Polymer Characterization (7)
- General Materials Science (6)

There were 87 oral contributions and 51 posters presented. As always, creativity and originality of presentations and discussions were important; there was no attempt to have a large number of participants. There were 171 delegates from 31 countries and 5 continents. 46 participants were students. Participants from countries other than South Africa came from Australia, Austria, Belgium, Brazil, Canada, China, Colombia, Croatia, Czech Republic, Egypt, France, Germany, India, Italy, Japan, Korea, Malaysia, Nepal, New Zealand, Nigeria, Poland, Portugal, Republic of Korea, Saudi Arabia, Sweden, Thailand, The Netherlands, Turkey, United Kingdom, and USA.

The contributions, oral and poster, covered a broad range of materials and their properties, application, and processing. There were several contributions on the nanocomposites, including the popular graphene-containing systems. Also drug delivery systems, water purification, field responsive materials, and morphology on the nanoscale were important subjects as well—plus tribology and wear and combinations of polymers and biological systems/materials.

Each year, it is very difficult to select those presentations that can be named in a short report. The program and all the abstracts are available at http://academic.sun.ac.za/POLYCHAR/speakers.html

The Short Course on Polymer Characterization consisted of 7 lectures and had 43 participants:

- Glass Transition and Disorder in Polymer Materials—How to Characterize What Happens at the Glass Transition, Jean-Marc Saiter, University of Rouen
- Comprehensive Analysis of Macromolecules by Chromatographic Methods, Peter Kilz, (PSS Polymer Standards Service, Darmstadt)
- Dynamic-Mechanical and Calorimetric Properties of Polymers, Michael Hess (University of Antioquia, Medellin)
- Electron Microscopy of Polymers, Sven Henning (Fraunhofer Institute for Mechanics of Materials, Halle)
- Characterization of Polymer Structure, Transitions and Reactions by Pressure-Volume-Temperature Measurements, Jürgen Pionteck (Leibnitz Institute for Polymer Research Dresden)
- Advanced Fractionation Techniques for the Analysis of Complex Polyolefines, Harald Pasch (University of Stellenbosch)
- Polymer Tribology: Witold Brostow (University of North Texas, Denton)

As usual, the Short Course was held the day before the conference lectures started to give the participants—in particular the students—an opportunity to update their knowledge.

The Conference was opened by the welcome address of Prof T.E. Cloete, Vice-Rector (Research and Innovation, University of Stellenbosch); Witold Brostow (University of North Texas, Denton), the President of the POLYCHAR Scientific Committee; and Michael Hess, the IUPAC Representative (Chosun University, Korea, and University of Antioquia, Medellin, Colombia).

Winner of the Paul J. Flory research Prize Eric Baer, with the Chair of the Prize Committee Jean-Jacques Pireaux, left, and the chair of POLYCHAR 22, Peter Mallon.

At the end of the Forum, the prestigious **Paul J. Flory Research Prize** was given ex aequo to **Eric Baer**, Herbert-Henry-Dow Professor of Science and Engineering, Case Western Reserve University, Cleveland, Ohio, for his impressive work on new nanofibers and nanolayered systems produced by solvent-free coextrusion processing and to **Andrew**

Whittaker, Australian Institute for Bioengineering and Nanotechnology, Institute for Advanced Imaging, The University of Queensland, St. Lucia, for his seminal work on NMR-based in vivo imaging, in particular 19F-molecular imaging used to track therapeutic particles and cells in vivo.

Winner of the Paul J. Flory Research Prize Andrew Whittaker,

Winner of the POLYCHAR International Materials Science Prize, **Chunye Xu**

The **International Materials Research Prize** was awarded to **Chunye Xu**, formerly University of Washington, Seattle, now at the Chinese Academy of Sciences Key Laboratory of Soft Matter, National Laboratory for Physical Sciences at Microscale, University of Science and Technology of China, Hefei, for her ingenious research in electro-responsive polymers, devices and their applications.

One of the prominent goals of POLYCHAR is to support young scientists, i.e. graduates not older than 32 years. This is reflected by the **Bruce-Hartmann-Young-Scientists Prize**, awarded ex aequo to **Marilia Horn**, Universidade de Sao Paulo, Sao Carlos, for her work on rheology of chitosan-containing Pequi oil

Two of the three winners of the IUPAC Student's Poster Prize, Jonas Daenicke (middle, left) and Qiong Wu (middle, right), missing is Aliza Janse van Rensburg, framed by Peter Mallon and Michael Hess (IUPAC representative).

gels (laboratory of Anna Maria de Guzzi Plepis) and to **Lola Olantunji**, Polymer & Textile Research Laboratory, Federal Institute of Industrial Research, Lagos, for her work on production and mechanical properties of penetration enhancers from natural polymers from fish scales.

The **Jürgen-Springer Young Scientists Price** went ex aequo to **Rueben Pfuka**, Stellenbosch University, for his work on nanostructures created by controlled hierarchical self-assembly of foldamers and to **Alexandre Dhotel**, Institut des Materiaux de Rouen, University of Rouen, for his work on molecular motions with self-assembled monolayers.

Three **IUPAC Students poster prizes** went to **Qiong Wu** (Royal Institute of Technology, Stockholm), for her work on a new type of flame retardant foam based on a sustainable biohybrid material of wheat gluten and silica, **Jonas Daenicke** (Friedrich Alexander University, Erlangen-Nuremberg) for his work on resilience of silicone breast implants: New insights by mapping the mechanical properties of implant, and **Aliza Janse van Rensburg**, (Cardiovascular Unit, Cape Town), for her work on heparin and heparan sulfate hydrogels for cardiovascular tissue regeneration.

After five days of concentrated work during the conference with many challenging contributions, discussions, and meetings that reinforced international contacts and cooperation, the Forum ended with a visit to Robben Island with the prisoner cell of Nelson Mandela, the Table Mountain and a drive down the South Coast to Houte Bay. The participants left for their home countries, again with the feeling of having

had an illuminating meeting of the POLYCHAR family. The scientific "children" and even "grandchildren" of the early participants from more than 20 years ago have come together. POLYCHAR 23 is scheduled for 11-15 May 2015 in Lincoln, Nebraska, hosted by Mehrdad Neghaban of the University of Nebraska–Lincoln and his team.

Thanks are due to Peter Mallon, his colleagues, and collaborators at the University of Stellenbosch for effective organization of the Course and the Forum. Good organization is a necessary condition for a creative and nice atmosphere, which was appreciated by the participants in Stellenbosch.

Global Experiments Spark International Years: Sharing Best Practices

International Years are both a celebration and an excellent opportunity to raise awareness about a wide range of topics. In the last decade, some of main branches of science including physics, astronomy, and chemistry have been recognized by the United Nations with International Years. During the 2011 International Year of Chemistry, IUPAC in partnership with UNESCO organized the Global Water Experiment [water.chemistry2011.org] as one of the flagship activities under the theme "Water: A Chemical Solution."[1] Comprised of four simple experiments about water quality and purification, hundreds of thousands of students took part in this massive global activity, reported their data online, and helped to build an interactive global map where anyone can see, compare, and analyze the data collected in the yearlong activity.[2]

This year, on 20 January 2014, at the opening ceremony of the International Year of Crystallography at the UNESCO headquarters in Paris, Maciej Nalecz, Director of the Division of Basic & Engineering Sciences at UNESCO, said, "The international year of chemistry introduced the global water experiment that became part of the school curriculum in many countries," adding that "crystallography has many possibilities for follow up, and I'm absolutely sure this will be a year to remember."[3] A few months later, the Royal Society of Chemistry launched the "Global Experiment 2014: The Art of Crystallisation," a crystal growth competition, also consisting of simple experiments, sharing the data online, and creating a global interactive map.[4]

During the 4th International Conference of Young Scientists & Annual General Meeting of the Global Young Academy "Natural Resources in a Finite World" held in Santiago de Chile from 21-23 May 2014, Javier Garcia Martinez, co-chair of the Global Water Experiment, gave the invited lecture "The Global Experiment of the International Year of Chemistry: Creating Online Communities for Learner-driven Education." Javier talked about the lessons learned and showed how to organize simple, safe activities adaptable to different age ranges to how to create online communities using the web and social media.[5] After his presentation, a discussion followed on best practices regarding global experiments, learner empowerment through technology and the opportunities offered by online education.

Angélica Bucio, Officer of ICSU Regional Office for Latin America and the Caribbean, gave a presentation on "ICSU & Future Earth: knowledge and support to accelerate our transformations to a sustainable world." She explained the role of ICSU and International Unions in organizing a wide range of activities from International Years to Future Earth in order to reach large audiences, raise public awareness about critical issues, and gather the best expertise to solve our more urgent issues.

Finally, Jorge Sequeira, Director of the UNESCO Office of Education for Latin America and the Caribbean gave the keynote talk "Natural Resources in a Finite World—UNESCO's commitment to supporting the efforts of young women and men in the sciences, education, culture and communication." Dr. Sequira focused on how to tackle global issues through better understanding of the scientific and technological challenges, a more effective education, and the empowerment of women.

Chemistry is the central science and therefore

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Javier Garcia Martinez presenting at the 4th International Conference of Young Scientists & Annual General Meeting of the Global Young Academy held in Santiago de Chile in May 2014.

touches with many other scientific and technical disciplines. The United Nations is providing us with an excellent opportunity through its International Years to promote a wide range of causes and topics.

Global Experiments is an exciting new tool thanks to which millions of young students from all around the world can be reached and connected. We can all learn from previous experiences about how to build successful and effective Global Experiments to engage with the new generations of scientists and inspire new scientific vocations.

www.iupac.org/project/2010-011-1-050

References

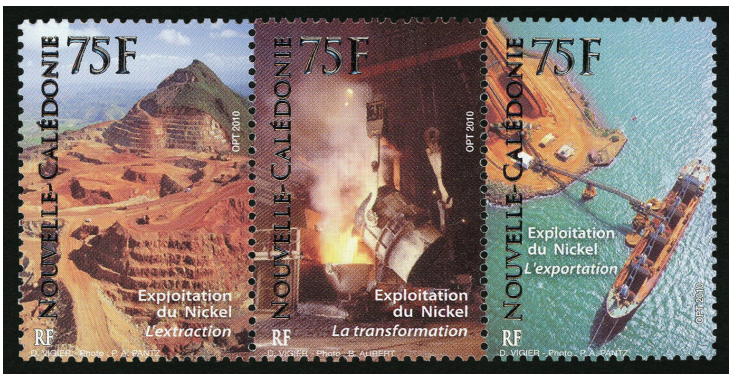
1. www.iupac.org/publications/ci/2012/3403/3_martinez.html
2. www.visualizing.org/full-screen/39174/embedlaunch
3. www.rsc.org/chemistryworld/2014/01/unesco-international-year-crystallography-opening-ceremony
4. http://rsc.li/ge2014
5. www.iupac.org/publications/ci/2010/3204/1_garcia-martinez.html

Nickel Mining in Paradise

New Caledonia, an overseas territory of France located approximately 1400 km east of Australia, has what most people would expect from a rather secluded archipelago in the southwestern Pacific Ocean, including a fascinating biodiversity and a mixed population of Melanesian and European descent. Discovered by the celebrated British navigator and explorer James Cook in 1774, the main island, Grande Terre, is surrounded by coral reefs and consists primarily of coastal plains, lush mountains, and valleys. A rich array of flora and fauna, beautiful beaches, a myriad of waterfalls and hiking trails, moderate weather, and a unique blend of indigenous and French cultures make it an appealing tourist destination.

However, it may come as a surprise to many that New Caledonia, which is only half the size of Taiwan and has a population of roughly a quarter of a million, is one of the world's top producers of nickel, together with Australia, Canada, Indonesia, Russia, Brazil, and the Philippines. The French engineer Jules Garnier first encountered green deposits of nickel-containing minerals in New Caledonia in 1864, and commercial mining operations in the main island began in 1875. The export of nickel ores and ferronickel alloys is today a major driver of the economy in New Caledonia, which boasts some 10-15% of the world reserves of the versatile metal.

The stamp triptych featured in this note was issued in 2010 to highlight the three key steps involved in the production of nickel in New Caledonia, namely the mining of mineral ores, the smelting process, and the transfer of the ensuing silvery-white metal for export. Nickel, often in combination with chromium or small quantities of other transition metals, is extensively used in electroplating applications and in the manufacture of stainless steel and a variety of nonferrous alloys, leading to the material's enhanced strength and corrosion resistance. Significant quantities of nickel are also used in rechargeable batteries and catalytic hydrogenation reactions. With world production and consumption of nickel on the rise, renewed efforts are made in New Caledonia and elsewhere to minimize the adverse environmental impact of mining and processing of nickel ores. Interestingly, "nickel" (five-cent) coins in the United States, in circulation since 1866, contain only 25% of the metal, the balance being actually copper!



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

Theoretical and Computational Chemistry

5-10 October 2014, Santiago, Chile

The World Association of Theoretical and Computational Chemists Congress WATOC 2014 is a premier forum for the presentation of research results on conceptual developments and application of theoretical and computational chemistry to a wide range of fields in chemistry, physics and biology.

WATOC 2014 will bring together leading researchers, students and scientists interested in the role of computational chemistry in the natural sciences. This will be an exciting opportunity to promote scientific exchange and discussion on electronic structure theory and computational tools in chemical and physical processes.

WATOC 2014, an interdisciplinary conference, will provide a stimulating and dynamic environment to examine issues and opportunities associated with the essential role of theoretical and computational chemistry in many chemical, biological and physical processes.

See program and details at watoc2014.com

Data Sharing and Integration for Global Sustainability

2–5 November 2014 in New Delhi, India

The International Conference on Data Sharing and Integration for Global Sustainability (SciDataCon) is motivated by the conviction that the most significant research challenges—and in particular the pressing issues relating to global sustainability—cannot be properly addressed without due attention to various issues relating to data. SciDataCon aims to make explicit the connection between concrete and specific challenges to ensure environmental protection, economic prosperity and social well being along with the research questions that arise from these challenges and the necessary role of data policy, management, and analysis in addressing these research questions. The effectiveness and credibility of research findings rely on the widest possible availability of quality-assessed and interoperable datasets.

Research data are essential to all scientific endeavours. The emerging cultures of data sharing and publication, open access to, and reuse of data are the positive signs of an evolving research environment. Nevertheless, several cultural and technological challenges are still preventing the research community from realizing the full benefits of these tendencies.

The Committee on Data for Science and Technology (CODATA) and the World Data System (WDS), interdisciplinary committees of the International Council for Science (ICSU) are together advancing this agenda by actively promoting effective data policies and good data management practices in the research community, to produce better science, which ultimately benefits society. As a major contribution to this effort, the two organizations are co-sponsoring and organizing a high profile international biennial conference, which will examine, in an integrated way, the data issues at the heart of the global research questions in a manner that will have tangible benefit for research and society.

SciDataCon will provide a unique platform bringing together international experts and practitioners in data sciences, technologies and management; researchers from the natural, social, health, and computer sciences; research funders and sponsors; and policymakers and advisors.

www.scidatacon2014.org

Environmental Horizon

9-11 January 2015, Karachi, Pakistan

The 3rd International Conference on Environmental Horizon (ICEH-2015) **Nurture Nature: Serve to Conserve** is going to be held on 9-11 January 2015 at Department of Chemistry, University of Karachi, Pakistan.

ICEH is mainly devoted to the development of scientific knowledge, its application and training in the field of interdisciplinary approaches to better understand the environmental segments. The conference aims to provide a forum for researchers, students, industrialists, and others working in diversified fields of environment.

Details are available at www.chemuok.edu.pk

For more information, please contact Erum Zahir, PhD Conference Secretary, Department of Chemistry University of Karachi, Karachi 75270 Pakistan Tel: + 92-21-99261300-6 Ext: 2290

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

2014 (after 15 October)

15-17 October 2014 • Bioinspired Materials • Nice, France
2nd International Conference on Bioinspired and Biobased Chemistry & Materials
Prof. Frédéric Guittard, Université de Nice, Sophia Antipolis, Groupe Surfaces & Interfaces, LPMC/UMR 7336, 28 Avenue Valrose, F-06100 Nice, France, E-mail: guittard@unice.fr, www.nice2014-conference.com

20-25 October 2014 • Natural Products • Shanghai, China
8th International Conference on Biodiversity and 28th International Symposium on the Chemistry of Natural Products (ICOB-8 & ISCNP-28)
Prof. Yang Ye, Chinese Academy of Sciences, Institute of Materia Medica, 555 Zu Chong Zi Road, Shanghai 201203, China, E-mail: yye@mail.shcnc.ac.cn, http://iupac.simm.ac.cn

21-24 October 2014 • Green Chemistry • Moscow, Russia
5th International Chemical Assembly: Green Chemistry
Ms. Olga V. Kamentseva, Business Programme Manager, Expocentre, 14, Krasnopresnenskaya Nab. RF-123100 Moscow, Russia, E-mail: kamentseva@expocentr.ru, http://chemistry-expo.ru/en/

26-29 October 2014 • Solvothermal & Hydrothermal based technologies • Bordeaux, France
4th International Solvothermal and Hydrothermal Association Conference (ISHA 2014)
Prof. Cyril Aymonier, Université de Bordeaux, ICMBC-CNRS, 87 Avenue de Dr. A. Schweitzer, F-33608 Pessac, France, E-mail: aymonier@icmcb-bordeaux.cnrs.fr, http://isha2014.univ-bordeaux.fr

27-31 October 2014 • Photodynamics • Oaxaca, México
8th International Meeting on Photodynamics and Related Aspects
Prof. Ramón Hernández, Universidad Autónoma del Estado de Morelos, Centro de Investigaciones Químicas, Avenida Universidad 1001, C.P. 62209, Col. Chamilpa, Cuernavaca, Morelos, México
E-mail: ramon@uaem.mx, www.photodynamics.hol.es

POSTPONED • Herbal Medicine • Dhaka, Bangladesh
ChemRAWN XX - International Conference on Herbal Medicine
Prof. Mohammed Mosihuzzaman, Bangladesh Institute of Health Sciences, International Center for Natural Product Chemistry (ICNPR), 125 Darussalam, Mirpur, Dhaka 1216 Bangladesh
E-mail: mmosihuzzaman@yahoo.com, www: tba

23-27 November 2014 • Molecular Architectures and Materials • Johannesburg, South Africa
7th International Symposium on Macro- and Supra-molecular Architectures and Materials (MAM-2014)
Dr. Robert Tshikhudo, DST/Mintek Nanotechnology Innovation Centre, 200 Malibongwe Drive, Private Bag X 3015, Randburg, South Africa, E-mail: robertt@mintek.co.za, www.MAM-14.com

2015

11-15 January 2015 • Bio-Organic Chemistry • Pune, India
10th International Conference on Bio-Organic Chemistry
Prof. Krishna N. Ganesh, Indian Institute of Science Education and Research, Homi Bhabha Road, Pune, Maharashtra 411 008, India, E-mail: isboc10-2015@iiserpune.ac.in, www.iiserpune.ac.in/isboc10

13-14 January 2015 • Quality of Chemical Analytical Results • Tel Aviv, Israel
International Workshop on Human Errors and Quality of Chemical Analytical Results
Dr. Ilya Kuselman, National Physical Laboratory of Israel, Givat Ram, IL-91904 Jerusalem, Israel
E-mail: ilya.kuselman@economy.gov.il, www.isranalytica.org.il

25-29 May 2015 • Transactinide Elements • Kitashiobara, Japan
5th International Conference on the Chemistry and Physics of the Transactinide Elements (TAN'15)
Dr. Hiromitsu Haba, RIKEN, Nishina Center for Accelerator Based Science, 2-1 Hirosawa, Wako, Saitama 351-0198, Japan, E-mail: haba@riken.jp, http://asrc.jaea.go.jp/conference/TAN15/

See more online at www.iupac.org/home/conferences

I U P A C

ADVANCING THE WORLDWIDE ROLE OF CHEMISTRY FOR THE BENEFIT OF MANKIND

MISSION

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

NATIONAL ADHERING ORGANIZATIONS

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Australian Academy of Science *(Australia)*
Österreichische Akademie der Wissenschaften *(Austria)*
Bangladesh Chemical Society *(Bangladesh)*
The Royal Academies for the Sciences and Arts of Belgium *(Belgium)*
Brazilian Chemical Society *(Brazil)*
Bulgarian Academy of Sciences *(Bulgaria)*
National Research Council of Canada *(Canada)*
Sociedad Chilena de Química *(Chile)*
Chinese Chemical Society *(China)*
Chemical Society located in Taipei *(China)*
Croatian Chemical Society *(Croatia)*
Sociedad Cubana de Química *(Cuba)*
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)*
Finnish Chemical Society *(Finland)*
Comité National Français de la Chimie *(France)*
Deutscher Zentralausschuss für Chemie *(Germany)*
Association of Greek Chemists *(Greece)*
Hungarian Academy of Sciences *(Hungary)*
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Royal Irish Academy *(Ireland)*
Israel Academy of Sciences and Humanities *(Israel)*
Consiglio Nazionale delle Ricerche *(Italy)*
Caribbean Academy of Sciences—Jamaica Chapter *(Jamaica)*
Science Council of Japan *(Japan)*
Jordanian Chemical Society *(Jordan)*
Korean Chemical Society *(Korea)*
Kuwait Chemical Society *(Kuwait)*
Fonds National de la Recherche *(Luxembourg)*
Institut Kimia Malaysia *(Malaysia)*
Academy of Sciences of Mozambique *(Mozambique)*
Nepal Polymer Institute (Nepal)
Koninklijke Nederlandse Chemische Vereniging *(Netherlands)*
Royal Society of New Zealand *(New Zealand)*
Chemical Society of Nigeria *(Nigeria)*
Norsk Kjemisk Selskap *(Norway)*
Chemical Society of Pakistan *(Pakistan)*
Polska Akademia Nauk *(Poland)*
Sociedade Portuguesa de Química *(Portugal)*
Colegio de Químicos de Puerto Rico *(Puerto Rico)*
Russian Academy of Sciences *(Russia)*
Serbian Chemical Society *(Serbia)*
Slovak Chemical Society *(Slovakia)*
Slovenian Chemical Society *(Slovenia)*
National Research Foundation *(South Africa)*
Ministerio de Educación y Ciencia *(Spain)*
Institute of Chemistry, Ceylon *(Sri Lanka)*
Svenska Nationalkommittén för Kemi *(Sweden)*
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Tanzania Chemical Society *(Tanzania)*
Ministry of Science and Technology *(Thailand)*
Société Chimique de Tunisie *(Tunisia)*
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